Mackey–Moore cohomology and topological extensions of Polish groups

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Topological group extensions with Abelian kernels are analyzed using factor sets and following the pattern of the work of Eilenberg and MacLane on extensions of groups without topology. In this analysis, the Eilenberg–MacLane cohomology is replaced by the Mackey–Moore one, whose cochains are Borel mappings and which is especially suitable in the case of Polish groups (Hausdorff second countable complete groups). The connection between cohomology groups of degree 2 and equivalence classes of topological group extensions with Abelian kernels is established. A fundamental sequence of cohomology groups and group homomorphisms is proven to be exact, and it is shown that, in some interesting cases, the low degree cohomology groups of topological semidirect products are determined by the corresponding cohomology groups of the factors.

1. INTRODUCTION

The occurrence of group extensions in the physical literature is quite a recent phenomenon that can be traced back to the lectures of Michel at the Istanbul Summer School in 1962.[1] However, group extensions were implicitly considered in the early days of quantum mechanics by Weyl[2] and later by Wigner.[3] In the work of Wigner, topological considerations are of primary importance for the handling of multipliers (or factors, as they are called by Wigner). The emphasis on the topology is even more manifest in Bargmann's paper,[4] where the study of continuous unitary projective representations is pursued in the case of an arbitrary topological group G, in particular of a Lie group. In this work the multipliers appear as factor sets of extensions of G by $\mathbf{U}(1)$ (the group of complex numbers of absolute value 1), and one is immediately faced with a difficulty: They can be chosen to be continuous in a neighborhood of $(1, 1)$, but, in general, they cannot be chosen to be continuous in $G \times G$. This is a typical pitfall of the theory of topological group extensions, where the discontinuity of factor sets is an unpleasant but unavoidable fact. However, using a result of Dixmier,[5] one can prove that it is always possible to choose Borel factor sets when G is a Polish group, i.e., a Hausdorff second countable and complete group.

The class of Polish groups contains all the second countable locally compact groups (in particular the finite-dimensional second countable real or complex Lie groups) and some groups of mappings, for instance the Abelian group of m-times continuously differentiable mappings of $\mathbf{R}^n$ into $\mathbf{R}$, where m and n are in $\mathbf{N}$. Many of these groups occur as symmetry groups in physics, where the interest in topological extensions of Polish groups arises especially in connection with the problem of projective representations.[4,6,7] The aim of this paper is to study some basic questions of the theory of topological extensions (with Abelian kernels) of Polish groups, following the track of Mackey[8] and Moore.[9,10,11] An application to a physical symmetry problem of the results obtained here is given in Ref. 12.

In Sec. 2 we introduce the Mackey-Moore cohomology, which is especially suitable for the study of topological extensions of Polish groups and which is obtained from the usual Eilenberg-MacLane cohomology by requiring that the cochains should be Borel mappings. We prove (Theorem 1 and its corollary) the exactness of an important sequence of group homomorphisms and of Mackey-Moore cohomology groups of a topological group G with values in a Polish G-module A_ψ. This generalizes the result of Moore[9] for G and A second countable and locally compact.

Topological group extensions with Abelian kernels are studied in Sec. 3, and the difficulty associated with the nonexistence of continuous factor sets is pointed out. If G is a group and A_ψ is a G-module, a well-known theorem of Eilenberg and MacLane[13,14] affirms the existence of an isomorphism of the group of equivalence classes of extensions of G by A_ψ onto the group of cohomology of degree 2 of G with values in A_ψ. We show (Theorem 2) that this result is partially valid also in the case where G is a Polish group, A_ψ is a Polish G-module, and only topological extensions of G by A_ψ are considered, provided one replaces the Eilenberg-MacLane cohomology by the Mackey-Moore one. By "partially valid" we mean that we are able only to prove the existence of an injective group homomorphism.

In Sec. 4 we use a generalization of a theorem of Mackey (Theorem 9.4 of Ref. 6) in order to derive some propositions on the low degree cohomology groups of topological semidirect products.

For the reader's convenience, few definitions and results in the theory of Borel, Baire, and Polish spaces are collected in Appendix A. In Appendix B the same is done for the cohomology theory of cochain complexes; the reader is referred to this appendix for the cohomological notation. In Appendix C we show that the notion of a Baer addition may also be introduced in the study of topological extensions of Polish groups.

NOTATION AND SOME BASIC DEFINITIONS

Let R be an equivalence relation in a given set E. We denote by $[x]$ the equivalence class of $x \in E$, tacitly understanding "modulo R" if no misinterpretation is possible. Given a mapping $f: A \to B$, a subset A' of A, and a subset B' of B such that $f(A') \subseteq B'$, we denote by $f \mid (A' \to B')$ the mapping deduced from f by passing to the subsets A' and B'. As it is usual, we write $f \mid A'$ for $f \mid (A' \to B)$. If A and B are topological spaces, then the continuity of $f \mid (A' \to B')$ has to be understood as the continuity in the induced topologies. The neutral element of a group G is denoted by 1 (resp. by 0) if the law of composition is written multiplicatively (resp. additively), and e_G stands for 1 or for 0. When topological groups are considered, the meaning of a "product group" (resp. of a "quotient group") is always that of a "topological product group" (resp. of a "topological quotient group"). We also write "locally compact" for "Hausdorff locally compact" throughout.

Let G be a group, let A be an Abelian group (resp. a vector space), and let Ψ be an operation (resp. a linear operation) of G on A. As is well known, this means that

$$\Psi: G \to \mathrm{Aut}(A)$$

is a group homomorphism. Then A, equipped with Ψ, is called a *G-module* (resp. a *linear G-module*) and we denote it by A_Ψ. Furthermore, A^S will stand for the subgroup (resp. the vector subspace) of A

$$\{a \mid a \in A \text{ and } \Psi(s)a = a \text{ for all } s \in S\},$$

where S is any subgroup of G. Let A_Ψ and $A'_{\Psi'}$ be two G-modules. A mapping $\alpha: A_\Psi \to A'_{\Psi'}$ is called a *G-module homomorphism* (or simply a *G-homomorphism*) if it is a group homomorphism and if

$$\alpha \circ \Psi(g) = \Psi'(g) \circ \alpha$$

for all $g \in G$.

Let G and A be topological groups, with A Abelian. An operation Ψ of G on A such that the mapping

$$(g, a) \mapsto \Psi(g)a = g \cdot a$$

of $G \times A$ into A is continuous (joint continuity) is said to be a *topological operation*. In this case the G-module A_Ψ is called a *topological G-module*. Suppose $A'_{\Psi'}$ is also a topological G-module and let $\alpha: A_\Psi \to A'_{\Psi'}$ be a G-homomorphism. If α is continuous, then it is called a *topological G-homomorphism*.

A *section* associated with a surjective group homomorphism $\rho: G \to G'$ is a mapping $\sigma: G' \to G$ such that $\rho \circ \sigma = \mathrm{Id}_{G'}$ (the identity mapping of G'). Obviously, it is an injective mapping; if $\sigma(e_{G'}) = e_G$, the section σ is said to be normalized. If G and G' are topological groups, then a section σ associated with ρ and which is a Borel (resp. a continuous) mapping (see Appendix A) is said to be a *Borel* (resp. a *continuous*) *section*.

2. THE EILENBERG-MACLANE AND MACKEY-MOORE COHOMOLOGIES

Let G be a topological group and let A_Ψ be a topological G-module. Many different cohomologies of G with values in A_Ψ have been proposed in the mathematical literature. We will consider here two of them which are relevant for our purposes.

(i) The *Eilenberg-MacLane cohomology*[13,14] is the cohomology of the Eilenberg-MacLane cochain complex $C^*(G, A_\Psi)$ with the cohomology groups $H^p(G, A_\Psi)$ of degree p ($p \in \mathbb{Z}$) of G with values in A_Ψ (see Appendix B).

(ii) If $p > 0$, let $C_b^p(G, A_\Psi)$ be the subgroup of $C^p(G, A_\Psi)$ of all the (normalized) Borel mappings of the product space G^p into A. Notice that this choice is meaningful because the Borel space associated with the product of p topological spaces is the product of the Borel spaces associated with the p factors.[15] If $p \leq 0$, put $C^p{}_b(G, A_\Psi) = C^p(G, A_\Psi)$. In this way we get a subcomplex $C_b^*(G, A_\Psi)$ of $C^*(G, A_\Psi)$, because $f \in C_b^*(G, A_\Psi)$ implies $\delta f \in C_b^*(G, A_\Psi)$ by well-known properties of Borel mappings (cf. Ref. 9, Proposition 1.2). We shall call $C_b^*(G, A_\Psi)$ a Mackey-Moore cochain complex and its cohomology the *Mackey-Moore cohomology*.[8-11] The relevant groups of $C_b^*(G, A_\Psi)$ will be denoted by the usual Eilenberg-MacLane symbols with an additional subscript "b".

Remark 1: A cochain complex $C_c^*(G, A_\Psi)$ may be defined as the subcomplex of $C_b^*(G, A_\Psi)$ obtained by requiring that, for any $p > 0$, the elements of $C_c^p(G, A_\Psi)$ be continuous mappings of G^p into A_Ψ. However, the cohomology of $C_c^*(G, A_\Psi)$ is, in general, not very useful for the group extension problem (cf. Sec. 3, Remark 3).

Remark 2: If G is a discrete group, then

$$C^*(G, A_\Psi) = C_c^*(G, A_\Psi) = C_b^*(G, A_\Psi)$$

because any mapping of a discrete space into an arbitrary topological space is continuous and hence Borel.

Remark 3: The Mackey-Moore cohomology is especially suitable in the case where G is a Polish group and A_Ψ a Polish G-module (see Appendix A and next section).

Let again G be a topological group and let $A^{(1)}_{\Psi(1)}$, $A^{(2)}_{\Psi(2)}, \ldots, A^{(n)}_{\Psi(n)}$ be topological G-modules. A diagram

$$A^{(1)}_{\Psi(1)} \xrightarrow{\alpha(1)} A^{(2)}_{\Psi(2)} \xrightarrow{\alpha(2)} \cdots \xrightarrow{\alpha(n-1)} A^{(n)}_{\Psi(n)}$$

is said to be an exact sequence of topological G-modules if

(1) all the $\alpha^{(i)}$ are topological G-homomorphisms,

(2) the diagram is exact, i.e., $\mathrm{Ker}\,\alpha^{(i+1)} = \mathrm{Im}\,\alpha^{(i)}$ for $1 \leq i \leq n-2$.

If all the $A^{(i)}_{\Psi(i)}$ are Polish G-modules, we shall say that we have an exact sequence of Polish G-modules.

Now consider an exact sequence

$$0 \longrightarrow A'_{\Psi'} \xrightarrow{\iota} A_\Psi \xrightarrow{\pi} A''_{\Psi''} \longrightarrow 0$$

of Polish G-modules. As A'' is Hausdorff and π is continuous, $\mathrm{Im}\,\iota = \mathrm{Ker}\,\pi$ is closed in A and thus $\iota(A'_{\Psi'})$ is a Polish G-module. By a theorem of Banach (Ref. 16, Satz 9; cf. also Ref. 17, §35, V), the mapping $\iota \mid (A' \to \iota(A'))$ is a homeomorphism and thus ι is a closed mapping. In addition π is an open mapping. In fact, let

$$A \xrightarrow{\pi'} A/\iota(A') \xrightarrow{\pi''} A''$$

be the canonical factorization of π, where π' and π'' are continuous group homomorphisms with π' the canonical surjection and with π'' bijective. As the quotient group $A/\iota(A')$ is Polish, we may apply the theorem of Banach quoted above and conclude that π is open because π'' is a homeomorphism.

Let $\alpha: A_\Psi \to A'_{\Psi'}$ be a topological G-homomorphism. We denote by $\tilde{\alpha}$ the homomorphism of cochain complexes

$$C^*(G, A_\Psi) \to C^*(G, A'_{\Psi'})$$

such that $\tilde{\alpha}(f) = \alpha \circ f$ for all $f \in C^p(G, A_\Psi)$ if $p > 0$ and $\tilde{\alpha}(f) = \alpha(f)$ for all $f \in A_\Psi$. Since α is continuous,

$$\tilde{\alpha}(C_b^*(G, A_\Psi)) \subseteq C_b^*(G, A'_{\Psi'}),$$

and we denote by $\tilde{\alpha}_b$ the homomorphism of cochain complexes

$$\tilde{\alpha} | (C_b^*(G, A_\Psi) \to C_b^*(G, A'_{\Psi'})).$$

Theorem 1: Let G be a topological group and let

$$\mathfrak{E}: 0 \longrightarrow A'_{\Psi'} \xrightarrow{\iota} A_\Psi \xrightarrow{\pi} A''_{\Psi''} \longrightarrow 0$$

be an exact sequence of Polish G-modules. Then

$$\tilde{\mathfrak{E}}: 0 \longrightarrow C^*(G, A'_{\Psi'}) \xrightarrow{\tilde{\iota}} C^*(G, A_\Psi) \xrightarrow{\tilde{\pi}} C^*(G, A''_{\Psi''}) \longrightarrow 0$$

and

$$\tilde{\mathfrak{E}}_b: 0 \longrightarrow C_b^*(G, A'_{\Psi'}) \xrightarrow{\tilde{\iota}_b} C_b^*(G, A_\Psi) \xrightarrow{\tilde{\pi}_b} C_b^*(G, A''_{\Psi''}) \longrightarrow 0$$

are exact sequences of cochain complexes.

Proof: The exactness of $\tilde{\mathfrak{E}}$ is well known,[14] and can easily be checked directly. In order to prove that $\tilde{\mathfrak{E}}_b$ is exact too, one has to show, for each $p \in \mathbf{Z}$, the exactness of the diagram

$$\tilde{\mathfrak{E}}_b^p: 0 \longrightarrow C_b^p(G, A'_{\Psi'}) \xrightarrow{\tilde{\iota}_b^p} C_b^p(G, A_\Psi) \xrightarrow{\tilde{\pi}_b^p} C_b^p(G, A''_{\Psi''}) \longrightarrow 0.$$

This is obvious if $p \leq 0$. If $p > 0$, we first notice that the injectivity of ι implies that of $\tilde{\iota}_b^p$; furthermore,

$$\tilde{\iota}_b^p(C_b^p(G, A'_{\Psi'})) \subseteq \operatorname{Ker}\tilde{\pi}_b^p$$

because $\pi \circ \iota = 0$. Let $f \in \operatorname{Ker}\tilde{\pi}_b^p$. As $f(G^p) \subseteq \iota(A'_{\Psi'})$, there is one and only one mapping $f' \in C^p(G, A'_{\Psi'})$ such that $f = \iota \circ f'$. But, ι being injective and continuous, the image under ι of any Borel set of A' is a Borel set of A (Ref. 18, §6, Cor. to Théorème 3) and therefore $f' \in C_b^p(G, A'_{\Psi'})$. On the other hand $\tilde{\iota}_b^p(f') = f$, so that $\operatorname{Ker}\tilde{\pi}_b^p \subseteq \operatorname{Im}\tilde{\iota}_b^p$ and hence $\operatorname{Ker}\tilde{\pi}_b^p = \operatorname{Im}\tilde{\iota}_b^p$. Now take $f'' \in C_b^p(G, A''_{\Psi''})$ and choose a normalized section σ associated with π as follows. Since $\iota(A')$ is a closed subgroup of A, there exists a Borel set B_0 of A such that, for each $a \in A$, $B_0 \cap (a + \iota(A'))$ is a set with one and only one element (Ref. 5, Lemma 3). Thus, if $B_0 \cap \iota(A') = a_0$, $B = B_0 - a_0$ is a Borel set of A with $B \cap \iota(A') = \{0\}$ and $B \cap (a + \iota(A'))$ is a set with one and only one element for all $a \in A$. There exists a unique mapping $\sigma: A'' \to A$ such that, for any $a \in A$,

$$(\sigma \circ \pi)(B \cap (a + \iota(A'))) = B \cap (a + \iota(A'))$$

and, obviously, σ is a normalized section associated with π. In addition σ is a Borel mapping: If C is any Borel set of A, then $B \cap C$ is a Borel set too and

$$\sigma^{-1}(C) = \sigma^{-1}(B \cap C) = \pi(B \cap C)$$

is a Borel set of A'' because $\pi | B$ is injective and continuous. Therefore $\sigma \circ f'' \in C_b^p(G, A_\Psi)$, $\tilde{\pi}_b^p(\sigma \circ f'') = f''$, and we conclude that $\tilde{\pi}_b^p$ is surjective. ■

By the theorem of Appendix B one gets

Corollary: Let G and $\mathfrak{E}$ be as in Theorem 1. Then

$$0 \longrightarrow H^0(G, A'_{\Psi'}) \xrightarrow{\tilde{\iota}_*^0} H^0(G, A_\Psi) \xrightarrow{\tilde{\pi}_*^0} H^0(G, A''_{\Psi''}) \xrightarrow{\delta_{\mathfrak{E}}^0} H^1(G, A'_{\Psi'}) \xrightarrow{\tilde{\iota}_*^1} \cdots$$
$$\cdots \xrightarrow{\delta_{\mathfrak{E}}^{p-1}} H^p(G, A'_{\Psi'}) \xrightarrow{\tilde{\iota}_*^p} H^p(G, A_\Psi) \xrightarrow{\tilde{\pi}_*^p} H^p(G, A''_{\Psi''}) \xrightarrow{\delta_{\mathfrak{E}}^p} H^{p+1}(G, A'_{\Psi'}) \xrightarrow{\tilde{\iota}_*^{p+1}} \cdots$$

and

$$0 \longrightarrow H_b^0(G, A'_{\Psi'}) \xrightarrow{(\tilde{\iota}_b)_*^0} H_b^0(G, A_\Psi) \xrightarrow{(\tilde{\pi}_b)_*^0} H_b^0(G, A''_{\Psi''}) \xrightarrow{\delta_{\mathfrak{E}b}^0} H_b^1(G, A'_{\Psi'}) \xrightarrow{(\tilde{\iota}_b)_*^1} \cdots$$
$$\cdots \xrightarrow{\delta_{\mathfrak{E}b}^{p-1}} H_b^p(G, A'_{\Psi'}) \xrightarrow{(\tilde{\iota}_b)_*^p} H_b^p(G, A_\Psi) \xrightarrow{(\tilde{\pi}_b)_*^p} H_b^p(G, A''_{\Psi''}) \xrightarrow{\delta_{\mathfrak{E}b}^p} H_b^{p+1}(G, A'_{\Psi'}) \xrightarrow{(\tilde{\iota}_b)_*^{p+1}} \cdots$$

are exact sequences of Abelian groups.

3. LOW DEGREE COHOMOLOGY AND TOPOLOGICAL GROUP EXTENSIONS WITH ABELIAN KERNELS

Let G and A be topological groups, where A is Abelian, and let Ψ be a topological operation of G on A. For $p = 0, 1, 2$, the groups $H^p(G, A_\Psi)$ and $H_b^p(G, A_\Psi)$ have the following simple interpretations.

(i) The groups $H^0(G, A_\Psi)$ and $Z^0(G, A_\Psi)$ (resp. $H_b^0(G, A_\Psi)$ and $Z_b^0(G, A_\Psi)$) may be trivially identified and then

$$H^0(G, A_\Psi) = H_b^0(G, A_\Psi) = A^G.$$

(ii) The elements of $Z^1(G, A_\Psi)$ are called crossed homomorphisms of G into A and the elements of $B^1(G, A_\Psi)$ are the principal crossed homomorphisms. Hence $H^1(G, A_\Psi)$ is the group of equivalence classes of crossed homomorphisms modulo the principal ones. If G is a Polish group and if A_Ψ is a Polish G-module, then

$$Z_b^1(G, A_\Psi) = Z_c^1(G, A_\Psi)$$

and so

$$H_b^1(G, A_\Psi) = H_c^1(G, A_\Psi).$$

This can be shown as follows, using an argument of Banach (Ref. 16, Satz 6 and Ref. 19, Chap. I, Théorème 4). If $f \in Z_b^1(G, A_\Psi)$, then there exists a meager subset M of G such that $f | G - M$ is continuous (Ref. 17, §28, I and II). Let $g \in G$ and let (g_n) be any sequence of elements of G converging to g. The set $\bigcup_n g_n^{-1}M = M'$ is meager too and there exists $g' \in G - M'$ because G is a Baire space (Appendix A). It follows that $g_n g' \in G - M$ for all $n \in \mathbf{N}$ and thus

$$\lim_{n\to\infty} f(g_n) = \lim_{n\to\infty} f(g_n g') - \lim_{n\to\infty} \Psi(g_n) f(g') = f(g).$$

This can be performed for any $g \in G$, and so f is continuous.

(iii) The cohomology groups $H^2(G, A_\Psi)$ and $H_b^2(G, A_\Psi)$ are related to equivalence classes of extensions of G by A.

We recall that an *extension of G by A* [20] is an exact sequence

$$\mathfrak{E}: 0 \longrightarrow A \xrightarrow{\iota} E \xrightarrow{\rho} G \longrightarrow 1 \qquad (3.1)$$

of groups.[21] This means that in diagram (3.1) E is a group and the arrows are group homomorphisms with ι injective, ρ surjective, and

$$\operatorname{Ker}\rho = \operatorname{Im}\iota.$$

We say that E is the group obtained from the extension $\mathfrak{E}$ of G by A. By the axiom of choice there exists a normalized section σ associated with ρ. Let Ψ be the group homomorphism of G into $\mathrm{Aut}(A)$ such that

$$\iota(\Psi(g)a) = \sigma(g)\iota(a)\sigma(g)^{-1} \tag{3.2}$$

for all $g \in G$ and all $a \in A$. Then A_Ψ is a G-module and, as Ψ is independent of the section σ chosen, one says that $\mathfrak{E}$ is an extension of G by A_Ψ (or, alternatively, an extension of G by A relative to Ψ). We shall identify A and $\iota(A)$ through ι and describe an extension of G by A as an ordered pair (E,ρ), where $\rho: E \to G$ is a surjective group homomorphism such that $\mathrm{Ker}\rho = A$.

Two extensions $\mathfrak{E}$ and $\mathfrak{E}'$ of G by A are said to be *equivalent* if there exists a group homomorphism γ such that the diagram

$$\begin{array}{ccccccccc} \mathfrak{E}: 0 & \longrightarrow & A & \xrightarrow{\iota} & E & \xrightarrow{\rho} & G & \longrightarrow & 1 \\ & & \downarrow \mathrm{Id}_A & & \downarrow \gamma & & \downarrow \mathrm{Id}_G & & \\ \mathfrak{E}': 0 & \longrightarrow & A & \xrightarrow{\iota'} & E' & \xrightarrow{\rho'} & G & \longrightarrow & 1 \end{array} \tag{3.3}$$

is commutative. Note that actually γ is a group isomorphism and that if $\mathfrak{E}$ is an extension of G by A_Ψ, then any extension of G by A equivalent to $\mathfrak{E}$ is an extension of G by A_Ψ too.

For any operation Ψ of G on A, the set $\mathrm{Ext}(G, A_\Psi)$ of equivalence classes of extensions of G by A_Ψ can be given the structure of an Abelian group with the so called Baer addition[14] as the law of composition.

A *topological extension*

$$\mathfrak{E}_t: 0 \longrightarrow A \xrightarrow{\iota} E \xrightarrow{\rho} G \longrightarrow 1$$

of G by A is a group extension with the following additional requirements:

(a) E is a topological group;

(b) $\iota \mid (A \to \iota(A))$ is a homeomorphism;

(c) ρ is continuous and open.

Notice that the mapping deduced from ρ by passing to the quotient by $\iota(A)$ is a homeomorphism by virtue of (c). The operation Ψ of G on A given by (3.2) is topological; thus we have a topological G-module A_Ψ and $\mathfrak{E}_t$ is said to be a topological extension of G by A_Ψ (or of G by A relative to Ψ). Again we shall identify A and $\iota(A)$ through ι and describe a topological extension of G by A as an ordered pair (E,ρ), where E is a topological group and $\rho: E \to G$ is a surjective, open, and continuous group homomorphism such that $\mathrm{Ker}\rho = A$.

Two topological extensions $\mathfrak{E}_t$ and $\mathfrak{E}_t'$ of G by A are said to be equivalent if there is a topological group isomorphism γ such that the diagram (3.3) is commutative.

Let G and A be Polish groups and let Ψ be an arbitrary topological operation of G on A. With the Baer addition as the law of composition (for details see Appendix C and Ref. 22), the set $\mathrm{Ext}_t(G, A_\Psi)$ of equivalence classes of topological extensions of G by A_Ψ becomes an Abelian group.

Note that if G and A are Polish groups, then E is a Polish group too: It is Hausdorff, second countable, and complete by Proposition 3.1 of Ref. 23 and thus metrizable (Ref. 18, §3, Prop. 1). Moreover, if G, E, and A are Polish, then the continuity of ι and ρ already implies that $\iota \mid (A \to \iota(A))$ is a homeomorphism (hence ι is closed) and that ρ is open. This can be shown by the same argument used in the case of an exact sequence of Polish G-modules (see Sec. 2).

Now, we come back to the cohomology groups $H^2(G, A_\Psi)$ and $H_b^2(G, A_\Psi)$. As is well known,[13,14] there exists a group isomorphism

$$\alpha: \mathrm{Ext}(G, A_\Psi) \to H^2(G, A_\Psi)$$

such that if $[(E,\rho)] \in \mathrm{Ext}(G, A_\Psi)$, then

$$\alpha([(E,\rho)]) = [f] \in H^2(G, A_\Psi),$$

where $f \in Z^2(G, A_\Psi)$ is the factor set of (E,ρ) defined by a normalized section σ associated with ρ, i.e., it is the mapping of $G \times G$ into A such that

$$f(g,g') = \sigma(g)\sigma(g')\sigma(gg')^{-1}.$$

The elements of the equivalence class $\alpha^{-1}([0])$ are said to be the *inessential extensions* of G by A_Ψ. If G is a Polish group and if A_Ψ is a Polish G-module, a weaker form of this result may be proven for topological group extensions as follows.

Lemma 1: Let E and G be Polish groups and let $\rho: E \to G$ be a continuous surjective group homomorphism. Then there exists a normalized Borel section associated with ρ.

Proof: Once we have noticed that $\mathrm{Ker}\rho$ is a closed subgroup of E, we apply Lemme 3 of Ref. 5 as in the proof of Theorem 1. ∎

Theorem 2: Let G be a Polish group and let A_Ψ be a Polish G-module. Then there exists an injective group homomorphism

$$\alpha_b: [(E,\rho)] \mapsto [f] \tag{3.4}$$

of $\mathrm{Ext}_t(G, A_\Psi)$ into $H_b^2(G, A_\Psi)$, where f is the (Borel) factor set of (E,ρ) defined by a normalized Borel section associated with ρ.

Proof: Let (E,ρ) be an arbitrary topological extension of G by A_Ψ. By Lemma 1 one has a normalized Borel section σ associated with ρ, and therefore, if f is the (Borel) factor set defined by σ, we may show the existence of the mapping α_b of (3.4) as in the case of group extensions without topology (see Ref. 14, Chap. IV, Theorem 4.1).

It suffices to notice that

(i) f' is the factor set of (E,ρ) defined by a normalized Borel section σ' associated with ρ if and only if

$$h: g \mapsto \sigma'(g)\sigma(g)^{-1}$$

is a Borel mapping of G into A such that $f' = f + \delta h$;

(ii) if $(E',\rho') \in [(E,\rho)]$ and if γ is the topological group isomorphism of the commutative diagram (3.3), then $\gamma \circ \sigma$ is a normalized Borel section associated with ρ' and f is the factor set of (E',ρ') defined by $\gamma \circ \sigma$.

Again, it is clear from the definition of the Baer addition that the mapping, α_b is a group homomorphism (cf. Appendix C). In order to prove the injectivity of α_b, let us first make two preliminary remarks.

(1) All the elements of the equivalence class $\alpha_b([(E,\rho)]) = [f]$ are Borel factor sets of (E,ρ) defined by normalized Borel sections associated with ρ [cf. (i) above].

(2) Suppose (E,ρ) is such that $\alpha_b([(E,\rho)]) = 0$ (the equivalence class [0]), and let σ be any normalized Borel section associated with ρ and defining the factor set 0. Then σ is a Borel group homomorphism of a Polish group into a Polish group and thus continuous by a theorem of Banach already mentioned. It follows that the surjective mapping $\beta: E \to A$ given by

$$\beta(e) = e\sigma(\rho(e))^{-1}$$

is continuous too. Furthermore, any element e of E may be written as $\beta(e)\sigma(\rho(e))$ and thus the bijection

$$e \mapsto (\beta(e), \sigma(\rho(e))) \tag{3.5}$$

of E onto $A \times \sigma(G)$ is a homeomorphism.

Now, let (E,ρ) and (E',ρ') be two extensions of G by A_Ψ such that

$$\alpha_b([(E,\rho)]) = \alpha_b([(E',\rho')]) = 0.$$

By virtue of the remark (1) above, we can choose two normalized Borel sections σ and σ' associated, respectively, with ρ and ρ' and defining the factor set 0. A group isomorphism $\gamma: E \to E'$ making commutative the diagram (3.3) is defined by

$$\gamma(e) = \beta(e)\sigma'(\rho(e)).$$

Using the homeomorphism (3.5), one sees easily that γ is continuous. The same argument shows the continuity of γ^{-1}, because

$$\gamma^{-1}(e') = \beta'(e')\sigma(\rho'(e'))$$

for all $e' \in E'$. ∎

Remark 1: Mackey has proven that if G and A are locally compact second countable groups, then α_b is a group isomorphism.[8] Moore claims that this is also true in the case of G locally compact second countable and A Polish.[11]

Remark 2: It follows from the proof of Theorem 2 that if (E,ρ) is any element of the equivalence class $\alpha_b^{-1}(0)$, then E is topologically isomorphic to $A \times_\Psi G$, the external topological semidirect product of G by A relative to Ψ.[24] The elements of $\alpha_b^{-1}(0)$ are the *inessential topological extensions* of G by A_Ψ.

Remark 3: If E, G, and ρ are as in Lemma 1, there is not, in general, a continuous section associated with ρ even if E and G are connected Lie groups.[22]

Remark 4: A topological extension (E,ρ) of G by A is said to be quasifibered[23] if there exists a normalized section σ associated with ρ and continuous at 1. For each topological operation Ψ of G on A, the set $\mathrm{Ext}_t^{QF}(G, A_\Psi)$ of equivalence classes of quasifibered extensions of G by A_Ψ is a subgroup of $\mathrm{Ext}_t(G, A_\Psi)$. If G and A are first countable and Hausdorff, then

$$\mathrm{Ext}_t(G, A_\Psi) = \mathrm{Ext}_t^{QF}(G, A_\Psi)$$

(Ref. 25, Theorem 2; cf. Ref. 23, Prop. 3.6).

4. LOW DEGREE COHOMOLOGY OF TOPOLOGICAL SEMIDIRECT PRODUCTS

Let G be a topological group, let K be a normal subgroup of G, and let A_Ψ be a topological G-module such that $\Psi(k) = \mathrm{Id}_A$ for all $k \in K$. Suppose that the group G operates on K by

$$(g,k) \mapsto g(k) = gkg^{-1},$$

and consider the operation $\hat{\Psi}^p$ of G on $C_b^p(K, A_{\Psi|K})$ ($p \in \mathbf{Z}$) such that $\hat{\Psi}^0 = \Psi$ and, if $p > 0$,

$$(\hat{\Psi}^p(g)f)(k_1, \ldots, k_p) = \Psi(g)f(g^{-1}(k_1), \ldots, g^{-1}(k_p))$$

for all $f \in C_b^p(K, A_{\Psi|K})$ and all $(k_1, \ldots, k_p) \in K^p$. For any $p \in \mathbf{Z}$ and any $g \in G$,

$$\delta^p \circ \hat{\Psi}^p(g) = \hat{\Psi}^{p+1}(g) \circ \delta^p; \tag{4.1}$$

thus $Z_b^p(K, A_{\Psi|K})$ is stable for $\hat{\Psi}^p$ and we can consider the operation

$$\hat{\Psi}_Z^p : g \mapsto \hat{\Psi}^p(g) \mid (Z_b^p \to Z_b^p)$$

of G on $Z_b^p(K, A_{\Psi|K})$ induced by $\hat{\Psi}^p$. Besides, (4.1) shows that we have also an operation $\hat{\Psi}_B^p$ of G on $B_b^p(K, A_{\Psi|K})$ induced by $\hat{\Psi}_Z^p$. By passing to the quotient we get an operation $\hat{\Psi}_*^p$ of G on $H_b^p(K, A_{\Psi|K})$. From now on these operations will be tacitly understood.

The following lemma is a generalization of a result of Mackey (Ref. 6, Theorem 9.4).

Lemma 2: Let G be a topological semidirect product of S by K and let A_Ψ be a topological G-module. Suppose that $\Psi(K) = \{\mathrm{Id}_A\}$. Then, if f' is any element of $Z_b^2(G, A_\Psi)$, there exist $f \in [f']$, $f_1 \in Z_b^2(K, A_{\Psi|K})$, a Borel mapping f_2 of $K \times S$ into A, and $f_3 \in Z_b^2(S, A_{\Psi|S})$ such that

$$f(ks, k's') = f_1(k, s(k')) + f_2(k', s) + f_3(s, s') \tag{4.2}$$

for all k, k' in K and all s, s' in S. The mappings f_1 and f_2 satisfy

(i) $f_1(s(k), s(k')) = \Psi(s)f_1(k, k') + f_2(kk', s) - f_2(k, s) - f_2(k', s)$

and

(ii) $f_2(k, ss') = f_2(s'(k), s) + \Psi(s)f_2(k, s')$

for all k, k' in K and all s, s' in S. Conversely, given $f_1 \in Z_b^2(K, A_{\Psi|K})$, a Borel mapping f_2 of $K \times S$ into A, and $f_3 \in Z_b^2(S, A_{\Psi|S})$ satisfying (i) and (ii), the mapping f of $G \times G$ into A defined by (4.2) belongs to $Z_b^2(G, A_\Psi)$.

Proof: Throughout this proof k, k', and k'' (resp. s, s', and s'') will denote arbitrary elements of K (resp. of S). Using repeatedly the fact that f' is a 2-cocycle and that $\Psi(K) = \{\mathrm{Id}_A\}$, we obtain

$$f'(ks, k's') = f'(k, s(k')) + f'(s, s') + f'(s, k') - f'(s(k'), s) - f'(k, s) - \Psi(ks)f'(k', s') + f'(ks(k'), ss').$$

Let f_2 be the Borel mapping of $K \times S$ into A given by

$$f_2(k, s) = f'(s, k) - f'(s(k), s). \tag{4.3}$$

As G is a semidirect product, there exists $h \in C_b^1(G, A_\Psi)$ such that

$$h(ks) = f'(k, s).$$

Hence

$$f'(ks,k's') = f_1(k, s(k')) + f_2(k', s) + f_3(s, s') - \delta h(ks, k's'),$$

where $f_1 = f' \mid K \times K$ and $f_3 = f' \mid S \times S$, and it follows that

$$f = (f' + \delta h) \in [f']$$

satisfies (4.2). Now

$$\begin{aligned}\delta f(ks, k's', k''s'') = &- f_1(k, s(k')) + \Psi(s)f_1(k', s'(k''))\\ &- f_1(ks(k'),(ss')(k''))+ f_1(k, s(k's'(k'')))\\ &- f_2(k', s) + \Psi(s)f_2(k'', s') - f_2(k'', ss')\\ &+ f_2(k's'(k''), s),\end{aligned} \tag{4.4}$$

and, by virtue of (4.3),

$$f_2 \mid K \times \{1\} = 0 \quad \text{and} \quad f_2 \mid \{1\} \times S = 0.$$

Since $\delta f = 0$ we see, by putting $k = s' = 1$ (resp. $k' = 1$) in (4.4), that f_1 and f_2 satisfy (i) [resp. f_2 satisfies (ii)].

Conversely, let $f_1 \in Z_b^2(K, A_{\Psi \mid K})$, let f_2 be a Borel mapping of $K \times S$ into A, and let $f_3 \in Z_b^2(S, A_{\Psi \mid S})$. Suppose that these mappings satisfy (i) and (ii). If f is defined by (4.2), then, using (i) and (ii) in (4.4) as well as the fact that f_1 is a 2-cocycle, we get $\delta f = 0$. ■

Remark: Condition (i) of Lemma 2 is equivalent to

(i′) $\hat{\Psi}_Z^2(s)f_1 = f_1 + \delta f_2^{(s)}$

for all $s \in S$, where the normalized Borel mapping $f_2^{(s)}: K \to A$ is given by

$$f_2^{(s)}(k) = - \Psi(s)f_2(k, s^{-1}). \tag{4.5}$$

Condition (ii) is equivalent to

(ii′) $f_2^{(ss')} = f_2^{(s)} + \hat{\Psi}^1(s)f_2^{(s')}$

for all s, s' in S.

Suppose that $f_1 \in Z_b^2(K, A_{\Psi \mid K})$ and a Borel mapping $f_2: K \times S \to A$ satisfy (i) and (ii). If $f_1' \in [f_1]$, then there exists $h \in C_b^1(K, A_{\Psi \mid K})$ such that $f_1' = f_1 + \delta h$ and we have, for each $s \in S$, a Borel mapping

$$f_2'^{(s)} = f_2^{(s)} + \hat{\Psi}^1(s)h - h$$

of K into A, where $f_2^{(s)}$ is given by (4.5). It is easy to check that f_1' and $f_2'^{(s)}$ $(s \in S)$ satisfy (i′) and (ii′). Hence $[f_1] \in H_b^2(K, A_{\Psi \mid K})^S$ and we conclude that

$$H_b^2(K, A_{\Psi \mid K})' = \left\{ [f_1] \,\middle|\, \begin{array}{l} f_1 \in Z_b^2(K, A_{\Psi \mid K}) \text{ and there exists} \\ \text{a Borel mapping } f_2: K \times S \to A \\ \text{such that } f_1 \text{ and } f_2 \text{ satisfy (i) and} \\ \text{(ii) of Lemma 2} \end{array} \right\}$$

is a subgroup of $H_b^2(K, A_{\Psi \mid K})^S$.

Proposition 1: Let G be a topological semidirect product of S by K and let A_Ψ be a topological G-module such that $\Psi(K) = \{\mathrm{Id}_A\}$. Then

(i) $H_b^0(G, A_\Psi) = H_b^0(K, A_{\Psi \mid K})^S$,

(ii) $H_b^1(G, A_\Psi) \approx H_b^1(K, A_{\Psi \mid K})^S \times H_b^1(S, A_{\Psi \mid S})$,

(iii) $H_b^2(G, A_\Psi) \approx H_b^2(K, A_{\Psi \mid K})' \times H_b^2(S, A_{\Psi \mid S})$, provided that

$$H^1(S, H_b^1(K, A_{\Psi \mid K})_{\hat{\Psi}_*^1 \mid S}) = \{0\}.$$

Proof: Throughout this proof again k, k' (resp. s, s') will denote arbitrary elements of K (resp. of S). Part (i) of the proposition is a consequence of $\Psi(K) = \{\mathrm{Id}_A\}$.

Proof of (ii): There is a mapping

$$\alpha: (f_1, f_2) \mapsto f$$

of $Z_b^1(K, A_{\Psi \mid K})^S \times Z_b^1(S, A_{\Psi \mid S})$ into $Z_b^1(G, A_\Psi)$ such that

$$f(ks) = f_1(k) + f_2(s).$$

In fact,

$$\begin{aligned}f(ksk's') &= f_1(ks(k')) + f_2(ss')\\ &= f_1(k) + \Psi(s)f_1(k') + f_2(s) + \Psi(s)f_2(s')\\ &= f(ks) + \Psi(ks)f(k's').\end{aligned}$$

Obviously α is a group homomorphism, and moreover it is surjective because, if $f \in Z_b^1(G, A_\Psi)$, then

$$(\hat{\Psi}_Z^1(s)f)(k) = \Psi(s)f(s^{-1}) + f(k) + f(s) = f(k),$$

and so $f = \alpha(f \mid K, f \mid S)$. Let R be the equivalence relation in $Z_b^1(K, A_{\Psi \mid K})^S \times Z_b^1(S, A_{\Psi \mid S})$ defined by the (normal) subgroup $\{0\} \times B_b^1(S, A_{\Psi \mid S})$, and let R′ be the equivalence relation in $Z_b^1(G, A_\Psi)$ defined by $B_b^1(G, A_\Psi)$. Note that

$$(f_1', f_2') \equiv (f_1'', f_2'') \pmod{\mathrm{R}}$$

implies

$$f_1' = f_1'' \quad \text{and} \quad f_2' = f_2'' + \delta a_2,$$

where $a_2 \in A$. Therefore,

$$\alpha(f_1', f_2')(ks) = f_1'(k) + f_2'(s) = \alpha(f_1'', f_2'')(ks) + \delta a_2(ks),$$

i.e., α is compatible with R and R′. By passing to the quotients, we get a surjective group homomorphism

$$\alpha_*: H_b^1(K, A_{\Psi \mid K})^S \times H_b^1(S, A_{\Psi \mid S}) \to H_b^1(G, A_\Psi).$$

We end the proof of (ii) by showing that α_* is injective too. Let $(f_1, f_2) \in Z_b^1(K, A_{\Psi \mid K})^S \times Z_b^1(S, A_{\Psi \mid S})$ be such that

$$\alpha_*([(f_1, f_2)]) = [0].$$

Then $\alpha(f_1, f_2) = \delta a$, where $a \in A$, i.e.,

$$f_1(k) + f_2(s) = - a + \Psi(s)a,$$

whence $f_1 = 0$, $f_2 \in B_b^1(S, A_{\Psi \mid S})$, and $[(f_1, f_2)] = [(0, 0)]$.

Proof of (iii): Consider the set E of all the ordered pairs (f_1, f_2) such that

(1) $f_1 \in Z_b^2(K, A_{\Psi \mid K})$ and $f_2: K \times S \to A$ is a Borel mapping,

(2) f_1 and f_2 satisfy (i) and (ii) of Lemma 2.

By Lemma 2 there is a mapping

$$\alpha: (f_1, f_2, f_3) \mapsto f$$

of $E \times Z_b^2(S, A_{\Psi \mid S})$ into $Z_b^2(G, A_\Psi)$ given by (4.2). Define an equivalence relation R in $E \times Z_b^2(S, A_{\Psi \mid S})$ as follows:

$$(f_1, f_2, f_3) \equiv (f_1', f_2', f_3') \pmod{\mathrm{R}} \tag{4.6}$$

if and only if

$$f_1 \equiv f_1' \ (\mathrm{mod} B_b^2(K, A_{\Psi|K})) \quad \text{and} \quad f_3 \equiv f_3' \ (\mathrm{mod} B_b^2(S, A_{\Psi|S})).$$

If R' is the equivalence relation defined by $B_b^2(G, A_\Psi)$ in $Z_b^2(G, A_\Psi)$, then we shall show that α is compatible with R and R$'$, i.e., that (4.6) implies

$$\alpha(f_1, f_2, f_3) \equiv \alpha(f_1', f_2', f_3') \ (\mathrm{mod}\ \mathrm{R}').$$

Put

$$\bar f = \alpha(f_1', f_2', f_3') - \alpha(f_1, f_2, f_3);$$

then

$$\bar f(ks, k's') = \delta h_1(k, s(k')) + \bar f_2(k', s) + \delta h_3(s, s'), \tag{4.7}$$

where $h_1 \in C_b^1(K, A_{\Psi|K})$, $\bar f_2 = f_2' - f_2$, and $h_3 \in C_b^1(S, A_{\Psi|S})$. The mappings $h_1, \bar f_2$, and h_3 satisfy the conditions

$$\hat\Psi_B^2(s)\delta h_1 = \delta h_1 + \delta \bar f_2^{(s)} \tag{4.8}$$

and

$$\bar f_2^{(ss')} = \bar f_2^{(s)} + \hat\Psi^1(s)\bar f_2^{(s')}, \tag{4.9}$$

where $\bar f_2^{(s)} : K \to A$ is given by

$$\bar f_2^{(s)}(k) = -\Psi(s)\bar f_2(k, s^{-1}).$$

We identify canonically $H_b^1(K, A_{\Psi|K})$ with $Z_b^1(K, A_{\Psi|K})$ and consider the mapping

$$h : s \mapsto \hat\Psi^1(s)h_1 - h_1 - \bar f_2^{(s)} \tag{4.10}$$

of S into $H_b^1(K, A_{\Psi|K})$. This is meaningful since

$$\delta(h(s)) = \hat\Psi_B^2(s)\delta h_1 - \delta h_1 - \delta \bar f_2^{(s)} = 0$$

by (4.8), i.e., $h \in C^1(S, H_b^1(K, A_{\Psi|K})_{\hat\Psi_*^1|S})$. Furthermore, $h \in Z^1(S, H_b^1(K, A_{\Psi|K})_{\hat\Psi_*^1|S})$, because

$$\delta h(s, s') = h(s) + \hat\Psi_*^1(s)h(s') - h(ss') = \bar f_2^{(ss')} - \bar f_2^{(s)} - \hat\Psi^1(s)\bar f_2^{(s')} = 0$$

on account of (4.9). By assumption, there is $h_1' \in H_b^1(K, A_{\Psi|K})$ such that

$$h(s) = -h_1' + \hat\Psi_*^1(s)h_1'$$

and thus, by virtue of (4.10),

$$\bar f_2(k, s) = (h_1' - h_1)(s(k)) - \Psi(s)(h_1' - h_1)(k).$$

We may choose $h' \in C_b^1(G, A_\Psi)$ such that $h' | S = 0$, $h' | K = h_1 - h_1'$, and $h'(ks) = h'(k)$; then

$$\delta h'(ks, k's') = \bar f_2(k', s) + \delta h_1(k, s(k')). \tag{4.11}$$

On the other hand, we may pick out an element h'' of $C_b^1(G, A_\Psi)$ such that $h''(ks) = h_3(s)$, and then

$$\delta h''(ks, k's') = \delta h_3(s, s'). \tag{4.12}$$

Therefore, by (4.7), (4.11), and (4.12) we see that the normalized Borel mapping $\bar h = h' + h''$ of G into A_Ψ satisfies $\delta \bar h = \bar f$, and thus α is compatible with R and R$'$. By passing to the quotients, we get a mapping

$$\alpha_* : H_b^2(K, A_{\Psi|K})' \times H_b^2(S, A_{\Psi|S}) \to H_b^2(G, A_\Psi)$$

which is surjective by Lemma 2. One can easily see that α_* is a group homomorphism; it remains to show its injectivity. For this, let $[f_1] \in H_b^2(K, A_{\Psi|K})'$, $[f_3] \in H_b^2(S, A_{\Psi|S})$, and suppose

$$\alpha_*([f_1], [f_3]) = [0].$$

Then there exist $h \in C_b^1(G, A_\Psi)$ and a Borel mapping $f_2 : K \times S \to A$ such that $(f_1, f_2) \in E$ and

$$\delta h(ks, k's') = f_1(k, s(k')) + f_2(k', s) + f_3(s, s'). \tag{4.13}$$

Putting $s = s' = 1$ in (4.13) we get $f_1 = \delta(h | K)$, and putting $k = k' = 1$ we get $f_3 = \delta(h | S)$; hence α_* is injective. ■

Remember the following definitions:

(1) An Abelian group A is said to be *divisible* if, for any $n \in \mathbf{N}^*$ (the set of all integers > 0), $nA = A$.

(2) One says that an Abelian group A is *torsion free* if, for any $a \in A$ different from 0, the relation $na = 0$ with n in $\mathbf{N}$ implies $n = 0$.

Proposition 2: Let G, K, S, and A_Ψ be as in Proposition 1. Suppose in addition that A is divisible and torsion free and that S is a finite group. Then

(i) $H_b^0(G, A_\Psi) = H_b^0(K, A_{\Psi|K})^S$;

(ii) $H_b^1(G, A_\Psi) \approx H_b^1(K, A_{\Psi|K})^S$;

(iii) $H_b^2(G, A_\Psi) \approx H_b^2(K, A_{\Psi|K})'$.

Proof: As S is finite and as A is divisible and torsion free, then

$$H_b^p(S, A_{\Psi|S}) = H^p(S, A_{\Psi|S}) = \{0\}$$

for all $p > 0$ (Ref. 14, Chap. IV, Corollary 5.4). The result follows from Proposition 1 once we have shown that

$$H^1(S, H_b^1(K, A_{\Psi|K})_{\hat\Psi_*^1|S}) = \{0\}.$$

We get this because the group $H_b^1(K, A_{\Psi|K}) = Z_b^1(K, A_{\Psi|K})$ is divisible and torsion free. For were not $Z_b^1(K, A_{\Psi|K})$ torsion free, then given $f \in Z_b^1(K, A_{\Psi|K})$, $f \neq 0$, we could find $n \in \mathbf{N}^*$ such that $nf = 0$ in contradiction with the assumption that A is torsion free. Now take any $f \in Z_b^1(K, A_{\Psi|K})$ and any $n \in \mathbf{N}^*$. Since A is divisible and torsion free, then, for every $k \in K$, there is a unique $a_k \in A$ such that $f(k) = na_k$. Besides, the mapping $f' : K \to A$ such that $f'(k) = a_k$ is an element of $Z_b^1(K, A_{\Psi|K})$. So, $f = nf'$ and $Z_b^1(K, A_{\Psi|K})$ is divisible. ■

Proposition 3: Let G be a topological semidirect product of S by K and suppose S finite. Let F be a field of characteristic 0 and let A_Ψ be an F-linear topological G-module such that $\Psi(K) = \{\mathrm{Id}_A\}$. Then

$$H_b^2(K, A_{\Psi|K})^S = H_b^2(K, A_{\Psi|K})'.$$

The proof rests on the following.

Lemma 3: Let G, K, S, F, and A_Ψ be as in Proposition 3. Then

$$H_b^p(K, A_{\Psi|K})^S \approx Z_b^p(K, A_{\Psi|K})^S / \delta C_b^{p-1}(K, A_{\Psi|K})^S$$

for all $p \in \mathbf{Z}$.

Proof: Throughout the proof p will denote an arbitrary element of $\mathbf{Z}$. The groups $C_b^p(K, A_{\Psi|K})$, $Z_b^p(K, A_{\Psi|K})$, and $B_b^p(K, A_{\Psi|K})$ are vector spaces over F in an obvious way and, furthermore, the F-linearity of A_Ψ implies the F-linearity of the G-modules $C_b^p(K, A_{\Psi|K})_{\hat{\Psi}^p}$, $Z_b^p(K, A_{\Psi|K})_{\hat{\Psi}_Z^p}$, and $B_b^p(K, A_{\Psi|K})_{\hat{\Psi}_B^p}$. Since S is finite, there are S-modules $(T_b^p)_{\hat{\Psi}_T^p|S}$ and $(U_b^p)_{\hat{\Psi}_U^p|S}$ such that

$$Z_b^p(K, A_{\Psi|K})_{\hat{\Psi}_Z^p|S} = B_b^p(K, A_{\Psi|K})_{\hat{\Psi}_B^p|S} \oplus (T_b^p)_{\hat{\Psi}_T^p|S} \tag{4.14}$$

and

$$C_b^p(K, A_{\Psi|K})_{\hat{\Psi}^p|S} = Z_b^p(K, A_{\Psi|K})_{\hat{\Psi}_Z^p|S} \oplus (U_b^p)_{\hat{\Psi}_U^p|S}, \tag{4.15}$$

where $\oplus$ denotes the direct sum of sub-S-modules (Ref. 26, Chap. XVIII, Theorem 1). The mapping

$$\beta: [f] \; (\mathrm{mod} B_b^p(K, A_{\Psi|K})^S) \mapsto [f] \; (\mathrm{mod} B_b^p(K, A_{\Psi|K}))$$

of $Z_b^p(K, A_{\Psi|K})^S / B_b^p(K, A_{\Psi|K})^S$ into $H_b^p(K, A_{\Psi|K})^S$ is an injective group homomorphism. It suffices to notice that if f, f' are in $Z_b^p(K, A_{\Psi|K})^S$, then $[f] = [f'] \; (\mathrm{mod} B_b^p(K, A_{\Psi|K}))$ implies $[f] = [f'] \; (\mathrm{mod} B_b^p(K, A_{\Psi|K})^S)$. We will show that β is surjective too. Let $f \in Z_b^p(K, A_{\Psi|K})$, and suppose $[f] \in H_b^p(K, A_{\Psi|K})^S$. This means that, for any $s \in S$, there is $h^{(s)} \in C_b^{p-1}(K, A_{\Psi|K})$ such that

$$\hat{\Psi}_Z^p(s) f = f + \delta h^{(s)}.$$

By virtue of (4.14) we have a (unique) decomposition

$$f = f_B + f_T,$$

where $f_B \in B_b^p(K, A_{\Psi|K})$ and $f_T \in T_b^p$. Moreover,

$$\hat{\Psi}_B^p(s) f_B + \hat{\Psi}_T^p(s) f_T = f_B + f_T + \delta h^{(s)}$$

implies

$$\hat{\Psi}_T^p(s) f_T = f_T$$

for all $s \in S$, i.e., $f_T \in Z_b^p(K, A_{\Psi|K})^S$. As

$$f_T \equiv f \; (\mathrm{mod} B_b^p(K, A_{\Psi|K})),$$

we conclude that β is surjective. We end the proof by showing that

$$B_b^p(K, A_{\Psi|K})^S = \delta C_b^{p-1}(K, A_{\Psi|K})^S.$$

For this purpose we consider $h \in C_b^{p-1}(K, A_{\Psi|K})$ such that $\delta h \in B_b^p(K, A_{\Psi|K})^S$.

By (4.15) there is a (unique) decomposition

$$h = h_Z + h_U,$$

where $h_Z \in Z_b^{p-1}(K, A_{\Psi|K})$ and $h_U \in U_b^{p-1}$. It follows that $h_U \in C_b^{p-1}(K, A_{\Psi|K})^S$.

In fact,

$$\delta(\hat{\Psi}^{p-1}(s) h - h) = 0$$

for all $s \in S$, and this implies

$$\delta(\hat{\Psi}_U^{p-1}(s) h_U - h_U) = 0,$$

whence

$$\hat{\Psi}_U^{p-1}(s) h_U = h_U$$

for all $s \in S$. As $\delta h_U = \delta h$, we conclude that

$$B_b^p(K, A_{\Psi|K})^S \subseteq \delta C_b^{p-1}(K, A_{\Psi|K})^S.$$

The inclusion

$$\delta C_b^{p-1}(K, A_{\Psi|K})^S \subseteq B_b^p(K, A_{\Psi|K})^S$$

is obvious. ■

Proof of Proposition 3: Let $f \in Z_b^2(K, A_{\Psi|K})$ and suppose $[f] \in H_b^2(K, A_{\Psi|K})^S$. By Lemma 3 there exists an element f' of $[f] \cap Z_b^2(K, A_{\Psi|K})^S$; hence $[f] \in H_b^2(K, A_{\Psi|K})'$ because $f_1 = f'$ and $f_2 = 0$ satisfy (i) and (ii) of Lemma 2. ■

A vector space over a field of characteristic 0 is divisible and torsion free; therefore we have the following.

Corollary: Let G, K, S, F, and A_Ψ be as in Proposition 3. Then

$$H_b^p(G, A_\Psi) \approx H_b^p(K, A_{\Psi|K})^S \approx Z_b^p(K, A_{\Psi|K})^S / \delta C_b^{p-1}(K, A_{\Psi|K})^S$$

for $p = 0, 1, 2$.

We emphasize the analogy of this result, based on the assumptions that S is finite and that A is a vector space over a field of characteristic 0, with a result in the cohomology theory of Lie algebras (Ref. 27, Theorem 1), where the role of S was played by a semisimple subalgebra.

Remark 1: If A_Ψ is an F-linear topological G-module, then the groups $H_b^p(G, A_\Psi)$ and $H_b^p(K, A_{\Psi|K})$ ($p \in \mathbf{Z}$) are (quotient) vector spaces over F and the isomorphisms in Lemma 3 and in the corollary to Proposition 3 are vector space isomorphisms.

Remark 2: Lemmas 2 and 3, Propositions 1, 2, and 3, and the corollary to Proposition 3 are also valid if we replace the Mackey-Moore by the Eilenberg-MacLane cohomology. Once the subscripts "b" have been taken away and "Borel mapping" has been replaced everywhere by "mapping," the statements and the proofs are verbatim the same. Obviously, in the Eilenberg-MacLane cohomology we obtain the same results also if we drop all the assumptions concerning the topology.

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APPENDIX A: BOREL, BAIRE, AND POLISH SPACES

Let E be a set. A *Borel structure* on E (or a σ-field of subsets of E) is a collection $\mathfrak{B}$ of subsets of E such that

(i) $E \in \mathfrak{B}$,

(ii) if $E' \in \mathfrak{B}$, then $E - E' \in \mathfrak{B}$,

(iii) if (E_n) is any sequence of elements of $\mathfrak{B}$, then $\bigcup_n E_n \in \mathfrak{B}$.

Let $\mathfrak{A}$ be any collection of subsets of E. The smallest

Borel structure on E containing $\mathfrak{A}$ is said to be the Borel structure generated by $\mathfrak{A}$. The set E endowed with a Borel structure $\mathfrak{B}$ is called a *Borel space* and the elements of $\mathfrak{B}$ are called the *Borel sets* of E. The concepts of induced Borel structure and Borel subspace (resp. product Borel structure and product Borel space, resp. quotient Borel structure and quotient Borel space) are defined in analogy with the corresponding topological concepts.[15,28] Let E and E' be Borel spaces. A mapping $f: E \to E'$ is said to be a *Borel mapping* if, for any Borel set B' of E', $f^{-1}(B')$ is a Borel set of E. Suppose now that E is a topological space and let $\mathfrak{C}$ be the collection of all closed sets of E. The set E endowed with the Borel structure generated by $\mathfrak{C}$ is called the Borel space associated with the topological space E. Whenever we refer to a topological space as a Borel space, we tacitly understand the associated Borel space. So we can freely speak of Borel mappings of a topological space into a topological space. Notice, in particular, that any continuous mapping is a Borel one. For details and results concerning Borel spaces and Borel mappings see Refs. 15, 17, 28.

A subset S of a topological space E is said to be *nowhere dense* (or *rare*) if $E - \overline{S}$ (the complement of the closure of S) is dense in E, and a subset M of E is said to be *meager* (or *of Baire I. category*) if it is the union of a countable family of nowhere dense sets. A topological space E such that $E - M$ is everywhere dense for each meager subset M of E is called a *Baire space*. Any locally compact space, as well as any metrizable space with a distance compatible with the topology and for which the space is complete, is a Baire space (Ref. 18, §5, Théorème 1).

A topological space P is said to be a *Polish space* if it is second countable, metrizable, and if there is a distance compatible with the topology and making P into a complete space. The product of a countable family of Polish spaces is Polish, as well as any closed subspace of a Polish space (Ref. 18, §6, Prop. 1). We say that a topological group G (resp. a topological G-module A_ψ) is a *Polish group* (resp. a *Polish G-module*) if the topological space G (resp. A) is Polish. In particular, any second countable locally compact group is Polish (Ref. 29, TG III, §3, Cor. 1 to Prop. 4 and Ref. 18, §3, Prop. 1). The quotient group of a Polish group by a closed normal subgroup is Polish. In fact it is metrizable and complete by Prop. 4, §3 of Ref. 18, and it is second countable because the canonical surjection is continuous and open.

APPENDIX B

1. THE COHOMOLOGY OF A COCHAIN COMPLEX

An Abelian group C^* (written additively) is called an (internally) **Z**-*graded group* if it is the direct sum of a family $(C^p)_{p\in\mathbf{Z}}$ of subgroups. We identify canonically C^* and the external direct sum $\bigoplus_{p\in\mathbf{Z}} C^p$. The elements of C^p are said to be the homogeneous elements of C^* of degree p. Let C'^* be also a **Z**-graded group and let $r \in \mathbf{Z}$. A group homomorphism $\alpha: C^* \to C'^*$ is said to be a **Z**-*graded group homomorphism of degree r* if $\alpha(C^p) \subseteq C'^{p+r}$ for all $p \in \mathbf{Z}$, and we denote $\alpha|(C^p \to C'^{p+r})$ by α^p. If $r = 0$, we say simply that α is a **Z**-graded group homomorphism. A *cochain complex* (of Abelian groups) is an ordered pair (C^*, δ), where C^* is a **Z**-graded group such that $C^p = \{0\}$ for all $p < 0$ and $\delta: C^* \to C^*$ (the *coboundary operator* of (C^*, δ)) is a **Z**-graded group homomorphism of degree 1 such that $\delta \circ \delta = 0$.

Then a homomorphism

$$\alpha: (C^*, \delta) \to (C'^*, \delta')$$

of cochain complexes is a **Z**-graded group homomorphism $\alpha: C^* \to C'^*$ satisfying

$$\alpha \circ \delta = \delta' \circ \alpha.$$

It is now clear what an exact sequence of cochain complexes is: a diagram

$$(C^*_{(1)}, \delta_{(1)}) \xrightarrow{\alpha_{(1)}} (C^*_{(2)}, \delta_{(2)}) \xrightarrow{\alpha_{(2)}} \cdots \xrightarrow{\alpha_{(n-1)}} (C^*_{(n)}, \delta_{(n)}),$$

where the $\alpha_{(i)}$ are homomorphisms of cochain complexes and

$$\mathrm{Ker}\,\alpha_{(i+1)} = \mathrm{Im}\,\alpha_{(i)} \quad \text{for } 1 \leqslant i \leqslant n-2.$$

A cochain complex (C'^*, δ') is said to be a *subcomplex* of (C^*, δ) if $C'^p \subseteq C^p$ for all $p \in \mathbf{Z}$ and if $\delta' = \delta \mid C'^*$.

Given a cochain complex (C^*, δ) we can define, for any $p \in \mathbf{Z}$, the (Abelian) group $Z^p = \mathrm{Ker}\,\delta^p$ of the *p-cochains* and the group $B^p = \mathrm{Im}\,\delta^{p-1}$ of the *p-coboundaries*. The quotient group $H^p = Z^p/B^p$ is said to be the *cohomology group of degree p* of (C^*, δ) and the family $(H^p)_{p\in\mathbf{Z}}$ (or equivalently $H^*(C^*, \delta) = \bigoplus_{p\in\mathbf{Z}} H^p$) is called the *cohomology* of (C^*, δ).

If $\alpha: (C^*, \delta) \to (C'^*, \delta')$ is a homomorphism of cochain complexes then, for any $p \in \mathbf{Z}$, $\alpha^p_Z = \alpha \mid (Z^p \to Z'^p)$ and $\alpha^p_B = \alpha \mid (B^p \to B'^p)$ are group homomorphisms. We denote by α^p_* the group homomorphism of H^p into H'^p deduced from α^p_Z by passing to the quotients. Given an exact sequence

$$\mathfrak{E}: 0 \longrightarrow (C'^*, \delta') \xrightarrow{\iota} (C^*, \delta) \xrightarrow{\pi} (C''^*, \delta'') \longrightarrow 0$$

of cochain complexes, one can define a **Z**-graded group homomorphism of degree 1

$$\delta_{\mathfrak{E}}: H^*(C''^*, \delta'') \to H^*(C'^*, \delta')$$

called the *connecting homomorphism for* $\mathfrak{E}$ (for a definition see Ref. 30, Chap. I, 2.1). Then $\delta^p_{\mathfrak{E}} = \delta_{\mathfrak{E}} \mid (H''^p \to H'^{p+1})$ is the connecting homomorphism of degree p.

Theorem: If

$$\mathfrak{E}: 0 \longrightarrow (C'^*, \delta') \xrightarrow{\iota} (C^*, \delta) \xrightarrow{\pi} (C''^*, \delta'') \longrightarrow 0$$

is an exact sequence of cochain complexes, then

$$0 \longrightarrow H'^0 \xrightarrow{\iota^0_*} H^0 \xrightarrow{\pi^0_*} H''^0 \xrightarrow{\delta^0_{\mathfrak{E}}} H'^1 \xrightarrow{\iota^1_*} \cdots$$

$$\cdots \xrightarrow{\delta^{p-1}_{\mathfrak{E}}} H'^p \xrightarrow{\iota^p_*} H^p \xrightarrow{\pi^p_*} H''^p \xrightarrow{\delta^p_{\mathfrak{E}}} H'^{p+1} \xrightarrow{\iota^{p+1}_*} \cdots$$

is an exact sequence of Abelian groups.

This theorem can be proved like Theorem 4.1, Chap. II of Ref. 14 (exact homology sequence). In order to obtain a proof for our case, it suffices to replace there homology by cohomology.

2. THE EILENBERG-MACLANE COHOMOLOGY

Let G be a group and let A_ψ be a G-module. A mapping $f: G^p \to A$ is said to be normalized if, for any $(g_1, \ldots, g_p) \in G^p$, $f(g_1, \ldots, g_p) = 0$ whenever $1 \in \{g_1, \ldots, g_p\}$. For any $p \in \mathbf{N}^*$, let $C^p(G, A_\psi)$ be the set of all normalized mappings of G^p into A. This set becomes an Abelian group by defining the addition as addition of values. For $p = 0$ let $C^0(G, A_\Psi) = A$, and put $C^p(G, A_\Psi) = \{0\}$ for all $p < 0$. Then

$$C^*(G, A_\Psi) = \bigoplus_{p \in \mathbf{Z}} C^p(G, A_\Psi)$$

is a Z-graded group. Consider the Z-graded group homomorphism δ of degree 1 of $C^*(G, A_\Psi)$ into itself such that, if $p > 0$λ

$$\delta f(g_1, \dots, g_{p+1}) = (-1)^{p+1} f(g_1, \dots, g_p) + \Psi(g_1) f(g_2, \dots, g_{p+1}) + \sum_{i=1}^{p} (-1)^i f(g_1, \dots, \hat{g}_i, g_i g_{i+1}, \dots, g_{p+1})$$

for all $f \in C^p(G, A_\Psi)$ and all $(g_1, \dots, g_{p+1}) \in G^{p+1}$ (here $\hat{g}_i$ means the omission of g_i). If $p = 0$, put

$$\delta f(g) = \Psi(g) f$$

for all $f \in A$ and all $g \in G$. One checks easily that $\delta \circ \delta = 0$; so $(C^*(G, A_\Psi), \delta)$ is a cochain complex called an *Eilenberg-MacLane cochain complex*. We use the same symbol δ, defined as above, for all Eilenberg-MacLane cochain complexes and for their subcomplexes, and so we write simply $C^*(G, A_\Psi)$ instead of $(C^*(G, A_\Psi), \delta)$. The groups Z^p, B^p, H^p, and $H^*(C^*(G, A_\Psi))$ of the cochain complex $C^*(G, A_\Psi)$ are usually denoted, respectively, by $Z^p(G, A_\Psi)$, $B^p(G, A_\Psi)$, $H^p(G, A_\Psi)$, and $H^*(G, A_\Psi)$.

APPENDIX C: THE BAER ADDITION

Let G be a Polish group, let A_Ψ be a Polish G-module, and let (E_1, ρ_1) and (E_2, ρ_2) be topological extensions of G by A_Ψ. Consider the (topological) subgroup

$$S = \{(e_1, e_2) \mid (e_1, e_2) \in E_1 \times E_2 \quad \text{and} \quad \rho_1(e_1) = \rho_2(e_2)\}$$

of the product group $E_1 \times E_2$. Since S is closed in $E_1 \times E_2$ (Ref. 29, TG I, §8, Prop. 2), it is a Polish group. Moreover,

$$A' = \{(a, -a) \mid a \in A\}$$

is a closed normal subgroup of S and so we can construct the Polish quotient group $E = S/A'$.

The group homomorphism

$$\rho' : (e_1, e_2) \mapsto \rho_1(e_1) = \rho_2(e_2)$$

of S onto G is continuous and open because the mapping $(e_1, e_2) \mapsto e_1$ of S onto E_1 is continuous and open. Moreover, ρ' is compatible with the equivalence relation defined by A' in S; so, by passing to the quotient, we get a continuous and open group homomorphism ρ of E onto G. Now let ι be the injective group homomorphism.

$$a \mapsto (a, 1)A'$$

of A into E. If ι' stands for the group isomorphism $a \mapsto (a, 1)$ of A onto $A \times \{1\}$, then $\iota = (\pi \mid A \times \{1\}) \circ \iota'$, where π is the canonical mapping of S onto S/A'. On the other hand, ι' and $\pi \mid (A \times \{1\} \to \iota(A))$ are homeomorphisms and therefore $\iota \mid (A \to \iota(A))$ is a homeomorphism too. We identify A and $\iota(A)$ through ι and notice that $\operatorname{Ker}\rho = A$. Furthermore, if σ_1 (resp. if σ_2) is a normalized section associated with ρ_1 (resp. with ρ_2), then we have that the mapping

$$\sigma : g \mapsto (\sigma_1(g), \sigma_2(g))A'$$

of G into E is a normalized section associated with ρ and that, for any $g \in G$ and any $a \in A$,

$$\sigma(g) a \sigma(g)^{-1} = (\sigma_1(g), \sigma_2(g))(a, 1)(\sigma_1(g)^{-1}, \sigma_2(g)^{-1})A' = (\Psi(g)a, 1)A' = \Psi(g)a.$$

Thus (E, ρ) is a topological extension of G by A_Ψ and the mapping

$$((E_1, \rho_1), (E_2, \rho_2)) \mapsto (E, \rho) = (E_1, \rho_1) \top (E_2, \rho_2)$$

is a law of composition on the set of all topological extensions of G by A_Ψ. Note that if f_1 (resp. if f_2) is the factor set of (E_1, ρ_1) (resp. of (E_2, ρ_2)) defined by σ_1 (resp. by σ_2), then $f = f_1 + f_2$ is the factor set of (E, ρ) defined by σ because

$$\sigma(g)\sigma(g')\sigma(gg')^{-1} = (f_1(g, g'), f_2(g, g'))A' = (f_1(g, g') + f_2(g, g'), 1)A' = f_1(g, g') + f_2(g, g')$$

for all $(g, g') \in G \times G$.

Exactly as in the case of extensions of groups without topology, one verifies[14] that the law $\top$ is commutative, associative, and compatible with the equivalence relation R defined by means of the commutative diagram (3.3) in the set of all topological extensions of G by A_Ψ. The *Baer addition* on $\operatorname{Ext}_t(G, A_\Psi)$ is then the quotient law of $\top$ by R, i.e., the law of composition

$$([(E_1, \rho_1)], [(E_2, \rho_2)]) \mapsto [(E_1, \rho_1)] + [(E_2, \rho_2)] = [(E_1, \rho_1) \top (E_2, \rho_2)].$$

Given a topological extension (E, ρ) of G by A_Ψ, we can consider the ordered pair (E^0, ρ^0), where E^0 is the opposite topological group of E (Ref. 29, TG III, §1, 1) and ρ^0 is the continuous and open group homomorphism $e \mapsto \rho(e^{-1})$ of E^0 onto G (with kernel A). So, (E^0, ρ^0) is a topological extension of G by A and one verifies, again as in the case of groups without topology, that it is an extension relative to Ψ. Furthermore,

$$[(E, \rho)] + [(E^0, \rho^0)] = [(A \times_\Psi G, \mathrm{pr}_2)].$$

In fact, put $(E, \rho) \top (E^0, \rho^0) = (\check{E}, \check{\rho})$ and consider the closed subgroup

$$\check{G} = \{(e^{-1}, e)A' \mid e \in E\}$$

of $\check{E}$. The mapping $\kappa = \check{\rho} \mid \check{G}$ is a topological group isomorphism of $\check{G}$ onto G because $\check{G}$ is a Polish group. Therefore, the group isomorphism

$$\gamma : (a, g) \mapsto a\kappa^{-1}(g)$$

of $A \times_\Psi G$ onto $\check{E}$ is a topological one. Moreover, it establishes the equivalence of $(A \times_\Psi G, \mathrm{pr}_2)$ and $(\check{E}, \check{\rho})$ (cf. Sec. 3) because $\gamma(a, 1) = a$ and $(\check{\rho} \circ \gamma)(a, g) = \mathrm{pr}_2(a, g)$ for all $a \in A$ and all $g \in G$. One easily verifies that

$$[(E, \rho)] + [(A \times_\Psi G, \mathrm{pr}_2)] = [(E, \rho)]$$

once we have noticed that, if $(E,\rho) \top (A \times_\Psi G, \mathrm{pr}_2) = (E',\rho')$, the mapping

$$(e, (0,\rho(e))A' \mapsto e$$

of E' into E is a topological group isomorphism. Summarizing, we have proven that $\mathrm{Ext}_t(G, A_\Psi)$, equipped with the Baer addition, is an Abelian group with neutral element $[(A \times_\Psi G, \mathrm{pr}_2)]$ and with

$$[(E,\rho)] = -[(E^0,\rho^0)].$$

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Coupling of space–time and electromagnetic gauge transformations

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A kind of topological extensions of a space–time group Q by an electromagnetic gauge group J are investigated in order to determine covariance groups of electrodynamics. Here Q stands for the Poincaré group, for the Galilei group, or for their neutral components, and J is the Abelian group of all real-valued functions of class C^m ($m \in \mathbb{N}$ or $m = \infty$) defined in space-time. The topological groups $J_\Phi f Q$ so obtained, already inportant in the study of charged particles in external electromagnetic fields, are analyzed and placed in the general context of combining different symmetry groups. They are characterized by a given operation Φ of Q on J and by factor sets f such that $f(q,q')$ is a constant gauge function for all $(q,q') \in Q \times Q$. It is shown that all these groups $J_\Phi f Q$ are topologically isomorphic to the external topological semidirect product of Q by J relative to Φ.

1. INTRODUCTION

According to the standard principles of relativistic mechanics and electrodynamics, the observables in the interaction with matter of a classical, i.e., nonquantized, electromagnetic field are covariants[1] of the operations of two groups, namely $\mathbf{P}_0$ (the connected component of the neutral element of the Poincaré group $\mathbf{P}$) and the electromagnetic gauge group J. It is also usually assumed that this still must be true if we are able to quantize the fields. So, we are interested in combining $\mathbf{P}_0$ and $\mathbf{J}$ into a single covariance group, i.e., in coupling space-time and electromagnetic gauge transformations. As this is a special case of quite a wide class of problems, we will put the present investigation in a more general frame by illustrating the guiding ideas with some well-known examples.

A natural way for coupling symmetries of different kinds is to construct a group in which they appear as ingredients. This can be done sometimes very easily in the case where these different symmetries can be made to operate on a given set.

As a first example we may mention the Poincaré group $\mathbf{P}$, which can be seen as a combination of the Lorentz group $\mathbf{L}$ and the group $\mathbf{T}$ of space-time translations. The elements of $\mathbf{L}$ and $\mathbf{T}$ are symmetries of relativistic physics and are transformations of the Minkowski space $\mathbf{M}$. The coupling arises by considering the set of all ordered pairs $p = (t, L)$ $(t \in \mathbf{T}, L \in \mathbf{L})$ of transformations of $\mathbf{M}$ (first L, then t) and by defining the products pp' as the result of successive transformations (first p', then p). This way leads uniquely to the Poincaré group $\mathbf{P}$ as the external topological semidirect product[2] of $\mathbf{L}$ by $\mathbf{T}$ relative to the natural operation of $\mathbf{L}$ on $\mathbf{T}$.

The coupling of Lorentz transformations and space-time translations is a minimal one, in the sense that $\mathbf{L}$ and $\mathbf{T}$ are canonically identified with subgroups of $\mathbf{P}$. However, in physics there are also nonminimal couplings of symmetries. This is the case in crystallography where, by coupling macroscopic point symmetries (which are orthogonal transformations forming the crystallographic point group K) and microscopic translations (forming the group U of lattice translations, also called primitive translations), one gets a space group G. Now, K may be canonically identified with a subgroup of G only if G is a so-called symmorphic space group.[3] For a nonsymmorphic space group this identification cannot be made.[3,4]

A symmorphic space group (resp. the Poincaré group) is obtained from an inessential extension[5] of K by U (resp. of $\mathbf{L}$ by $\mathbf{T}$), and so we can say that the coupling is inessential. In a nonsymmorphic space group the coupling is said to be essential, because such a space group is obtained from an essential extension of K by U. Note that, *a priori*, even with an inessential extension we could have the case where the crystallographic point group K is not canonically identified with a subgroup of the space group G and therefore get a nonminimal coupling. In fact, K is embedded in G by choosing a complete set of (right) coset representatives, and the answer to the relevant question if this arbitrariness gives rise to a nonminimal coupling depends on whether different sections[5] are physically equivalent or not. In the case of symmorphic space groups there is a physical equivalence of all sections and the coupling is minimal.[6]

Returning to our particular problem, we note that the electromagnetic gauge group can be seen as an internal symmetry group because gauge transformations do not act on space-time. Therefore, we have a particular case of the problem of combining space-time and internal symmetry groups.[7,8,9] Furthermore, even if the coupling is a minimal one, the group obtained is not purely of academic interest and can give rise to a deeper physical insight. This is shown by a well-known example: The study of the continuous unitary projective representations of $\mathbf{P}_0$ gives results which are unexpected if one considers $\mathbf{L}_0$ and $\mathbf{T}$ as two independent groups.

The construction adopted in this paper for combining $\mathbf{P}_0$ and J follows closely the one used for the combination of $\mathbf{L}$ and $\mathbf{T}$ into the Poincaré group $\mathbf{P}$. We take as electromagnetic gauge group J the Abelian group of three-times continuously differentiable mappings of the Minkowski space $\mathbf{M}$ into $\mathbf{R}$ (cf. Sec. 2). As both $\mathbf{P}_0$ and J operate in a well-known manner on the space of Maxwell potentials, we consider the set of all ordered pairs $g = (\lambda, p)(\lambda \in J, p \in \mathbf{P}_0)$ with an action on this space obtained by letting p act first and then λ. The new fact is that, by requiring that the set $J \times \mathbf{P}_0$ should form a group operating on the space of Maxwell potentials, we do not get a unique group as in the case of $\mathbf{P}$. Instead, we obtain a whole collection $\{J_{\Phi_0} f \mathbf{P}_0\}$ of groups characterized by the operation Φ_0 of $\mathbf{P}_0$ on J and by well-defined maps f of $\mathbf{P}_0 \times \mathbf{P}_0$ into J such that, for any $(p,p') \in \mathbf{P}_0 \times \mathbf{P}_0$, $f(p,p')$ is a constant gauge function.

All the groups $J_{\Phi_0} f \mathbf{P}_0$ are candidates as covariance groups of relativistic electrodynamics (classical and quantum). They are obtained from extensions of $\mathbf{P}_0$ by J_{Φ_0} with factor sets f (Ref. 5); therefore, one has to find all equivalence classes of such extensions, pick out the groups $J_{\Phi_0} f \mathbf{P}_0$ having a physical meaning, and partition these groups in classes of physically equivalent covariance groups. In the present paper this program is not completely realized. We hope to be able to do it in a subsequent publication.

We will restrict ourselves to consider only topological extensions of $\mathbf{P}_0$ by J_{Φ_0}, after having endowed J with an appropriate topology. There are strong reasons justifying this restriction. First of all, a group $J_{\Phi_0} f \mathbf{P}_0$ obtained from a nontopological extension could have a very complicated structure. Without the support of topology we are not able to discuss its mathematical properties, and therefore also unable to find the classes of physically equivalent covariance groups. Secondly, in all the examples we know of combination of different symmetry groups, only topological groups appear. At the present state of knowledge, the physical relevance of nontopological group extensions seems to be very doubtful.

The main result of this paper is that any topological extension of $\mathbf{P}_0$ by J_{Φ_0} with a factor set f such that $f(p,p')$ is a constant mapping for all $(p,p') \in \mathbf{P}_0 \times \mathbf{P}_0$ is inessential (and therefore one can say that the corresponding coupling of space-time and electromagnetic gauge transformations is inessential). This means that the groups obtained from such extensions are topologically isomorphic (i.e., isomorphic and homeomorphic) to $J \times_{\Phi_0} \mathbf{P}_0$, the external topological semidirect product of $\mathbf{P}_0$ by J relative to Φ_0. Note that in the minimal coupling case one precisely gets a topological semidirect product.

Even at the present stage, and without going into details, it is important to think of the physical implications of the (possible) existence of covariance groups obtained by a nonminimal coupling of space-time and electromagnetic gauge transformations. One can argue that in such a case a relativistically non-covariant formulation of electrodynamics would be required.

In this paper, calculations are performed not only for $\mathbf{P}_0$ but also for the Poincaré group $\mathbf{P}$ and for the corresponding nonrelativistic space-time groups, namely for the Galilei group $\mathbf{G}$ and for $\mathbf{G}_0$, the connected component of its neutral element. Moreover, we consider other possibilities in the choice of J. In particular, we take as electromagnetic gauge group the (Abelian) group of all the mappings of class C^m ($m \in \mathbf{N}$ or $m = \infty$) of $\mathbf{M}$ into $\mathbf{R}$ with suitable operations of the space-time groups on it. Beside the intrinsic interest they represent, some of these cases also play a role in problems of charged particles in external electromagnetic fields.[10] However, the result that we get is always the same, namely groups which are topologically isomorphic to external topological semidirect products of the space-time groups by the electromagnetic gauge groups.

Our paper is organized as follows: In Sec. 2 we derive the rule for the combination of $\mathbf{P}_0$ and J. The associated extension problem is formulated in precise mathematical terms in Sec. 3 and generalized by considering different space-time and electromagnetic gauge groups with appropriate operations. We prove that all the topological group extensions considered are inessential. Some comments on recent publications on related topics are given in Sec. 4, where the analogies with our work are emphasized. In the Appendix we prove that the operation Φ of Q on J is topological.

For notations and definitions concerning the cohomology of groups and group extensions the reader is referred to Ref. 5. Whenever a finite-dimensional vector space is considered it has to be understood as a topological vector space with the canonical topology.

2. THE GROUP EXTENSION ASSOCIATED WITH A COMBINATION OF P_0 AND J

In order to state our problem in a proper mathematical form, we have to be precise on the electromagnetic gauge functions that we will consider. Let $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$ ($m \in \mathbf{N}$ or $m = \infty$) stand for the vector space over $\mathbf{R}$ of all the mappings of class C^m of $\mathbf{R}^4$ into $\mathbf{R}$. In other words, the elements of $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$ are continuous functions if $m = 0$, m-times continuously differentiable functions if $m > 0$, and indefinitely differentiable functions if $m = \infty$. We equip $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$ with the C^m-topology (cf. Sec. 3), and so it becomes a topological vector space. Basing our choice on the example of a classical electromagnetic field, we take as electromagnetic gauge group J the Abelian topological group $\mathcal{C}^3_{\mathbf{R}}(\mathbf{R}^4)$ [identified with $\mathcal{C}^3_{\mathbf{R}}(\mathbf{M})$ in an obvious way]. This preference is rather arbitrary: There are a lot of more or less reasonable candidates for the electromagnetic gauge group and a definitive choice may be made only *a posteriori*. Using $\mathcal{C}^3_{\mathbf{R}}(\mathbf{R}^4)$ we are able to put forward some ideas and draw some conclusions; however, our results apply to many other possible choices of the gauge group (cf. the end of this section and Remark 2 of Sec. 3).

Again from the example of a classical electromagnetic field, we get a scalar operation

$$\Phi_0 : \mathbf{P}_0 \to \mathrm{Aut}(J)$$

of $\mathbf{P}_0$ on J such that, for all $\lambda \in J$ and all $x \in \mathbf{R}^4$,

$$(\Phi_0(p)\lambda)(x) = \lambda(p^{-1} \cdot x), \tag{2.1}$$

where the dot stands for the natural operation of $\mathbf{P}_0$ on $\mathbf{R}^4$.

Consider the vector space $\mathcal{C}^2(\mathbf{R}^4;\mathbf{R}^4)$ of all the mappings of class C^2 of $\mathbf{R}^4$ into $\mathbf{R}^4$; endowed with the C^2-topology it is a topological vector space. The group $\mathbf{P}_0$ operates on $\mathcal{C}^2(\mathbf{R}^4;\mathbf{R}^4)$ by the law $(p,\alpha) \mapsto p\cdot\alpha = (t,L)\cdot\alpha$ such that

$$(p\cdot\alpha)_\mu(x) = \Lambda(L^{-1})^\nu_\mu\, \alpha_\nu(p^{-1}\cdot x) \quad (0 \leqslant \mu \leqslant 3) \tag{2.2}$$

for all $x \in \mathbf{R}^4$, where Λ is the natural operation of $\mathbf{L}_0$ on $\mathbf{R}^4$. The Maxwell potentials, i.e., the solutions of class C^2 of Maxwell equations, belong to $\mathcal{C}^2(\mathbf{R}^4;\mathbf{R}^4)$. Let us denote by $\mathbf{MP}$ the subspace of $\mathcal{C}^2(\mathbf{R}^4;\mathbf{R}^4)$ (with the induced topology) of all Maxwell potentials. This topological space is stable for the operation of $\mathbf{P}_0$ on $\mathcal{C}^2(\mathbf{R}^4;\mathbf{R}^4)$ given by (2.2), and the electromagnetic gauge group J operates on it by

$$(\lambda, A) \mapsto \lambda \cdot A = A + \partial\lambda. \tag{2.3}$$

Now we proceed as in the case of the combination of the Lorentz and space-time translation groups into $\mathbf{P}$:

(i) We form the ordered pairs (λ, p) with $\lambda \in J$ and $p \in \mathbf{P}_0$;

(ii) We define an action of (λ, p) on **MP** by

$$((\lambda, p), A) \mapsto (\lambda, p)\cdot A = p\cdot A + \partial\lambda; \qquad (2.4)$$

(iii) We require that the following conditions be satisfied:

(1) The product set

$$J \times \mathbf{P}_0 = \{(\lambda, p) \mid \lambda \in J \text{ and } p \in \mathbf{P}_0\}$$

is a topological group operating on **MP** by (2.4);

(2) $(\lambda, 1)(0, p) = (\lambda, p)$

and

$(0, p)(\lambda, 1) = (\Phi_0(p)\lambda, p)$ for all

$\lambda \in J$ and all $p \in \mathbf{P}_0$;

(3) $\{(\lambda, 1) \mid \lambda \in J\}$ is a subgroup identified with J through the topological group isomorphism $(\lambda, 1) \mapsto \lambda$;

(4) The group homomorphism $(\lambda, p) \mapsto p$ is continuous and open.

The neutral element of the new group is $(0, 1)$ and its multiplication is such that, for any $A \in \mathbf{MP}$,

$$((\lambda, p)(\lambda', p'))\cdot A = (\lambda, p)\cdot((\lambda', p')\cdot A). \qquad (2.5)$$

From (2.5) we get the law of composition[10]

$$(\lambda, p)(\lambda', p') = (\lambda + \Phi_0(p)\lambda' + c, pp').$$

Here, $c \in J$ is a constant mapping arising because, in (2.3), $\lambda\cdot A = (\lambda + c)\cdot A$. *A priori*, c depends on λ, λ', p, p'; however, it is easy to see that it depends only on p and p' [using (iii), one gets $c = (0, p)(0, p')(0, pp')^{-1}$]. So we can write

$$(\lambda, p)(\lambda', p') = (\lambda + \Phi_0(p)\lambda' + f(p, p'), pp'), \qquad (2.6)$$

where, for all p, p' in $\mathbf{P}_0$,

$$f : \mathbf{P}_0 \times \mathbf{P}_0 \to J$$

is such that $f(p, p')$ is a constant mapping and

$$f(p, 1) = f(1, p) = 0.$$

In addition, f satisfies a relation imposed by the associativity of the group multiplication [which implies that $f \in Z^2(\mathbf{P}_0, J_{\Phi_0})$]; the class of admissible f is also restricted by the requirement that the group $J_{\Phi_0} f \mathbf{P}_0$ of the ordered pairs (λ, p) with multiplication (2.6) should be a topological one. Note that, for any $p \in \mathbf{P}_0$ and any $\lambda \in J$:

$$(\Phi_0(p)\lambda, 1) = (0, p)(\lambda, 1)(0, p)^{-1}.$$

From the classical case just described we abstract the rule for the combination of $\mathbf{P}_0$ and the electromagnetic gauge group $J = \mathcal{C}^3_{\mathbf{R}}(\mathbf{R}^4)$: We unite $\mathbf{P}_0$ and J into a topological group $J_{\Phi_0} f \mathbf{P}_0$ whose elements are the ordered pairs $(\lambda, p)(\lambda \in J,\ p \in \mathbf{P}_0)$ and the law of composition is given by (2.6). The values of the mapping f of $\mathbf{P}_0 \times \mathbf{P}_0$ into J are assumed to be constant mappings of $\mathbf{R}^4$ into $\mathbf{R}$, and the mappings $\iota : \lambda \mapsto (\lambda, 1)$ of J into $J_{\Phi_0} f \mathbf{P}_0$ and $\rho : (\lambda, p) \mapsto p$ of $J_{\Phi_0} f \mathbf{P}_0$ onto $\mathbf{P}_0$ are assumed to be continuous group homomorphisms with ι closed and ρ open.

In the next section we will show that the ordered pairs $(J_{\Phi_0} f \mathbf{P}_0, \rho)$ are topological extensions of $\mathbf{P}_0$ by J relative to Φ_0, and so we shall be led to solve the problem of finding such extensions. The result that we shall get is very simple: For any admissible f, $J_{\Phi_0} f \mathbf{P}_0$ is topologically isomorphic to $J_{\Phi_0} 0 \mathbf{P}_0 = J \times_{\Phi_0} \mathbf{P}_0$. Actually, this will come out as a particular case of a more general extension problem. The generalization is threefold:

(a) We take an arbitrary group $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$ ($m \in \mathbf{N}$ or $m = \infty$) as a possible electromagnetic gauge group J;

(b) In the nonrelativistic case we use $\mathbf{G}_0$ and the appropriate operation on J instead of $\mathbf{P}_0$ and Φ_0;

(c) Together with $\mathbf{P}_0$ and $\mathbf{G}_0$ we consider $\mathbf{P}$ (resp. $\mathbf{G}$) and a class of operations of $\mathbf{P}$ (resp. $\mathbf{G}$) on J which generalize Φ_0.

The detail of this problem will be given in the next section.

3. THE INESSENTIAL COUPLING OF SPACE-TIME AND ELECTROMAGNETIC GAUGE TRANSFORMATIONS

In the previous section we said that $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$ ($m \in \mathbf{N}$ or $m = \infty$), endowed with the C^m-topology, is a topological vector space. Let us now give some details about the C^m-topology.[11,12,13,14] Consider a 4-multi-index $r = (r_0, r_1, r_2, r_3) \in \mathbf{N}^4$ of total degree $|r| = r_0 + r_1 + r_2 + r_3$. Let D^r, $|r| > 0$, stand for the partial differentiation operator

$$\frac{\partial^{|r|}}{(\partial x^0)^{r_0}(\partial x^1)^{r_1}(\partial x^2)^{r_2}(\partial x^3)^{r_3}}$$

and let D^0 be the identity mapping. There exists an increasing sequence $(K_l)_{l\in\mathbf{N}}$ of compact subsets of $\mathbf{R}^4$ such that $\mathbf{R}^4 = \bigcup_{l\in N} K_l$ and, for any $l \in \mathbf{N}$, $K_l \subset \mathring{K}_{l+1}$ (the interior of K_{l+1}). For each pair l, s of integers with $1 \geq 0$, $0 \leq s \leq m$ if $m \in \mathbf{N}$ and $s \geq 0$ if $m = \infty$, the mapping

$$p_{s,l} : \lambda \mapsto \sup_{|r| \leq s, x \in K_l} |D^r\lambda(x)|$$

of $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$ into $\mathbf{R}$ is a seminorm. The topology defined by the family of seminorms $(p_{s,l})$ is the C^m-topology. Let I be the index set of the family $(p_{s,l})$. The collection $\mathfrak{S}_m$ of all the sets

$$W_m((\alpha_i); \epsilon) = \{\lambda \mid \lambda \in \mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4) \text{ and } p_{\alpha_i}(\lambda) < \epsilon \text{ for } 1 \leq i \leq N\}, \qquad (3.1)$$

where $(\alpha_i)_{1\leq i\leq N}$ is any finite family of elements of I and ϵ is any real number greater than 0, is a fundamental system of neighborhoods of 0 in $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$.

Equipped with the C^m-topology, $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$ ($m \in \mathbf{N}$ or $m = \infty$) is a Fréchet space, i.e., a locally convex metrizable and complete topological vector space; moreover it is separable. In fact, $\mathcal{C}^m_{\mathbf{C}}(\mathbf{R}^4)$ is separable by (12.14.6.

2) of Ref. 11 and by (17.1.2) of Ref. 12, and the real topological vector space underlying $\mathcal{C}_{\mathbf{C}}^{m}(\mathbf{R}^4)$ is the topological direct sum

$$\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4) \oplus {}_t i\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4).$$

Since a separable metrizable topological space is second countable, $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ is Polish (see Appendix A of Ref. 5).

Now, consider a topological linear operation ϕ of a topological group Q on the vector space $\mathbf{R}$ such that $\phi(Q_0) = \{\mathrm{Id}_{\mathbf{R}}\}$, where Q_0 is the connected component of the neutral element of Q. If Q/Q_0 is a finite group, the condition that ϕ is topological is redundant. If ψ is any given linear topological operation of Q on $\mathbf{R}^4$, we can define a linear operation Φ of Q on $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ ($m \in \mathbf{N}$ or $m = \infty$) such that

$$(\Phi(q)\lambda)(x) = \phi(q)\lambda(\psi(q^{-1})x) \tag{3.2}$$

for all $\lambda \in \mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ and all $x \in \mathbf{R}^4$. In the Appendix we prove that if Q is second countable and locally compact, then Φ is topological. Note that if $Q = \mathbf{P}_0$, if $m = 3$, and if ψ is the natural operation of $\mathbf{P}_0$ on $\mathbf{R}^4$, then Φ coincides with the operation Φ_0 defined by (2.1). If $Q = \mathbf{P}$ (resp. $Q = \mathbf{G}$), if $m = 3$, and if ψ is again the natural operation of $\mathbf{P}$ (resp. of $\mathbf{G}$) on $\mathbf{R}^4$, then the operation Φ with $\phi(q) = -1$ for all antichronous q and $\phi(q) = 1$ for all orthochronous q is the one occuring in the invariance group problem considered by Janner and Janssen[10] (see Sec. 4).

In the sequel, we will determine the topological extensions (G,ρ) of the Polish group $Q \in \{\mathbf{P}_0, \mathbf{P}, \mathbf{G}_0, \mathbf{G}\}$ by the Polish group $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ ($m \in \mathbf{N}$ or $m = \infty$) relative to the topological operation Φ of Q on $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ defined by (3.2) and satisfying the following condition:

(RE) There is a normalized Borel section σ associated with ρ such that, if f is the factor set defined by σ, then $f(q,q') \in \mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ is a constant mapping of $\mathbf{R}^4$ into $\mathbf{R}$ for all $(q,q') \in Q \times Q$.

The restriction (RE) is suggested by the results of Sec. 2. As was mentioned at the end of that section, the ordered pairs $(J_{\Phi_0} f \mathbf{P}_0, \rho)$ are topological extensions of $\mathbf{P}_0$ by J_{Φ_0}. In fact, $\mathbf{P}_0$ and J are Polish groups, Φ_0 is topological, and the mappings $\rho:(\lambda,p) \mapsto p$ and $\iota:\lambda \mapsto (\lambda,1)$ are assumed to be continuous, with ρ open and ι closed. Note that the mapping $\sigma: p \mapsto (0,p)$ of $\mathbf{P}_0$ into $J_{\Phi_0} f\mathbf{P}_0$ is a normalized section associated with ρ and that f is the factor set defined by σ. Remembering that $f \in Z^2(\mathbf{P}_0, J_{\Phi_0})$, that $f(p,p') \in J$ is a constant mapping for all $(p,p') \in \mathbf{P}_0 \times \mathbf{P}_0$, and using Theorem 2 of Ref. 5, it is easy to prove the existence of an element f' of $Z_b^2(\mathbf{P}_0, J_{\Phi_0})$ which is in the same equivalence class of f modulo $B^2(\mathbf{P}_0, J_{\Phi_0})$ and is such that $f'(p,p')$ too is a constant mapping for all $(p,p') \in \mathbf{P}_0 \times \mathbf{P}_0$. It suffices to notice that

$$\{(\lambda,p) \mid (\lambda,p) \in J_{\Phi_0} f\mathbf{P}_0 \text{ and } \lambda \text{ constant}\}$$

is a closed subgroup of $J_{\Phi_0} f\mathbf{P}_0$ and hence Polish.

Summarizing, we are faced with the following problem:

(PR) Find the topological extensions (G,ρ) of Q by $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi$ ($m \in \mathbf{N}$ or $m = \infty$) satisfying (RE), where $Q \in \{\mathbf{P}_0, \mathbf{P}, \mathbf{G}_0, \mathbf{G}\}$ and Φ is defined by (3.2).

In the sequel we will apply ourselves to solve this problem, and Q and Φ will be always assumed as in (PR).

First, notice that if a topological extension (G,ρ) of Q by $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi$ satisfies condition (RE), then any topological extension of Q by $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi$ equivalent to (G,ρ) satisfies (RE) too. Thus, we have to find the subgroup of $\mathrm{Ext}_t(Q, \mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi)$

$$\mathrm{Ext}_t^{\mathrm{RE}}(Q, \mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi) = \{[(G,\rho)] \mid [(G,\rho)] \in \mathrm{Ext}_t(Q, \mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi) \text{ and } (G,\rho) \text{ satisfies (RE)}\}.$$

For this purpose we need some preliminary results.

A. An exact sequence of Polish Q-modules

Consider the following mappings:

(1) The injection $\iota: r \mapsto \lambda_r$ of $\mathbf{R}$ into $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ such that

$$\lambda_r(x) = r \quad \text{for all } x \in \mathbf{R}^4;$$

(2) The (continuous) canonical mapping π of $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ onto the (topological) quotient vector space $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)/\iota(\mathbf{R})$;

(3) The unique linear operation Φ' of Q on $\mathbf{R}$ which makes the following diagram commutative for each $q \in Q$:

$$\begin{array}{ccc} \mathbf{R} & \xrightarrow{\iota} & \mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4) \\ {\scriptstyle \Phi'(q)}\downarrow & & \downarrow{\scriptstyle \Phi(q)} \\ \mathbf{R} & \xrightarrow[\iota]{} & \mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4). \end{array}$$

Note that $\Phi' = \phi$;

(4) The quotient of Φ, i.e., the linear operation Φ'' of Q on $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)/\iota(\mathbf{R})$ such that

$$(q, \pi(\lambda)) \mapsto \Phi''(q)\pi(\lambda) = \pi(\Phi(q)\lambda).$$

Thus $(\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)/\iota(\mathbf{R}))_{\Phi''}$ is the quotient Q-module $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi/\iota(\mathbf{R}_{\Phi'})$.

Lemma: Let Q and $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi$ be as in (PR), and let $\iota, \pi, \Phi', \Phi''$ be defined by (1)-(4). The diagram

$$\mathfrak{E}: 0 \to \mathbf{R}_{\Phi'} \xrightarrow{\iota} \mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)_\Phi \xrightarrow{\pi} (\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)/\iota(\mathbf{R}))_{\Phi''} \to 0$$

is an exact sequence of Polish Q-modules.

Proof: The diagram $\mathfrak{E}$ is exact by definition. The bijective linear mapping $r \mapsto \iota(r)$ of $\mathbf{R}$ onto $\iota(\mathbf{R})$ is a homeomorphism because $\mathbf{R}$ is finite-dimensional. Moreover, $\iota(\mathbf{R})$ is closed in $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ [Ref. 11, (12.13.2)]; so ι is a closed continuous mapping and Φ' is topological. As π is open, the operation Φ'' is topological too (Ref. 2, TG III, Sec. 2, Prop. 11). Finally, $\mathbf{R}$ and $\iota(\mathbf{R})$ are Polish spaces, as well as $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4)$ and the quotient space $\mathcal{C}_{\mathbf{R}}^{m}(\mathbf{R}^4/\iota(\mathbf{R})$ (see Appendix A of Ref. 5).

B. The cohomology group $H_b^2(Q, \mathbf{R}_\phi)$

Let ϕ be the same mapping as in (3.2), i.e., a continuous (linear) representation of Q on $\mathbf{R}$ such that $\phi(Q_0) = \{\mathrm{Id}_{\mathbf{R}}\}$. Consider the subgroup $V = \{e, \bar{e}, e', \bar{e}'\}$ of $Q \neq Q_0$,

Table I. Character χ_i of the representation ξ_i of V on $\mathbf{R}$ ($1 \leq i \leq 4$)

$\chi_i \backslash v$	e	$\bar{e}$	e'	$\bar{e}'$
χ_1	1	1	1	1
χ_2	1	1	−1	−1
χ_3	1	−1	1	−1
χ_4	1	−1	−1	1

where $e(=1)$ is the neutral element, $\bar{e}$ is the space inversion, e' is the time inversion, and $\bar{e}'$ is the space-time inversion. It is well known that Q is a Lie group and that $Q \neq Q_0$ is the topological semidirect product of V by Q_0. The characters of the representations of V on $\mathbf{R}$ are given in Table I. Without going into details, we show how the cohomology group $H^2_b(Q, \mathbf{R}_\phi)$ is determined using the following three results:

(i) Let G be a locally compact second countable group, let K be a closed normal subgroup of G, and let A_Ψ be a locally compact second countable topological G-module. Then, there exists an exact sequence of groups[15]

$$0 \longrightarrow H^1_b(G/K, (A^K)_{\check{\Psi}}) \xrightarrow{\inf^1} H^1_b(G, A_\Psi) \xrightarrow{\mathrm{res}^1} H^1_b(K, A_{\Psi|K})^G$$

$$(K, A_{\Psi|K})^G \xrightarrow{\mathrm{tg}^1} H^2_b(G/K, (A^K)_{\check{\Psi}}) \xrightarrow{\inf^2} H^2_b(G, A_\Psi), \quad (3.3)$$

where

$$\check{\Psi}: G/K \to \mathrm{Aut}(A^K)$$

is the topological operation with the law

$$(Kg, a) \mapsto \check{\Psi}(Kg)a = \Psi(g)a.$$

Here inf, res, and tg denote, respectively, the inflation, restriction, and transgression group homomorphisms. For a definition of these mappings see, for instance, Ref. 16, Chap. XI, Sec. 9. The exact sequence (3.3) is called the *inflation-restriction sequence*.

(ii) Let $\tilde{Q}_0$ be the universal covering group of Q_0 and let $L(\tilde{Q}_0)$ be its Lie algebra. Denote by 1 a trivial group operation and by 0 a trivial Lie algebra operation. Applying Theorem 4.1 and Theorem 5.1 of Ref. 17 to the simply connected Lie group $\tilde{Q}_0$, we see that $H^2_c(\tilde{Q}_0, \mathbf{R}_1)$ and the Chevalley-Eilenberg cohomology space[18] $H^2(L(\tilde{Q}_0), \mathbf{R}_0)$ are isomorphic vector spaces. Then, using the result of Mackey mentioned in Remark 1, Sec. 3 of Ref. 5 and Theorem 3.2 of Ref. 19, one can easily show that

$$H^2_b(\tilde{Q}_0, \mathbf{R}_1) \approx H^2(L(\tilde{Q}_0), \mathbf{R}_0) \quad (3.4)$$

(vector space isomorphism).

(iii) Take $Q = \mathbf{G}$ and consider the usual identification (choice of a coordinate system) of each element g of $\mathbf{G}$ with a 5-tuple $(\epsilon_g, t^0_g, \mathbf{t}_g, \mathbf{v}_g, O_g)$, where $\epsilon_g \in \{1, -1\}$, $t^0_g \in \mathbf{R}$, $\mathbf{t}_g \in \mathbf{R}^3$, $\mathbf{v}_g \in \mathbf{R}^3$, $O_g \in \mathbf{O}(3, \mathbf{R})$ are, respectively, the time inversion, time translation, space translation, Galilean boost, and orthogonal transformation parameters. Let $f \in C^2_b(\mathbf{G}, \mathbf{R}_\phi)$ [actually $f \in C^2_c(\mathbf{G}, \mathbf{R}_\phi)$] be given by

$$f(g, g') = \chi(gg')\mathbf{t}_g \cdot O_g\mathbf{v}_{g'} - t^0_g(\tfrac{1}{2}\mathbf{v}^2_{g'} + \chi(g')\mathbf{v}_g \cdot O_g\mathbf{v}_{g'}), \quad (3.5)$$

where the dot denotes the inner product on $\mathbf{R}^3$ and χ is the character of ϕ. If $\phi = \phi_2$ (see Tables I and II), then[10,17] $f \in Z^2_b(\mathbf{G}, \mathbf{R}_{\phi_2})$ and the vector space

$$H_f(\mathbf{G}) = \{\lambda[f] \,|\, \lambda \in \mathbf{R}\} \approx \mathbf{R}$$

is a subspace of $H^2_b(\mathbf{G}, \mathbf{R}_{\phi_2})$. Analogously, the vector space

$$H_f(\mathbf{G}_0) = \{\lambda[f_0] \,|\, \lambda \in \mathbf{R} \quad \text{and} \quad f_0 = f\,|\mathbf{G}_0 \times \mathbf{G}_0\} \approx \mathbf{R}$$

is a subspace of $H^2_b(\mathbf{G}_0, \mathbf{R}_1)$.

Table II. Cohomology group $H^2_b(Q, \mathbf{R}_\phi)(Q \in \{\mathbf{P}_0, \mathbf{P}, \mathbf{G}_0, \mathbf{G}\}; \phi \in \{\phi_1, \phi_2, \phi_3, \phi_4\}$, where $\phi_i(Q_0) = \{\mathrm{Id}_{\mathbf{R}}\}$ and $\phi_i | V = \xi_i \ (1 \leq i \leq 4))$

$H^2_b(\mathbf{P}_0, \mathbf{R}_1)$	$\{0\}$			
$H^2_b(\mathbf{G}_0, \mathbf{R}_1)$	$\approx \{\mathbf{R}\}$			
	ϕ_1	ϕ_2	ϕ_3	ϕ_4
$H^2_b(\mathbf{P}, \mathbf{R}_{\phi_i})$	$\{0\}$	$\{0\}$	$\{0\}$	$\{0\}$
$H^2_b(\mathbf{G}, \mathbf{R}_{\phi_i})$	$\{0\}$	$\approx \mathbf{R}$	$\{0\}$	$\{0\}$

Now we can determine $H^2_b(Q, \mathbf{R}_\phi)$(cf. Table II) as follows. Suppose first $Q = Q_0$ and consider the inflation-restriction sequence (3.3) with $G = \tilde{Q}_0$, $K = Z(\tilde{Q}_0)$ (the center of $\tilde{Q}_0$), $A = \mathbf{R}$, and Ψ the trivial operation. As $Z(\tilde{Q}_0)$ is finite of order 2,

$$H^1_b(Z(\tilde{Q}_0), \mathbf{R}_1) = \{0\}$$

(Ref. 16, Chap. IV, Corollary 5.4) and $\inf^2$ is injective. On the other hand,[17,20,21]

$$H^2(L(\tilde{\mathbf{P}}_0), \mathbf{R}_0) = \{0\}$$

and

$$H^2(L(\tilde{\mathbf{G}}_0), \mathbf{R}_0) \approx \mathbf{R};$$

therefore, by (3.4),

$$H^2_b(\mathbf{P}_0, \mathbf{R}_1) = \{0\}$$

and there exists an injective vector space homomorphism of $H^2_b(\mathbf{G}_0, \mathbf{R}_1)$ into $\mathbf{R}$. From (iii) it follows that

$$H^2_b(\mathbf{G}_0, \mathbf{R}_1) = H_f(\mathbf{G}_0) \approx \mathbf{R}.$$

If $Q \in \{\mathbf{P}, \mathbf{G}\}$, the result of Table II is obtained by application of the corollary to Proposition 3 of Ref. 5. We get immediately

$$H^2_b(\mathbf{P}, \mathbf{R}_\phi) = \{0\}.$$

Let $Q = \mathbf{G}$. It suffices to check that, if $f_0 = f\,|\mathbf{G}_0 \times \mathbf{G}_0$ with $f \in C^2_b(\mathbf{G}, \mathbf{R}_\phi)$ given by (3.5) and if $\phi = \phi_2$, then $f_0 \in Z^2_b(\mathbf{G}_0, \mathbf{R}_1)^V$, while if $\phi = \phi_1$

$$\hat{\phi}^2_Z(e')f_0 = \hat{\phi}^2_Z(\bar{e}')f_0 = -f_0,$$

if $\phi = \phi_3$

$$\hat{\phi}^2_Z(\bar{e})f_0 = \hat{\phi}^2_Z(e')f_0 = -f_0,$$

and if $\phi = \phi_4$

$$\hat{\phi}^2_Z(\bar{e})f_0 = \hat{\phi}^2_Z(\bar{e}')f_0 = -f_0.$$

Thus, in the case where $\phi = \phi_2$,

$$H^2_b(\mathbf{G}, \mathbf{R}_\phi) = H_f(\mathbf{G}) \approx \mathbf{R},$$

and in the case where $\phi \in \{\phi_1, \phi_3, \phi_4\}$,

$$H^2_b(\mathbf{G}, \mathbf{R}_\phi) = \{0\}.$$

C. The group $\mathrm{Ext}^{\mathrm{RE}}_t(Q, \mathfrak{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi)$

Equipped with the results of the subsections A and B, we now can solve (**PR**).

Theorem: If Q and $\mathfrak{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi$ are as in (PR), then

$$\mathrm{Ext}^{\mathrm{RE}}_t(Q, \mathfrak{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi) = \{0\}.$$

Proof: By the corollary to Theorem 1 of Ref. 5, and on account of the lemma proved above, the following diagram is an exact sequence of groups:

$$\cdots \xrightarrow{\delta^1 \tilde{\mathfrak{E}}_b} H_b^2(Q, \mathbf{R}_{\Phi'}) \xrightarrow{(\tilde{\iota}_b)^2_*} H_b^2(Q, \mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi)$$

$$\xrightarrow{(\tilde{\pi}_b)^2_*} H_b^2(Q, (\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)/\iota(\mathbf{R}))_{\Phi''}) \xrightarrow{\delta^2 \tilde{\mathfrak{E}}_b} \cdots.$$

Let (G, ρ) be any topological extension of Q by $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi$ satisfying (RE), and let α_b be the injective group homomorphism of $\mathrm{Ext}_t(Q, \mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi)$ into $H_b^2(Q, \mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi)$ of Theorem 2 of Ref. 5. Then

$$((\tilde{\pi}_b)^2_* \circ \alpha_b)([G, \rho]) = 0,$$

i.e.,

$$\alpha_b([(G, \rho)]) \in \mathrm{Ker}(\tilde{\pi}_b)^2_* = \mathrm{Im}\,(\tilde{\iota}_b)^2_*.$$

If $Q \in \{\mathbf{P}_0, \mathbf{P}\}$, or if $Q = \mathbf{G}$ with $\Phi' \in \{\phi_1, \phi_3, \phi_4\}$, we conclude that

$$\mathrm{Ext}^{\mathrm{RE}}_t(Q, \mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi) = \{0\}$$

using the results of Table II. If $Q = \mathbf{G}_0$, take $f_0 = f \mid \mathbf{G}_0 \times \mathbf{G}_0$ with $f \in C_b^2(\mathbf{G}, \mathbf{R}_{\Phi'})$ given by (3.5). There exists a real number γ such that

$$\alpha_b([(G, \rho)]) = (\tilde{\iota}_b)^2_*(\gamma[f_0]);$$

choosing $h_0 \in C_b^1(\mathbf{G}_0, \mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi)$ such that

$$h_0(g)(x) = \gamma(\tfrac{1}{2}\mathbf{v}_g^2 x^0 - \mathbf{v}_g \cdot \mathbf{x})$$

for all $x = (x^0, \mathbf{x}) \in \mathbf{R}^4$, one checks easily that $\delta h_0 = \iota \circ \gamma f_0$. This implies

$$(\tilde{\iota}_b)^2_*(\gamma[f_0)] = 0,$$

hence $\alpha_b([(G, \rho)]) = 0$ and thus

$$\mathrm{Ext}^{\mathrm{RE}}_t(\mathbf{G}_0, \mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi) = \{0\}.$$

If $Q = \mathbf{G}$ and if $\Phi' = \phi_2$, the proof is the same as in the case where $Q = \mathbf{G}_0$ but with h_0 replaced by $h \in C_b^1(\mathbf{G}, \mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi)$ such that

$$h(g)(x) = \gamma(\tfrac{1}{2}\mathbf{v}_g^2 x^0 - \chi(g)\mathbf{v}_g \cdot \mathbf{x})$$

for all $x \in \mathbf{R}^4$. ∎

It follows from the theorem just proved that, if (G, ρ) is any topological extension of $Q \in \{\mathbf{P}_0, \mathbf{P}, \mathbf{G}_0, \mathbf{G}\}$ by $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)_\Phi$ ($m \in \mathbf{N}$ or $m = \infty$) satisfying (RE), with Φ given by (3.2), then G is topologically isomorphic to $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4) \times_\Phi Q$. This is the result already quoted in Secs. 1 and 2.

Remark 1: The lemma and the theorem of this section are also valid if $Q \in \{\tilde{\mathbf{P}}_0, \tilde{\mathbf{G}}_0\}$ and Φ is again defined by (3.2) (with $\phi(Q) = \{\mathrm{Id}_{\mathbf{R}}\}$).

Remark 2: It is easy to see that the choice, instead of $\mathcal{C}^m_{\mathbf{R}}(\mathbf{R}^4)$ ($m \in \mathbf{N}$ or $m = \infty$), of another topological vector space, say $\mathfrak{A}_{\mathbf{R}}(\mathbf{R}^4)$, of mappings of $\mathbf{R}^4$ into $\mathbf{R}$ does not change the result of the above theorem provided

(a) $\mathfrak{A}_{\mathbf{R}}(\mathbf{R}^4)$ is Polish;
(b) $\mathfrak{A}_{\mathbf{R}}(\mathbf{R}^4)$ contains the constant mappings;
(c) the operation Φ of Q on $\mathfrak{A}_{\mathbf{R}}(\mathbf{R}^4)$ given by (3.2) is topological.

Moreover, the result does not change either if, instead of Φ, we take another topological operation Ω such that $\Omega(q)\lambda = \Phi(q)\lambda$ for all $q \in Q$ and all constant mappings λ of $\mathbf{R}^4$ into $\mathbf{R}$.

4. CONCLUDING REMARKS

The problem of the union of a relativistic space-time group and an electromagnetic gauge group into a covariance group of quantum electrodynamics was translated by Rideau[22] too into a study of topological group extensions. Under different assumptions concerning the gauge group [taken as the Abelian group underlying a real (separable) Hilbert space carrying the continuous unitary representation of spin and mass zero of $\tilde{\mathbf{P}}_0$] and the extensions considered (all the topological ones having a continuous factor set), Rideau's result is exactly like ours.

In a more recent work,[23] Rideau adopts the view that electromagnetic gauge transformations of the first kind are not already included in those of the second kind, so that he faces the subsequent problem of combining different gauge groups together and with a space-time group. Here, however, we considered the first kind of electromagnetic gauge transformations as a special case of the second one. This point of view is supported by previous investigations where, instead of covariance groups of electrodynamics, invariance groups of Hamiltonians or Lagrangians yielding equations of motion of charged particles in external (classical) electromagnetic fields were considered.[10] There also, one was naturally led to the coupling of electromagnetic gauge and space-time transformations.

Another point of view is that of Schrader,[24] who investigated a covariance group of Dirac and Klein-Gordon particles in constant uniform external electromagnetic fields. His covariance group (the Maxwell group) operates on the product of the Minkowski space and the set of all these fields. The Maxwell group is obtained from an essential extension of the Poincaré group by the Abelian group of all skew-symmetric real 4×4-matrices.

Continuous unitary projective representations of the space-time invariance groups of (nonzero) constant uniform external electromagnetic fields have been considered by Bacry et al.[25] in order to describe properties of charged particles. They were able to derive the additivity and the superselection rule of the electric charge.

In the work of Janner and Janssen,[10] the starting point is the remark that, generally, electromagnetic potentials and not fields occur in Hamiltonians or Lagrangians. Now, the space-time invariance group of a given electromagnetic potential A is a subgroup only (possibly an improper one) of the space-time invariance group of the field derived from A; therefore, space-time operators leaving the field invariant need not leave invariant the Hamiltonian or the Lagrangian considered. However, these are well invariant under the action of the ordered pairs (λ, q) ($\lambda \in J$ and $q \in Q$, where $Q \in \{\mathbf{P}, \mathbf{G}\}$) which leave invariant A. The problem of giving to the set of all the (λ, q) a group structure is again complicated by the fact that the group multiplication determined by the action of the (λ, q) is not unique. A way out is to consider these ordered pairs as elements of a covariance group $J_\Phi f Q$, where Φ is given by (3.2) with $\phi = \phi_2$ (see Tables I and II) and with the natural operation of Q on space-time, and where the factor set f undergoes the usual restriction. Adopting this point of view, Janner and Janssen got an invariance group $I_f^Q(A)$ as the subgroup of $J_\Phi f Q$ which operates trivially on A.[26] The groups $I_f^Q(A)$ are very useful in studying the states of a charged particle in the external electromagnetic field derived from A. As expected, different choices of the gauge of the electromagnetic potential simply lead to isomorphic invariance groups.

The situation of $I_0^Q(A)$ with respect to $J \times_\Phi Q$ is much the same as that of a space group G (an invariance group of a given crystal) with respect to a three-dimensional Euclidean group $\mathbf{E}(3)$ (a covariance group of crystal physics). Indeed,

$$\mathbf{E}(3) = \mathbf{T}(3) \times_\psi \mathbf{O}(3)$$

[where $\mathbf{T}(3)$, $\mathbf{O}(3)$, and ψ have a manifest meaning] is a transformation group of a three-dimensional Euclidean space E_3. It is obtained from an inessential topological extension of $\mathbf{O}(3)$ by $\mathbf{T}(3)_\psi$, and $\mathbf{O}(3)$[resp. $\mathbf{T}(3)$] is canonically identified with a subgroup of $\mathbf{E}(3)$ through the continuous section $O \mapsto (0, O)$ [resp. through $t \mapsto (t, 1)$]. The choice of another section with the property of being again a group homomorphism merely corresponds to a change of the origin of the affine space canonically attached to E_3. Now comparing $\mathbf{E}(3)$ with $J \times_\Phi Q$ and G with $I_0^Q(A)$, one arrives at the conclusion that translations correspond to gauge transformations, primitive translations (lattice translations) to gauge transformations of the first kind, and the choice of the origin to the choice of the gauge. In the opinion of the authors this analogy is not a superficial one and deserves further investigation.

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APPENDIX

The operation Φ is topological

Lemma 1: Let G and A be Polish groups and suppose A Abelian. If Ψ is an operation of G on A such that the mapping $g \mapsto \Psi(g)a$ of G into A is continuous for all $a \in A$ and the mapping $a \mapsto \Psi(g)a$ of A into A is continuous for all $g \in G$, then Ψ is topological.

Proof: Let us first notice that the law of operation

$$f: (g, a) \to \Psi(g)a$$

is a Borel mapping (Ref. 27, § 27,V) and that $G \times A$ is a Baire space. Since $G \times A$ and A are Polish, there is a meager subset M of $G \times A$ such that $f \mid G \times A - M$ is continuous (Ref. 27, § 28, II). Let (g, a) be any element of $G \times A$ and consider an arbitrary sequence (g_n, a_n) of elements of $G \times A$ converging to (g, a). The set

$$M' = \bigcup_n M(g_n^{-1}, a_n)$$

is meager and thus $G \times A - M' \neq \emptyset$ (because $G \times A$ is a Baire space). Let $(g', a') \in G \times A - M'$. Then

$$(g'g_n, a' + a_n) \in G \times A - M$$

for all $n \in \mathbf{N}$ and it follows from the continuity of $f \mid G \times A - M$ that

$$\lim_{n\to\infty} \Psi(g'g_n)(a' + a_n) = \Psi(g'g)(a' + a).$$

On account of the continuity of the partial mappings determined by f, we get

$$\lim_{n\to\infty} \Psi(g_n)(a'+a_n) = \Psi(g')^{-1} \lim_{n\to\infty} \Psi(g'g_n)(a'+a_n) = \Psi(g)(a'+a)$$

and

$$\lim_{n\to\infty} \Psi(g_n)a_n = \lim_{n\to\infty} \Psi(g_n)(a' + a_n) - \lim_{n\to\infty} \Psi(g_n)a' = \Psi(g)a,$$

whence the continuity of f. ■

Lemma 2: Let G be a topological group, let X be a metric space, and let Ψ be a topological operation of G on X. Suppose K is a compact subset of X, let r be a real number > 0, and let g be any element of G. If, for each $x \in K$, $B(\Psi(g)x; r)$ is the open ball of center $\Psi(g)x$ and radius r, then there exists a neighborhood $V(g)$ of g such that

$$\Psi(V(g))x \subset B(\Psi(g)x; r) \quad \text{for all } x \in K.$$

Proof: As Ψ is topological, there exist, for each $x \in K$, an open x-nbd (neighborhood of x) $W_g(x)$ and a g-nbd $V_x(g)$ such that

$$\Psi(V_x(g))W_g(x) \subseteq B(\Psi(g)x; \tfrac{1}{2}r).$$

Note that the x-nbd $W_g(x)$ [resp. the g-nbd $V_x(g)$] is dependent on g (resp. on x). By the Borel-Lebesgue axiom, we may extract from the open covering $(W_g(x))_{x\in K}$ of K a finite subcovering $(W_g(x_i))_{x_i \in I}$ ($I \subseteq K$ and finite). If

$$V(g) = \bigcap_{x_i \in I} V_{x_i}(g),$$

then

$$\Psi(V(g))x \subset B(\Psi(g)x; r) \quad \text{for all } x \in K. \quad ■$$

Proposition: Let Q be a second countable locally compact group. The operation Φ of Q on $\mathcal{C}_{\mathbf{R}}^m(\mathbf{R}^4)$ ($m \in \mathbf{N}$ or $m = \infty$) defined by (3.2) is topological.

Proof: On account of Lemma 1 we have only to show that the partial mappings determined by $(q, \lambda) \mapsto \Phi(q)\lambda$ are continuous. Throughout this proof we shall keep m fixed but arbitrarily chosen.

(1) Continuity of $q \mapsto \Phi(q)\lambda = \phi(q) \circ \lambda \circ \psi(q^{-1})$

Let $p_{s,l}$ be a seminorm of the family which defines the $\mathbf{C}^m$-topology on $\mathcal{C}_{\mathbf{R}}^m(\mathbf{R}^4)$ (cf. Sec. 3), let r be a 4-multi-index with $|r| \leqslant s$, and let $q_0 \in Q$. If $x \in \mathbf{R}^4$ and $q \in Q$, then

$$\begin{aligned}|D^r(\Phi(q)\lambda - \Phi(q_0)\lambda)(x)| &\leqslant \sum_{r(i)} |\chi(q)\eta_{r(i)}(q)D^{r(i)}\lambda(\psi(q^{-1})x) \\ &\quad - \chi(q_0)\eta_{r(i)}(q_0)D^{r(i)}\lambda(\psi(q_0^{-1})x)|,\end{aligned}$$

where χ is the character of the representation ϕ of Q on $\mathbf{R}$, $r(i)$ is a 4-multi-index of total degree $|r|$, $\eta_{r(i)}(q)$ is a monomial of degree $|r|$ in the matrix elements of the Jacobian matrix of $\psi(q^{-1})$ at x [independent of x because of the linearity of $\psi(q^{-1})$], and the summation is extended to all $4^{|r|}$ r-tuples formed with $\partial/\partial x^0$, $\partial/\partial x^1$, $\partial/\partial x^2$, and $\partial/\partial x^3$. Hence,

$$\begin{aligned}|D^r(\Phi(q)\lambda - \Phi(q_0)\lambda)(x)| &\leqslant \sum_{r(i)} |\chi(q)\eta_{r(i)}(q)| |D^{r(i)}\lambda(\psi(q^{-1})x) - D^{r(i)}\lambda(\psi(q_0^{-1})x)| \\ &\quad + \sum_{r(i)} |\chi(q)\eta_{r(i)}(q) - \chi(q_0)\eta_{r(i)}(q_0)| |D^{r(i)}\lambda(\psi(q_0^{-1})x)|. \qquad \text{(A1)}\end{aligned}$$

Let ϵ be every real number >0. The operations ϕ and ψ are topological, so there is a compact q_0-nbd $V'(q_0)$ such that, for any $q \in V'(q_0)$,

$$\sup_{|r|\leq s,\, x\in K_l} \sum_{r(i)} |\chi(q)\eta_{r(i)}(q) - \chi(q_0)\eta_{r(i)}(q_0)| \, |D^{r(i)}\lambda(\psi(q_0^{-1})x)| < \epsilon/2. \quad \text{(A2)}$$

Now let

$$\sup_{|r|\leq s,\, q\in V'(q_0)} \sum_{r(i)} |\chi(q)\eta_{r(i)}(q)| = k_s \quad \text{(A3)}$$

and put

$$t_s = \sum_{|r|\leq s} 4^{|r|}.$$

As $D^{r(i)}\lambda$ is continuous and ψ is topological, for each $r(i)$ and each $x \in K_l$ there exists a q_0-nbd $V_x^{r(i)}(q_0)$ such that

$$|D^{r(i)}\lambda(\psi(q^{-1})x) - D^{r(i)}\lambda(\psi(q_0^{-1})x)| < \frac{\epsilon'}{2t_s k_s} < \frac{\epsilon}{2t_s k_s} \quad \text{(A4)}$$

for all $q \in V_x^{r(i)}(q_0)$. Moreover, by Lemma 2, we can find a q_0-nbd $V^{r(i)}(q_0)$ such that (A4) is satisfied for all $x \in K_l$ and all $q \in V^{r(i)}(q_0)$. Take

$$V''(q_0) = \bigcap_{|r(i)|\leq s} V^{r(i)}(q_0);$$

then

$$\sup_{|r|\leq s,\, x\in K_l} \sum_{r(i)} |D^{r(i)}\lambda(\psi(q^{-1})x) - D^{r(i)}\lambda(\psi(q_0^{-1})x)| < \frac{\epsilon}{2k_s} \quad \text{(A5)}$$

for all $q \in V''(q_0)$. Finally, for any q in the q_0-nbd $V_{(s,l)}^{(\epsilon)}(q_0) = V'(q_0) \cap V''(q_0)$,

$$p_{s,l}(\Phi(q)\lambda - \Phi(q_0)\lambda) < \epsilon$$

by (A1), (A2), (A3), and (A5). This can be done for any seminorm of the family $(p_{s,l})$ and for any real number $\epsilon > 0$. Using the fundamental system of neighborhoods of $\Phi(q_0)\lambda$

$$\{\Phi(q_0)\lambda + W_m((\alpha_i);\epsilon) \mid W_m((\alpha_i);\epsilon) \in \mathfrak{S}_m\},$$

where $\mathfrak{S}_m$ is as in Sec. 3 [cf. (3.1)], one easily concludes that $q \mapsto \Phi(q)\lambda$ is continuous for all $\lambda \in \mathfrak{C}_{\mathbf{R}}^m(\mathbf{R}^4)$.

(2) Continuity of $\lambda \mapsto \Phi(q)\lambda$

The mapping is linear; thus we have only to prove its continuity at the point 0. Keeping the notation of (1) we obtain, for any $\lambda \in \mathfrak{C}_{\mathbf{R}}^m(\mathbf{R}^4)$ and any seminorm $p_{s,l}$,

$$p_{s,l}(\Phi(q)\lambda) \leq h_s(q) \sup_{|r|\leq s,\, x\in K_l} \sum_{r(i)} |D^{r(i)}\lambda(\psi(q^{-1})x)|,$$

where

$$h_s(q) = \sup_{|r|\leq s} \sum_{r(i)} |\chi(q)\eta_{r(i)}(q)|.$$

As $\psi(q^{-1})K_l$ is a compact set, it follows from the Borel-Lebesgue axiom the existence of a compact set $K_{l'} \supseteq \psi(q^{-1})K_l$ in the sequence (K_l) covering $\mathbf{R}^4$ of Sec. 3. Therefore

$$p_{s,l}(\Phi(q)\lambda) \leq h_s(q) t_s p_{s,l'}(\lambda),$$

and this is valid for any seminorm of $(p_{s,l})$, whence the continuity of $\lambda \mapsto \Phi(q)\lambda$ for all $q \in Q$.

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[1]We give to the terms "covariant," "covariance," and "covariance group" a more general meaning than is usual: Together with the familiar space-time covariance groups, we consider also internal symmetry covariance (in particular invariance) groups and combinations of both types. Obviously, a precise definition of covariance is possible only in the context of a specific theory. For a definition of a space-time covariance in the frame of an algebraic theory of local systems see, for instance, R. Haag and D. Kastler, J. Math. Phys. **5**, 848 (1964), or G. G. Emch, *Algebraic Methods in Statistical Mechanics and Quantum Field Theory* (Wiley-Interscience, New York, 1972).

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Coherent states and Lie algebras*

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The Bloch coherent states for a spin or a system of spins and the Glauber coherent states for bosons are examined from the viewpoint of Lie algebras. It is pointed out that the Bloch coherent states are vectors in the space spanned by the basis functions for an irreducible representation of the unitary unimodular group $SU(2)$, and that the Glauber coherent states are vectors in the space spanned by the basis functions for the infinite-dimensional irreducible representation of a contracted group of $SU(2)$. A deeper understanding of many of the useful properties of these coherent states is gained.

1. INTRODUCTION

It has been a common practice which has become almost routine, when one encounters the boson creation and annihilation operators $a^\dagger$ and a and the spin operators $\mathbf{S}^z, \mathbf{S}^+$, and $\mathbf{S}^-$ for a spin, or a system of spins of total angular momentum $[S(S+1)]^{1/2}$, to associate them with the basis functions $|n\rangle, n = 0, 1, 2, \ldots$ (for the bosons) and $|S, m\rangle, m = -S, S+1, \ldots, S$ (for the spin). As is well known, the analytical forms of the basis functions $|n\rangle$ and $|S,m\rangle$ are expressible in terms of the Hermite polynomials and the spherical harmonics, respectively. More recently, however, the use of the so-called Glauber coherent states[1,2] $|\alpha\rangle$ for the bosons and the Bloch coherent states[3,4] $|\mu\rangle$ for the spin system has become more wide spread as these states have been shown to provide a useful alternative for the description of the respective systems. Of considerable interest were some recent results[5,6] which showed that the coherent states $|\alpha\rangle$ and $|\mu\rangle$ provide a natural basis for the calculations of the thermodynamic and phase transition properties of the Dicke model of superradiance and the BCS model of superconductivity. More significantly, consideration of these coherent states led to a useful new approach to the study of equilibrium quantum systems.[7]

The Glauber coherent states[1,2] $|\alpha\rangle$ and the Bloch coherent states[3,4] $|\mu\rangle$ are formally defined in terms of the traditionally used basis functions $|n\rangle$ and $|S,m\rangle$ by

$$|\alpha\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{(n!)^{1/2}} |n\rangle, \tag{1.1}$$

$$|\mu\rangle = \frac{1}{(1+|\mu|^2)^S} \sum_{p=0}^{2S} \left(\frac{(2S)!}{p!(2S-p)!}\right)^{1/2} \mu^p |S,p\rangle. \tag{1.2}$$

The considerable usefulness of these coherent states naturally prompted one to pose questions regarding the origins of these coherent states and the deep connections which lie behind the algebraic identities formally relating these coherent states to the traditional basis functions $|n\rangle$ and $|S,m\rangle$. The problem is best looked upon from the viewpoint of Lie algebras, as we shall see in the following sections.

2. BLOCH COHERENT STATES AND THE LIE ALGEBRA $\mathcal{G}$

Consider a Lie algebra $\mathcal{G}$ which has generators $\mathcal{S}^z, \mathcal{S}^+$, and $\mathcal{S}^-$ such that

$$[\mathcal{S}^z, \mathcal{S}^\pm] = \pm \mathcal{S}^\pm, \quad [\mathcal{S}^+, \mathcal{S}^-] = 2\mathcal{S}^z, \quad [\mathcal{S}^i, \mathcal{I}] = 0 \quad \text{for } i = z, + \text{ or } -, \tag{2.1}$$

where $\mathcal{I}$ in the third relation is the identity. A realization of the generators of this algebra is given by (we shall write $\mathbf{S}^i$ for a realization of the generator $\mathcal{S}^i$)

$$\mathbf{S}^\pm = \mathbf{S}^x \pm i\mathbf{S}^y = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \pm i\left[-i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\right]$$

and

$$\mathbf{S}^z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right). \tag{2.2}$$

The corresponding Lie group associated with $\mathcal{G}$ with the above realization of the generators of $\mathcal{G}$ is obviously the three-dimensional rotation group $O(3)$. The basis functions for the $(2S+1)$-dimensional irreducible representation of $O(3)$ are, as is well known, the functions $|S,m\rangle$ or for integral values of S, the spherical harmonics $Y_m^S(\theta,\phi), m = -S, -S+1, \ldots, S$.

Suppose we consider another realization of the generators of the same algebra $\mathcal{G}$ given by

$$\mathbf{S}^+ = z\frac{\partial}{\partial \zeta}, \quad \mathbf{S}^- = \zeta\frac{\partial}{\partial z},$$

and

$$\mathbf{S}^z = \tfrac{1}{2}\left(z\frac{\partial}{\partial z} - \zeta\frac{\partial}{\partial \zeta}\right), \tag{2.3}$$

where ζ and z are arbitrary complex variables. This realization was used by Bargmann[8] and in the operator form by Schwinger,[9] and it was also suggested in the author's previous work[7] dealing with the problem of expressing a general Hamiltonian equation in terms of the coherent states. We now wish to show the following: (i) the corresponding Lie group directly associated with the above realization (2.3) of the generators of $\mathcal{G}$ is the unitary unimodular group $SU(2)$ (which is, of course, isomorphic to the $O(3)$ group), (ii) the Bloch coherent states $|\mu\rangle$ are some linear combinations of the basis functions for an irreducible representation of $SU(2)$. It is more instructive to illustrate these points in reverse as follows: Given the group $SU(2)$, we ask what are the "infinitesmal transformation operators" for the corresponding Lie algebra? As is well known, the group $SU(2)$ is characterized by the transformations[10]

$$u' = au + bv \quad (aa^* + bb^* = 1), \qquad v' = -b^*u + a^*v, \tag{2.4}$$

where the parameters a's and b's and the variables u's and v's are generally complex. Let the three independent parameters in (2.4) be a, b, and b^* while let a^* be expressed by $a^* = (1-bb^*)/a$. In the neighborhood of the identity, we have

$$a \approx 1 + \delta a, \quad b \approx \delta b, \quad b^* \approx \delta b^*, \tag{2.5}$$

and

$$a^* \approx 1 - \delta a.$$

Thus we get

$$u' = (1 + \delta a)u + \delta b v, \quad (2.6)$$

$$v' = (1 - \delta a)v - \delta b^* u, \quad (2.7)$$

so the infinitesimal operators of the group are

$$X_1 = u\frac{\partial}{\partial u} - v\frac{\partial}{\partial v}, \quad X_2 = v\frac{\partial}{\partial u}, \quad \text{and } X_3 = -u\frac{\partial}{\partial v} \quad (2.8)$$

or if we define $\mathbf{S}^+ = -X_3, \mathbf{S}^- = X_2$, and $\mathbf{S}^z = \frac{1}{2}X_1$ we obtain (2.3).[11]

The basis functions for the $(2S + 1)$-dimensional representation of the $SU(2)$ group are $u^{2S}, u^{2S-1}v, u^{2S-2}v^2, \ldots, v^{2S}$. To see how the Bloch coherent states $|\mu\rangle$ are directly related to the basis functions of this form, let us observe the results of multiplying $|\mu\rangle$ by the spin operators. We have

$$\begin{aligned}(\mathbf{S}^-)^k|\mu\rangle &= \frac{1}{(1+|\mu|^2)^S}\sum_p\left(\frac{(2S)!}{p!(2S-p)!}p(p-1)\cdots(p-k+1)\right.\\ &\quad\left.\times(2S-p+1)(2S-p+2)\cdots(2S-p+k)\right)^{1/2}\mu^p|S,p-k\rangle\\ &= \frac{1}{(1+|\mu|^2)^S}\sum_p\left(\frac{(2S)!}{p!(2S-p)!}\right)^{1/2}\\ &\quad\times(2S-p)(2S-p-1)\cdots(2S-p-k+1)\,\mu^{p+k}|S,p\rangle\\ &= \frac{1}{(1+|\mu|^2)^S}\sum_p\left(\frac{(2S)!}{p!(2S-p)!}\right)^{1/2}\left(\mu\frac{\partial}{\partial v}\right)^k v^{2S-p}\mu^p|S,p\rangle\Big|_{v=1}. \end{aligned} \quad (2.9)$$

Similarly, we have

$$(\mathbf{S}^+)^k|\mu\rangle = \frac{1}{(1+|\mu|^2)^S}\sum_p\left(\frac{(2S)!}{p!(2S-p)!}\right)^{1/2}\left(v\frac{\partial}{\partial\mu}\right)^k \times v^{2S-p}\mu^p|S,p\rangle\Big|_{v=1} \quad (2.10)$$

and

$$(\mathbf{S}^z)^k|\mu\rangle = \frac{1}{(1+|\mu|^2)^S}\sum_p\left(\frac{(2S)!}{p!(2S-p)!}\right)^{1/2} \times\left[\frac{1}{2}\left(v\frac{\partial}{\partial v} - \mu\frac{\partial}{\partial\mu}\right)\right]^k v^{2S-p}\mu^p|S,p\rangle\Big|_{v=1}. \quad (2.11)$$

Thus, re-writing the definition of Bloch coherent states $|\mu\rangle$ as

$$|\mu\rangle = \frac{1}{(1+|\mu|^2)^S}\sum_{p=0}^{2S}\left(\frac{(2S)!}{p!(2S-p)!}\right)^{1/2} v^{2S-p}\mu^p|S,p\rangle\Big|_{v=1}, \quad (2.12)$$

clearly shows that $|\mu\rangle$ can be viewed as some linear combination of the basis functions for the $(2S + 1)$-dimensional representation of the $SU(2)$ group, namely, $|\mu\rangle$ is a vector in the space spanned by the basis functions for the $(2S + 1)$-dimensional representation of the $SU(2)$ group. From this viewpoint, we also have the consistent results that the spin operators are given in the form (2.3). It is easy to see why v (or μ) can be set equal to 1 for practical purposes after being operated on. This is because the spin operators preserve the homogeneity of the basis functions $v^{2S}, v^{2S-1}\mu, v^{2S-2}\mu^2, \ldots, \mu^{2S}$ in such a way that the sum of the powers of v and μ in every term of (2.9)–(2.11) remains equal to $2S$ [this is why the set $v^{2S-p}\mu^p, p = 0, 1, \ldots, 2S$ provides a basis for the $(2S + 1)$-dimensional representation of the unitary group] and therefore the power of v is completely determined by the power of its "companion" variable μ or vice versa.

It was shown in Ref. 7 that if, in the Hamiltonian equation

$$H(\mathbf{S}^z, \mathbf{S}^+, \mathbf{S}^-)|E\rangle = E|E\rangle \quad (2.13)$$

the spin operators are represented in terms of the differential operators by the substitutions (2.3), the corresponding eigenfunctions $f(\zeta, z)$ in the transformed Hamiltonian equation

$$H\left(\frac{1}{2}\left(z\frac{\partial}{\partial z} - \zeta\frac{\partial}{\partial\zeta}\right), z\frac{\partial}{\partial\zeta}, \zeta\frac{\partial}{\partial z}\right)f(\zeta, z)\Big|_{\zeta=1} = Ef(\zeta, z)\Big|_{\zeta=1} \quad (2.14)$$

are given by

$$f(\zeta, z) = \sum_n c_n\zeta^{2S-n}z^n. \quad (2.15)$$

It is now clear to us that (2.15) simply states that the eigenfunctions in (2.14) can be expanded as some linear combinations of the basis functions corresponding to an irreducible representations of the $SU(2)$ group, in the same way as that if the spin operators in (2.13) are represented by the substitutions (2.2), the eigenfunctions in (2.13) can be expanded in terms of the spherical harmonics which are, of course, the basis functions for the irreducible representations of the three-dimensional rotation group $O(3)$.

The important points of this section can thus be summarized as follows:

The Bloch coherent states $|\mu\rangle$ are normally viewed as certain linear combinations of the spherical harmonics. Not previously noted, however, is the fact that $|\mu\rangle$ can be viewed as certain linear combinations of the basis functions for the irreducible representations of the $SU(2)$ group, i.e., the states $|\mu\rangle$ are vectors in the space spanned by $v^{2S-K}\mu^K$, $K = 0, 1, \ldots, 2S$. It is from this latter point of view that some of the useful and distinctive properties of the Bloch coherent states can be better understood.

3. GLAUBER COHERENT STATES AND THE LIE ALGEBRA $\mathcal{H}$

Consider the harmonic oscillator Lie algebra $\mathcal{H}$ which has the generators $\mathfrak{X}^z$, $\mathfrak{X}^+$ and $\mathfrak{X}^-$ such that

$$[\mathfrak{X}^z, \mathfrak{X}^\pm] = \pm\,\mathfrak{X}^\pm, \quad [\mathfrak{X}^+, \mathfrak{X}^-] = -1,$$
and
$$[\mathfrak{X}^i, \mathfrak{I}] = 0 \quad \text{where } i = z, + \text{ or } -, \quad (3.1)$$

$\mathfrak{I}$ in the third relation being the identity. A realization of the generators of this algebra is well known and is given by (we write X^i for a realization of the generator $\mathfrak{X}^i$)

$$X^+ = a^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right), \quad X^- = a = \frac{1}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right),$$
$$X^z = a^\dagger a = \tfrac{1}{2}\left(x^2 - \frac{\partial^2}{\partial x^2} - 1\right), \quad (3.2)$$

where $a^\dagger$ and a are the boson creation and annihilation operators. The corresponding Lie group associated with $\mathcal{H}$ with the above realization of the generators of $\mathcal{H}$ will be refered to as H. The basis functions for the irreducible representation (of infinite dimensions) of H are the states $|n\rangle$, or $e^{-x^2/2}H_n(x)$, $n = 0, 1, 2, \ldots$ where $H_n(x)$ is the Hermite polynomial of degree n.

Consider another realization of the generators of the same algebra $\mathcal{K}$ given by

$$X^+ = \alpha,$$
$$X^- = \frac{\partial}{\partial\alpha}, \qquad (3.3)$$

and

$$X^z = \alpha\frac{\partial}{\partial\alpha},$$

where α is an arbitrary complex variable. This realization was used by Fock[12] and Bargmann[13] and it was also suggested by the author's previous work[7] dealing with the problem of expressing a general Hamiltonian equation in terms of the coherent states. The corresponding Lie group associated with the above realization (3.3) of the generators of $\mathcal{K}$ will be called H' which must, of course, be isomorphic to H.

It is well known that the algebra $\mathcal{K}$ is a contraction[4,14] of the algebra $\mathcal{G}$. However, in all previous work,[4] the contraction is discussed in terms of the contraction of the group $O(3)$ into the group H. Here let us consider the contraction in terms of the contraction from the group $SU(2)$ into the group H'. Let us assume that the limits, as $S\to\infty$, of the following operators

$$\mathbf{S}^+/(2S)^{1/2}, \quad \mathbf{S}^-/(2S)^{1/2}, \quad \text{and } \mathbf{S}^z/(2S) \qquad (3.4)$$

exist. Consider the function

$$f = \sum_K c_K \nu^{2S-K}\mu^K. \qquad (3.5)$$

Let

$$\alpha = \mu/\xi, \qquad (3.6)$$

where

$$\xi = \nu/(2S)^{1/2}. \qquad (3.7)$$

Then we obtain, using the substitutions given by (2.3) for the spin operators (replacing z by ν and ζ by μ), as $S\to\infty$,

$$\frac{1}{(2S)^{1/2}}\,\nu\frac{\partial}{\partial\mu}f = \frac{\partial}{\partial(\mu/\xi)}f = \frac{\partial}{\partial\alpha}f, \qquad (3.8)$$

$$\frac{1}{(2S)^{1/2}}\,\mu\frac{\partial}{\partial\nu}f = (2S)^{1/2}\nu^{-1}\mu f = \alpha f, \qquad (3.9)$$

and

$$\frac{1}{2S}\,\tfrac{1}{2}\left(\nu\frac{\partial}{\partial\nu} - \mu\frac{\partial}{\partial\mu}\right)f = \tfrac{1}{2}\left(1 - \frac{1}{2S}\,\alpha\frac{\partial}{\partial\alpha}\right)f = \tfrac{1}{2}f. \qquad (3.10)$$

The function f given by (3.5) can be seen to reduce to the Bloch coherent states $|\mu\rangle$ if we let $\nu = 1$ and

$$c_K = \frac{1}{(1+|\mu|^2)^S}\left\{\frac{(2S)!}{K!(2S-K)!}\right\}^{1/2}|S,K\rangle \qquad (3.11)$$

for any given S. In the limit $S\to\infty$, f becomes the Glauber coherent states $|\alpha\rangle$ given by

$$|\alpha\rangle = e^{-|\alpha|^2/2}\sum_n \frac{\alpha^n}{(n!)^{1/2}}\,|n\rangle \qquad (3.12)$$

if we let c_K be given by (3.11), $\nu = 1$ and

$$|\infty, n\rangle \to |n\rangle, \qquad (3.13)$$

$$\mu \to \frac{\alpha}{(2S)^{1/2}}. \qquad (3.14)$$

We see from Eqs. (3.8)–(3.10) that, in contracting the $SU(2)$ group into the group H', we have the following transformations:

$$\frac{\mathbf{S}^+}{(2S)^{1/2}} = \frac{1}{(2S)^{1/2}}\,\nu\frac{\partial}{\partial\mu} \to X^- = \frac{\partial}{\partial\alpha}, \qquad (3.15)$$

$$\frac{\mathbf{S}^-}{(2S)^{1/2}} = \frac{1}{(2S)^{1/2}}\,\mu\frac{\partial}{\partial\nu} \to X^+ = \alpha, \qquad (3.16)$$

and

$$\frac{\mathbf{S}^z}{2S} = \frac{1}{2S}\,\tfrac{1}{2}\left(\nu\frac{\partial}{\partial\nu} - \mu\frac{\partial}{\partial\mu}\right) \to \tfrac{1}{2}. \qquad (3.17)$$

We also see that the Bloch coherent states $|\mu\rangle \to$ the Glauber coherent states $|\alpha\rangle$, and that the Galuber coherent states $|\alpha\rangle$ can be viewed as certain linear combinations of the basis functions corresponding to the infinite-dimensional irreducible representation of the group H' which are given by $\alpha^k, k = 0, 1, 2, \ldots$.

It was shown in Ref. 7 that if the Hamiltonian equation

$$H(a^\dagger, a)|E\rangle = E|E\rangle \qquad (3.18)$$

is represented by

$$H\left(z, \frac{\partial}{\partial z}\right)f(z) = Ef(z), \qquad (3.19)$$

the corresponding eigenfunctions $f(z)$ are given by

$$f(z) = \sum_n c_n z^n. \qquad (3.20)$$

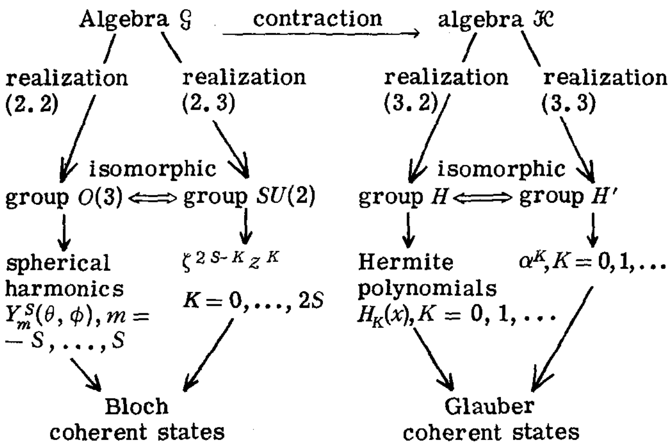
It is now clear to us that (3.20) simply states that the eigenfunctions in (3.19) can be expanded as some linear combinations of the basis functions corresponding to the infinite–dimensional irreducible representation of the group H', in the same way as that if the boson operators in (3.18) are represented by the Schrödinger representation $a^\dagger = (p + ix)/\sqrt{2}$ and $a = (p - ix)/\sqrt{2}$, the corresponding eigenfunctions can be expanded in terms of the Hermite polynomials (with the Gaussian factors) which are the basis functions for the infinite–dimensional irreducible representation for the group H.

4. SPECIAL FUNCTIONS AND COHERENT STATES

It is well known that the Hermite polynomials and the associated Legendre polynomials turned up in physics in the study of the problems of harmonic oscillators and the angular momentum (spin), respectively. It is also known that the theory of Lie algebras provides a unified view of the theory of not only the Hermite and the Legendre polynomials but also of various other special functions in mathematical physics.[15] It is clear from the preceding sections, however, that the above mentioned special functions would arise only if certain particular realizations of the generators of the algebras were used. The realizations which give rise to the Hermite and the Legendre polynomials are "physical" in the sense that the variables x, y, and z are physical quantities. On the other hand, the realizations given by (2.3) and (3.3) corresponding to the groups $SU(2)$ and H' involve complex variables which do not have any direct physical interpretation. However, the resulting "special functions" $\zeta^{2S-K}z^K, K = 0, 1, \ldots, 2S$, and α^K, $K = 0, 1, \ldots,$ have the distinct advantage of being simple, so simple that one would not call them special functions. If we call the space spanned by the basis functions (special functions) of the d-dimensional representation of a group G, say, by $\mathcal{S}^{(d)}(G)$, then a Bloch coherent state may be viewed as a vector in $\mathcal{S}^{(2S+1)}(O(3))$ or as a vector in $\mathcal{S}^{(2S+1)}(SU(2))$. Similarly, a Glauber coherent state may be viewed as a vector in $\mathcal{S}^{(\infty)}(H)$ or as a vector in $\mathcal{S}^{(\infty)}(H')$. However, many of the useful properties of the coherent states can be better understood from the second point of view, as was made clear in the preceding sections. The use of coherent states in place of the traditionally used basis functions might be compared with the situation in which it is more convenient to do the angular momentum problems by considering the group $SU(2)$ rather than the group $O(3)$ because, among other things, the basis functions for $SU(2)$ are easier to manipulate than the basis functions for $O(3)$.

5. SUMMARY

The main results of this paper can be briefly summarized by the following chart:



The direct connection of the Bloch coherent states with the basis functions for the irreducible representations of the $SU(2)$ group and the relation of the $SU(2)$ group with the algebra $\mathcal{G}$ through realization (2.3) were explicitly made in the text, and also for the corresponding case of the Glauber coherent states. We have also pointed out that the distinction between using the groups $SU(2)$ and $O(3)$ concerns the comparative advantages and disadvantages of handling the basis functions for the irreducible representations of the respective groups. All this had not been noted or clearly stated by the previous authors.[4,16] In fact, some authors[4] retain the angular parameters θ and ϕ in the application of the Bloch coherent states which somewhat confuses if not actually defeats the purpose of using these states, for any advantage of using the coherent states rather than the traditionally used basis functions is gained through expressing every function and every relation of interest in terms of the two complex variables constituting the basis functions for the irreducible representations of $SU(2)$. The reader is refered to Ref. 7 for some interesting applications of this concept.

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[11]Care must, of course, be exercised in dealing with algebra involving complex elements. The important thing is to see that the generators satisfy the structure, i.e., the basic commutation relations of the algebra considered. For example, if we consider the pseudo-unitary unimodular group $SU(1,1)$ characterized by [see A. O. Barut and L. Girardello, Commun. Math. Phys. **21**, 41 (1971)]

$$u' = au + bv, \quad v' = b^*u + a^*v, \quad (aa^* - bb^* = 1),$$

the infinitesmal operators of the group can be seen to be obtainable from the operators

$$X_1 = u\frac{\partial}{\partial u} - v\frac{\partial}{\partial v}, \quad X_2 = v\frac{\partial}{\partial u}, \text{ and } X_3 = u\frac{\partial}{\partial v}.$$

Here we must define $S^+ = iX_3$, $S^- = iX_2$, and $S^z = \frac{1}{2}X_1$ such that the basic commutation relations characterizing the algebra

$$[S^z, S^\pm] = \pm S^\pm, \quad [S^+, S^-] = -2S^z$$

are satisfied. $SU(1,1)$ is a noncompact group. The coherent states defined by Barut and Girardello will not be discussed in this paper.
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Invariants of Born reciprocity theory*

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In an attempt to use Born reciprocity theory as a possible scheme for explaining elementary particles we calculate all the invariants of this theory. It turned out that all the invariants are functions of the operator (x^2+p^2). Thus there is only one independent invariant which characterizes this theory.

1. INTRODUCTION

In an attempt to explain elementary particles, Born and his collaborators[1,2,3,4] used the principle of reciprocity as a postulate. This principle states that the laws of nature are symmetrical with regard to space-time and momentum-energy. Mathematically, the principle asserts that the laws of nature are invariant under the following transformations

$$x_\mu \to \pm p_\mu, \quad p_\mu \to \mp x_\mu. \tag{1}$$

Indeed the canonical equations of classical mechanics

$$\dot{x}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial x_i}, \quad (i = 1, 2, 3)$$

are invariant under transformation (1). These equations also hold in operator form of quantum mechanics. The commutations relations($\hbar = c = 1$)

$$x_\mu p_\nu - p_\nu x_\mu = i g_{\mu\nu} \quad (\mu = 0, 1, 2, 3)$$

as well as the component of angular momentum

$$m_{\mu\nu} = x_\mu p_\nu - x_\nu p_\mu$$

exhibit the same invariance.

These examples suggested strongly to Born the principle of reciprocity. In his paper, (1949) Born[1] assumed that the masses of elementary particles are the roots of a self reciprocal function $f(p)$ where self reciprocity is expressed by saying that $f(x)$ is its own Fourier transform, i.e.,

$$f(x) = (2\pi)^{-1/2} \int f(p) e^{-ipx} dp.$$

Furthermore, he showed that every self reciprocal function is an eigenfunction of a reciprocally invariant operator and vice versa; i.e.,

$$S(x,p) f(p) = s f(p)$$

where

$$S(x,p) = S(\pm p, \mp x).$$

To find $f(p)$ Born chose the simplest reciprocally and relativistically invariant operator, namely

$$G = x^2 + p^2. \tag{2}$$

Shin[5] in a different approach to elementary particles interpreted the eigenvalues of G as the masses of elementary particles and got a linear mass formula which closely predicted some of the masses of elementary particles.

As can be seen from the work of Shin,[6] the operator G commutes with all reciprocally invariant operators and hence is an invariant of reciprocity theory. Thus it would be interesting to see if there exist any other independent invariants of this theory, i.e., operators commuting with all reciprocally invariant operators.

In Sec. 2 we review the reciprocally invariant operators and their algebriac structure and in Sec. 3 we calculate the invariants of reciprocity theory.

2. RECIPROCALLY INVARIANT OPERATOR

The principle of reciprocity restricts the number of reciprocally invariant operators considerably. Shin[6] considered all bilinear operators in x_μ and p_μ and found that only 16 of these in addition to the metric tensor $g_{\mu\nu}$ of Minkowski space are reciprocally invariant. Furthermore, all higher order reciprocally invariant operators can be constructed from these. The 16 reciprocally invariant operators are

$$G_{\mu\nu} = G_{\nu\mu} = x_\mu x_\nu + p_\mu p_\nu, \tag{3}$$

$$m_{\mu\nu} = -m_{\nu\mu} = x_\mu p_\nu - x_\nu p_\mu, \tag{4}$$

and

$$g_{\mu\nu} = -i[x_\mu, p_\nu]. \tag{5}$$

Since Eq. (5) is trivial it will not be considered any further. $G_{\mu\nu}$ and $m_{\mu\nu}$ have the following commutations relations:

$$[m_{\mu\nu}, m_{\rho\sigma}] = -i[g_{\nu\rho} m_{\mu\sigma} + g_{\mu\rho} m_{\sigma\nu} - g_{\mu\sigma} m_{\rho\nu} - g_{\nu\sigma} m_{\mu\rho}], \tag{6}$$

$$[m_{\mu\nu}, G_{\rho\sigma}] = -i[g_{\nu\rho} G_{\mu\sigma} + g_{\nu\sigma} G_{\mu\rho} - g_{\mu\rho} G_{\nu\sigma} - g_{\mu\sigma} G_{\nu\rho}], \tag{7}$$

$$[G_{\mu\nu}, G_{\rho\sigma}] = -i[g_{\mu\rho} m_{\sigma\nu} + g_{\mu\sigma} m_{\nu\rho} - g_{\nu\rho} m_{\mu\sigma} - g_{\nu\sigma} m_{\mu\rho}]. \tag{8}$$

We take the following linear combination

$$\Gamma_{\mu\nu} = \alpha G_{\mu\nu} + \beta m_{\mu\nu}$$

and demand the closure of Γ; i.e.,

$$[\Gamma, \Gamma] \sim \Gamma.$$

Using the commutations relations (6), (7), and (8), we find

$$\begin{aligned}[\Gamma_{\mu\nu}, \Gamma_{\rho\sigma}] = &-i g_{\mu\rho}(\alpha^2 + \beta^2) m_{\sigma\nu} + i g_{\nu\sigma}(\alpha^2 + \beta^2) m_{\mu\rho} \\ &+ g_{\nu\rho}[i(\alpha^2 - \beta^2) m_{\mu\sigma} - 2i\alpha\beta G_{\mu\sigma}] \\ &- g_{\mu\sigma}[i(\alpha^2 - \beta^2) m_{\rho\nu} - 2i\alpha\beta G_{\rho\nu}].\end{aligned}$$

Thus the closure will be satisfied provided

$$(\alpha^2 + \beta^2) = 0, \quad i(\alpha^2 - \beta^2) = \beta, \quad \text{and} \quad -2i\alpha\beta = \alpha.$$

These have the solutions:

$$\alpha = \pm \tfrac{1}{2}, \quad \beta = i/2.$$

Taking $+\frac{1}{2}$ for α we find

$$[\Gamma_{\mu\nu}, \Gamma_{\rho\sigma}] = g_{\nu\rho}\Gamma_{\mu\sigma} - g_{\mu\sigma}\Gamma_{\rho\nu}, \tag{9}$$

where

$$\Gamma_{\mu\nu} = \tfrac{1}{2}(G_{\mu\nu} + im_{\mu\nu}). \tag{10}$$

The commutations relations (9) are those of $U(1,3)$ algebra. Since $\Gamma_{\mu\nu}$ are given by linear combinations of reciprocally invariant operators, all 16 independent components of $\Gamma_{\mu\nu}$ are also reciprocally invariant. $G_{\mu\nu}$ and $m_{\mu\nu}$ are given in terms of $\Gamma_{\mu\nu}$ simply as

$$G_{\mu\nu} = \Gamma_{\mu\nu} + \Gamma_{\nu\mu},$$

$$m_{\mu\nu} = i(\Gamma_{\nu\mu} - \Gamma_{\mu\nu}).$$

Thus all other reciprocally invariant operators can be constructed from $\Gamma_{\mu\nu}$ and hence belong to the enveloping algebra of $U(1,3)$.

3. THE INVARIANTS OF RECIPROCITY

Since all higher order reciprocally invariant operators belong to the enveloping algebra of $U(1,3)$, it follows that the Casimir operators of $U(1,3)$ form a basic set of invariants for reciprocity theory. All other invariants are functions of the Casimir operators. Hence the problem of invariants is reduced to finding the Casimir operators of $U(1,3)$ in the special representation (10) of the generators $\Gamma_{\mu\nu}$.

There are four Casimir operators, since $U(1,3)$ is a group of rank 4. From expressions like

$$\Gamma^\alpha_\alpha,\ \Gamma^\beta_\alpha\Gamma^\alpha_\beta,\quad \Gamma_{\alpha\beta}\Gamma^{\beta\gamma}\Gamma^\alpha_\gamma,\quad \text{and}\quad \Gamma_{\alpha\beta}\Gamma^{\beta\gamma}\Gamma_{\gamma\delta}\Gamma^{\delta\alpha},$$

we can construct the four Casimir operators c_1, c_2, c_3, and c_4 which commute with all reciprocally invariant operators.

The first Casimir operator c_1 *is:*

$$c_1 = \Gamma_\mu{}^\mu = \tfrac{1}{2}G_\mu{}^\mu = \tfrac{1}{2}G = \tfrac{1}{2}(x^2 + p^2). \tag{11}$$

Thus as we asserted in the introduction the operator G commutes with all reciprocally invariant operators.

The second Casimir operator c_2 *is:*

$$c_2 = \Gamma_\mu{}^\nu\Gamma_\nu{}^\mu = \tfrac{1}{4}(G_{\mu\nu}G^{\nu\mu} - m^{\mu\nu}m_{\nu\mu}).$$

Using Eqs. (3) and (4) we find the following relation:

$$G_{\mu\nu}G^{\nu\mu} - m^{\mu\nu}m_{\nu\mu} = G^2 - 12. \tag{12}$$

Therefore

$$c_2 = \tfrac{1}{4}(G^2 - 12). \tag{13}$$

Hence c_2 depend entirely on G.

The third Casimir operator c_3 *is:*

$$c_3 = \Gamma_{\mu\nu}\Gamma^{\nu\rho}\Gamma_\rho{}^\mu = \tfrac{1}{8}\begin{pmatrix} G^{\alpha\rho}G_\rho{}^\beta G_{\beta\alpha} + i(G^{\alpha\rho}m_{\rho\beta}G^\beta{}_\alpha + m^{\alpha\rho}G_{\rho\beta}G^{\beta\alpha} + G^{\alpha\rho}G_{\rho\beta}m^\beta{}_\alpha) \\ -(G^{\alpha\rho}m_{\rho\beta}m^\beta{}_\alpha + m^{\alpha\rho}G_{\rho\beta}m^\beta{}_\alpha + m^{\alpha\rho}m_{\rho\beta}G^\beta{}_\alpha) - im^{\alpha\rho}m_{\rho\beta}m^\beta{}_\alpha \end{pmatrix}.$$

Using the symmetry properties of $G_{\mu\nu}$ and $m_{\mu\nu}$, we find that the second term in the above expression reduces to

$$i(G^{\alpha\rho}m_{\rho\beta}G^\beta{}_\alpha + m^{\alpha\rho}G_{\rho\beta}G^\beta{}_\alpha + G^{\alpha\rho}G_{\rho\beta}m^\beta{}_\alpha) = i(G^{\alpha\rho}G_{\rho\beta}m^\beta{}_\alpha + [G^{\alpha\rho}, m_{\rho\beta}]G^\beta{}_\alpha).$$

By elementary algebra we find the following generalization of Eq. (12)

$$G^{\alpha\rho}G_{\rho\beta} = m^\alpha{}_\nu m^\nu{}_\beta + GG^\alpha{}_\beta + 4im^\alpha{}_\beta - 3g^\alpha{}_\beta. \tag{14}$$

Using the commutations relations, Eqs. (12) and (14), we find that the above term reduces to

$$i(G^{\alpha\rho}m_{\rho\beta}G^\beta{}_\alpha + m^{\alpha\rho}G_{\rho\beta}G^\beta{}_\alpha + G^{\alpha\rho}G_{\rho\beta}m^\beta{}_\alpha) = 3G^2 + im_{\alpha\nu}m^\nu{}_\beta m^\beta{}_\alpha - 48.$$

Similarly, the third term reduces to

$$-(G^{\alpha\rho}m_{\rho\beta}m^\beta{}_\alpha + m^{\alpha\rho}G_{\rho\beta}m^\beta{}_\alpha + m^{\alpha\rho}m_{\rho\beta}G^\beta{}_\alpha) = -\tfrac{3}{2}Gm_{\alpha\beta}m^{\beta\alpha};$$

also the first term becomes

$$G^{\alpha\rho}G_\rho{}^\beta G_\beta{}^\alpha + \tfrac{3}{2}Gm_{\alpha\beta}m^{\beta\alpha} + G^3 - 15G.$$

Adding all the terms in c_3, we finally find

$$c_3 = \tfrac{1}{8}[G^3 + 3G^2 - 15G - 48]. \tag{15}$$

Thus the third Casimir operator is given entirely in terms of G.

The fourth Casimir operator: The fourth casimir operator is more complicated and the calculations are lengthy. Here we find a need to generalize Eqs. (12) and (14) further. By elementary algebra we find the following generalization:

$$G^{\mu\nu}G_{\alpha\rho} - G_\alpha{}^\nu G^\mu{}_\rho - m^{\mu\nu}m_{\alpha\rho} + m_\alpha{}^\nu m^\mu{}_\rho = i(g^{\mu\nu}m_{\rho\alpha} + g^\nu{}_\alpha m^\mu{}_\rho + g_{\rho\alpha}m^{\mu\nu} + g_\rho{}^\mu m^\nu{}_\alpha) + g_{\rho\alpha}g^{\mu\nu} + g_\rho{}^\mu g_\alpha{}^\nu. \tag{16}$$

Equations (12) and (14) are produced by repeated contractions over one and two of the indices, respectively, in Eq. (16). c_4 is given by

$$c_4 = \Gamma^{\mu\nu}\Gamma_{\nu\rho}\Gamma^{\rho\alpha}\Gamma_{\alpha\mu}.$$

Using Eqs. (12) and (14) and the commutations relations, c_4 becomes

$$c_4 = \frac{1}{16}\begin{pmatrix} G^2m_{\mu\nu}m^{\nu\mu} + G^4 - 18G^2 - 16m_{\mu\rho}m^{\rho\mu} + 6G^3 - 96G + 36 \\ -(G_{\mu\nu}m^\nu{}_\rho m^{\rho\sigma}G_\sigma{}^\mu + G_{\mu\nu}m^\nu{}_\rho G^\rho{}_\sigma m^{\sigma\mu} + m_{\mu\nu}G^{\nu\rho}m_{\rho\sigma}G^{\sigma\mu} + m_{\mu\nu}G^{\nu\rho}G_{\rho\sigma}m^{\sigma\mu}) \end{pmatrix}$$

With the aid of Eqs. (12), (14), (16) and the commutations relations the last term in c_4 reduces to

$$\begin{aligned} &-(G_{\mu\nu}m^\nu{}_\rho m^{\rho\sigma}G_\sigma{}^\mu + G_{\mu\nu}m^\nu{}_\rho G^\rho{}_\sigma m^{\sigma\mu} + m_{\mu\nu}G^{\nu\rho}m_{\rho\sigma}G^{\sigma\mu} + m_{\mu\nu}G^{\nu\rho}G_{\rho\sigma}m^{\sigma\mu}) \\ &= 12G^2 + 16m_{\mu\alpha}m^{\alpha\mu} - 192 - 4m_{\nu\alpha}m^{\mu\nu}m^{\alpha\sigma}m_{\sigma\mu} + 4m_{\mu\sigma}m^{\sigma\mu} + 2m_{\nu\alpha}m^{\alpha\nu}m_{\mu\sigma}m^{\sigma\mu} - G^2m^{\alpha\beta}m_{\beta\alpha}. \end{aligned}$$

Now by straightforward calculations which involve several hundred terms we find that the m's satisfy the following equation:

$$4m_{\nu\alpha}m^{\mu\nu}m^{\alpha\sigma}m_{\sigma\mu} = 2m_{\nu\alpha}m^{\alpha\nu}m_{\mu\sigma}m^{\sigma\mu} + 4m_{\mu\sigma}m^{\sigma\mu}. \tag{17}$$

Adding all the terms and using Eq. (17), c_4 finally reduces to

$$c_4 = \frac{1}{16}[G^4 + 6G^3 - 6G^2 + 96G - 156]. \tag{18}$$

Thus we see that c_4 is again given entirely in term of G.

4. CONCLUSIONS

The invariants of reciprocity theory are functions of the Casimir operators of the group $U(1, 3)$ in the special representation (10) of its generators. It turned out that all the Casimir operators are polynomials in the operator G of Born[1] and Shin.[5] Thus the reciprocity theory is characterized by one invariant and hence insufficient at the present for the explanations of the invariants occurring in physics, namely: the mass, charge, spin, hypercharge, baryon numbers, lepton numbers, etc.

One may extend the principle of reciprocity by adopting the group $U(1, 3)$ as the symmetry group of elementary particles. In that case a more general representation whose invariants are independent of each other might prove useful for the classifications of elementary particles.

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Behavior of distribution functions in the thermodynamic limit

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Ruelle has proven that the solutions of the Kirkwood–Salsburg equation for a finite volume Λ become, in the limit as $\Lambda \to \infty$, the solutions to the Kirkwood–Salsburg equation for an infinite volume, i.e.,

$\lim_{\Lambda \to \infty} \rho_\Lambda \to \rho + \lim_{\Lambda \to \infty} \epsilon(\Lambda)$, $\lim_{\Lambda \to \infty} \epsilon(\Lambda) \to 0$.

The form of ϵ is not obtained. We show that for the first order contribution to the solution of the Kirkwood–Salsburg equations obtained via a perturbation scheme developed in an earlier paper that

$\epsilon(\Lambda) \leqslant \lim_{R \to \infty} \epsilon^{-k'_a R}$,

where k'_a is a positive real constant which can be specified and R is the minimum distance from the container walls to the particles of the system.

I. INTRODUCTION

Equilibrium thermodynamics can be rigorously obtained from statistical mechanics, but only in the thermodynamic limit. Experiments, of course, are always done in finite volumes. An obvious question is: What do the formulae of statistical mechanics, in the limit of infinite volume, say about finite volume experiments? The answer is that if the volume is large enough and the measurements to be performed are taken far enough from the walls of the container that the difference between experiment (finite volume) and theory (infinite volume) is negligible.

There are several objections to the above which can be characterized by the following questions. What is "large enough" and "far enough"? Is there a "large enough" or "far enough" in the coexistence region? Is there long-range order in the crystalline phase which transmits the effect of the walls over infinite distances? Is this long-range effect of the walls also felt at the critical point?

These questions are quite difficult to answer rigorously. This paper is a first step in employing a method of solution developed by the author[1] to try to answer, rigorously, some of the above questions. In this first paper we will treat the effect of the walls in the region of very low activity.

In a previous paper[1] referred to as (I) the author has proven that the Kirkwood–Salsburg[2] equation (K–S)

$$\rho = z + zPK\rho,$$

where

$$\rho = \begin{bmatrix} \rho_1(x_1) \\ \cdot \\ \cdot \\ \cdot \\ \rho_N(\{x_N\}) \end{bmatrix}$$

and zPK is defined by

$$\rho' = zPK\rho$$

$$\rho_1'(x_1) = z\sum_{n=1}^{\infty} \frac{1}{n!} \int \rho_n(x_2 \cdots x_{n+1}) \prod_{j=2}^{n+1} f_{ij}\, dx_j,$$

$$\rho_N'(\{x_N\}) = P_N z \prod_{j=2}^{N} (1+f_{ij})[\rho_{N-1}(x_2 \cdots x_N) + \sum_{n=1}^{\infty} \frac{1}{n!} \int \rho_{N+n-1}(x_2 \cdots x_{N+n}) \prod_{j=N+1}^{N+n} f_{ij}\, dx_j] \qquad \text{(I. 1)}$$

can be solved for potentials with a hard core and a finite range. The solution is obtained by decomposing the operator zPK into an unperturbed part PK_0

$$zPK_0 = \rho',$$

$$\rho_1'(x_1) = z\sum_{n=1}^{\infty} \frac{1}{n!} \int \rho_n(x_2 \cdots x_{n+1}) \prod_{j=2}^{n+1} f_{ij}\, dx_j,$$

$$\rho_N'(\{x_N\}) = zP_N \prod_{j=2}^{N} (1+f_{ij}) \sum_{n=1}^{\infty} \frac{1}{n!} \int \rho_{N+n-1}(x_2 \cdots x_{N+n}) \otimes \prod_{j+N+1}^{N+n} f_{ij}\, dx_j,$$

and a perturbation

$$PK'\rho = \rho',$$

$$\rho_1'(\{x_1\}) = 0,$$

$$\rho_N'(\{x_N\}) = P_N \prod_{j=2}^{N} (1+f_{ij})\rho_{N-1}(x_2 \cdots x_N),$$

expanding ρ in a power series in the perturbation parameter ϵ

$$\rho = \sum_n \epsilon^n \phi_n \qquad \text{(I. 2)}$$

and inserting the series into

$$\rho = z + zPK_0\rho + z\epsilon PK'\rho.$$

Equating powers of ϵ gives the recursion relations

$$\phi_0 = z + zPK_0\phi_0, \qquad \phi_N = zPK'\phi_{N-1} + zPK_0\phi_N. \qquad \text{(I. 3)}$$

The operator P is a modification to the K–S equation defined as

$$P = \begin{bmatrix} 1 & 0 & 0 & 0 & 0\ldots \\ 0 & 1 & 0 & 0 & 0\ldots \\ 0 & 0 & P_2(x_{23}) & 0 & 0\ldots \\ 0 & 0 & 0 & P_3(x_{23}, x_{24}, x_{34}) & 0\ldots \end{bmatrix},$$

where $P_N(x_2 \ldots x_N)$ is a projection operator which is 0 if any of the particles $2\ldots N$ overlap their hard cores and one otherwise.

It was proven in (I) that Eqs. (I. 3) have unique solutions and that (I. 2) converges uniformly for $\epsilon = 1$ and

$$|z| < [e^{\beta B'} eC(\beta)]^{-1},$$

where B' is a positive constant such that

$$P_N \prod_{j=2}^{N} (1 + f_{ij}) \leq e^{\beta B'} \ \forall N,$$

$$C(\beta) = \int |f_{ij}| \, dx_{ij},$$

and

$$f_{ij} = e^{-\beta \phi(x_{ij})} - 1.$$

Ruelle[3] has shown that the solution of the K–S equation, derived from an iterative approach, has the property that

$$\lim_{\Lambda \to \infty} \rho_\Lambda \to \rho + \lim_{\lambda \to \infty} \epsilon(\lambda): \lim_{\lambda \to \infty} \epsilon(\lambda) \to 0,$$

where Λ is the volume of a finite box, ρ_Λ is the distribution function vector for the box and $\epsilon(\lambda)$ is a function which depends on the size of Λ through λ which $\lim_{\Lambda \to \infty}$ implies $\lambda \to \infty$. The form of the function $\epsilon(\lambda)$ is not specified. In this paper we will begin to employ the new method of solution developed in (I) to specify the form of the function $\epsilon(\lambda)$.

It was shown in (I) that the first nonzero contribution, generated by the recursion relations (I. 3), to each of the distribution functions could be obtained by solving the set of equations.

$$\rho_{1S}(x_1) = z + z \int \rho_1(x_2) f_{12} dx_2,$$

$$\rho_{NS}(\{x_N\}) = z \prod_{j=2}^{N} (1 + f_{ij}) P_N[\rho_{N-1}(x_2 \ldots x_N) + \int \rho_{NS}(x_{N+1}, x_2 \ldots x_N) f_{1,N+1} dx_{N+1}],$$

which was called the strip operator (S-O) hierarchy. As the solution to the S–O hierarchy is a good approximation to the exact hierarchy solution for low z it is of some interest to examine the S-O solutions for information which might be mirrored in the solution of the exact hierarchy. It is also necessary to obtain this result as it is an integral part of the more general considerations.

We will prove that for

$$|z| < [e^{\beta B'} C(\beta) e]^{-1}$$

the solutions $\rho_{N\Lambda}(\{x_N\})$ of the S-O hierarchy for finite volumes

$$\rho_{1S_\Lambda}(x_1) = \chi(\Lambda)[z + z \int \rho_{1S_\Lambda}(x_2) f_{12} dx_2],$$

$$\rho_{NS_\Lambda}(\{x_N\}) = z\chi(\Lambda) \prod_{j=2}^{N} (1 + f_{ij}) P_N[\rho_{N-1S_\Lambda}(x_2 \ldots x_N) + \int \rho_{NS_\Lambda}(x_{N+1}, x_2 \ldots x_N) f_{1,N+1} dx_{N+1}]$$

tend in the limit as $\Lambda \to \infty$ as

$$\lim_{\Lambda \to \infty} \rho_{NS_\Lambda}(\{x_N\}) \to \rho_{NS}(\{x_N\}) + O(e^{ik'_{\alpha_0} R}) \times (C(\beta))^{-N},$$

where R is the minimum distance between the container walls and the cluster of particles $\{x_N\}$ (assumed to be large) and k'_{α_0} is the imaginary part of k_{α_0}, the root with the smallest positive imaginary part of

$$1 - z\hat{f}(k) = 0,$$

and $\chi(\Lambda)$ is the characteristic function of the volume Λ.

II. LARGE R BEHAVIOR FOR $\rho_{lS_\Lambda}(x_l)$

The thermodynamic[3] limit of the system is to be taken in the following way.

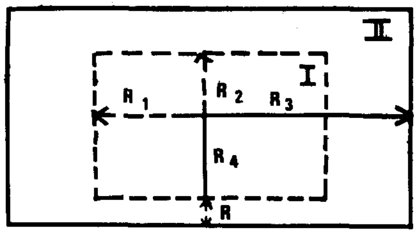

Fig. 1.

$R_1, R_2, R_3, R_4 \to \infty$ and $R \to \infty$, where R is the minimum distance between the two volumes. The set of particles $\{x_N\}$ which is the set whose correlation function $\rho_N(\{x_N\})$ is being considered is restricted to volume I. By definition the average particle density remains constant in the limiting process.

The proof of the postulated limiting property will proceed by induction.

First we will prove that

$$\lim_{\Lambda \to \infty} \rho_{1S_\Lambda}(x_1) \rho_{1S}(x_1) + O(\exp(ik'_{\alpha_0} R))$$

Proof: (We will drop the $1S$ subscripts in the proof)

$$\rho_\Lambda(x_1) = \chi(\Lambda)[z + z \int \rho_\Lambda(x_2) f_{12} dx_2].$$

Dividing both sides of the above equation by $\chi(\Lambda)$ yields

$$\rho'_\Lambda(x_1) = z[1 + \int \rho_\Lambda(x_2) f_{12} dx_2],$$

$$\rho'_\Lambda(x_1) = \rho_\Lambda(x_1)/\chi(\Lambda)$$

$\rho'_\Lambda(x_1)$ can be written as

$$\rho'_\Lambda(x_1) = \rho'_\Lambda(x_1)_0 + \rho'_\Lambda(x_1)_\mathrm{I},$$

where $\rho'_\Lambda(x_1)_0$ is nonzero only if particle 1 is outside the volume Λ (the volume Λ is the larger box marked II in Fig. 1) and $\rho'_\Lambda(x_1)_\mathrm{I}$ is nonzero only if particle I is inside Λ. By definition

$$\rho'_\Lambda(x_1)_0 = \rho_\Lambda(x_1). \tag{II. 1}$$

Therefore

$$\rho'_\Lambda(x_1)_0 + \rho_\Lambda(x_1)_\mathrm{I} = z + z \int \rho_\Lambda(x_2) f_{12} dx_2.$$

Taking the Fourier transform of both sides with respect to x_1 gives

$$\hat{\rho}_\Lambda(k)_\mathrm{I}(1 - z\hat{f}(k)) = z\delta(k) - \hat{\rho}'_\Lambda(k)_0.$$

Dividing by $(1 - z\hat{f}(k))$ and taking the inverse transform yields

$$\rho_\Lambda(x_1)_\mathrm{I} = [z/(1 - z\hat{f}(0))] - \int \rho'_\Lambda(x_2)_0 F(|x_1 - x_2|) \, dx_2, \tag{II. 2}$$

where

$$F(|x_1 - x_2|) = \int e^{ik \cdot x_{12}} [1 - z\hat{f}(k)]^{-1} dk.$$

Since

$$|z| < (e^{\beta B' + 1} C(\beta))^{-1}$$

and

$$\forall k, \text{ real}, \hat{f}(k) = \int f(x) e^{-ik \cdot x} dx < \int |f(x)| dx = C(\beta)$$

clearly

$$1 - z\hat{f}(k) > 0 \quad \forall k \text{ real}.$$

From (I) it is clear that

$$z/(1 - z\hat{f}(0))$$

is the solution to the infinite volume S-O hierarchy equation for $\rho_1(x_1)$. The properties of

$$\lim_{\Lambda\to\infty} \int \rho_\Lambda(x_2)_0 \, F(x_1 - x_2)\, dx_2$$

must be examined.

First we will rewrite $F(x_1 - x_2)$ as

$$F(x_1 - x_2) = \delta(x_{12}) + F'(x_{12}),$$

where

$$\begin{aligned}\int e^{ik\cdot x_{12}} \left[1 + \frac{z\hat{f}(k)}{1 - z\hat{f}(k)}\right] dk &= \delta(x_{12}) + \int \frac{z\hat{f}(k)}{1 - z\hat{f}(k)}\, e^{ik\cdot x_{12}}\, dk, \\ &= \delta(x_{12}) + F'(x_{12}).\end{aligned} \qquad \text{(II. 3)}$$

Inserting (II. 3) into (II. 2) gives

$$\rho_\Lambda(x_1)_\mathrm{I} = [z/(1 - z\hat{f}(0))] - \rho'_\Lambda(x_1)_0 - \int \rho'_\Lambda(x_2)_0 F'(x_1 - x_2) dx^2$$

since x_1 can be chosen at will and we are interested in the configurations in which x_1 is in Λ

$$\rho'_\Lambda(x_1)_0 = 0,$$

$\rho_\Lambda(x_1)$ is a bounded function (by assumption). In the space of bounded functions

$$z \int \rho_\Lambda(x_2) f_{12} dx_2$$

is a bounded operator. Consequently $\rho_\Lambda(x_1)_0$ is also bounded.

In (I) two theorems were proven that will be useful here. The first is that

$$F'(x) = \int \frac{z\hat{f}(k)}{1 - z\hat{f}(k)}\, e^{ik\cdot x}\, dk$$

is a bounded function of x for all x real. The second is that for $|x|$ greater than the range of the potential

$$F'(|x|) = f(|x|) + \sum_\alpha \frac{e^{ik\alpha|x|}}{|x|} A_\alpha, \qquad \text{(II. 4)}$$

where the fact that $F'(x)$ depends only on $|x|$ has been made explicit and

$$\sum_\alpha \frac{e^{ik\alpha|x|}}{|x|} A_\alpha$$

converges uniformly in the required range of $|x|$. We will now prove that

$$\int \left| \int \frac{z\hat{f}(k)}{1 - z\hat{f}(k)}\, e^{ik\cdot x}\, dk \right| dx = \int \left| F'(x) \right| dx$$

is also bounded.

For the values of $|z|$ considered,

$$\begin{aligned}F'(|x_{12}|) &= \int \frac{z\hat{f}(k)}{1 + z\hat{f}(k)}\, e^{ik\cdot x_{12}} dk \\ &= zf(x_{12}) + z^2 \int f(x_1 - x_3) f(x_2 - x_3) dx_3 \\ &\quad + z^3 \int f(x_1 - x_3) f(x_3 - x_4) f(x_4 - x_2) dx_3 dx_4 + \dots \\ &= \sum_{n=1}^{\infty} z^n (f^*)^n,\end{aligned} \qquad \text{(II. 5)}$$

where $(f^*)^n$ is the nth convolution of the f's and $(f^*) = f$. The term by term integration is justified by the uniform bounded convergence of the series.[4]

Clearly,

$$\left|\sum_{n=1}^{\infty} z^n (f^*)^n\right| \le \sum_{n=1}^{\infty} |z|^n (|f|^*)^n$$

so that

$$\begin{aligned}\int \left|F'(x_{12})\right| dx_{12} &\le \sum_n \int dx_{12}\, |z|^n (|f|^*)^n \\ &\le \sum_{n=1}^{\infty} |z|^n (C(\beta))^n.\end{aligned} \qquad \text{(II. 6)}$$

Since

$$|z| < [e^{\beta B'+1} C(\beta)]^{-1}$$

and

$$\sum_{n=1}^{\infty} |z|^n (C(\beta))^n = \frac{|z| C(\beta)}{1 - |z| C(\beta)}$$

it follows that

$$\int |F'(x)| dx \le \frac{|z| C(\beta)}{1 - |z|\, C(\beta)} \qquad \text{(II. 7)}$$

and the boundedness of the integral is proven. We are now in a position to examine

$$\lim_{\Lambda\to\infty} \rho_\Lambda(x_1)_\mathrm{I} = \frac{z}{1 - z\hat{f}(0)} - \lim_{\Lambda\to\infty} \int \rho_\Lambda(x_2)_0 F'(x_1 - x_2) dx_2. \qquad \text{(II. 8)}$$

Since $\rho_\Lambda(x_1)_0$ is 0 if x_2 is not outside Λ (i.e., Λ_II in Fig. 1) and we demand that x_1 is in Λ_I then

$$|x_1 - x_2| \ge R$$

over the entire range of integration. Using the uniform convergence of the integral in (II. 8) to interchange limit and integral we increase Λ in the prescribed manner until

$$R > \lambda,$$

where

λ = range of potential.

At this point we have

$$\begin{aligned}F'(x_1 - x_2) &= f(x_1 - x_2) + \sum_\alpha \frac{e^{ik\alpha|x_{12}|}}{|x_{12}|} A_\alpha \\ &= \sum_\alpha \frac{e^{ik\alpha|x_{12}|}}{x_{12}} A_\alpha.\end{aligned}$$

If k'_{α_0} is the imaginary part of the root with the smallest imaginary (positive) part then

$$F'(|x_{12}|) = \exp(ik'_{\alpha_0}|x_{12}|_{F''}) (|x_1 - x_2|),$$

where $f''(|x_1 - x_2|)$ is a bounded function. Therefore if

$$\sup_{\forall x_1} |\rho_\Lambda(x_1)_0| < A$$

and

$$\sup_{\forall x_1, x_2} |F''(|x_1 - x_2|)| < B,$$

then

$$\int \rho_\Lambda(x_1)_0 F(x_1 - x_2) dx_2 \le 4\pi AB \int_R^\infty x^2 \exp(ik_{\alpha_0} x) dx$$

which goes to 0 as

$$\exp(ik'_{\alpha_0}R)$$

in the limit as

$$R \to \infty.$$

III. LARGE R BEHAVIOR FOR $\rho_{NS}(\ x_N\ )$

In this section we will prove that the solution to an arbitrary S-O equation has the postulated property. Proceeding with the proof by induction we assume that

$$\rho_{N-1_{\Lambda S}}(\{x_{N-1}\}') = \rho_{(N-1)S}(\{x_{N-1}\}') + G_\Lambda(\{x_{N-1}\}'),$$

where

$$\{x_{N-1}\}' = \{x_2 \ldots x_N\}$$

and

$$\lim_{\Lambda\to\infty} G_\Lambda(\{x_{N-1}\}') \to O(\exp(ik'_{\alpha_0}R)(C(\beta))^{-N}$$

if $\{x_{N-1}\}'$ are restricted to Λ_I. We have

$$\rho_\Lambda(\{x_N\}) = z\chi(\Lambda)\prod_{j=2}^{\infty}(1+f_{ij})P_N[\rho_\Lambda(\{x_{N-1}\}') + \int \rho_\Lambda(x_{N+1}, \{x_{N-1}\}')f_{1,N+1}dx_{N+1}].$$

The subscripts have been dropped for the sake of simplicity and the order N of the function can be inferred from the variable dependence.

Therefore,

$$\rho_\Lambda(\{x_N\}) = \Theta_N^{-1}(\rho(\{x_{N-1}\})z\prod_{j=2}^{N}(1+f_{ij})\chi(A)) + \Theta_N^{-1}(G_\Lambda(\{x_{N-1}\})z\prod_{j=2}^{N}(1+f_{ij})\chi(\Lambda)) \quad \text{(III. 1)}$$

where

$$\Theta_N\rho(\{x_N\}) = \rho\{x_N\} - P_{N\chi(\Lambda)}\prod_{j=2}^{N}(1+f_{ij})\int f_{1,N+1} \otimes \rho_N(x_{N+1}, \{x_{N-1}\}')dx_{N+1}.$$

From (I) it is clear that Θ^{-1} exists and is bounded for the range of z considered. Therefore, the second term on the right-hand side of (III. 1) will clearly approach 0 in the same manner as $G_\Lambda(\{x_{N-1}\}')$, or faster, when $\{x_N\}$ is restricted to Λ_I and Λ_I and $\Lambda\to\infty$. We turn our attention therefore to the term

$$\phi_\Lambda(\{x_N\}) = \Theta_N^{-1}(z\rho(\{x_{N-1}\})\prod_{j=2}^{N}(1+f_{ij})\chi(\Lambda)).$$

That is we want to investigate the behavior of the solution of

$$\phi_\Lambda(\{x_N\}) = z\chi(\Lambda)P_N\prod_{j=2}^{N}(1+f_{ij})[\rho(\{x_{N-1}\}) + \int \phi_\Lambda(x_{N+1}, \{x_{N-1}\})f(x_1 - x_{N+1})dx_{N+1}]. \quad \text{(III. 2)}$$

If we divide both sides of Eq. (III. 2) by

$$\chi(\Lambda)\prod_{j=2}^{N}(1+f_{ij})P_N$$

we have

$$\phi'_\Lambda(\{x_N\}) = z\rho(\{x_{N-1}\}') + z\int \phi_\Lambda(x_{N+1}, \{x_{N-1}\}')f(x_1 - x_{N+1})dx_{N+1}, \quad \text{(III. 3)}$$

where

$$\phi'_\Lambda(\{x_N\}) = \frac{\phi(\{x_N\})}{\chi(\Lambda)\prod_{j=2}^{N}(1+f_{ij})P_N}.$$

Multiplying both sides of (III. 3) by $(C(\beta))^{-N}$ and defining

$$\bar\phi_\Lambda(\{x_N\}) = \phi_\Lambda(\{x_N\})/(C(\beta))^{-N},$$

we have

$$\bar\phi'_\Lambda(\{x_N\}) = z\rho(\{x_{N-1}\}')(C(\beta))^{-N} + z\int \bar\phi_\Lambda(x_{N+1}, \{x_{N-1}\}')f(x_1 - x_{N+1})dx_{N+1}. \quad \text{(III. 4)}$$

From (I) it is clear that $\bar\phi_\Lambda$, $\bar\phi'_\Lambda$, and $\rho(\{x_{N-1}\}')(C(\beta))^{-N}$ are bounded by numbers independent of N. $\bar\phi'_\Lambda$ can be decomposed into a number of functions with disjoint support.

$$\bar\phi'_\Lambda(\{x_N\}) = \bar\phi'_{\Lambda_{\underline{0}}}(\{x_N\}_0) + \bar\phi''_\Lambda(\{x_N\}_0) + \bar\phi'_{\Lambda_{\underline{0}}}(\{x_N\}_I) + \bar\phi'_{\Lambda_{\underline{I}}}(\{x_N\}_I') + \bar\phi'_{\Lambda_{\underline{0}}}(x_{1_0}(\{x_{N-1}\}_I') + \bar\phi'_{\Lambda_{\underline{I}}}(x_{1_0}(\{x_{N-1}\}'). \quad \text{(III. 5)}$$

The subscripts within the parentheses (with one exception) refer to whether the subscripted variables are inside or outside of Λ. The underlined subscripts in (III. 5) refer to whether particle 1 is within the potential range of at least one of the particles in $\{x_{N-1}\}'$. For example, if particle one was not within the potential range of one of the particles $\{x_{N-1}\}'$ then

$$\bar\phi'_{\Lambda_{\underline{I}}}(\{x_N\}) = 0$$

independent of the positions of the $\{x_N\}$ particles relative to Λ. The one exception mentioned above is $\bar\phi''_\Lambda(\{x_N\}_0)$ which is 0 if any of the particles in $\{x_N\}_0$ is outside Λ. $\bar\phi_\Lambda(\{x_N\})$ has a similar decomposition,

$$\bar\phi_\Lambda(\{x_N\}) = \bar\phi_{\Lambda_{\underline{0}}}(\{x_N\}_I) + \bar\phi_{\Lambda_{\underline{I}}}(\{x_N\}_I). \quad \text{(III. 6)}$$

Clearly

$$\bar\phi'_{\Lambda_{\underline{0}}}(\{x_N\}_I) = \bar\phi_{\Lambda_{\underline{0}}}(\{x_N\}_I). \quad \text{(III. 7)}$$

Taking the Fourier transform of both sides of (III. 4) with respect to x_1 and employing Eqs. (III. 5), (III. 6), and (III. 7) one obtains after some algebraic manipulation and taking the inverse Fourier transform,

$$\bar\phi_{\Lambda_{\underline{0}}}(\{x_N\}_I) = -\int F(x_1 - x_{N+1})[\bar\phi''_\Lambda(x_{N+1_0}, \{x_{N-1}\}_0') + \bar\phi'_{\Lambda_{\underline{I}}}(x_{N+1_I}, \{x_{N-1}\}_I') + \bar\phi'_{\Lambda_{\underline{I}}}(x_{N+1_0}, \{x_{N-1}\}_I') + \bar\phi'_{\Lambda_{\underline{0}}}(x_{N+1_0}, \{x_{N-1}\}_I') + \bar\phi'_{\Lambda_{\underline{0}}}(x_{N+1_0}, \{x_{N-1}\}_0')] \times dx_{N+1} + \int F'(x_1 - x_{N+1})\bar\phi_{\Lambda_{\underline{I}}}(x_{N+1_I}, \{x_{N-1}\}_I')dx_{N+1} + z(C(\beta))^{-N}\frac{\rho(\{x_{N-1}\}')}{1 - z\hat f(0)}. \quad \text{(III. 8)}$$

As discussed in sec. II,

$$F(x_1 - x_3) = \delta(x_1 - x_3) + F'(x_1 - x_3). \quad \text{(III. 9)}$$

Employing (III. 9) and restricting particles $\{x_N\}$ to Λ_I gives

$$\bar\phi_{\Lambda_{\underline{0}}}(\{x_N\}_I) + \bar\phi'_{\Lambda_{\underline{I}}}(\{x_N\}_I) = -\int F'(x_1 - x_{N+1}) \times [\bar\phi'_{\Lambda_{\underline{I}}}(x_{N+1_I}, \{x_{N-1}\}_I') + \bar\phi'_{\Lambda_{\underline{I}}}(x_{N+1_0}, \{x_{N-1}\}_I') + \bar\phi'_{\Lambda_{\underline{0}}}(x_{N-1_0}, \{x_{N-1}\}_I') - \bar\phi_{\Lambda_{\underline{I}}}(x_{N+1_I}, \{x_{N-1}\}_I')](dx_{N+1}) + z(C(\beta))^{-N}\frac{\rho(\{x_{N-1}\}')}{1 - z\hat f(0)}. \quad \text{(III. 10)}$$

If we multiply both sides of (III. 10) by a function Δ which equals 1 if particle 1 is within the potential range of at least one of the particles $\{x_{N-1}\}'$ and is 0 otherwise then

$$\bar{\phi}'_{\Lambda_I}(\{x_N\}_I) - \Delta \int F'(x_1 - x_{N+1})\,(1 - \prod_{j=2}^{N}(1+f_{ij})) \otimes \bar{\phi}'_{\Lambda_I}(x_{N+1_I}, \{x_{N-1}\}'_I)dx_{N+1} = -\Delta \int F'(x_1 - x_{N+1})[\bar{\phi}'_{\Lambda_I}(x_{N+1_0}, \{x_{N-1}\}_I) \bar{\phi}'_{\Lambda_0}(x_{N+1_0}, \{x_{N-1}\}'_I)]dx_{N+1} + \frac{z(C(\beta))^{-N}\rho(\{x_{N-1}\}')}{1 - z\hat{f}(0)}. \tag{III.11}$$

We define an operator W such that

$$W\rho_N(\{x_N\}) = \rho_N(\{x_N\}) - \int F'(x_1 - x_{N+1})(1 - \prod_{j=2}^{N}(1 + f_{N+1,j})) \times \rho_N(x_{N+1}, \{x_{N-1}\}')\,dx_{N+1}.$$

From equation (II. 7) it is clear that for the range of z considered, W has a bounded inverse.

Employing the uniform convergence of all the integrals in (III. 11) we have

$$\lim_{\Lambda\to\infty}\bar{\phi}'_{\Lambda_I} = W^{-1}[\lim_{\Lambda\to\infty}\Delta\frac{z(C(\beta))^{-N}\rho(\{x_{N-1}\}')}{1 - z\hat{f}(0)} + \Delta\int dx_{N+1}\lim_{\Lambda\to\infty}F'(x_1 - x_{N+1})\{\bar{\phi}'_{\Lambda_I}(x_{N+1_0}, \{x_{N-1}\}_I) + \bar{\phi}'_{\Lambda_0}(x_{N+1_0}, \{x_{N-1}\}'_I)\}]. \tag{III.12}$$

From (I) it can be seen that the first term on the r.h.s. of (III. 12) is the solution of the infinite volume S-O equation for $(C(\beta))^{-N}\bar{\phi}'_I(\{x_N\})$. The remaining terms can, by considerations identical to those of Sec. II, be shown to damp in the proposed manner. Each time a S-O equation is solved the residue of the infinite volume limiting procedure contains an additional term. The question remains whether the residue remains finite for R small and still damps in the proposed manner for R large in the limit as N, the order of the S-O solution, becomes infinite. That this is in fact the case can be seen by noting that each term that is added is of the form

$$T_N + \gamma T_N = \gamma' T_N,$$

where γ is a bounded operator and T_N is a function of such a form that $(C(\beta))^{-N}T_N$ is bounded for all N. From equation III. 1 it can be seen that the Nth S–O distribution function has a damped term which is bounded by

$$\sum_{n=1}^{N}\left(\frac{ze^{\beta B'}}{1 - ze^{\beta B'}C(\beta)}\right)^{n}T, \tag{III.13}$$

where

$$\left\|\prod_{j=1}^{N}(1 + f_{ij})\right\| < e^{\beta B'} \quad \nabla N$$

and

$$\|\phi_N^{-1}\| < (1 - ze^{\beta B'}C(\beta))^{-1}.$$

For the range of z considered

$$\frac{ze^{\beta B'}}{1 - ze^{\beta B'}C(\beta)} < 1$$

and (III. 13) converges in the limit as $n \to \infty$. This concludes the proof of the form of the residue of the infinite volume limiting procedure of the S-O distributions.

RESULTS AND CONCLUSIONS

Although the form of the residue of the infinite volume limiting procedure was derived for an approximate hierachy it is clear that this form should be a good approximation for very small z.

As was argued in (I) and mentioned in the introduction of this paper, the solution of the entire hierarchy, via the perturbation expansion, involves solving equations identical to those of the S-O hierarchy except for the inhomogeneous term. The methods, therefore, employed in this paper, and their results, are those tools which are needed to generalize this result to perturbation solutions of the exact hierarchy.

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Proof of Zwanzig's rule of "planar" graphs

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A rigorous proof is given of Zwanzig's conjecture that only planar graphs contribute to the virial coefficients of discreet-orientation models for a fluid of long thin rods. The proof makes use of relations between connected graphs and "trees"—the simplest type of connected graphs.

1. INTRODUCTION

Zwanzig[1] has introduced a simple model-a system of long rectangular parallelepipeds allowed to point in only three mutually perpendicular directions-for the study of the liquid crystal phase transition in a gas of long thin rods. (This first order transition was first predicted by Onsager[2]). Within this model, it is feasible to calculate, well beyond the second virial approximation, Onsager's series for the Helmholtz free energy of a gas of long rods.[2] The virial coefficients in this series are given by the formula[1,3]

$$B(n_1, n_2, n_3) = \frac{1}{V\Pi(n_i!)} \int (\sum \Pi f) d^3r_1 \ldots d^3r_N \quad (N = \sum_1^3 n_i), \tag{1}$$

where $\sum \Pi f$ is a sum of products of Mayer f functions taken over all irreducible graphs with n_i molecules pointing in direction i, $i = 1, 2, 3$. The number of virial coefficients that need to be computed was greatly reduced by Zwanzig by means of the conjecture that only "planar" graphs make nonvanishing contributions to the integral $(1/V) \int \sum \Pi f$ in the limit

$$l \to \infty, \quad l^2 d = \text{const} \tag{2}$$

(l = length, $d \times d$ = square cross section of parallelepipeds). The planar graphs are those in which all the molecular long axes are parallel to the same plane. [Therefore, the only nonvanishing virial coefficients are of the form $B(n_1, n_2, 0)$].

In this article we give a rigorous proof of Zwanzig's conjecture; i.e., it is shown that any nonplanar, irreducible graph G of N points $N \geqslant 3$, has a vanishing integral in the limit (2):

$$\int' \Pi_G f = 0 \quad \text{[in limit (2)]}, \qquad G = \text{nonplanar, irreducible graph.} \tag{3}$$

(The prime means integration over only $N - 1$ molecules.) The proof, although presented for Zwanzig's case, will be seen to apply to any model with a finite number of allowed directions for the molecular long axes.[4] To our knowledge, (3) has not been proven before (see also Sec. 4).

Further work along the lines of Zwanzig has been done by Runnels and Colvin.[5]

2. PRELIMINARIES AND DEFINITIONS

For the sake of clarity, we adopt, to some extent, the mathematical style of presentation. Thus, we have definitions, theorems, etc.

The concepts of graph, connected graph and irreducible graph are assumed known.[6]

Our proof in the next section, although quite simple, makes use of the existence of a certain type of graphs—which we call "trees"—and some elementary theorems about these graphs. The following definitions introduce the idea of a tree and several related concepts needed to understand Theorems A1 and A2 of the Appendix. We use capitals to denote graphs and sets in general and lower case letters, or numerals, to denote points of a graph. Recall that a graph is a set $\{a_i\} \cup \{a_j a_k\}$ of points a_i and lines (or "bonds") $a_j a_k$ joining some pairs of points.

Definition 1: We say there is a path $P = P(a_1, a_m) = \{a_1 a_2, a_2 a_3, \ldots a_{m-1} a_m\}$, connecting points a_1 and a_m of a graph G, if $a_i a_{i+1}$ is a bond of G, for $i = 1, 2, \ldots, m-1$, and all the points a_j are different.

Definition 2: A tree, T, is a connected graph such that any point of T is connected to a point o, of T, by a *unique* path. The point o is called the origin of T (see Fig. 1).

Definition 3: We say a graph G can be reduced to the graph G' if: (i) G' and G have the same set of points; (ii) set of bonds of $G' \subseteq$ set of bonds of G.

Definition 4: A mixed graph is a graph whose bonds are divided into several types or "colors".

Definition 5: Let G be a mixed graph and M be a maximal set of points of G connected by bonds of color x (regardless of bonds of other colors). Then the connected subgraph consisting of M and the bonds of color x is called an island of type x.

Definition 6: A terminal point of a graph is a point with one and only one attached bond.

It may be useful to point out that when we form a new graph by removing a point P from a graph, it is, of course, implied that all bonds attached to P are also removed. On the other hand, when a bond is removed from a graph its end points need not; unless otherwise stated, it is understood that the end points are not removed.

We give now a few simple theorems which are helpful in clarifying the concept of a tree. In particular, Theorem 5 shows why trees are useful to us.

Theorem 1: Any point of a tree serves equally well as origin of the tree.

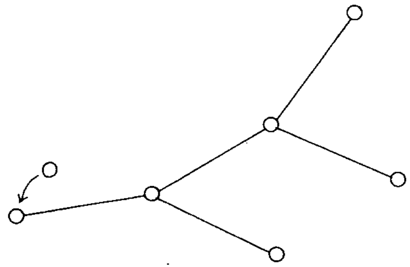

FIG. 1. Example of a tree. The point "o" is the chosen origin.

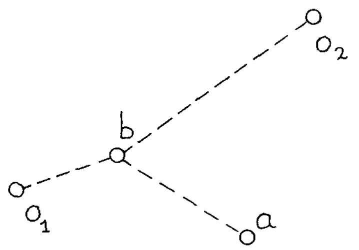

FIG. 2. Diagram for the proof of Theorem 1.

Proof: Let o_1 be the given origin of a nontrivial tree T (i.e., T contains more than one point). Pick some other point o_2 of T as candidate for origin of T. We show that there exists a unique path from o_2 to any point a ($\neq o_2$) of T.

By assumption, there exist unique paths $P(o_1, o_2)$ and $P(o_1, a)$. Let $P(o_1, b) = P(o_1, a) \cap P(o_1, o_2)$ [$b = o_2$, or $b = o_1$, are allowed; if $b = o_1$ then $P(o_1, b)$ is the empty set ϕ]. Then $P(o_1, o_2) = P(o_1, b) \cup P(b, o_2)$ and $P(o_1, a) = P(o_1, b) \cup P(b, a)$, where $P(b, a)$ is a path from b to a (see Fig. 2). Therefore, $P(o_2, a) = P(o_2, b) \cup P(b, a)$ is a path from o_2 to a. This path is unique. For, suppose there exists a $P'(o_2, a) \neq P(o_2, a)$. Then, by an argument similar to the above, it follows there exists a $P'(o_1, a) \neq P(o_1, a)$, contradicting the fact that T is a tree with origin o_1.

Theorem 2: (Composition of trees): (a) Let T_1, T_2 be two trees. Then the connected composite graph T_3 obtained by identifying any given pair of points of T_1 and T_2 is a tree; (b) Let T_3 be a nontrivial tree and pick an arbitrary point a of T_3. Suppose a (the "linkage" point) is bonded to points b_i, $i = 1, 2, \ldots, p$ (and no others). Let $1 \leq r \leq p$. Then the subgraph T_1 containing a, and all the points of T_3 connected to a through the bonds ab_i, $i = 1, 2, \ldots, r$, is a tree. Similarly, the subgraph T_2 containing a and the points connected to a through ab_i, $i = r + 1, \ldots, p$, is a tree (if $r = p$, define $T_2 = \{a\}$). Note: $T_3 = T_1 \cup T_2$ in both (a) and (b).

Proof: (a) Let o_1 and o_2 be the points of T_1 and T_2 that are to be identified. Choose o_i as origin of T_i. Then $o_1 = o_2 \equiv o$, is, by Definition 2, and origin for T_3.

(b) Choose a as origin of T_3. Then, obviously, a is an origin for both T_1 and T_2.

Theorem 3: Let T be a tree with N points, $1 < N < \infty$, with chosen origin o. Then T has at least one terminal point, $t, t \neq o$.

Proof: Consider a sequence of lengthening paths $P(o, a_n) = \{oa_1, a_1a_2, \cdots, a_{n-1}a_n\}, n = 1, 2, \cdots$. Because $N > 1$, $P(o, a_1)$ exists. Now suppose $P(o, a_n)$ exists. If a_n is connected to some point b other than a_{n-1}, then $b \neq a_i$ for $i = 0, 1, \ldots, n-1$ (for otherwise there would exist two different paths from o to a_n). Therefore, we can form $P(o, a_{n+1}) = \{oa_1, \cdots, a_{n-1}a_n, a_na_{n+1}\}$ $(a_{n+1} = b)$. But T is finite ($N < \infty$); therefore, there must exist a path $P(o, a_m)$, with $m < N - 1$, such that a_m is only connected to a_{m-1}. Thus, we can take $t = a_m (\neq o)$.

Theorem 4: The number of bonds in a tree of N points is $N - 1$.

Proof: If $N = 1$ the proposition is obviously true. Suppose the proposition is true for a tree with N points. Consider a tree T with $N + 1$ points, and let o denote its origin. By Theorem 3, T has a terminal point b with unique bond ab. Then, by Theorem 2(b), the subgraph T' containing all points of T other than b is a tree. T' has N points and, by the induction hypothesis, $N - 1$ bonds. Therefore, $T = T' \cup \{b\} \cup \{ab\}$ has $(N - 1) + 1 = (N + 1) - 1$ bonds. The proof is completed by mathematical induction.

Theorem 5: Let T be a finite tree (number of points $N < \infty$) with origin o. Then T can be collapsed down to the origin o by successive removal of terminal points (and their single bonds).

Proof: If $N = 1$, there is nothing to prove. If $N > 1$, T has a terminal point $t_1 (\neq o)$, by Theorem 3. Thus, we can remove t_1 (and its single bond) from T to get the graph T_1. By Theorem 2(b), T_1 is a tree. T_1 has $N - 1$ points. If $N - 1 > 1$, the argument can be repeated to form T_2 which has $N - 2$ points; and so on. The process ends with T_{N-1} which has only one point, namely the origin o.

In the integral of a graph, the integration over a terminal point can be carried out immediately as a single particle integral $\int f d^3R$. Therefore, by Theorem 5 and 4, the integral of a tree is computed very simply as the product of $N - 1$ single particle integrals. Letting a bond correspond to $-f$, which is nonnegative and dominated by 1 in the case of repulsive interactions, we can obtain an upper bound to the integral of a graph by reducing the graph to a tree (see the Appendix). This procedure is used heavily in the next section.

3. PROOF

Step 1: First we show that any connected graph G with at least one pair of parallel molecules joined by a bond has a vanishing integral in the limit (2).

Let molecules 1 and 2 be parallel and joined by bond 12. Let us say that the bond 12 is "red" while all the other bonds of G are "white". By the corollary of Theorem 2 of the Appendix, we can reduce the mixed graph G to a tree T with the red bond 12 appearing in T. Since the number of bonds in T is no greater than the number of bonds in G, and since $-f_{ij} = 0$ or 1 for hard core interactions, we have

$$0 \leq \Pi_G(-f_{ij}) \leq \Pi_T(-f_{ij}). \tag{4}$$

The single particle integral is given by[1]

$$\int (-f_{ij}) d^3r_i = \begin{cases} 2(l+d)^2 d & \text{for } i \text{ and } j \text{ perpendicular,} \\ 8ld^2 & \text{for } i \text{ and } j \text{ parallel.} \end{cases} \tag{5}$$

Therefore, taking molecule 1 as the origin of T, one gets, in the limit (2) (with N = number of points in G),

$$\begin{aligned} \int d^3r_2 \cdots d^3r_N \, \Pi_T(-f_{ij}) &\leq (2l^2d)^{N-2} \int d^3r_2(-f_{12}) \\ &\leq 4(2l^2d)^{N-1} d/l \\ &\xrightarrow[\lim (2)]{} 0. \end{aligned} \tag{6}$$

Combining (6) and (4), we have the desired result. It is sufficient, therefore, to consider graphs G where only perpendicular molecules are joined by a bond.

Step 2: Let G be a nonplanar, irreducible graph of N points, $N \geq 3$. Pick a triplet of mutually perpendicular molecules, labeled 0, 1, and 2, say, and connected by bonds 01, 12 (see Fig. 3). (It is easy to see that G must contain such a triplet. For, consider molecules a and b, joined to each other by bond ab and, to a third molecule, 3, perpendicular to both, by path $P = \{ab, \ldots, x3\}$. Such molecules, a, b, 3 and path P exist because G is nonplanar and connected. Further, we can suppose 3 is the first molecule perpendicular to both a and b that is encountered along P—otherwise take a shorter P. Then molecule 3 and the two molecules preceeding it in P form a connected triplet of mutually perpendicular molecules—remember only perpendicular molecules are joined by a bond). Because G is irreducible, there exists a path $P' = \{23, 34, \ldots, (M-1)M, M0\}$, from 2 to 0, different from the path $P = \{21, 10\}$. Let us take the bonds 01, 12, 23, ..., $(M-1)M$ as "red" and all the remaining bonds of G as "white" (see Fig. 3). By the corollary of Theorem 2 of the Appendix, G can be reduced to a tree T which includes all of the "red" bonds.

The integral of T, however, is not a useful upper bound for the integral of G. A better bound is obtained by inserting back the bond $M0$ into T to give the graph T'. We can integrate off the points of T', except those in the *closed* path $\{01, 12, \ldots, (M-1)M, M0\}$, in the same fashion as for T:

$$\int' \Pi d^3r\, \Pi_G(-f_{ij}) \leq \int' \Pi d^3r\, \Pi_{T'}(-f_{ij}) = [2(l+d)^2 d]^{N-M-1} I_M, \tag{7}$$

where

$$I_M \equiv \int \prod_{i=1}^{M} d^3r_i (-f_{01})(-f_{12})\cdots(-f_{M0}). \tag{8}$$

The Mayer f function for Zwanzig's model can be written

$$-f_{ij} = \theta_r(x_i - x_j)\theta_p(y_i - y_j)\theta_q(z_i - z_j), \tag{9}$$

where

$$\theta_s(\zeta) = \begin{cases} 1, & |\zeta| < s, \\ 0, & |\zeta| > s, \end{cases}$$

and r, p, q depend on the orientations of molecules i and j; e.g., if i and j are both parallel to the X axis then $r = l$, $p = q = d$. With this notation, I_M becomes a product of integrals in the x, y, and z variables:

$$\begin{aligned} I_M = &\int \prod_1^M dx_i \underline{\theta_L(x_0 - x_1)}\theta_d(x_1 - x_2)\theta_{r_3}(x_2 - x_3)\ldots\theta_{r_{M+1}}(x_M - x_0) \\ &\times \int \prod_1^M dy_i \underline{\theta_L(y_0 - y_1)}\theta_L(y_1 - y_2) \\ &\times \theta_{p_3}(y_2 - y_3)\ldots\theta_{p_{M+1}}(y_M - y_0) \\ &\times \int \prod_1^M dz_i \theta_d(z_0 - z_1)\underline{\theta_L(z_1 - z_2)} \\ &\times \theta_{q_3}(z_2 - z_3)\ldots\theta_{q_{M+1}}(z_M - z_0). \end{aligned} \tag{10}$$

Here $L = (l + d)/2$ and, for each i, two of r_i, p_i, q_i are equal to L and one is equal to d (since only perpendicular molecules are joined by a bond).

An upper bound for I_M may be obtained by replacing the integrand of each *factor* in (10) by a tree; we do this by dropping in each factor the least restrictive of the two (one-dimensional) bonds attached to molecule 1 [these are the underlined bonds in (10)]. Because molecule 1 is "doubly-restricted," i.e., restricted to an interval of $2d$ in *two* directions by the combined action of its neighbors, the integration over $\mathbf{r}_1$ gives a factor $(2d)^2 2L$:

$$I_M \leq (2d)^2 2L \int \prod_2^M d^3r_i (-f_{23})\cdots(-f_{M0}) = (8Ld^2)(8L^2d)^{M-1}. \tag{11}$$

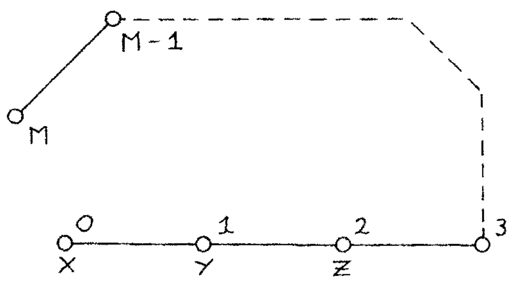

FIG. 3. The subset of red bonds in the nonplanar graph G (see Sec. 3, Step 2).

Combining (11) and (7), and recalling $L = (l + d)/2$, gives

$$\begin{aligned} 0 &\leq \int' \Pi d^3r\, \Pi_G(-f_{ij}) \leq (8L^2d)^{N-2} 8Ld^2 \\ &= (8L^2d)^{N-1} d/L \\ &\xrightarrow[\lim (2)]{} 0. \end{aligned} \tag{12}$$

which is the desired final result.

4. COMMENTS

The above proof can be adapted to the case where the molecules have more than three (but finitely many) allowed directions.[4] The single particle integral, Eq. (5), is given—in the limit (2)—by $(2l^2d)\sin\theta_{ij}$, where θ_{ij} is the angle between the long axes of molecules i and j. This is again zero for molecules i and j parallel. Molecules 0, 1, and 2 of the proof (see Fig. 3) are now, in general, a nonplanar, oblique triplet. The Mayer f functions for a given triplet can be written in the form (9) with the coordinates x_i, y_i, z_i referred to oblique axes parallel to the three molecular directions. The volume elements dV_i contain, when expressed in terms of dx_i, dy_i, dz_i, a constant factor depending on the angles between the oblique axes. The main thing is, that after removal of the three least restrictive one-dimensional bonds attached to molecule 1 in

$$\begin{aligned} I_M = \text{const} \times \int' \Pi\, dx_i dy_i dz_i \theta_L(x_0 - x_1)\theta_d(x_1 - x_2) \\ \theta_L(y_0 - y_1)\theta_L(y_1 - y_2) \\ \times \theta_d(z_0 - z_1)\theta_L(z_1 - z_2)(-f_{23})\cdots(-f_{M0}), \end{aligned}$$

The integral over $\mathbf{r}_1$ is proportional to Ld^2. Therefore, we again get $I_M \propto (L^2d)^M d/L$ and the result (12) for nonplanar graphs G.

After completing the above work we found the article by Runnels and Colvin, reference 5, which contains an argument to show that the integral of a non-planar graph vanishes in the limit (2). We wish to note that their argument contains much of the basic geometry of the problem, but does not quite constitute a rigorous proof. They did not have a method for estimating upper bounds of integrals of graphs and their argument makes no use of the fact that one is dealing with irreducible graphs. It is easy to see, however, that the result (3) can only be asserted in general for graphs G that are irreducible [e.g., if T is a tree of N points, then $\int' \Pi\, d^3r\, \Pi_T(-f) = (8L^2d)^{N-1}$, regardless of whether the graph is planar or not, provided that bonds join only perpendicular molecules].

ACKNOWLEDGMENTS

I am grateful to Dr. Baez Duarte of the Mathematics Department of IVIC for suggesting the proof by induction of Theorem A1 of the Appendix.

APPENDIX

Theorem A1: Any finite connected graph can be reduced to a tree.

Proof: Let G_N denote an arbitrary connected graph of N points. The theorem is obviously true for $N = 1, 2$. Suppose that the proposition is true for N. Now consider a G_{N+1}, and pick $a \in G_{N+1}$; by removing a and all its bonds ab_i, $i = 1, 2 \ldots p$, from G_{N+1} we obtain a graph G_N. (Since G_{N+1} is connected, $p \geq 1$). By assumption, G_N can be reduced to a tree T_N. Let $T_{N+1} = T_N \cup \{a, b_1\} \cup \{ab_1\}$. T_{N+1} contains all the points of G_{N+1} (obvious) and is a tree (by Theorem 2(a) in the text). Also, bonds of $T_{N+1} \subseteq$ bonds of G_{N+1} (since bonds of $T_N \subseteq$ bonds of G_N). Therefore, G_{N+1} can be reduced to the tree T_{N+1}. The theorem follows by induction.

Notation: given a connected graph G, the symbol G^T denotes any tree to which G can be reduced (by Theorem A1, G^T exists).

Theorem A2: Let G be a finite, mixed graph with white and red bonds. Suppose G contains red islands I_i, $i = 1, 2 \ldots, L$. Then G can be reduced to a tree T which contains subtrees I_i^T, $i = 1, 2, \ldots, L$.

Proof: We prove the theorem by mathematical induction on L.

Case $L = 1$

Let $G_1 \subset G$ be the graph obtained from G by removing all points of I_1; G_1 contains the points of G which have only white bonds attached. If $G_1 = \phi$, then I_1 contains all the points of G and $T = I_1^T$ satisfies the theorem.

Suppose $G_1 \neq \phi$. Then

$$G_1 = \bigcup_{i=1}^{M} K_i (K_i \cap K_j = \phi), \qquad 1 \leq M < \infty,$$

where the K_i are finite, connected graphs with white bonds. Let $\{a_j'\}$ be the set of points of I_1 which have, in G, white bonds attached. Because G is connected, we can select from $\{a_j'\}$ a subset $\{a_i\}_{i=1}^{M}$ such that a_i is joined to a point $k_i \in K_i$ by the bond $a_i k_i$. Some of the points a_i may be the same. Using Theorem A1, we know I_1, K_i can be reduced to trees I_1^T, K_i^T. By repeated application of Theorem 2(a) in the text, noting $k_i \in K_i^T$, $a_i \in I_1^T$ and that $\{a_i, k_i\} \cup \{a_i k_i\}$ is a tree, it follows

$$T = I_1^T \cup \left[\bigcup_{i=1}^{M} K_i^T \cup \{a_i, k_i\} \cup \{a_i k_i\} \right]$$

is a tree. (Also, the fact $I_1 \cap K_i = \phi$, has been used.)

Obviously, T contains all the points of G (since $p \in G$ means $p \in I_1$ or $p \in G_1$) and, bonds of $T \subseteq$ bonds of G; i.e., we have shown that G can be reduced to the tree T containing I_1^T.

Case of general L

Suppose the proposition is true for L. Let G be a mixed graph with $L + 1$ red islands I_i. Because G is connected, we can find a pair of islands, say I_L and I_{L+1}, such that they are connected by a path (of white bonds) $P = P(a, b) = \{ac_1, c_1 c_2, \ldots c_m b\}$ where only the endpoints $a \in I_L$ and $b \in I_{L+1}$ belong to an island. Now let us, momentarily, include the bonds of P among the red bonds. Then

$$J_L = I_L \cup I_{L+1} \cup \{c_i\}_{i=1}^{m} \cup P$$

is a single red island. Therefore, by hypothesis, G can be reduced to a tree T containing subtrees $I_1^T, I_2^T, \ldots, I_{L-1}^T, J_L^T$. Obviously, J_L^T contains all the points c_i and all the bonds of P (otherwise J_L^T would not be connected). By application of Theorem 2(b) in the text, to linkage points a and b, it follows that J_L^T contains subtrees I_L^T, I_{L+1}^T and $\{c_i\} \cup P$:

$$J_L^T = I_L^T \cup I_{L+1}^T \cup [\{c_i\}_{i=0}^{m+1} \cup P] (c_0 \equiv a, c_{m+1} \equiv b).$$

Therefore, G has been reduced to a tree T containing subtrees $I_1^T, I_2^T, \ldots, I_L^T$, and I_{L+1}^T. Mathematical induction completes the proof of the theorem.

Corollary: If I_i is already a tree, then all the bonds of I_i appear in T.

Proof: By Definition 2 it is immediate that the removal of any bond from a tree results in a disconnected graph. Therefore, a tree cannot be reduced further, i.e., $I_i^T = I_i$, if I_i is a tree. Hence, I_i appears in T.

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Note on space-times that admit constant electromagnetic fields*

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All space–times that admit a covariantly constant, test, electromagnetic field are constructed. All solutions to the Einstein–Maxwell equations with constant electromagnetic field are given.

1. INTRODUCTION

Honig, Schücking, and Vishveshwara recently gave an elegant discussion[1] of the motion of a charged test particle in any space-time $(M, \mathbf{g})$ with a covariantly constant (hence source-free) electromagnetic field $\mathbf{F}$. But they did not address the question: Which $(M, \mathbf{g})$ admit such an $\mathbf{F}$, even a test field $\mathbf{F}$? This note answers this question. The argument will be familiar to mathematicians, but physicists may find it novel. For simplicity, we will confine the work to some local neighborhood in $(M, \mathbf{g})$.

2. HOLONOMY OF SPACE-TIME

Choose any point $p \in M$ in space-time. Fix, once and for all, a simply connected neighborhood U of p. Parallelly carry an orthonormal tetrad O_p around any closed path in U beginning and ending at p, yielding some new tetrad O'_p: $O'_p = \Lambda O_p$, where Λ is some homogeneous Lorentz transformation depending only on the choice of path. The set of all such Λ at p for all possible paths forms Cartan's (local) *holonomy group*[2,3,4] $H(p)$. $H(p)$ is a subgroup of the homogeneous Lorentz group L; $H(p)$ is in fact independent of $p \in U$. Roughly, the higher the symmetry of $(M, \mathbf{g})$, the *smaller* $H(p)$ is.

Let $\mathbf{T}$ be any geometric-object field on $(M, \mathbf{g})$ for which covariant differentiation ∇ is defined. Can there exist in U a covariantly constant $\mathbf{T}$, $\nabla\mathbf{T} = 0$? If so, $\mathbf{T}$ can be uniquely constructed by giving its value $\mathbf{T}(p)$ at *one* point $p \in U$, and then carrying $\mathbf{T}$ parallelly all over U along paths in U. This construction must be path-independent; equivalently, $\mathbf{T}(p)$ must be left invariant at p when it is carried parallelly around any closed path beginning and ending at p. That is, $\mathbf{T}(p)$ must be invariant under the action of $H(p)$:

Lemma (see e.g., Schouten[2]): $(M, \mathbf{g})$ (locally) admits a covariantly constant, test, field $\mathbf{T}$ iff there exists $\mathbf{T}(p)$ at any point $p \in M$, invariant under the holonomy group $H(p)$.

3. CONSTANT, TEST, ELECTROMAGNETIC FIELD

The differential problem, "solve $\nabla\mathbf{F} = 0$," is thus reduced to an algebraic problem (Cartan's favorite trick!): Choose a point p; find an electromagnetic field tensor $\mathbf{F}(p) \neq 0$ such that its invariance group $G[\mathbf{F}(p)]$,

$$G[\mathbf{F}(p)] \equiv \left\{ \Lambda \in L \mid \Lambda\mathbf{F}(p) = \mathbf{F}(p) \right\},$$

contains the holonomy group: $H(p) \subseteq G[\mathbf{F}(p)] \subseteq L$.

Choose a favored observer at p with tetrad $O_p = (\mathbf{e}_{\hat{t}}, \mathbf{e}_{\hat{x}}, \mathbf{e}_{\hat{y}}, \mathbf{e}_{\hat{z}})$ so that the tetrad components $F_{\mu\nu}$ of $\mathbf{F}(p)$ reduce to one of two canonical forms[5]: "$\mathbf{F}(p)$ null" or "$\mathbf{F}(p)$ nonnull."

(A) $\mathbf{F}(p)$ null: $F_{\hat{t}\hat{x}} = -F_{\hat{x}\hat{t}} = F_{\hat{x}\hat{z}} = -F_{\hat{z}\hat{x}} = A = \text{const}$, other components vanish. $G[\mathbf{F}(p)]$ is generated by the two null rotations[6] which leave invariant the null direction defined by $\mathbf{k} = \mathbf{e}_{\hat{t}} + \mathbf{e}_{\hat{z}}$. Define the spinor[7] $o^A(p)$ by $o^A(p)\bar{o}^{\dot{A}}(p) = k^{A\dot{A}}$; then $G[\mathbf{o}^A(p)] = G[\mathbf{F}(p)]$. Therefore (by lemma) $(M, \mathbf{g})$ must admit a covariantly constant spinor field $\mathbf{o}^A$ (equivalently, a covariantly constant, complex, null bivector field $\mathbf{F} + i^*\mathbf{F}$). By a result of Ehlers and Kundt,[8] it is necessary and sufficient that in some local coordinates

$$\mathbf{g} = 2K(u,x,y)du^2 + 2du\,dv + dx^2 + dy^2, \qquad (1a)$$

and

$$\mathbf{F} = 2^{1/2}A\,du \wedge dx. \qquad (1b)$$

(B) $\mathbf{F}(p)$ nonnull: $F_{\hat{t}\hat{z}} = -F_{\hat{z}\hat{t}} = A\cos\theta = \text{const.}$, $F_{\hat{x}\hat{y}} = -F_{\hat{y}\hat{x}} = A\sin\theta = \text{const.}$, other components vanish. $G[\mathbf{F}(p)]$ is the direct product of the one-parameter group of boosts in the (tz) plane with the commuting one-parameter group of rotations in the (xy) plane. It is a fundamental result[3] that if the tangent space T_p is reducible under $H(p)$, then $(M, \mathbf{g})$ is correspondingly reducible into the direct product of (pseudo-) Riemannian manifolds of lower dimension. Here, T_p reduces to the (tz) and (xy) planes under $H(p)$, so $(M, \mathbf{g}) = (M_+, \mathbf{g}_+) \otimes (M, g_-)$, where $(M_+, \mathbf{g}_+)$ is a Lorentzian 2-manifold and $(M_-, \mathbf{g}_-)$ is a Riemannian 2-manifold. The vector fields $\mathbf{e}_{\hat{t}}$ and $\mathbf{e}_{\hat{z}}$ lie entirely in $(M_+, \mathbf{g}_+)$; $\mathbf{e}_{\hat{x}}$ and $\mathbf{e}_{\hat{y}}$ lie entirely in $(M_-, \mathbf{g}_-)$. In some coordinates,

$$\mathbf{g} = \mathbf{g}_+ + \mathbf{g}_-, \qquad (2a)$$

where

$$\mathbf{g}_+ = g_{+ab}(t,z)dx^a dx^b, \quad x^a \equiv (t,z), \qquad (2b)$$

$$\mathbf{g}_- = g_{-ij}(x,y)dx^i dx^j, \quad x^i \equiv (x,y), \qquad (2c)$$

and

$$\mathbf{F} = A\cos\theta(-g_+)^{1/2}dt \wedge dz + A\sin\theta(g_-)^{1/2}dx \wedge dy. \qquad (2d)$$

Equations (1) and (2) give all space-times $(M, \mathbf{g})$, and all test fields $\mathbf{F}$, that solve $\nabla\mathbf{F} = 0$.

4. ELECTROVAC SOLUTIONS

Now impose the Einstein-Maxwell equations for a nontest $\mathbf{F}$, to find all solutions with covariantly constant $\mathbf{F}$. The resulting electrovac space-times are well known.

(A) $\mathbf{F}$ null: The Einstein-Maxwell equations for Eqs. (1) read

$$(\partial_x^2 + \partial_y^2)K(u,x,y) = -4A^2. \qquad (3)$$

The general solution K is a linear superposition, $K = K_{\text{em}} + K_{\text{grav}}$, where K_{em} is the particular solution,

$$K_{\text{em}} = -A^2(x^2 + y^2),$$

and K_{grav} is any homogeneous solution,

$$(\partial_x^2 + \partial_y^2)K_{\rm grav}(u,x,y) = 0.$$

$K_{\rm em}$ represents the transverse, "monopole," always focusing gravitational disturbance due to **F**; this disturbance is homogeneous for local observers (despite the dependence of $K_{\rm em}$ on x and y). $K_{\rm grav}$ represents an arbitrary "plane-fronted gravitational wave with parallel rays"[8] ("pp wave"). So the electrovac space-time given by Eqs. (1) and (3) describes an arbitrary, gravitational pp wave traversing a region of constant, null **F**, such that the wave direction is everywhere parallel to the Poynting vector.

(B) F nonnull: The Einstein-Maxwell questions for Eqs. (2) imply that (M_+, g_+) is a two-dimensional anti-deSitter space-time[9] of radius A^{-1}, and that (M_-, g_-) is a 2-sphere of radius A^{-1}. This solution is the "Bertotti-Robinson magnetic universe"; for discussions see Bertotti,[10] Robinson,[11] and Lindquist,[12] and Exercise 32.1 of Misner, Thorne, and Wheeler.[13]

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Exact nearest neighbor degeneracy for dumbbells on a one-dimensional lattice space

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Relationships are developed which describe exactly the degeneracy associated with nearest neighbor pairs of occupied sites (1 — 1), mixed sites (0 — 1), and vacant sites (0 — 0) for dumbbells distributed on a one-dimensional lattice space. The first moments of these statistics are calculated, thereby permitting an evaluation of the error inherent in the use of the Bragg–Williams approximation for this situation.

I. INTRODUCTION

A statistical mechanical treatment of adsorption, elasticity, alloys, magnetism, and other cooperative phenomena which involve the nearest neighbor approximation, i.e., in which the total interaction energy E_i is written

$$E_i = n_{11}V_{11} + n_{01}V_{01} + n_{00}V_{00} \tag{1}$$

(where n_{11}, n_{01}, and n_{00} are the number of occupied, mixed, and vacant nearest neighbor pairs respectively and V_{11}, V_{01} and V_{00} are the related potential energies of interaction), requires knowledge of the degeneracy associated with each type of nearest neighbor pair.

For simple particles, each of which occupies a single lattice site, the question of nearest neighbor pair degeneracy for a one-dimensional lattice space has been considered in a previous paper.[1] The purpose of the present paper is to extend these previously reported results to situations in which dumbbells (particles which occupy two adjacent sites) are distributed on a one-dimensional lattice space. The treatment of the adsorption of homonuclear, diatomic molecules involving nearest neighbor interaction represents one application of the statistics to be developed herein. Obviously, the subscripts 0 and 1 could refer to electronic spin or chemical species as well as occupation.

If one neglects the end compartments of the lattice space, the numbers n_{11}, n_{01}, and n_{00} are related by

$$2q = 2n_{11} + n_{01}, \tag{2}$$

$$2(N-2q) = 2n_{00} + n_{01}, \tag{3}$$

where q is the number of dumbbells and N is the number sites of which the lattice space is composed.

Equations (2) and (3) may be derived on the basis of the following reasoning (see Fig. 1). If a line is drawn from each occupied site to its nearest neighbor (see Fig. 1A), there will be $4q$ lines. The total number of lines can also be determined by noting that between the two parts of a dumbbell there are two lines, between occupied nearest neighbor pairs there are two lines, and between mixed nearest neighbor pairs there is one line. Thus

$$4q = 2q + 2n_{11} + n_{01},$$

which is given in Eq. (2).

Next draw a line from every empty site to each of its nearest neighbors (see Fig. 1B); there will be $2(N-2q)$ lines. Of these, two lines will be between each vacant nearest neighbor pair and one line will be between a mixed nearest neighbor pair. Hence Eq. (3).

Thus from Eqs. (2) and (3) any of the numbers n_{11}, n_{01} or n_{00} can be determined approximately in terms of another number, the number of dumbbells, and the number of lattice sites.

II. OCCUPIED NEAREST NEIGHBOR DEGENERACY

In this Section we will calculate $A[n_{11}\,|\,q,N]$, the number of ways of arranging q indistinguishable dumbbells on a one-dimensional lattice space of N equivalent compartments in such a way as to create exactly n_{11} occupied nearest neighbor pairs.

It has been shown[2] that $A[q,N]$, the total number of independent arrangements arising when q indistinguishable dumbbells are arranged in all possible ways on a one-dimensional lattice space of N equivalent sites, is given by

$$A[q,N] = \binom{N-q}{q}. \tag{4}$$

If we consider the subset of the $A(q,N)$ arrangements which contains only those arrangements in which exactly n_{11} occupied nearest neighbor pairs occur, then we find that the selected arrangements always contain $q - n_{11}$ "units" (see Fig. 2). This arises because there are $q-1$ separations between the q dumbbells. Of these, n_{11} separations are between occupied nearest neighbor pairs, so that $q - 1 - n_{11}$ separations are not between nearest neighbor pairs. Thus there are $q - n_{11}$ "units." Such "units" consist of one or more pairs of occupied sites together with a single vacancy (if one is needed) to isolate a "unit" from other dumbbells and/or other vacancies. Thus the number of separating vacancies is one less than the number of "units." For purposes of the following argument we will consider initially each of these "units" to be identical, regardless of the number of particles incorporated in it or whether or not it is terminated by a vacancy.

There are $N - 2q$ vacancies but not all of these are permutable, i.e., not all of the $N-2q$ vacancies can be

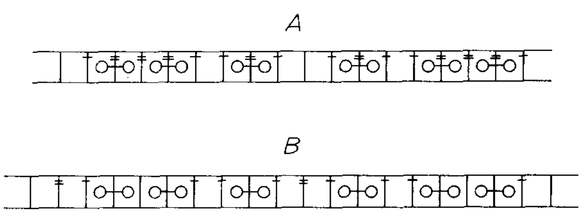

FIG. 1(A). Figure used in deriving Eq. (1). A line is drawn from each occupied site to each of its nearest neighbor sites. (B) Figure utilized in deriving Eq. (2). A line is drawn from each vacant site to each of its nearest neighbor sites.

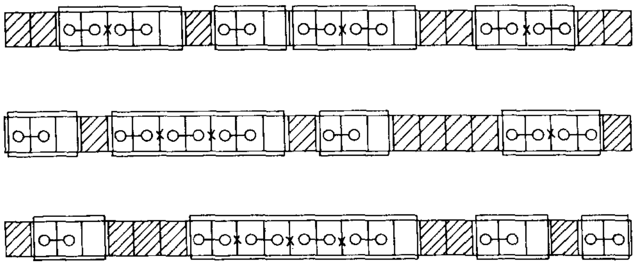

FIG. 2. $q = 7$ indistinguishable dumbbells are arranged on a one-dimensional lattice space of $N = 24$ equivalent sites to yield exactly $n_{11} = 3$ occupied nearest neighbor pairs (represented by crosses). Regardless of the arrangements there are $q - n_{11} = 4$ "units" (unshaded). These units can be permuted with $N - 3q + n_{11} = 7$ vacancies (shaded). There are $\binom{11}{4}$ independent ways of arranging the "units" and the permutable vacancies. This figure shows three possible arrangements in which the indistinguishable "units" are composed of all the possible groupings of occupied nearest neighbor pairs, that is, the nearest neighbor pairs are in (1) different "units", (2) one in one "unit" and two in another, and (3) all nearest neighbor pairs are in the same "unit."

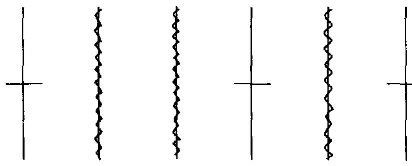

FIG. 3. The seven dumbbells illustrated at the top of Fig. 2 have six separations between them. Of the six separations, $n_{11} = 3$ are between occupied nearest neighbor pairs, (short horizontal lines) and 3 are not (jagged lines). Figure 3 represents the arrangement shown at the top of Fig. 2. There are $\binom{6}{3}$ ways of arranging the separations between the seven dumbbells with the constraint that three of the separations are between nearest neighbor pairs.

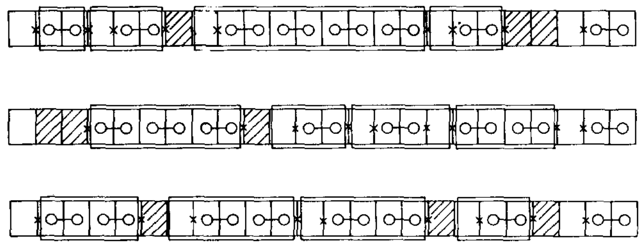

FIG. 4. Eight indistinguishable dumbbells are arranged on a one-dimensional lattice space of $N = 24$ equivalent sites to yield $n_{01} = 9$ mixed nearest neighbor pairs (represented by crosses). Regardless of the arrangement there are $[(n_{01} - 1)/2] = 4$ permutable "units" (unshaded) and $N - 2q - 1 - [(n_{01} - 1)/2] = 3$ permutable vacancies (shaded). Thus there are $\binom{7}{4}$ ways of arranging the "units" with the permutable vacancies.

interchanged to form additional independent arrangements. Because one of the "units" on an end does not need a vacancy to isolate it, there are $q - n_{11} - 1$ vacancies which must be utilized to separate the $q - n_{11}$ "units." Thus the number of indistinguishable, permutable vacancies is $N - 2q - (q - n_{11} - 1) = N - 3q + n_{11} + 1$.

Consequently, the total number of individual objects is just the sum of the number of "units" and the number of permutable vacancies, i.e., $(q - n_{11}) + (N - 3q + n_{11} + 1) = N - 2q + 1$. Now the number of ways of arranging $N - 2q + 1$ things of which $q - n_{11}$ are one kind (indistinguishable) and $N - 3q + n_{11} + 1$ are another (indistinguishable) is the binomial coefficient

$$\binom{N - 2q + 1}{q - n_{11}} = \binom{N - 2q + 1}{N - 3q + n_{11} + 1}.$$

We have assumed that all the "units" are identical. Clearly this is not correct. To remove this constraint and to ascertain $A[n_{11} \mid q, N]$, we must determine the number of ways the dumbbells can be arranged to form the $q - n_{11}$ "units." There are $q - 1$ separations between the q dumbbells of which the "units" are composed (see Fig. 3); n_{11} of these separations constitute nearest neighbor pairs and $q - n_{11} - 1$ separations do not involve nearest neighbor pairs. There are

$$\binom{q-1}{n_{11}} = \binom{q-1}{q-1-n_{11}}$$

ways of arranging the $q - 1$ separations where n_{11} of the separations are between nearest neighbor pairs,

$A[n_{11} \mid q, N]$ is thus given by the product of the number of possible arrangements of the "units" and the number of possible ways in which the "units" can be constituted, i.e.,

$$A[n_{11} \mid q, N] = \binom{q-1}{n_{11}} \binom{N - 2q + 1}{q - n_{11}}. \tag{5}$$

If $A[n_{11} \mid q, N]$ is summed over all values of n_{11}, $[0 \le n_{11} \le q - 1]$ the result, by Vandermonde theorem[3] is $\binom{N-q}{q}$ [see Eq. (4)].

III. MIXED NEAREST NEIGHBOR DEGENERACY

Here we are concerned with nearest neighbor pairs, one of which is occupied and one of which is vacant. An approximate solution for the degeneracy of mixed nearest neighbors when simple particles are involved was determined by Ising.[4] To determine $A[n_{01} \mid q, N]$, we must consider two situations: when n_{01} is odd and when it is even.

1. n_{01} odd

When n_{01} is odd, one and only one end compartment is occupied (see Fig. 4). If the occupied end compartment is on the right-hand side, we construct "units" consisting of a single dumbbell or contiguous group of dumbbells and the adjacent vacancy (if one is needed) just to the left to isolate the "unit" from other dumbbells and vacancies. Initially we consider these "units" to be indistinguishable, one from the other, regardless of their composition or configuration. We observe that there are always $[(n_{01} - 1)/2]$ of these permutable "units."

This arises because one of the n_{01} mixed nearest neighbor pairs is associated with the dumbbell on the end of the array. Two nearest neighbor pairs are then involved in each permutable unit. Thus there are $[(n_{01} - 1)/2]$ "units." These indistinguishable, permutable "units" may be permuted with the indistinguishable, permutable vacancies to form independent arrangements.

There are $N - 2q$ vacancies, but not all of them can be permuted with "units" to form independent arrangements. The number of vacancies which are required to form the "units" is $(n_{01} - 1)/2$. Thus there are $N - 2q - [(n_{01} - 1)/2] - 1$ indistinguishable permutable vacancies because one vacancy is required at the end of the array for a total of $N - 2q - [(n_{01} - 1)/2] - 1 + (n_{01} - 1)/2 = N - 2q - 1$ objects. These can be arranged in

$$\binom{N - 2q - 1}{(n_{01} - 1)/2} = \binom{N - 2q - 1}{N - 2q - 1 - [(n_{01} - 1)/2]}$$

independent ways.

The "units" are not, of course, indistinguishable; the dumbbells may be arranged in various ways to form "units" consisting of a range of numbers of dumbbells, subject only to the constraint that there be n_{01} mixed nearest neighbor pairs. To determine the number of ways q indistinguishable dumbbells may be arranged to form $[(n_{01}-1)/2]$ "units," we consider the $q-1$ separations between the q dumbbells (see Fig. 5). $[(n_{01}-1)/2]$ of these are the separations of the dumbbells by two mixed nearest neighbor pairs and $q-1-[(n_{01}-1)/2]$ separate adjacent dumbbells. These separations may be arranged in $\binom{q-1}{[(n_{01}-1)/2]}$ ways. This is just the number of ways q indistinguishable dumbbells can be arranged to form $[(n_{01}-1)/2]$ "units."

Consequently, if we require the compartment on the right end of the array to be occupied while the end compartment on the left is vacant then there are $\binom{N-2q-1}{(n_{01}-1)/2}\binom{q-1}{(n_{01}-1)/2}$ independent arrangements possible. Of course, with equal probability the end compartment on the left could have been occupied while the end compartment on the right could have been empty, so that in general if n_{01} is odd we obtain

$$A[n_{01}\,|\,q,n] = 2\binom{N-2q-1}{(n_{01}-1)/2}\binom{q-1}{(n_{01}-1)/2} \qquad (n_{01}\text{ odd}) \tag{6}$$

2. n_{01} even

If n_{01} is even, then in any single arrangement one of two situations exist:

(a) Both end compartments are vacant (see Fig. 6), or

(b) both end compartments are occupied (see Fig. 7).

If there are n_{01} mixed nearest neighbor pairs and if both end compartments are vacant, then there are always $[n_{01}/2]$ "units," each of which consists of a dumbbell or a contiguous group of dumbbells together with a vacancy (if one is needed) to isolate the "unit" from other "units." Regardless of their composition, we initially regard these units as identical, indistinguishable entities which can be permuted with some of the vacancies.

Not all of the $N-2q$ vacancies are permutable, i.e., they cannot all be positioned indiscriminately to form new arrangements. Because one and only one of the end units requires a vacancy to isolate it from the interior units, only $[(n_{01}-2)/2]$ of the vacancies are required to form mixed nearest neighbor pairs. Furthermore, two additional vacancies, one at either end, are not permutable. Thus there are $N-2q-[(n_{01}-2)/2]-2=N-2q-[n_{01}/2]-1$ permutable vacancies or a total of $[n_{01}/2]+N-2q-[n_{01}/2]-1=N-2q-1$ permutable objects. These can be arranged in

$$\binom{N-2q-1}{n_{01}/2}=\binom{N-2q-1}{N-2q-1-[n_{01}/2]}$$

independent ways.

Clearly, the "units," contrary to our initial assumption, are not identical. There are $\binom{q-1}{(n_{01}/2)-1}$ ways of arranging the q dumbbells in the $[n_{01}/2]$ units. This can be demonstrated by the following reasoning. There are $q-1$ lines which can symbolize the separation of the q dumbbells (see Fig. 8). Of these lines, $[(n_{01}-2)/2]$ represent separations of the dumbbells by two mixed nearest pairs and $q-1-[(n_{01}-2)/2]$ lines separate adjacent dumbbells. These $q-1$ lines can be arranged in $\binom{q-1}{[(n_{01}/2)-1]}$ independent ways. This represents the number of ways the q dumbbells can be arranged to form $[n_{01}/2]$ "units" when both end compartments are empty.

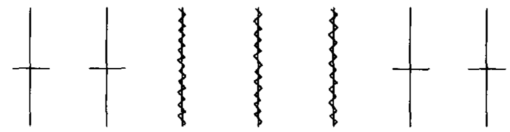

FIG. 5. Figure 5 considers the particular arrangement shown in the top arrangement in Fig. 4. There are $q-1=7$ separations between the eight dumbbells. Of these separations $[(n_{01}-1)/2]=4$ are separations between vacant and occupied sites, i.e., between mixed nearest neighbor pairs (short horizontal lines) and $q-1-[(n_{01}-1)/2]=3$ are separations between two dumbbells (jagged lines). Thus there are $\binom{7}{3}$ ways in which the seven separations may be arranged to form the four "units."

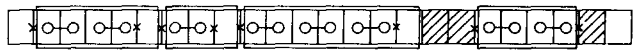

FIG. 6. Eight indistinguishable dumbbells are arranged in such a way that both end sites are empty and that there are eight mixed nearest neighbor pairs. There are $[n_{01}/2]=4$ "units" (unshaded) and $N-2q-[n_{01}/2]-1=3$ permutable vacancies (shaded).

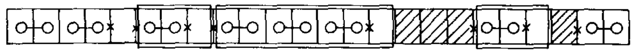

FIG. 7. Eight indistinguishable dumbbells are arranged in such a way that both end compartments are occupied and that $n_{01}=8$. There are $[(n_{01}/2)-1]=3$ permutable "units" (unshaded) and 4 permutable vacancies (shaded).

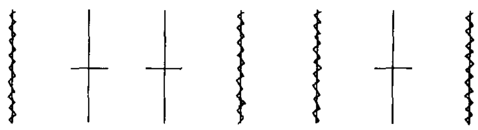

FIG. 8. This figure represents the situation illustrated in Fig. 6. There are seven separations between the eight dumbbells; $[n_{01}/2]=3$ separations involving mixed nearest neighbor pairs (short horizontal lines) and $q-1-[n_{01}/2]=4$ are separations between dumbbells (jagged lines).

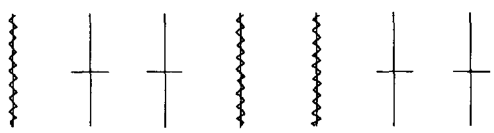

FIG. 9. This figure represents the situation illustrated in Fig. 7. Of the seven separations between the eight dumbbells 4 (short horizontal lines) are separations involving mixed nearest neighbor pairs and $q-1-n_{01}/2=3$ are separations between dumbbells (jagged lines).

Thus

$$\binom{N-2q-1}{n_{01}/2}\binom{q-1}{(n_{01}/2)-1}$$

represents the number of ways q particles can be arranged to form exactly n_{01} mixed nearest neighbor pairs under the constraint that both end compartments are vacant.

If situation (b) exists, in which both end compartments are occupied, then there are $[(n_{01}/2)-1]$ permutable "units" each composed of a dumbbell or group of dumbbells and a vacancy to isolate a "unit" from adjacent "units" (see Fig. 7). There are $N-2q-1-[(n_{01}/2)-1]$ permutable vacancies or a total of $N-2q-1$ objects which can be permuted. These objects can be arranged in $\binom{N-2q-1}{(n_{01}/2)-1}$ ways.

There are $q-1$ lines symbolizing the separation of the q dumbbells (see Fig. 9); of these lines, $[n_{01}/2]$, constitute separation by two mixed nearest neighbor pairs and $q-1-[n_{01}/2]$ are separations between adjacent dumbbells. Thus the number of ways that q indistinguishable dumbbells can be arranged among the "units" and the dumbbell groups on the end is $\binom{q-1}{n_{01}/2}$.

Consequently, when both end compartments are occupied, the q dumbbells can be arranged in $\binom{N-2q-1}{(n_{01}/2)-1}\binom{q-1}{n_{01}/2}$ ways to form exactly n_{01} mixed nearest neighbor pairs.

$A[n_{01}\mid q,N]$, the total number of independent arrangements which contain exactly n_{01} mixed nearest neighbor pairs (when n_{01} is even), is then the sum of those arrangements in which both end compartments are empty and in which both end compartments are occupied, is given by

$$A[n_{01}\mid q,N] = \binom{N-2q-1}{n_{01}/2}\binom{q-1}{(n_{01}/2)-1} + \binom{N-2q-1}{(n_{01}/2)-1}\binom{q-1}{n_{01}/2}$$

$$= 2\left[\frac{N-q-n_{01}}{n_{01}}\right]\binom{N-2q-1}{(n_{01}/2)-1}\binom{q-1}{(n_{01}/2)-1} \qquad (n_{01}\ \text{even}) \qquad (7)$$

The normalization for $A[n_{01}\mid q,N]$ can be shown to be

$$\sum_{n_{01}} A[n_{01}\mid q,N] = \binom{N-q}{q}, \qquad (8)$$

where $A[n_{01}\mid q,N]$ is given alternately by Eqs. (6) and (7) as the sum proceeds over all values of n_{01}.

IV. VACANT NEAREST NEIGHBOR DEGENERACY

We now calculate $A[n_{00}\mid q,N]$, the number of independent ways of arranging q indistinguishable dumbbells on a one-dimensional lattice space consisting of N equivalent sites in such a way as to create exactly n_{00} pairs of vacant nearest neighbors.

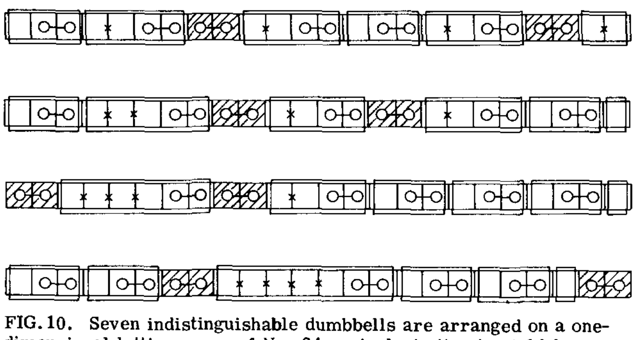

FIG. 10. Seven indistinguishable dumbbells are arranged on a one-dimensional lattice space of $N = 24$ equivalent sites to yield four vacant nearest neighbor pairs (represented by crosses). Regardless of the arrangement there are $N - 2q - n_{00} = 6$ "units" (unshaded). These "units" are permuted with $q - (N - 2q - n_{00} - 1) = 3q - N + n_{00} + 1 = 2$ dumbbells (shaded). There are $\binom{8}{2} = 28$ independent ways of arranging the "units" and the permutable dumbbells. This figure shows four possible arrangements in which the indistinguishable "units" are composed of all the possible groupings of vacant nearest neighbor pairs.

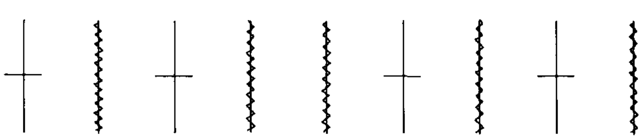

FIG. 11. Figure 11 deals with the top arrangement shown in Fig. 10. The ten vacancies illustrated in Fig. 10 have $N - 2q - 1 = 9$ separations between them. Of the nine separations, $n_{00} = 4$ are between vacant nearest neighbor pairs (short horizontal lines) and 5 are not (jagged lines). There are $\binom{9}{4} = 126$ ways of arranging the separations between the vacancies to form six "units."

Any arrangement of q indistinguishable dumbbells on a one-dimensional lattice space contains $N - 2q - n_{00}$ "units" (See Fig. 10). These "units" consist of a group of one or more contiguous vacant sites and a dumbbell (occupying two adjacent lattice sites) if one is needed to isolate the group of vacancies from other vacancies and/or other dumbbells. We initially consider these "units" to be indistinguishable one from another, regardless of their composition or configuration. Thus the number of dumbbells necessary to separate the "units" is $N - 2q - n_{00} - 1$, or one less than the number of "units."

There are q indistinguishable dumbbells; however, not all of these can be permuted to form additional independent arrangements; some of the dumbbells must be employed to separate a "unit" from the rest of the array. Because $N - 2q - n_{00} - 1$ dumbbells are required to isolate the "units," there are $q - (N - 2q - n_{00} - 1) = 3q + n_{00} - N + 1$ indistinguishable permutable dumbbells remaining to be permuted with the "units." Consequently, there are always $q + 1$ objects to be permuted, $N - 2q - n_{00}$ "units" and $3q + n_{00} - N + 1$ permutable dumbbells. These objects can be arranged in

$$\binom{q+1}{N-2q-n_{00}} = \binom{q+1}{3q+n_{00}-N+1}$$

independent ways.

The "units" are initially considered to be indistinguishable; in reality, however, vacancies can be moved from one "unit" to another to form new arrangements. To determine $A[n_{00}\mid q,N]$, we must ascertain the number of independent ways that "units" can be constituted, subject to the constraint that the number of "units" does not change.

We note that there are $N - 2q$ vacancies with $N - 2q - 1$ separations between them (see Fig. 11). Of these separations, n_{00} are indistinguishable from each other and separate nearest neighbor pairs of vacancies, and $N - 2q - 1 - n_{00}$ separate pairs of vacant nearest neighbors. These separations may be permuted in

$$\binom{N-2q-1}{n_{00}} = \binom{N-2q-1}{N-2q-1-n_{00}}$$

independent ways.

$A[n_{00}\mid q,N]$ is then determined to be the product of the number of independent ways the "units" can be arranged and the number of independent ways in which the "units" may be constructed. Thus

$$A[n_{00}\mid q,N] = \binom{q+1}{N-2q-n_{00}}\binom{N-2q-1}{n_{00}} \qquad (9)$$

is the desire quantity.

$A[n_{00}\mid q,N]$ is summed over all values of n_{00}, $[0 \le n_{00} \le N - 2q - 1]$ the result from the Vandermonde Theorem[3] is $\binom{N-q}{q}$, in accordance with Eq. (4).

V. THE FIRST MOMENT

With the degeneracy expressions for nearest neighbor pairs, Eq. (5), Eq. (6) or Eq. (7) and Eq. (8), it is possible to calculate the moment of these statistics and thereby determine the nature and magnitude of the error introduced by the Bragg-Williams approximation.

First to determine $\langle n_{11}\rangle$ as a function of coverage, θ, where $\lim_{N\to\infty}(2q/N) \equiv \theta$, we proceed as follows: From Eq. (5)

$$\frac{\sum_{n_{11}=0}^{q-1} n_{11}A[n_{11}|q,N]}{\sum_{n_{11}=0}^{q-1} A[n_{11}\,|\,q,N]} = (N-q-1)\binom{N-q-2}{q-2}\binom{N-q}{q}^{-1}. \quad (10)$$

Then the ensemble average density of occupied nearest neighbor pairs is

$$\lim_{N\to\infty}(\langle n_{11}\rangle/N) = \theta^2/2(2-\theta). \quad (11)$$

Similar calculations for n_{01} and n_{00} yield

$$\lim_{N\to\infty}(\langle n_{01}\rangle/N) = 2\theta[1-\theta]/(2-\theta) \quad (12)$$

and

$$\lim_{N\to\infty}(\langle n_{00}\rangle/N) = 2(1-\theta)^2/(2-\theta). \quad (13)$$

Thus for dumbbells, on a one-dimensional lattice space, the relationship

$$4\langle n_{00}\rangle\langle n_{11}\rangle = \langle n_{01}\rangle^2 \quad (14)$$

describes the "reaction"

$$2(01) \rightleftarrows (11) + (00). \quad (15)$$

Equation (10) may also be interpreted in terms of the concept of the "range" or order.[5] σ, the short-range order, is defined as

$$\sigma \equiv \langle 4n_{11}\rangle/N - 1 \quad (-1 \le \sigma \le 1). \quad (16)$$

Then

$$\sigma = 2\theta^2/(2-\theta) - 1. \quad (17)$$

Because L, the long range order, is defined as

$$L \equiv 4q/N - 1 = 2\theta - 1 \quad (-1 \le L \le 1), \quad (18)$$

the relation between the short range order and the long range order can be shown to be

$$\sigma = (L+1)^2/(3-L) - 1. \quad (19)$$

Equation (16) may be compared to the Bragg-Williams approximation,[6]

$$\sigma_{BW} = \tfrac{1}{2}(L+1)^2 - 1 \quad (20)$$

and thereby permit an estimate of the magnitude of error introduced through the use of the Bragg-Williams approximation. The Bragg-Williams approximation is only valid at $L \simeq 1$, i.e., when $\theta \simeq 1$.

It should also be noted from Eq. (11), that the value of θ which maximizes $\langle n_{01}\rangle/N$ is

$$\theta_{\max} = 2 - \sqrt{2} \simeq 0.586 \quad (21)$$

and the value of $\langle n_{01}\rangle/N$ at $\theta_{\max}$ is

$$\langle n_{01}\rangle/N = 2[3 - 2\sqrt{2}\,] \simeq 0.344\,. \quad (22)$$

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Gel'fand-pattern technique applied to the physically important $SU(3)\otimes SU(2)\subset SU(6)$ decomposition of $SU(6)$

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Explicit and easily computable formulas for the *physical* quantum numbers I_3, Y, and S_3, and also two additional quantum numbers for all states spanning an arbitrary irreducible representation of $SU(6)$ are obtained by using Gel'fand-pattern technique. This result is accomplished by establishing a correspondence between the 3 diagonal $SU(3)\otimes SU(2)$ generators + 2 "quark-spin" generators, and the 5 "canonical" generators $H_1 - H_5$, the eigenvalues of which are given by the Gel'fand patterns of $SU(6)$ in the ordinary way. The $SU(3)\otimes SU(2)\subset SU(6)$ content of the $SU(6)$ representations taken as examples is displayed explicitly. The possibility of doing this suggests that Gel'fand patterns may be useful even in a nonmaximal decomposition, although the patterns are intrinsically linked to the "canonical" chain of decomposition: $SU(n)\supset U_1(1)\otimes SU(n-1)\supset U_1(1)\otimes U_2(1)\otimes SU(n-2)\supset\cdots$ etc. The procedure developed in the case of $SU(6)$ is generalized to the twofold nonmaximal decomposition of $SU(mn)\supset SU(m)\otimes SU(n)$.

I. INTRODUCTION

The Gelfand pattern technique[1,2,3] establishes an elegant solution to the problem of uniquely constructing an orthonormal basis of the irreducible representations (IR) of $(S)U(n)$. The labeling of states within an IR is based on the "canonical" decomposition $SU(n)\supset U_1(1)\otimes SU(n-1)\supset U_1(1)\otimes U_2(1)\otimes SU(n-2)\ldots$ etc. In the case of $SU(6)$ the *physical* decomposition chain is, however, $SU(6)\supset SU(3)\otimes SU(2)$, and this is the reason why the "pattern method" has been thought of as nonapplicable in the study of the physical $SU(6)$ symmetry.[4] The usual prescription for reading off the quantum numbers from the Gelfand pattern of $SU(6)$ does not reveal anything of physical interest. The Gelfand patterns, however, contain a maximal amount of information, and furnish the eigenvalues of 20 diagonal operators, 5 of which are the Casimir[5,6] invariants of $SU(6)$. Of the remaining 15 operators, 5 are just the diagonal *generators* of $SU(6)$, and the 10 others may be chosen[7] as the Casimir invariants of the subgroups in the "canonical" chain of decomposition. The eigenvalues of the Casimir invariants of the $SU(m)$ subgroup are polynomials [deg $LEQ(m)\,GEQ(2)$] of the entries in the mth row of the Gelfand pattern. These entries themselves constitute an equivalent set of classifying numbers, and the possibility of constructing other sets are clearly conceivable. The present paper will give indications that in the case of $SU(6)$, the 3 Casimir invariants of the subgroups in the decomposition $SU(3)\otimes SU(2)$ [2 for $SU(3)$, 1 for $SU(2)$] may be part of another set. The additional information contained in the Gelfand patterns might be exploited to solve the technical questions involved in the nonmaximal decomposition of $SU(6)$ generally, and particularly in the one of physical significance. After the completion of this work, by a communication of M. Hamermesh, the author was made aware of some papers that have previously escaped his attention. J. D. Louck,[8] Biedenharn, Louck and Giovannini,[9] J. D. Louck,[10] and Brody, Moshinsky, and Renero[11] have published papers on tensor operators and generalized Wigner coefficients of $(S)U(n)$ which mathematically represent a wide generalization of some of the aspects of the present paper, but in other respects the present paper is concerned with problems that are essentially different from those of Refs. 8–11. References 8 and 9 are concerned with the coupling of two IR's of the *same* group $U(n)$ and the reduction of the direct product involved into the direct sum of IR's of $U(n)$ once again. In order to obtain the generalized Wigner coefficients, the embedding of $U(n)\otimes U(n)\subset U(n^2)$ is taken into consideration. The nice and very general results cannot be compared directly to the results of the present paper, because it is concerned with the $SU(6)$ content of the direct product of two *different* groups, namely $SU(3)$ and $SU(2)$.

T. A. Brody *et.al.*[11] take into consideration the IR's of $SU(n)$ as part of $U(nr)\supset U(n)\otimes U(r)$, $r\geqslant n-1$, and introduce the concept of "auxiliary Wigner coefficients." Taking $n=3$, $r=3-1=2$, the $SU(6)$ case may be handled within the framework of Ref. 11, but the examples given in the paper are just $SU(3)$ and $SU(4)$, not $SU(6)$. Furthermore, T. A. Brody *et.al.* also are *primarily* concerned with the Wigner coefficients of the reduction of direct products of the IR's of $SU(n)$ into direct sums of IR's of the *same* group. J. D. Louck[10] gives an excellent survey of the theory of tensor operators in the unitary groups, using Gelfand patterns throughout his paper and thus recommending this elegant scheme for wider use.

The present paper is primarily concerned with a group of paramount physical importance, namely $SU(6)$ [$SU(6)_N$ is now enjoying a re-birth] and gives results that are immediately applicable. The generalization of the procedure to $SU(mn)\supset SU(m)\otimes SU(n)$ puts no restraint on m and n (cf. Ref. 11: $U(nr)\supset U(n)\otimes U(r)$, with the restraint $r\geqslant n-1$).

II. CORRESPONDENCE BETWEEN THE "QUARK-SPIN" GENERATORS AND THE GENERATORS H_1-H_5

The Gelfand pattern of $SU(6)$ is:

$$\begin{array}{lccccccccccc}
\text{6th row:} & m_{16} & & m_{26} & & m_{36} & & m_{46} & & m_{56} & & m_{66}=0\\
\text{5th row:} & & m_{15} & & m_{25} & & m_{35} & & m_{45} & & m_{55} & \\
\text{4th row:} & & & m_{14} & & m_{24} & & m_{34} & & m_{44} & & \\
\text{3rd row:} & & & & m_{13} & & m_{23} & & m_{33} & & & \\
\text{2nd row:} & & & & & m_{12} & & m_{22} & & & & \\
\text{1st row:} & & & & & & m_{11} & & & & &
\end{array} \tag{1}$$

where $m_{i,j} \geq m_{i,j-1} \geq m_{i+1,j}$ ("in betweenness rule"). When the diagonal generators in the defining (quark) representation are taken to be the set

$$(A)\begin{cases} h_1 = \tfrac{1}{2}\,\text{diag}\,(1,-1,0,0,0,0), & (2)\\ h_2 = \dfrac{1}{2.3}\,\text{diag}\,(1,1,-2,0,0,0), & (3)\\ h_3 = \dfrac{1}{3.4}\,\text{diag}\,(1,1,1,-3,0,0), & (4)\\ h_4 = \dfrac{1}{4.5}\,\text{diag}\,(1,1,1,1,-4,0), & (5)\\ h_5 = \dfrac{1}{5.6}\,\text{diag}\,(1,1,1,1,1,-5), & (6)\end{cases}$$

and these are generalized to the diagonal generators H_1–H_5 in a general IR {proceeding for example by the Schwinger[12] boson-operator realization for *all* the generators [35 in the case of $SU(6)$]}, the eigenvalues of the diagonal generators are simply the difference between the average of two adjacent rows in the Gelfand-pattern[13]:

$$H_i \to M_i = \frac{1}{i}\sum_{j=1}^{i} m_{i,j} - \frac{1}{i+1}\sum_{j=1}^{i+1} m_{i+1,j}. \qquad (7)$$

These numbers, however, do not reveal the desired physical information.[14] This situation is remedied by considering the generators of $SU(3)\otimes SU(2)$, three of which are diagonal, namely $\mathbb{I}_3 = F_3 \otimes 1$, $\mathbb{Y} = (2/\sqrt{3})F_8 \otimes 1$, and $\mathbb{S}_3 = 1 \otimes S_3$, when the eight generators of $SU(3)$ are denoted $F_1, F_2, \ldots, F_8$, and those of $SU(2)$ are S_1, S_2 and S_3. The 8 + 3 generators of $SU(3)\otimes SU(2)$ are extended by the 24 "quark-spin" generators $Q_{ij} = F_i S_j$ giving a set of 35 generators for the $SU(6)$. Two "quark-spin" generators are diagonal, those are Q_{33} and Q_{83}. We now choose the Gell-Mann matrices[15] as the generators of $SU(3)$ in the defining representation, and the Pauli matrices analogously for the $SU(2)$. The resulting diagonal $SU(6)$ generators are:

$$(B)\begin{cases} \mathbb{I}_3 = \tfrac{1}{2}\,\text{diag}\,(1,1,-1,-1,0,0), & (8)\\ \mathbb{Y} = \tfrac{1}{3}\,\text{diag}\,(1,1,1,1,-2,-2,), & (9)\\ \mathbb{S}_3 = \tfrac{1}{2}\,\text{diag}\,(1,-1,1,-1,1,-1), & (10)\\ Q_{33} \equiv F_3S_3 = \tfrac{1}{4}\,\text{diag}\,(1,-1,1,-1,0,0), & (11)\\ \dfrac{2}{\sqrt{3}}Q_{83} \equiv YS_3 = \tfrac{1}{6}\,\text{diag}\,(1,-1,1,-1,-2,2). & (12)\end{cases}$$

[the whole set of $SU(6)$ generators developed from the $SU(3)\otimes SU(2)$ and quark-spin generators will be denoted the α-set and their explicit representation in the 6 dimensional matrices just defined will be denoted the α-representation hereafter.] A solution of the relevant set of 25 linear equations now establishes the correspondence between the sets (A) and (B) of generators through the transformation

$$(C)\begin{cases} \mathbb{I}_3 = 2(H_2 + H_3), & (13)\\ \mathbb{Y} = 4(H_4 + H_5), & (14)\\ \mathbb{S}_3 = H_1 - H_2 + 2(H_3 - H_4) + 3H_5, & (15)\\ Q_{33} = \dfrac{1}{2}(H_1 + H_2) - H_3, & (16)\\ Q_{83} = \dfrac{\sqrt{3}}{2}\{\tfrac{1}{3}(H_1 - H_2 + 2H_3 + 4H_4) - 2H_5\}. & (17)\end{cases}$$

[The same notation is used for the $SU(3)\otimes SU(2)$ relevant generators both in the defining representation and after generalization to the general IR of $SU(6)$.]

A check confirms the linear independence of the set defined in (C) given the linear independence of H_1-H_5.

III. EXPLICIT FORMULAS FOR THE PHYSICAL QUANTUM NUMBERS I_3, Y, AND S_3. TWO ADDITIONAL QUANTUM NUMBERS

The correspondence (C) now makes Eq. (7) applicable in calculating the physical quantum numbers I_3, Y, S_3, interpreted as the third component of isospin, the hypercharge, and the third component of the intrinsic (angular momentum) spin, respectively, of the states (particles) spanning the IR of $SU(6)$. One also gets two additional quantum numbers, which in some cases [i.e., in the defining (quark) representation] turns out to be just proportional to the products I_3S_3 and YS_3 of the physical quantum numbers just defined. In other cases, the physical interpretation of the additional quantum numbers is not that clear, but frequently they may serve the purpose of lifting a degeneracy of I_3, Y, and S_3 within an IR. Using Eq. (7), one gets these formulas for the "new" quantum numbers

$$I_3 = m_{12} + m_{22} - \tfrac{1}{2}(m_{14} + m_{24} + m_{34} + m_{44}), \qquad (18)$$

$$Y = m_{14} + m_{24} + m_{34} + m_{44} - \tfrac{2}{3}(m_{16} + m_{26} + m_{36} + m_{46} + m_{56} + 0), \qquad (19)$$

$$\begin{aligned} S_3 = {} & m_{11} - (m_{12} + m_{22}) + m_{13} + m_{23} + m_{33}\\ & - (m_{14} + m_{24} + m_{34} + m_{44}) + m_{15} + m_{25}\\ & + m_{35} + m_{45} + m_{55}\\ & - \tfrac{1}{2}(m_{16} + m_{26} + m_{36} + m_{46} + m_{56} + 0), \end{aligned} \qquad (20)$$

$$Q_{33} = \tfrac{1}{2}(m_{11} - (m_{13} + m_{23} + m_{33})) + \tfrac{1}{4}(m_{14} + m_{24} + m_{34} + m_{44}). \qquad (21)$$

$$\begin{aligned} \frac{2}{\sqrt{3}}Q_{83} = {} & \tfrac{1}{3}\{m_{11} - (m_{12} + m_{22}) + m_{13} + m_{23}\\ & + m_{33} + \tfrac{1}{2}(m_{14} + m_{24} + m_{34} + m_{44})\\ & - 2(m_{15} + m_{25} + m_{35} + m_{45} + m_{55})\\ & + m_{16} + m_{26} + m_{36} + m_{46} + m_{56} + 0\}. \end{aligned} \qquad (22)$$

Inspecting Eq. (20), we note that the spin of the particles is integer whenever the sum of the entries $m_{16} - m_{56}$ is even, and half-(odd) integer when this sum is odd. The entries $m_{16} - m_{56}$ ($m_{66} = 0$) determine the IR of $SU(6)$. We thus directly see whether the particles of an IR are bosons or fermions whenever the IR of $SU(6)$ is specified.

From Eq. (19), we see that *within* an IR, the hypercharge is determined by the 4th row in the Gelfand pattern, and Eq. (18) reveals the dependence of the 2nd and the 4th row only for I_3. In fact, if one makes the identification

$$m'_{11} = m_{12} + m_{22}, \qquad (23)$$

$$m'_{12} + m'_{22} = \sum_{i=1}^{4} m_{i4} \qquad (24)$$

$$m'_{13} + m'_{23} + 0 = \sum_{i=1}^{6} m_{i6} \quad (m_{66} = 0), \qquad (25)$$

one may establish a $SU(3)$ Gelfand pattern

$$\begin{matrix} m'_{13} & & m'_{23} & & 0 \\ & m'_{12} & & m'_{22} & \\ & & m'_{11} & & \end{matrix} \tag{26}$$

where the formulas (18) and (19) in terms of the primed entries just represent the ordinary way of reading off the quantum numbers I_3 and Y from the $SU(3)$ Gelfand pattern (26).

In the case of some low lying IR's of $SU(6)$, the three quantum numbers I_3, Y, and S_3 display the $SU(3) \otimes SU(2)$ decomposition right away. In general, one has to use the α-set of generators expressed in terms of the E_{ij} operators of Ref. 1, 2 and establish the Casimir invariants (C_2 and C_3) and S^2, respectively, of the $SU(3)$ and $SU(2)$ subgroups in the decomposition $SU(6) \supset SU(3) \otimes SU(2)$ and also the invariant I^2 of the isospin $[SU(2)]$ subgroup of $SU(3)$.

IV. APPLICATION TO SOME IMPORTANT $SU(6)$ REPRESENTATIONS

(a) The defining (quark) representation is specified by $m_{16} = 1, m_{26} = m_{36} = m_{46} = m_{56} = m_{66} = 0$.

There are six possible Gelfand patterns, describing six orthonormal states $|1\rangle \to |6\rangle$:

$$\begin{matrix} 1\ 0\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0 \\ 1\ 0\ 0 \\ 1\ 0 \\ 1 \end{matrix} \to |1\rangle, \qquad \begin{matrix} 1\ 0\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0 \\ 1\ 0\ 0 \\ 1\ 0 \\ 0 \end{matrix} \to |2\rangle,$$

$$\begin{matrix} 1\ 0\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0 \\ 1\ 0\ 0 \\ 0\ 0 \\ 0 \end{matrix} \to |3\rangle, \qquad \begin{matrix} 1\ 0\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0 \\ 0\ 0\ 0 \\ 0\ 0 \\ 0 \end{matrix} \to |4\rangle,$$

$$\begin{matrix} 1\ 0\ 0\ 0\ 0\ 0 \\ 1\ 0\ 0\ 0\ 0 \\ 0\ 0\ 0\ 0 \\ 0\ 0\ 0 \\ 0\ 0 \\ 0 \end{matrix} \to |5\rangle, \qquad \begin{matrix} 1\ 0\ 0\ 0\ 0\ 0 \\ 0\ 0\ 0\ 0\ 0 \\ 0\ 0\ 0\ 0 \\ 0\ 0\ 0 \\ 0\ 0 \\ 0 \end{matrix} \to |6\rangle.$$

Using formulas (18)–(22) one gets the following quantum numbers (notation: $|\gamma_i, I_3, Y, S_3, Q_{33}, (2/\sqrt{3})Q_{83}\rangle$, the last five symbols representing the eigenvalues of the diagonal α-set generators, γ_i representing all other quantum numbers):

$$|1\rangle = |\gamma_1, +\tfrac{1}{2}, +\tfrac{1}{3}, , +\tfrac{1}{2}, , \tfrac{1}{4}, \tfrac{1}{6}\rangle,$$
$$|2\rangle = |\gamma_2, +\tfrac{1}{2}, +\tfrac{1}{3}, , -\tfrac{1}{2}, , -\tfrac{1}{4}, -\tfrac{1}{6}\rangle,$$
$$|3\rangle = |\gamma_3, -\tfrac{1}{2}, +\tfrac{1}{3}, , +\tfrac{1}{2}, , -\tfrac{1}{4}, +\tfrac{1}{6}\rangle,$$
$$|4\rangle = |\gamma_4, -\tfrac{1}{2}, +\tfrac{1}{3}, , -\tfrac{1}{2}, , +\tfrac{1}{4}, -\tfrac{1}{6}\rangle,$$
$$|5\rangle = |\gamma_5, 0, -\tfrac{2}{3}, , +\tfrac{1}{2}, , 0, -\tfrac{1}{3}\rangle,$$
$$|6\rangle = |\gamma_6, 0, -\tfrac{2}{3}, , -\tfrac{1}{2}, , 0, +\tfrac{1}{3}\rangle.$$

By inspection, we may sort out the $SU(3) \otimes SU(2)$ decomposition, namely $\mathbf{6} = (\mathbf{3}, \tfrac{1}{2})$.

These results are well known of course, and we don't bother to plot the two $SU(3)$ weight diagrams of $S_3 = +\tfrac{1}{2}$ and $S_3 = -\tfrac{1}{2}$, respectively.

(b) The representation conjugate to the quark-representation is described by $m_{16} = m_{26} = m_{36} = m_{46} = m_{56} = 1$, $m_{66} = 0$. Here also we get six Gelfand patterns and the formulas (18)–(22) give the following states described by their quantum numbers:

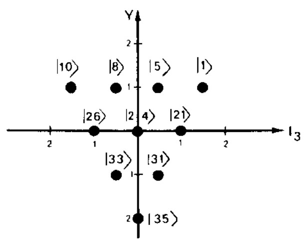
$$|\bar{1}\rangle = |\bar{\gamma}_1, 0, \tfrac{2}{3}, , \tfrac{1}{2}, , 0, -\tfrac{1}{3}\rangle,$$
$$|\bar{2}\rangle = |\bar{\gamma}_2, 0, \tfrac{2}{3}, , -\tfrac{1}{2}, , 0, \tfrac{1}{3}\rangle,$$
$$|\bar{3}\rangle = |\bar{\gamma}_3, -\tfrac{1}{2}, -\tfrac{1}{3}, , \tfrac{1}{2}, , -\tfrac{1}{4}, \tfrac{1}{6}\rangle,$$
$$|\bar{4}\rangle = |\bar{\gamma}_4, -\tfrac{1}{2}, -\tfrac{1}{3}, , -\tfrac{1}{2}, , \tfrac{1}{4}, -\tfrac{1}{6}\rangle,$$
$$|\bar{5}\rangle = |\bar{\gamma}_5, \tfrac{1}{2}, -\tfrac{1}{3}, , \tfrac{1}{2}, , \tfrac{1}{4}, \tfrac{1}{6}\rangle,$$
$$|\bar{6}\rangle = |\bar{\gamma}_6, \tfrac{1}{2}, -\tfrac{1}{3}, , -\tfrac{1}{2}, , -\tfrac{1}{4}, -\tfrac{1}{6}\rangle.$$

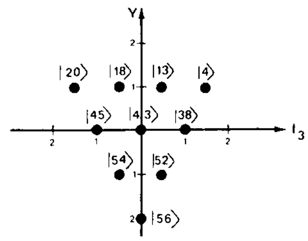
The quantum numbers I_3, Y, S_3 themselves immediately give the $SU(3) \otimes SU(2)$ decomposition.

(c) The 56-dimensional representation is described by $m_{16} = 3, m_{26} = m_{36} = m_{46} = m_{56} = m_{66} = 0$. Starting with

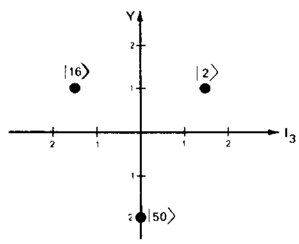
$$|1\rangle \quad \begin{matrix} 3\ 0\ 0\ 0\ 0\ 0 \\ 3\ 0\ 0\ 0\ 0 \\ 3\ 0\ 0\ 0 \\ 3\ 0\ 0 \\ 3\ 0 \\ 3, \end{matrix}$$

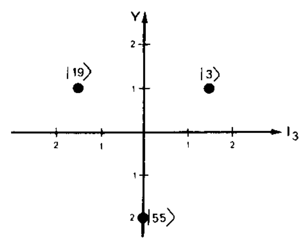
we enumerate the states corresponding to the Gelfand patterns from $|1\rangle$ to $|56\rangle$. The "key" is given in the Appendix and also the quantum numbers calculated by using formulas (18)–(22). By inspecting, one gets the following $SU(3)$ weight diagrams for states all having $S_3 = +\tfrac{3}{2}$ and $S_3 = -\tfrac{3}{2}$:



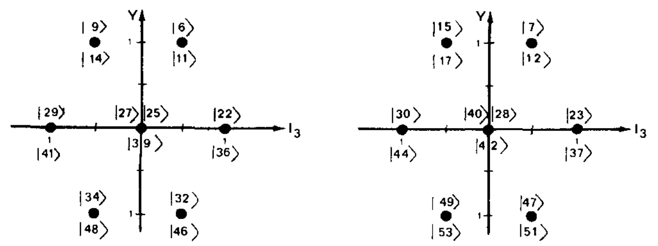


Six more states are nondegenerate and may be plotted as follows:





Let us plot all the candidates to the vacant places in $SU(3)$ weight diagrams:



Knowledge of the IR's of $SU(3)$ now gives uniquely the decomposition:

$$56 = (10, 3/2) \oplus (8, 1/2).$$

The problem of how to single out the individual states requires the additional tools mentioned earlier in Sec. III.

V. GENERALIZATION TO A TWOFOLD, NONMAXIMAL DECOMPOSITION OF $SU(mn) \supset SU(m) \otimes SU(n)$

There are $(m^2 - 1) + (n^2 - 1)$ traceless generators of $SU(m) \otimes SU(n)$. These are extended by the $(m^2 - 1) \cdot (n^2 - 1)$ "product" generators, furnishing $(m^2 - 1)n^2 + n^2 - 1 = (m \cdot n)^2 - 1$ traceless generators which may be taken as the α-set generators of $SU(mn)$. Given explicit matrix representations of the generators in the defining representations of $SU(m)$ and $SU(n)$ [this may be, for example, those connected with the Gelfand patterns for $SU(m)$ and $SU(n)$, respectively], the α-set generators of $SU(mn)$ may be expressed by the $H_1 - H_{mn-1}$ and the E_{ij} generators. This establishes the link to the Gelfand patterns of $SU(mn)$.

VI. CONCLUDING REMARKS

Adaption of Gelfand patterns to the physically important case of $SU(6) \supset SU(3) \otimes SU(2)$ opens possibilities in several directions. One is the use of tensor operators[3,9,10,13] in a "dynamic" theory, involving both $SU(6)$ symmetry-conserving and symmetry-breaking interactions. The theoretical predictions might then be compared with experiment.[16]

ACKNOWLEDGMENT

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APPENDIX

Enumeration of states corresponding to the Gelfand patterns of **56**:

$$|1\rangle \to \begin{matrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & \\ 3 & 0 & 0 & 0 & & \\ 3 & 0 & 0 & & & \\ 3 & 0 & & & & \\ 3 & & & & & \end{matrix}$$

$|2\rangle$, $|3\rangle$, and $|4\rangle$ are produced by lowering m_{11} in steps of one. Then

$$|5\rangle \to \begin{matrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & \\ 3 & 0 & 0 & 0 & & \\ 3 & 0 & 0 & & & \\ 2 & 0 & & & & \\ 2 & & & & & \end{matrix}$$

$|6\rangle$ and $|7\rangle$ follow by reducing m_{11} in steps of one.

$$|8\rangle \to \begin{matrix} 3 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & \\ 3 & 0 & 0 & 0 & & \\ 3 & 0 & 0 & & & \\ 1 & 0 & & & & \\ 1 & & & & & \end{matrix}$$

$|9\rangle$ follows by reducing m_{11} to zero.

$|10\rangle$ follows by setting both m_{11} and m_{12} to zero.

TABLE I. The eigenvalues of the diagonal α-set generators for the **56** representation of $SU(6)$, calculated from the Gelfand patterns using the formulas (18)–(22).

State no.	I_3	Y	S_3	Q_{33}	$(2/\sqrt{3})Q_{83}$
1	$\frac{3}{2}$	1	$\frac{3}{2}$	$\frac{3}{4}$	$\frac{1}{2}$
2	$\frac{3}{2}$	1	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{6}$
3	$\frac{3}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{4}$	$-\frac{1}{6}$
4	$\frac{3}{2}$	1	$-\frac{3}{2}$	$-\frac{3}{4}$	$-\frac{1}{2}$
5	$\frac{1}{2}$	1	$\frac{3}{2}$	$\frac{1}{4}$	$\frac{1}{2}$
6	$\frac{1}{2}$	1	$\frac{1}{2}$	$-\frac{1}{4}$	$\frac{1}{6}$
7	$\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{3}{4}$	$-\frac{1}{6}$
8	$-\frac{1}{2}$	1	$\frac{3}{2}$	$-\frac{1}{4}$	$\frac{1}{2}$
9	$-\frac{1}{2}$	1	$\frac{1}{2}$	$-\frac{3}{4}$	$\frac{1}{6}$
10	$-\frac{3}{2}$	1	$\frac{3}{2}$	$-\frac{3}{4}$	$\frac{1}{2}$
11	$\frac{1}{2}$	1	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{1}{6}$
12	$\frac{1}{2}$	1	$-\frac{1}{2}$	$\frac{1}{4}$	$-\frac{1}{6}$
13	$\frac{1}{2}$	1	$-\frac{3}{2}$	$-\frac{1}{4}$	$-\frac{1}{2}$
14	$-\frac{1}{2}$	1	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{6}$
15	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$-\frac{1}{4}$	$-\frac{1}{6}$
16	$-\frac{3}{2}$	1	$\frac{1}{2}$	$-\frac{1}{4}$	$\frac{1}{6}$
17	$-\frac{1}{2}$	1	$-\frac{1}{2}$	$\frac{3}{4}$	$-\frac{1}{6}$
18	$-\frac{1}{2}$	1	$-\frac{3}{2}$	$\frac{1}{4}$	$-\frac{1}{2}$
19	$-\frac{3}{2}$	1	$-\frac{1}{2}$	$\frac{1}{4}$	$-\frac{1}{6}$
20	$-\frac{3}{2}$	1	$-\frac{3}{2}$	$\frac{3}{4}$	$-\frac{1}{2}$
21	1	0	$\frac{3}{2}$	$\frac{1}{2}$	0
22	1	0	$\frac{1}{2}$	0	$-\frac{1}{3}$
23	1	0	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{2}{3}$
24	0	0	$\frac{3}{2}$	0	0
25	0	0	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{3}$
26	−1	0	$\frac{3}{2}$	$-\frac{1}{2}$	0
27	0	0	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{3}$
28	0	0	$-\frac{1}{2}$	0	$-\frac{2}{3}$
29	−1	0	$\frac{1}{2}$	0	$-\frac{1}{3}$
30	−1	0	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{3}{2}$
31	$\frac{1}{2}$	−1	$\frac{3}{2}$	$\frac{1}{4}$	$-\frac{1}{2}$
32	$\frac{1}{2}$	−1	$\frac{1}{2}$	$-\frac{1}{4}$	$-\frac{1}{6}$
33	$-\frac{1}{2}$	−1	$\frac{3}{2}$	$-\frac{1}{4}$	$-\frac{1}{2}$
34	$-\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{4}$	$-\frac{5}{6}$
35	0	−2	$\frac{3}{2}$	0	−1
36	1	0	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{3}$
37	1	0	$-\frac{1}{2}$	0	$\frac{1}{3}$
38	1	0	$-\frac{3}{2}$	$-\frac{1}{2}$	0
39	0	0	$\frac{1}{2}$	0	$\frac{2}{3}$
40	0	0	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{3}$
41	−1	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{2}{3}$
42	0	0	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{3}$
43	0	0	$-\frac{3}{2}$	0	0
44	−1	0	$-\frac{1}{2}$	0	$\frac{1}{3}$
45	−1	0	$-\frac{3}{2}$	$\frac{1}{2}$	0
46	$\frac{1}{2}$	−1	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{6}$
47	$\frac{1}{2}$	−1	$-\frac{1}{2}$	$-\frac{1}{4}$	$-\frac{1}{6}$
48	$\frac{1}{2}$	−1	$\frac{1}{2}$	$-\frac{1}{4}$	$\frac{1}{6}$
49	$-\frac{1}{2}$	−1	$-\frac{1}{2}$	$\frac{1}{4}$	$-\frac{1}{6}$
50	0	−2	$\frac{1}{2}$	0	$-\frac{1}{3}$
51	$\frac{1}{2}$	−1	$-\frac{1}{2}$	$\frac{1}{4}$	$\frac{5}{6}$
52	$\frac{1}{2}$	−1	$-\frac{3}{2}$	$-\frac{1}{4}$	$\frac{1}{2}$
53	$-\frac{1}{2}$	−1	$-\frac{1}{2}$	$-\frac{1}{4}$	$\frac{5}{6}$
54	$-\frac{1}{2}$	−1	$-\frac{3}{2}$	$\frac{1}{4}$	$\frac{1}{2}$
55	0	−2	$-\frac{1}{2}$	0	$\frac{1}{3}$
56	0	−2	$-\frac{3}{2}$	0	1

$$|11\rangle \rightarrow \begin{array}{c} 3\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0 \\ 3\ \ 0\ \ 0\ \ 0\ \ 0 \\ 3\ \ 0\ \ 0\ \ 0 \\ 2\ \ 0\ \ 0 \\ 2\ \ 0 \\ 2 \end{array}\ .$$

The states $|12\rangle \rightarrow |16\rangle$ now follow just as the states $|6\rangle \rightarrow |10\rangle$ are produced starting with $|5\rangle$.

$$|17\rangle \rightarrow \begin{array}{c} 3\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0 \\ 3\ \ 0\ \ 0\ \ 0\ \ 0 \\ 3\ \ 0\ \ 0\ \ 0 \\ 1\ \ 0\ \ 0 \\ 1\ \ 0 \\ 1 \end{array}\ .$$

and $|18\rangle$, $|19\rangle$, and $|20\rangle$ follow by setting m_{11} to zero, then also m_{12} and finally all three entries, m_{11}, m_{12}, and m_{13} equal to zero.

$$|21\rangle \rightarrow \begin{array}{c} 3\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0 \\ 3\ \ 0\ \ 0\ \ 0\ \ 0 \\ 2\ \ 0\ \ 0\ \ 0 \\ 2\ \ 0\ \ 0 \\ 2\ \ 0 \\ 2 \end{array}\ .$$

The procedure which started in passing from $|11\rangle \rightarrow |12\rangle$ is now repeated, giving the sequence $|22\rangle \rightarrow |30\rangle$.

$$|31\rangle \rightarrow \begin{array}{c} 3\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0 \\ 3\ \ 0\ \ 0\ \ 0\ \ 0 \\ 1\ \ 0\ \ 0\ \ 0 \\ 1\ \ 0\ \ 0 \\ 1\ \ 0 \\ 1 \end{array}\ .$$

$|32\rangle \rightarrow |35\rangle$ are produced by putting the 1's to 0 starting with m_{11}.

$$|36\rangle \rightarrow \begin{array}{c} 3\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0 \\ 2\ \ 0\ \ 0\ \ 0\ \ 0 \\ 2\ \ 0\ \ 0\ \ 0 \\ 2\ \ 0\ \ 0 \\ 2\ \ 0 \\ 2 \end{array}\ .$$

Proceeding as from $|21\rangle$ to $|35\rangle$, one gets the sequence $|37\rangle \rightarrow |50\rangle$.

$$|50\rangle \rightarrow \begin{array}{c} 3\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0 \\ 2\ \ 0\ \ 0\ \ 0\ \ 0 \\ 0\ \ 0\ \ 0\ \ 0 \\ 0\ \ 0\ \ 0 \\ 0\ \ 0 \\ 0 \end{array}\ . \qquad |51\rangle \rightarrow \begin{array}{c} 3\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0 \\ 1\ \ 0\ \ 0\ \ 0\ \ 0 \\ 1\ \ 0\ \ 0\ \ 0 \\ 1\ \ 0\ \ 0 \\ 1\ \ 0 \\ 1 \end{array}\ .$$

$|52\rangle \rightarrow |56\rangle$ are produced by putting the 1's to zero, again starting with m_{11}.

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Some observations on the operator $H = -(1/2)d^2/dx^2 + m^2x^2/2 + g/x^2$ *

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In the present work we study the differential operator $H = -(1/2)d^2/dx^2 + m^2x^2/2 + g/x^2$. This operator known as the Hamiltonian of the quantal oscillator has been a matter of study since the beginning of quantum mechanics. Recently, it has become again actual after the paper of Calogero where the correspondent N body problem (developed in many works) is studied. Parisi and the author have used H as Hamiltonian, studying the anomalous dimensions in one-dimensional quantum field theory. Finally, Klauder, using H as a simple degree of freedom example, has studied some qualitative features of quantum theories with singular interaction potentials. In the following work we are going to study H, showing that H is equivalent to "half an harmonic oscillator" for the odd and even eigenspaces separately.

It is well known[1-5] that from the formal differential operator H is possible to construct a self-adjoint operator $\tilde{H}$ acting in $L^2(R)$, that is bounded below if $g \geq -1/8$.[6] An intuitive argument for this condition on g is the following:

Using the Heisenberg uncertainty principle

$$\overline{(\Delta x)^2}\ \overline{(\Delta p)^2} \geq \tfrac{1}{4} \quad (\hbar = 1)$$

and considering a wave function finite in some small region of radius r_0 about the origin and equal to zero outside this region, the mean value of the kinetic energy in this state is of the order of $1/8r^2$ and the mean value of the potential energy is of the order of g/r^2.

Then the Hamiltonian is bounded below only if the sum:

$$1/8r_0^2 + g/r_0^2 \qquad (1)$$

is bounded below when $r_0 \to 0$; that is: $g \geq -\frac{1}{8}$.

Now assuming $g \geq -\frac{1}{8}$, the eigenvalue problem

$$\tilde{H}u = \lambda u \qquad (2)$$

has the following solutions:

$$\lambda_n = m(2n + a + 1),$$
$$u_n(x) = C_n(mx^2)^{(2a+1)/4} \quad \exp(-mx^2/2)L_n^a(mx^2), \qquad (3)$$

where c_n are normalization constants, $a = \frac{1}{2}\sqrt{1 + 8g}$, n is a nonnegative integer, and $L_n^a(mx^2)$ are the generalized Laguerre polynomials.[7]

It is easy to verify that if $g \geq 0$ also, then

$$v_n(x) = \theta(x)u_n(x) - \theta(-x)u_n(x)$$

are eigenfunctions of the problem (2) with the same eigenvalue where $\theta(x)$ is the usual θ function.

So that u_n, v_n are a complete orthonormal system of L^2.

We consider the operator

$$H_0 - \frac{1}{2}\frac{d^2}{dx^2} + \frac{m^2x^2}{2},$$

that is the Hamiltonian of the harmonic oscillator, the eigenvalue problem for H_0, has the following solutions[8]:

$$\lambda_n' = m(n + \tfrac{1}{2}),$$
$$\psi_n = c_n' H_n(mx) \exp\left(-\frac{mx^2}{2}\right),$$

where $H_n(mx)$ are the Hermite-Tchebycheff polynomials.

We note that the ψ_n are a complete orthonormal set for $L^2(R)$. If we consider the operator $\tilde{H}$ restricted over the space generated by its eigenfunctions $\{u_n\}$ and the operator H_0 restricted over the space generated by $\{\psi_{2n}\}$, we can show there is a real number β such that H_0 and $\tilde{H} + \beta I$ are unitarily equivalent.

In fact, let H_0 and $\tilde{H} + \beta I$ be as defined above, then there is a unitary operator W and a real number β such that

$$WH_0W^* = \tilde{H} + \beta I.$$

We define W: $\psi_{2n} \to u_n$, W is obviously an unitary map from the Hilbert space generated by $\{\psi_{2n}\}$ to the Hilbert space generated by $\{u_n\}$. We have

$$[WH_0W^* - (\tilde{H} + \beta I)]u_n = \{m(2n + \tfrac{1}{2}) - m(2n + a + 1 + \beta)\}u_n.$$

If $\beta = -(a + \frac{1}{2})$ this expression is equal to zero and we are done.

We note that if $g > 0$ also $\tilde{H} + \beta I$ restricted to the subspaces generated by v_n is unitarily equivalent to an "half harmonic oscillator" so that H is the direct sum of two "half harmonic oscillators."

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Irreducible tensorial sets within the group algebra of a compact group

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For compact topological groups (discrete or continuous) a basis of the group algebra is defined which consists of irreducible tensors only. This tensor basis is generally discussed and compared with similar constructions for finite groups and $SU(2)$.

1. INTRODUCTION

The object of this paper is the definition of a special orthogonal basis of $\mathfrak{A}(\mathcal{G})$, the group algebra of a compact group $\mathcal{G}$. The basis is adapted to the decomposition of the semisimple algebra $\mathfrak{A}(\mathcal{G})$ into simple constituents (and thus to all irreducible representations of $\mathcal{G}$) being the union of bases of the simple algebras. (We call a basis with this property convenient; otherwise, inconvenient). Furthermore, this basis is adapted to a group of automorphisms of $\mathfrak{A}(\mathcal{G})$ homomorphic to $\mathcal{G}$ because its elements transform under these automorphisms according to unitary irreducible matrix representations (unirreps) of $\mathcal{G}$. (We denote orthogonal bases with this property tensor bases).

Tensor bases were proposed by several authors: for finite groups (inconvenient ones) by Gamba,[1] Killingbeck,[2] and de Vries;[3] for $SU(2)$ (essentially the one given here) by Racah[4] and Corio.[5]

Tensor bases can be of physical interest because they define in the carrier space of an irreducible unitary representation of $\mathcal{G}$ a set of irreducible tensor operators complete with respect to all operators defined in this Hilbert space and, if the basis is convenient, even orthonormalized in a certain way. These operators are therefore especially suited for operator equivalences.[6,7]

For every finite-dimensional unitary representation of $\mathcal{G}$ orthonormalized sets of irreducible tensor operators exist which are complete with respect to all operators of this carrier space. But in case of a reducible representation some of these operators certainly do not represent elements of $\mathfrak{A}(\mathcal{G})$. It is therefore tempting to extend this reducible representation of $\mathcal{G}$ to an irreducible unitary representation of a larger compact group $\mathcal{G}' \supset \mathcal{G}$. In this case the complete set of tensor operators (with respect to $\mathcal{G}$) can be considered to represent (part of) a tensor basis of $\mathfrak{A}(\mathcal{G}')$. An example of a group extension leading to tensor operators with transformation properties impossible for an element of $\mathfrak{A}(\mathcal{G})$ was given by de Vries.[8]

In case the representation of $\mathcal{G}$ is infinite-dimensional a similar procedure would require a non compact group $\mathcal{G}'$. We do not deal with this problem. If the representation of $\mathcal{G}$ is infinite-dimensional, we consider only the bounded operators representing elements of $\mathfrak{A}(\mathcal{G})$ and unbounded ones intimately connected with them (generators, etc.).

The basic definitions and some general conclusions are given in Sec. 2. In Sec. 2A the definition of the group algebra $\mathfrak{A}(\mathcal{G})$ is outlined. In Sec. 2B a group of automorphisms of $\mathfrak{A}(\mathcal{G})$ is introduced as the "tensor representation" of $\mathcal{G}$. Two theorems stating necessary and sufficient conditions for irreducible representations to be contained in the tensor representation are proven in Sec. 2C. Our tensor basis is defined in Sec. 2D. There is also discussed what is needed to construct, for a given unitary representation of $\mathcal{G}$, the set of operators representing the tensor basis. Section 2E deals with group extensions leading to complete sets of irreducible tensor operators.

The general results of Sec. 2 are specialized for finite groups in Sec. 3. In Sec. 3A a formula is derived for the number of times (zero included) a given irreducible representation appears in the tensor representation. In Sec. 3B some special results for double point groups are mentioned. In Sec. 3C our tensor basis is compared with the one used up to now exclusively for finite groups. In Sec. 3D group extensions are reconsidered for finite groups.

Section 4 deals with the consequence following from the results of Sec. 2 for $SU(n)$, especially in case $n = 2$. In Sec. 4A modifications possible for Lie groups (Lie algebra instead of the group, universal enveloping algebra instead of the group algebra) are mentioned. In Sec. 4B necessary and sufficient conditions for an irreducible representation to appear in the tensor representation of $SU(n)$ are stated. Finally the tensor basis of $\mathfrak{A}(SU(2))$ is explicitly given in terms of operators representing elements of the group and/or the Lie algebra.

2. GENERAL THEORY

A. The group algebra $\mathfrak{A}(\mathcal{G})$

The definition of the group algebra $\mathfrak{A}(\mathcal{G})$ of a compact group $\mathcal{G}$ and its properties are extensively dealt with in mathematical textbooks.[9,10] Similar treatments exist for finite groups[11,12] and $SU(2)$[13] also in the physical literature. In the following we therefore accentuate only the propositions not to be found there stating the other facts in a less formal way.

If a group is compact an invariant integral

$$M[f] = M_x[f(x)] = M_x[f(yxz)] \quad \text{for all } y, z \in \mathcal{G} \tag{2.1}$$

exists for all complex-valued continuous functions defined on $\mathcal{G}$. We assume it to be normalized ($M[1] = 1$). The set of these functions forms a linear space. It is a unitary space if the scalar product is defined by

$$\langle f, g \rangle_1 = M_x[f^*(x) g(x)] \tag{2.2}$$

Completion gives the *Hilbert space $L^2(\mathcal{G})$ of complex valued square-integrable functions on $\mathcal{G}$.*

In $L^2(\mathcal{G})$ a group $\mathfrak{U}(\mathcal{G})$ of unitary operators $\mathbf{y}$ is defined by

$$\mathbf{y} f(x) = f(y^{-1}x), \qquad y \in \mathcal{G}, \mathbf{y} \in \mathfrak{U}(\mathcal{G}), f \in L^2(\mathcal{G}). \tag{2.3}$$

$\mathfrak{U}(\mathcal{G}) \cong \mathcal{G}$ and the mapping $\mathcal{G} \to \mathfrak{U}(\mathcal{G})$ is called the *regular representation* of $\mathcal{G}$.

By

$$\langle f, \mathbf{a}g\rangle_1 = M_x[a(x)\langle f, \mathbf{x}g\rangle_1] \quad \text{for all } f,g \in L^2(\mathcal{G}) \tag{2.4}$$

a bounded linear operator is defined for every $a \in L^2(\mathcal{G})$. The set

$$\mathfrak{A}(\mathcal{G}) = \{\mathbf{a} : a \in L^2(\mathcal{G})\} \tag{2.5}$$

is a Hilbert space isometric to $L^2(\mathcal{G})$ if the scalar product in $\mathfrak{A}(\mathcal{G})$ is defined by

$$\langle \mathbf{a}, \mathbf{b}\rangle_2 = \langle a, b\rangle_1 \tag{2.6}$$

$\mathfrak{A}(\mathcal{G})$ is a symmetric ring if the product $\mathbf{ab}$ is defined by the successive action of the operators and the involution as the mapping $\mathbf{a} \to \mathbf{a}^+$, $\mathbf{a}^+$ being the adjoint operator. In the following the term *group algebra* is used for the *symmetric Hilbert ring* $\mathfrak{A}(\mathcal{G})$.

Every representation $x \to U(x)$ of $\mathcal{G}$ by unitary operators $U(x)$ in a Hilbert space $\mathcal{H}$ can be extended by

$$\langle \psi, B(\mathbf{a})\varphi\rangle_{\mathcal{H}} = M_x[a(x)\langle \psi, U(x)\varphi\rangle_{\mathcal{H}}] \quad \text{for all } \psi, \varphi \in \mathcal{H} \tag{2.7}$$

to a representation $\mathbf{a} \to B(\mathbf{a})$ of $\mathfrak{A}(\mathcal{G})$ which is symmetric $[B(\mathbf{a}^+) = B^+(\mathbf{a})]$. Although the extension of a unitary representation of $\mathcal{G}$ to a symmetric one of $\mathfrak{A}(\mathcal{G})$ is always possible in principle, it is practicable only if the following condition is satisfied:

Condition 1: The group elements are parametrized by a set of real variables and the invariant integral is expressed as a sum and/or integral over these parameters.

To point out the connection (2.7) between representations of $\mathcal{G}$ and $\mathfrak{A}(\mathcal{G})$ which may be traced back to Eq. (2.4), we introduce instead of the definition (2.4) the shorter *symbolic notation*

$$\mathbf{a} = M_x[a(x)\mathbf{x}] \tag{2.8}$$

for the elements of $\mathfrak{A}(\mathcal{G})$. Equations in which this notation is used have always to be understood in the sense of Eq. (2.4).

From Eqs. (2.1)-(2.4) follows

$$\mathbf{ya} = M_x[a(y^{-1}x)\mathbf{x}] \tag{2.9}$$

The mappings $\mathbf{a} \to \mathbf{ya}$ therefore define a representation of $\mathcal{G}$ isomorphic to the regular one.

B. The tensor representation of $\mathcal{G}$

We introduce a second representation of $\mathcal{G}$ by

Definition 1: The *tensor representation* of $\mathcal{G}$ is the homomorphism $y \to (\mathbf{a} \to \mathbf{yay}^{-1})$; $y \in \mathcal{G}$; $\mathbf{y} \in \mathcal{U}(\mathcal{G})$; $\mathbf{a}, \mathbf{yay}^{-1} \in \mathfrak{A}(\mathcal{G})$.

Using Eqs. (2.1), (2.6), and (2.2), it is easily verified that

$$\mathbf{yay}^{-1} = M_x[a(y^{-1}xy)\mathbf{x}] \tag{2.10}$$

is an element of $\mathfrak{A}(\mathcal{G})$ if $\mathbf{a} \in \mathfrak{A}(\mathcal{G})$, and that the mapping $\mathbf{a} \to \mathbf{yay}^{-1}$ defines a unitary operator in the Hilbert space $\mathfrak{A}(\mathcal{G})$. [This unitary operator for which we do not introduce a new symbol must not be confused with the one defined by Eq. (2.9)]. Since the mapping $\mathbf{a} \to \mathbf{yay}^{-1}$ is also an automorphism of the symmetric ring $\mathfrak{A}(\mathcal{G})$ it is an automorphism of the Hilbert ring $\mathfrak{A}(\mathcal{G})$.

Because of Eq. (2.10) an element of the center

$$\mathfrak{z}[\mathcal{G}] = \{z : z \in \mathcal{G}; xz = zx \text{ for all } x \in \mathcal{G}\} \tag{2.11}$$

induces the identical transformation $\mathbf{a} \to \mathbf{a}$, but the reverse is also true (see the following section).

C. Units

$\mathfrak{A}(\mathcal{G})$ is a semisimple algebra decomposing into a direct orthogonal sum of finite-dimensional, symmetric, and simple algebras $\mathfrak{A}^\alpha(\mathcal{G})$:

$$\mathfrak{A}(\mathcal{G}) = \sum_\alpha \oplus\, \mathfrak{A}^\alpha(\mathcal{G}), \quad \mathfrak{A}^\alpha(\mathcal{G}) \text{ simple and symmetric,} \tag{2.12}$$

$$\text{dimension of } \mathfrak{A}^\alpha(\mathcal{G}) = n_\alpha^2 < \infty \tag{2.13}$$

Equation (2.12) implies a unique decomposition

$$\mathbf{a} = \sum_\alpha \mathbf{a}^\alpha, \quad \mathbf{a}^\alpha \in \mathfrak{A}^\alpha(\mathcal{G}), \tag{2.14}$$

of all elements into pairwise annihilating and orthogonal components:

$$\alpha \neq \beta \Rightarrow \mathbf{a}^\alpha\mathbf{b}^\beta = 0 \quad \text{and} \quad \langle \mathbf{a}^\alpha, \mathbf{b}^\beta\rangle_2 = 0. \tag{2.15}$$

If an irreducible unitary representation of $\mathcal{G}$ is extended to a symmetric (irreducible) representation of $\mathfrak{A}(\mathcal{G})$, then the ring of operators representing the elements of $\mathfrak{A}(\mathcal{G})$ is isomorphic to one of the subrings $\mathfrak{A}^\alpha(\mathcal{G})$. Therefore,

$$A = \{\alpha\} = \text{index set of equivalence classes of unirreps of } \mathcal{G}, \tag{2.16}$$

$$n_\alpha = \text{dimension of the unirrep } D^\alpha. \tag{2.17}$$

Every simple algebra $\mathfrak{A}^\alpha(\mathcal{G})$ is isomorphic to the algebra of $n_\alpha \times n_\alpha$ matrices. This implies the existence of a basis $\{\mathbf{e}^\alpha_{jk} : \mathbf{e}^\alpha_{jk} \in \mathfrak{A}(\mathcal{G}); \alpha \in A; j,k = 0,\ldots,n_\alpha - 1\}$ the elements of which sometimes,[14] and in the following called *units*, satisfy

$$\mathbf{e}^{\alpha+}_{jk} = \mathbf{e}^\alpha_{kj} \tag{2.18}$$

$$\mathbf{e}^\alpha_{jk}\mathbf{e}^\beta_{lm} = \delta_{\alpha\beta}\delta_{kl}\mathbf{e}^\alpha_{jm}, \tag{2.19}$$

$$\mathbf{a} = \sum_{\alpha jk} \langle \mathbf{e}^\alpha_{jk}, \mathbf{a}\rangle_2 \frac{1}{n_\alpha} \mathbf{e}^\alpha_{jk} \quad \text{for all } \mathbf{a} \in \mathfrak{A}(\mathcal{G}), \tag{2.20}$$

$$\mathbf{y}\mathbf{e}^\alpha_{jk} = \sum_l D^\alpha_{lj}(y)\mathbf{e}^\alpha_{lk} \quad \text{for all } \mathbf{y} \in \mathcal{U}(\mathcal{G}). \tag{2.21}$$

Equation (2.20) implies that the basis is orthogonal, and that the elements $\mathbf{e}^\alpha_{jk}$ are normalized to $n_\alpha^{1/2}$. Equation (2.21) shows that the regular representation of $\mathcal{G}$ decomposes into a direct sum of irreducible representations appearing with multiplicities equal to their dimensions.

The set $\{\mathbf{e}^\alpha_{jk}\}$ is an example for a basis of $\mathfrak{A}(\mathcal{G})$ which is the union of bases of the subalgebras $\mathfrak{A}^\alpha(\mathcal{G})$. Any such basis has two convenient properties:

(1) Its (nonvanishing) elements remain linearly independent in every representation.

(2) They may be defined by successively defining bases of the finite-dimensional subspaces $\mathfrak{A}^\alpha(\mathcal{G})$.

We accentuate these properties by

Definition 2: A basis of $\mathfrak{A}(\mathcal{G})$ is *convenient* if it is the union of bases of the subalgebras $\mathfrak{A}^\alpha(\mathcal{G})$; otherwise it is *inconvenient*.

A basis of a subalgebra $\mathfrak{A}^{\alpha}(\mathcal{G})$ can also be obtained via a matrix representation $\mathbf{a}^{\alpha} \to M^{\alpha}(\mathbf{a}^{\alpha})$. If $\{M^{\alpha}(i): i = 1, \ldots, n_{\alpha}^2\}$ is a set of n_{α}^2 linearly independent $n_{\alpha} \times n_{\alpha}$ matrices, then the set $\{\mathbf{a}_i^{\alpha} = \sum_{jk} M_{jk}^{\alpha}(i)\mathbf{e}_{jk}^{\alpha}: i = 1, \ldots, n_{\alpha}^2\}$ constitutes a basis of $\mathfrak{A}^{\alpha}(\mathcal{G})$. Because of

$$\langle \mathbf{a}^{\alpha}, \mathbf{b}^{\alpha}\rangle_2 = n_{\alpha}\, \mathrm{trace} M^{\alpha+}(\mathbf{a}^{\alpha}) M^{\alpha}(\mathbf{b}^{\alpha}) \tag{2.22}$$

[following from Eq. (2.20) and the bilinearity of the scalar product] this basis can be orthonormalized even without detailed knowledge of the invariant integration. The operators $B(\mathbf{a}_i^{\alpha})$ onto which the elements $\mathbf{a}_i^{\alpha}$ are mapped are completely determined by the matrices $M^{\alpha}(i)$ if in $\mathcal{K}$, the carrier space of the unitary representation of $\mathcal{G}$, a basis $\{\psi_{\alpha j w}\}$ is known the elements of which transform according to unirreps of $\mathcal{G}$. If such a basis is not known it has to be constructed or what amounts to the same the operators $B(\mathbf{e}_{jk}^{\alpha})$ have to be won from the unitary operators $U(y)$.

Because of

$$\mathbf{e}_{jk}^{\alpha} = M_x[n_{\alpha} D_{jk}^{\alpha *}(x)\mathbf{x}] \tag{2.23}$$

such a construction presupposes a knowledge of

$$\Delta = \{D_{jk}^{\alpha}(x): x \in \mathcal{G}; \alpha \in A; j, k = 0, 1, \ldots, n_{\alpha} - 1\}$$
$$= \text{a complete set of unirreps of } \mathcal{G} \tag{2.24}$$

To make the construction of the operators $B(\mathbf{e}_{jk}^{\alpha})$ practicable, the following condition must be fulfilled.

Condition 2: All matrix elements $D_{jk}^{\alpha}(x) \in \Delta$ have to be given as known functions of the real parameters mentioned in Condition 1.

From Eqs. (2.10), (2.23), and (2.21), follows

$$\mathbf{y}\mathbf{e}_{jk}^{\alpha}\mathbf{y}^{-1} = \sum_{lm} D_{lj}^{\alpha}(y) D_{mk}^{\alpha *}(y)\mathbf{e}_{lm}^{\alpha}. \tag{2.25}$$

From this results

Theorem 1: The tensor representation of $\mathcal{G}$ is a faithful representation of $\mathcal{G}/\mathfrak{z}[\mathcal{G}]$.

Proof: $\mathbf{y}\mathbf{a}\mathbf{y}^{-1} = \mathbf{a}$ for all $\mathbf{a} \in \mathfrak{A}(\mathcal{G})$ is equivalent to $\mathbf{y}\mathbf{e}_{jk}^{\alpha}\mathbf{y}^{-1} = \mathbf{e}_{jk}^{\alpha}$ for all α, j, k. This implies $D_{lj}^{\alpha}(y) D_{mk}^{\alpha *}(y) = \delta_{lj}\delta_{mk}$ which is only possible if $D^{\alpha}(y) = \omega_y E^{\alpha}$, $|\omega_y| = 1$, $E^{\alpha} = n_{\alpha} \times n_{\alpha}$ 1-matrix. Therefore, $D^{\alpha}(y) D^{\alpha}(x) = D^{\alpha}(x) D^{\alpha}(y)$ for all $x \in \mathcal{G}$. Since this holds for all unirreps, the same relation is true for the regular representation. But the latter is faithful; hence $y \in \mathfrak{z}[\mathcal{G}]$.

Theorem 1 comprises a necessary condition for an irreducible representation of type β to be contained in the tensor representation: The subduced representation $D^{\beta} \downarrow \mathfrak{z}[\mathcal{G}]$ [15] has to be the identical representation. Theorem 1 does not imply that the tensor representation necessarily contains all irreducible representations of $\mathcal{G}/\mathfrak{z}[\mathcal{G}]$ but only sufficiently many to make the representation faithful. Note however the following sufficient condition:

Theorem 2: If $\mathcal{G}$ has a faithful unirrep D^{α} then every irreducible representation of $\mathcal{G}/\mathfrak{z}[\mathcal{G}]$ is contained in the tensor representation.

Proof: A similar argumentation as in the proof of Theorem 1 shows that the Kronecker product $D^{\alpha} \times D^{\alpha *}$ ($\sim D^{\alpha *} \times D^{\alpha}$) is a faithful finite-dimensional representation of $\mathcal{G}/\mathfrak{z}[\mathcal{G}]$ if D^{α} is a faithful unirrep of $\mathcal{G}$. From this it follows[16] that the $2n$-fold Kronecker products $D^{\alpha} \times D^{\alpha *} \times \cdots \times D^{\alpha} \times D^{\alpha *}$ $(n = 1, 2, \cdots)$ contain all unirreps of $\mathcal{G}/\mathfrak{z}[\mathcal{G}]$. Therefore, only elements have to be found which transform according to these Kronecker products. But this is done by the elements of $\mathfrak{A}(\mathcal{G})$ corresponding to the n-fold products $D_{j_1k_1}^{\alpha *}(x) D_{j_2k_2}^{\alpha *}(x) \cdots D_{j_nk_n}^{\alpha *}(x) \in L^2(\mathcal{G})$ as can be seen from Eq. (2.10)

D. The tensor basis

Like every other unitary representation of $\mathcal{G}$ the tensor representation decomposes into a direct sum of finite-dimensional irreducible representations. As the decomposition of the regular representation is clearly visible if the units are taken as basis of $\mathfrak{A}(\mathcal{G})$, the decomposition of the tensor representation can be made obvious by the choice of a suitable basis.

Definition 3: A set $\{\mathbf{z}_{\beta r}: \mathbf{z}_{\beta r}(\neq 0) \in \mathfrak{A}(\mathcal{G}); \beta \in A; r = 0, \ldots, n_{\beta} - 1\}$ is an *irreducible tensorial set* (*ITS*), its elements are the *components*, and β is the *type* of the ITS, if for all $\mathbf{y} \in \mathfrak{U}(\mathcal{G})$

$$\mathbf{y}\mathbf{z}_{\beta r}\mathbf{y}^{-1} = \sum_s D_{sr}^{\beta}(y)\mathbf{z}_{\beta s}, \quad D^{\beta} \in \Delta. \tag{2.26}$$

Invariants are ITS's of type $\beta = 0$ $[D^0(y) = 1$ for all $y \in \mathcal{G}]$.

Theorems 1 and 2 can be restated as conditions for the types of ITS's.

Definition 4: A *tensor basis* is an orthogonal basis of $\mathfrak{A}(\mathcal{G})$ the elements of which are components of ITS's.

Definition 5: *Coupling coefficients* $[\alpha j \bar{\beta} l \mid v\gamma r]$ are complex numbers satisfying

$$D_{jk}^{\alpha}(y) D_{lm}^{\beta *}(y) = \sum_{v\gamma rs} [\alpha j \bar{\beta} l \mid v\gamma r] D_{rs}^{\gamma}(y) [\alpha k \bar{\beta} m \mid v\gamma s]^*$$

$$\sum_{jklm} [\alpha j \bar{\beta} l \mid v\gamma r]^* D_{jk}^{\alpha}(y) D_{lm}^{\beta *}(y) [\alpha k \bar{\beta} m \mid w\epsilon s] = \delta_{vw}\delta_{\gamma\epsilon} D_{rs}^{\gamma}(y) \tag{2.27}$$

for $D^{\alpha}, D^{\beta}, D^{\gamma} \in \Delta$ and all $y \in \mathcal{G}$.

The indices

$$v, w = 0, 1, \ldots, m_{\alpha\bar{\beta}\gamma} - 1$$
$$m_{\alpha\bar{\beta}\gamma} = \text{multiplicity of } D^{\gamma} \text{ in } D^{\alpha} \times D^{\beta *} \tag{2.28}$$

distinguish unirreps occuring more than once. If $m_{\alpha\bar{\beta}\gamma} = 1$, which always holds for simply reducible groups,[17] $v = w = 0$ can be omitted.

Theorem 3: Every set $\{[\alpha j \bar{\alpha} k \mid v\beta r]: \alpha, \beta \in A; j, k = 0, \ldots, n_{\alpha} - 1; v = 0, \ldots, m_{\alpha\bar{\alpha}\beta} - 1; r = 0, \ldots, n_{\beta} - 1\}$ of coupling coefficients defines uniquely a convenient tensor basis the elements belonging to $\mathfrak{A}^{\alpha}(\mathcal{G})$ being normalized to $n_{\alpha}^{1/2}$; and vice versa.

Corollary: ITS's of type β exist if and only if $m_{\alpha\bar{\alpha}\beta} \geq 1$ for some $\alpha \in A$.

Proof: (a) Assume the coupling coefficients to be given and set

$$\mathbf{z}_{v\beta r}^{\alpha} = \sum_{jk} [\alpha j \bar{\alpha} k \mid v\beta r]\mathbf{e}_{jk}^{\alpha}; \tag{2.29}$$

then $\mathbf{z}_{v\beta r}^{\alpha} \in \mathfrak{A}^{\alpha}(\mathcal{G})$.

$$\mathbf{e}_{jk}^{\alpha} = \sum_{\beta r v} [\alpha j \bar{\alpha} k \mid v\beta r]^* \mathbf{z}_{v\beta r}^{\alpha} \tag{2.30}$$

is the inverse transformation of (2.29), as follows from Eqs. (2.27), y = 1-element of $\mathcal{G}$. Since the **z**'s are obtained from the **e**'s by a unitary transformation, they are like these orthonormalized and a basis of $\mathfrak{A}(\mathcal{G})$. The required transformation properties (2.26) follow from Eqs. (2.29), (2.25), (2.30), and (2.27).

(b) Assume the tensor basis to be given. Its elements must permit a labelling by α (convenient basis), βr (components of ITS's), and an index v if $\mathfrak{A}^{\alpha}(\mathcal{G})$ contains more than one linearly independent ITS of type β. Furthermore, the elements have to be orthogonal (Definition 4) and normalized like the **e**'s (Theorem 3). This implies that unitary transformations like (2.29) and (2.30) exist. That the expansion coefficients appearing there satisfy Eqs. (2.27) is a consequence of the transformation properties (2.25) and (2.26) of the **e**'s and the **z**'s.

(c) The corollary follows from the completeness of the basis (2.29).

Both aspects of Theorem 3 may be of practical interest.

Condition 3: The coupling coefficients $[\alpha j\bar{\alpha}k \mid v\beta r]$ are tabulated or calculable by means of algorithms.

If Condition 3 is satisfied, the linear combinations (2.29) can be calculated at least successively. If also Conditions 1 and 2 are fulfilled, all bounded operators $\mathbf{z}^{\alpha}_{v\beta r}$ $[B(\mathbf{z}^{\alpha}_{v\beta r})]$ may be expressed as "linear combinations" of the unitary operators $\mathbf{x}$ $[U(x)]$. A better estimation of Condition 3 may be gained noting that the coupling coefficients $[\alpha j\bar{\beta}l \mid v\gamma r]$ are related to the usual Clebsch-Gordan (CG) coefficients[18] $(\alpha j\beta l \mid v\gamma r)$ by

$$[\alpha j\bar{\beta}l \mid v\gamma r] = \sum_{l'} (\alpha j\beta l' \mid v\gamma r)U^{\beta}_{ll'}, \tag{2.31}$$

the unitary $n_\beta \times n_\beta$ matrix U^β being defined by

$$D^{\beta *}(y) = U^{\beta}D^{\bar{\beta}}(y)U^{\beta +}, \quad D^{\beta}, D^{\bar{\beta}} \in \Delta. \tag{2.32}$$

The only thing that can be said about the coupling coefficients without further knowledge of the group refers to the identical representation ($\beta = 0, r = s = 0$):

$$m_{\alpha\bar{\alpha}0} = 1, \qquad [\alpha j\bar{\alpha}k \mid 000] = n_{\alpha}^{-1/2}\omega_{\alpha}\delta_{jk}, \quad |\omega_{\alpha}| = 1. \tag{2.33}$$

Equation (2.33) shows that every subalgebra $\mathfrak{A}^{\alpha}(\mathcal{G})$ contains just one linearly independent invariant.

The second part of Theorem 3 is of interest if a convenient tensor basis is constructed successively by means of matrix representations $M^{\alpha}(\mathbf{z}^{\alpha}_{v\beta r})$ (cf. Sec. 2.C). The postulated transformation properties of the matrices follow from Eq. (2.26) by substituting $\mathbf{y} \to D^{\alpha}(y)$, $\mathbf{z}_{\beta r} \to M^{\alpha}(\mathbf{z}_{\beta r})$. It is of advantage to satisfy them first because matrices transforming differently ($\beta r \neq \beta' r'$) are already orthogonal with respect to the scalar product defined on the right side of Eq. (2.22). The elements of the matrices so constructed are then coupling coefficients because of Theorem 3. If the matrices U^{α} are known, the CG coefficients $(\alpha j\bar{\alpha}k \mid v\beta r)$ are obtained as "by-product" of such a construction.

E. Tensor operators

It follows from Eqs. (2.10), (2.7), (2.1), and (2.26) that

$$U(y)B(\mathbf{z}_{\beta r})U(y^{-1}) = \sum_{s} D^{\beta}_{sr}(y)B(\mathbf{z}_{\beta s}). \tag{2.34}$$

As was to be expected, ITS's are represented by *tensor operators*.[19] If the carrier space $\mathcal{H}$ of a unitary representation is irreducible, then the algebra of its operators is isomorphic to one of the algebras $\mathfrak{A}^{\alpha}(\mathcal{G})$. In this case the operators $B(\mathbf{z}^{\alpha}_{v\beta r})$ offer a complete set of orthonormalized irreducible tensor operators. If $\mathcal{H}$ is reducible, then irreducible tensor operators which are not linear combinations of the operators $B(\mathbf{z}^{\alpha}_{v\beta r})$ always exist. Nevertheless, even then complete sets of orthonormalized tensor operators exist if the representation is finite-dimensional.

Theorem 4: (a) Every finite-dimensional unitary representation of a compact group $\mathcal{G}$ can be extended to an irreducible representation of a compact group $\mathcal{G}' \supset \mathcal{G}$.

(b) There exist tensor bases of $\mathfrak{A}(\mathcal{G}')$ represented in this irreducible representation of $\mathcal{G}'$ by operators which are irreducible tensor operators not only with respect to $\mathcal{G}'$ but also to $\mathcal{G}$.

Proof: (a) The n-dimensional Hilbert space engenders an irreducible representation of $\mathcal{G}' = U(n)$. [This does not exclude that $\mathcal{H}$ may also be irreducible for proper (compact) subgroups $\mathcal{G}' \subset U(n)$.]

(b) Choose a set Δ' of unirreps of $\mathcal{G}'$ for which the subduced representations $D' \downarrow \mathcal{G}$ are direct sums of unirreps $D \in \Delta$.

Theorem 4 may be satisfying from an esthetic point of view. However, a group $\mathcal{G}'$ will be of more than academic interest only if it has a rather simple multiplication law and/or admits physical interpretation. If one is only interested in a complete set of orthonormalized tensor operators, this can be obtained far easier by a direct construction.

(*Hint*: Choose a basis $\{\psi_{w\alpha j}\}$ for which

$$U(y)\psi_{w\alpha j} = \sum_{k} D^{\alpha}_{kj}(y)\psi_{w\alpha k}. \tag{2.35}$$

Define operators $E_{w\alpha j, w'\alpha' j'}$ by

$$E_{w\alpha j, w'\alpha' j'}\psi_{w''\alpha'' j''} = \delta_{w'w''}\delta_{\alpha'\alpha''}\delta_{j'j''}\psi_{w\alpha j}. \tag{2.36}$$

The set of operators

$$Z_{w\alpha w'\alpha' v\beta r} = \sum_{jj'} [\alpha j\bar{\alpha}' j' \mid v\beta r]E_{w\alpha j, w'\alpha' j'} \tag{2.37}$$

is then the desired one. Since their matrix elements in the symmetry adapted basis (2.35) are just the coupling coefficients defined by Eqs. (2.27), the operators (2.37) are quite similar to the Wigner operators introduced by Biedenharn.[20])

3. FINITE GROUPS

A. Total multiplicity

For finite groups (with discrete topology) $\mathfrak{A}(\mathcal{G})$ is $|\mathcal{G}|$-dimensional. This allows to strengthen the Corollary of Theorem 3.

Theorem 5: For finite $\mathcal{G}$ the number of linearly independent ITS's of type β is

$$m_{\beta} = \sum_{\alpha} m_{\alpha\bar{\alpha}\beta} = \sum_{\mu} \chi^{\beta}_{\mu}. \tag{3.1}$$

Proof:

$$m_{\alpha\bar{\alpha}\beta} = \sum_{\mu} \frac{|\mathcal{C}_{\mu}|}{|\mathcal{G}|} \chi^{\alpha}_{\mu}\chi^{\alpha *}_{\mu}\chi^{\beta}_{\mu}, \tag{3.2}$$

$$\sum_{\alpha} \frac{|\mathcal{C}_\mu|}{|\mathcal{G}|} \chi_\mu^\alpha \chi_{\mu'}^{\alpha *} = \delta_{\mu\mu'}. \quad (3.3)$$

The first part of Eq. (3.1) was proved by de Vries[3] under the restriction $\alpha = \bar{\alpha}$. The extremely useful form as a sum of primitive characters was given by Gamba[1] without proof.

In Eqs. (3.1)-(3.3)

$$\{\mu\} = \{0, 1, \ldots, |A| - 1\} = \text{class parameter} \quad (3.4)$$

and $\mathcal{C}_\mu$ is a class of conjugate elements.

B. Special results and explicit constructions

As an example for the application of the Theorems 1 and 2 we note

Theorem 6: In the group algebra $\mathcal{A}(\mathcal{G}^*)$ of a non-Abelian double point group $\mathcal{G}^*$ ITS's of type β exist if an only if D^β is a unirrep of the adjoint point group $\mathcal{G}$.

Proof: (a) If: Every double point group $\mathcal{G}^*$ being a finite subgroup of $SU(2)$ is defined by a faithful two-dimensional representation.[21] If this is reducible $\mathcal{G}^*$ is Abelian; if not, Theorem 2 applies and $\mathfrak{z}[\mathcal{G}^*] = \mathfrak{z}[SU(2)]$. But $\mathcal{G}^*/\mathfrak{z}[SU(2)] \cong \mathcal{G}$.

(b) Only if: Theorem 1.

To express the elements of the tensor basis as linear combinations of the elements $\mathbf{x}$ raises no difficulties. Condition 1 is always satisfied for finite groups by a parametrization with $i = 0, \ldots, |\mathcal{G}| - 1$ and

$$M[f] = (1/|\mathcal{G}|) \sum_i f(x_i). \quad (3.5)$$

For finite groups appearing in physical problems numerous tables[22] exist so that for a certain group only small calculations are necessary to satisfy also Conditions 2 and 3. Examples of tensor bases for the double point groups O^* and T^* constructed according to Eq. (2.29) were given by Blümelhuber and Mühl.[23]

C. Another tensor basis

These exist infinitely many tensor bases definable in different ways. In this section our definition (2.29) is compared with the one used up to now exclusively for finite groups.

Its definition is based on the following facts:

$$U(\mathcal{G}) \subset \mathcal{A}(\mathcal{G}), \quad \text{if } \mathcal{G} \text{ is finite}, \quad (3.6)$$

$$\langle \mathbf{x}, \mathbf{y} \rangle_2 = |\mathcal{G}| \delta_{xy}. \quad (3.7)$$

If the group elements are labelled by the class parameter (3.4) and by

$$\{\nu\} = \{0, 1, \ldots, |\mathcal{C}_\mu| - 1\} = \text{in-class parameters}, \quad (3.8)$$

then, as was noted by Gamba,[1] the mappings $\mathbf{a} \to \mathbf{yay}^{-1}$ induce permutations $\mathbf{x}_{\mu\nu} \to \mathbf{x}_{\mu\nu'}$. By choosing a basis $\{\mathbf{x}_{00}; \mathbf{x}_{10}, \ldots, \mathbf{x}_{1,|\mathcal{C}_1|-1}; \mathbf{x}_{20}, \ldots, \mathbf{x}_{2,|\mathcal{C}_2|-1}; \ldots\}$ Gamba obtained a decomposition of the tensor representation into a direct sum of $|\mathcal{C}_\mu|$-dimensional permutation representations. These so-called class representations may be reducible. By decomposing all of them into irreducible constituents a tensor basis can be defined. It suggests itself to achieve the decomposition by projecting the irreducible representations out of the class representations.[24] But if an irreducible representation is contained more than once in a class representation, then immediately the question arises: How are the projection operators and the elements of $\mathcal{A}(\mathcal{G})$ onto which they act to be chosen so that the ITS's resulting from the projection are orthogonal? This problem was solved essentially by de Vries[3] and completely by Gilmore[25] (and independently by the authors). Before giving this solution we explain the notation used therein.

The $|A|$ groups

$$\mathfrak{z}_\mu = \{x : x \in \mathcal{G}; x x_{\mu 0} = x_{\mu 0} x\}$$
$$= \text{centralizer of } x_{\mu 0} \quad (3.9)$$

of order

$$|\mathfrak{z}_\mu| = |\mathcal{G}| / |\mathcal{C}_\mu| \quad (3.10)$$

are special subgroups of $\mathcal{G}$. For their unirreps we introduce the symbols

$$A_\mu = \{\alpha_\mu\} = \text{index set of equivalence classes of unirreps of } \mathfrak{z}_\mu, \quad (3.11)$$

$$n_{\alpha_\mu} = \text{dimension of the unirrep } D^{\alpha_\mu}, \quad (3.12)$$

$$D_{00}^{\alpha_\mu = 0}(x) = 1 \quad \text{for all } x \in \mathfrak{z}_\mu. \quad (3.13)$$

Beside the unirreps $D^\alpha \in \Delta$ we need equivalent unirreps $D^{\alpha(\mu)}$ of $\mathcal{G}$ which subduce direct sums of unirreps D^{α_μ} of $\mathfrak{z}_\mu$:

$$D^{\alpha(\mu)}(x) = W^{\alpha(\mu)+} D^\alpha(x) W^{\alpha(\mu)}, \quad (3.14)$$

$$[W^{\alpha(\mu)}]^{-1} = W^{\alpha(\mu)+}, \quad (3.15)$$

$$D^{\alpha(\mu)} \downarrow \mathfrak{z}_\mu = \text{direct sum of unirreps } D^{\alpha_\mu} \text{ of } \mathfrak{z}_\mu, \quad (3.16)$$

$$m_{\alpha\alpha_\mu} = \text{multiplicity of } D^{\alpha_\mu} \text{ in } D^\alpha \downarrow \mathfrak{z}_\mu, \quad (3.17)$$

$$\{v(\alpha\alpha_\mu)\alpha_\mu j_\mu : \alpha \in A; \alpha_\mu \in A_\mu, m_{\alpha\alpha_\mu} \neq 0;$$
$$v(\alpha\alpha_\mu) = 0, 1, \ldots, m_{\alpha\alpha_\mu} - 1; j_\mu = 0, 1, \ldots, n_{\alpha_\mu} - 1\}$$
$$= \text{row index of } D^{\alpha(\mu)}. \quad (3.18)$$

Theorem 7: The set $\{\mathbf{z}^\mu_{v(\beta O)\beta r} : \mu = 0, \ldots, |A| - 1; \beta \in A; r = 0, \ldots, n_\beta - 1; v(\beta O) = 0, \ldots, m_{\beta O} - 1\}$ of elements

$$\mathbf{z}^\mu_{v(\beta O)\beta r} = \sum_{v(\beta\alpha_\mu)\alpha_\mu j_\mu} W^{\beta(\mu)}_{r, v(\beta\alpha_\mu)\alpha_\mu j_\mu}$$
$$\times \frac{1}{|\mathcal{G}|} \sum_y n_\beta D^{\beta(\mu)*}_{v(\beta\alpha_\mu)\alpha_\mu j_\mu, v(\beta O)OO}(y) \mathbf{y} \mathbf{x}_{\mu O} \mathbf{y}^{-1} \quad (3.19)$$

constitutes an inconvenient tensor basis, where the elements (3.19) are normalized to $(n_\beta |\mathfrak{z}_\mu|)^{1/2}$.

Proof: (a) The elements (3.19) are components of ITS's: Substitute $\mathbf{yx} \to \mathbf{x}$ in $\mathbf{y}\mathbf{z}_{v(\beta O)\beta r}\mathbf{y}^{-1}$ and use the representation properties of $D^{\beta(\mu)}(x)$ and Eqs. (3.14), (3.15).

(b) The elements (3.19) are orthogonal and normalized to $(n_\beta |\mathfrak{z}_\mu|)^{1/2}$: They are orthogonal in μ because of $\mathbf{z}^\mu_{v(\beta' O)\beta' r'} \in \mathcal{C}_\mu$ and Eq. (3.7). In calculating $\langle \mathbf{z}^\mu_{v(\beta' O)\beta' r'}, \mathbf{z}^\mu_{v(\beta O)\beta r} \rangle_2$, take into account Eq. (3.7), the equivalence

$$x x_{\mu O} x^{-1} = y x_{\mu O} y^{-1} \iff x^{-1} y \in \mathfrak{z}_\mu, \quad (3.20)$$

the multiplication properties, the orthogonality relations,[26] and the special form (3.16) of the unirreps $D^{\beta(\mu)}$, and Eqs. (3.10), (3.15).

(c) There are $|\mathcal{G}|$ different elements (3.19): For fixed $\mu\beta r$ there exist

$$m_{\beta 0} = \frac{|\mathcal{C}_\mu|}{|\mathcal{G}|} \sum_{y_\mu \in \mathfrak{z}_\mu} \chi^\beta(y_\mu) \tag{3.21}$$

and therefore because of Eq. (3.3) altogether

$$\sum_{\mu\beta} m_{\beta 0} n_\beta = \sum_\mu |\mathcal{C}_\mu| = |\mathcal{G}| \tag{3.22}$$

different elements.

(d) Inconvenience: Convenience implies the invariants to be multiples of the elements $\mathbf{z}^{\alpha}_{000}$ [see remark following Eq. (2.33)]. But

$$\mathbf{z}^{\mu}_{000} = \frac{1}{|\mathcal{C}_\mu|} \sum_\nu \mathbf{x}_{\mu\nu} = \sum_\alpha \chi^{\alpha}_{\mu}\omega_\alpha n_\alpha^{-1/2} \mathbf{z}^{\alpha}_{000}. \tag{3.23}$$

The tensor basis (3.19) has several disadvantages compared to the one proposed by us [Eq. (2.29)]:

(1) The defining equations (3.19) make sense only for finite groups. (If class and in-class parameters[27] are known, it is possible also for continuous groups to define something similar to Gamba's class representations if one considers functions defined on the in-class parameters and square-integrable with respect to them. But these representations cannot be constituents of the tensor representation.)

(2) The basis is inconvenient. Therefore, if its elements are represented by operators, linear dependences not existing within $\mathfrak{A}(\mathcal{G})$ appear in general.

(3) In most cases the construction of this basis entails calculational efforts not worthwhile in view of its application. Because to give the $\mathbf{z}$'s as linear combinations of the $\mathbf{x}$'s one has not only to determine the $|A|$ subgroups $\mathfrak{z}_\mu$ but also all the matrices $W^{\beta(\mu)}$. What is of interest in applications are the matrix elements of the corresponding operators in symmetry adapted bases (Wigner-Eckart theorem). But there appear automatically CG coefficients (or, depending on the definition of the reduced matrix element, coupling coefficients) and therefore these have to be calculated also in this case now at the latest.

D. Group extensions

As mentioned in Sec. 2E, it may be of interest to extend a reducible representation of $\mathcal{G}$ to an irreducible one of $\mathcal{G}'$ ($\supset \mathcal{G}$). The desired simplicity of the multiplication law suggests to look primarily for finite extensions if $\mathcal{G}$ is finite. Such ones exist if the suppositions of Theorem 4 (a) are somewhat limited.

Theorem 8: Every n-dimensional permutation representation of a finite group $\mathcal{G}$ can be extended to an irreducible unitary representation of a finite group $\mathcal{G}' \supset \mathcal{G}$, where $\mathcal{G}' \cong \mathcal{G}_1' \circledS \mathcal{G}_2'$ (semidirect product), $\mathcal{G}_1' \subset \mathcal{C}_n \otimes \cdots \otimes \mathcal{C}_n$ (n-fold direct product of the cyclic group of order n), $\mathcal{G}_2' \subset \mathcal{S}_n$ (symmetric group of order $n!$).

Proof: (a) Definition of $\mathcal{G}'$: Define $\mathcal{G}'$ by the matrix group generated by the permutation matrices $P(x)$, $x \in \mathcal{G}$, and the matrices

$$A = \begin{pmatrix} 1 & 0 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & \nu & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & \nu^2 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & \cdot & \nu^{n-1} \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & 1 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & 0 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & \cdot & 1 \\ 1 & 0 & 0 & \cdot & \cdot & \cdot & 0 \end{pmatrix}, \tag{3.24}$$

$$\nu = \text{primitive } n\text{th root of } 1 \tag{3.25}$$

(b) Irreducibility: A and B generate a unirrep of a subgroup of order n^3.[28] Therefore the whole set of matrices generated by A, B, and the $P(x)$'s, is a unirrep of $\mathcal{G}'$, faithful per definition.

(c) Definition and structure of $\mathcal{G}_1'$: $\mathcal{G}_1'$ is the subgroup of $\mathcal{G}'$ represented in this n-dimensional representation by diagonal matrices. As is shown below [see (e)] all diagonal elements are powers of ν. Therefore, $\mathcal{G}_1'$ may be identified with a subgroup of the n-fold direct product $\mathcal{C}_n \otimes \cdots \otimes \mathcal{C}_n$ represented in this n-dimensional representation by the diagonal matrices with elements $D_{kk} = \nu^{i_k}$, $k, i_k = 1, \ldots, n$.

(d) Definition and structure of $\mathcal{G}_2'$: $\mathcal{G}_2'$ is the subgroup of $\mathcal{G}'$ represented in this n-dimensional representation by permutation matrices generated by the matrices B and $P(x)$, $x \in \mathcal{G}$. Since every such permutation matrix defines a permutation of n objects $\mathcal{G}_2'$ may be identified with a subgroup of $\mathcal{S}_n$.

(e) Structure of $\mathcal{G}'$: If a permutation matrix P is multiplied by a power of A the resulting matrix X has the same structure as P, i.e., X and P have zeros and nonvanishing matrix elements on the same places. The only difference is that the elements different from zero are 1's for P and powers of ν for X. The product X_1X_2 of two matrices X_1 and X_2 having the structure of P_1 and P_2, respectively, has the structure of P_1P_2. Therefore, every matrix X representing an element of $\mathcal{G}'$ has the structure of a permutation matrix P_X representing an element of $\mathcal{G}_2'$ ($\subset \mathcal{G}'$). P_X is uniquely determined by X and thus also the diagonal matrix $XP_X^{-1} = D_X$ representing an element of $\mathcal{G}_1'$. Hence every $x' \in \mathcal{G}'$ has a unique decomposition $x' = x_1'x_2'$, $x_1' \in \mathcal{G}_1'$, $x_2' \in \mathcal{G}_2'$. $\mathcal{G}_1'$ is a normal subgroup since PDP^{-1} is diagonal if D is a diagonal and P a permutation matrix.

In his thesis[29] de Vries raised the question how to extend a finite group $\mathcal{G}$ to a finite group $\mathcal{G}'$ so that for all $\alpha \in A$ elements of $\mathfrak{A}(\mathcal{G}')$ can be found which transform according to D^α under the automorphisms corresponding to $\mathcal{G}$.

Corollary: All types $\alpha \in A$ of irreducible representations of a finite group $\mathcal{G}$ can be realized within the group algebra of a finite extension $\mathcal{G}'$ with $|\mathcal{G}'| \leq |\mathcal{G}|^{|\mathcal{G}|}|\mathcal{G}|!$.

Proof: (a) Choose as permutation representation the regular matrix representation (basis $\{\mathbf{x}\}$). Theorem 8 shows that this $|\mathcal{G}|$-dimensional representation can be extended to a unirrep of a group $\mathcal{G}'$ with $|\mathcal{G}'| \leq |\mathcal{G}|^{|\mathcal{G}|}|\mathcal{G}|!$.

(b) The $|\mathcal{G}|$-dimensional unirrep $D^{1'} \in \Delta'$ may be chosen to be of such a form that $D^{1'} \downarrow \mathcal{G}$ is a direct sum of unirreps $D^{\alpha} \in \Delta$ [cf. Sec. 2E, Theorem 4 (b)]. The units related to $D^{1'}$ are then the elements $\mathbf{e}^{1'}_{\alpha jk, \alpha' j' k'} \in \mathfrak{A}^{1'}(\mathcal{G}')$, $\alpha, \alpha' \in A, j, k = 0, \ldots, n_{\alpha} - 1, j', k' = 0, \ldots, n_{\alpha'} - 1$.

(c) For every $\alpha \in A$ the subalgebra $\mathfrak{A}^{1'}(\mathcal{G}')$ contains elements transforming according to D^{α} because of [cf. Eq. (2.25)]

$y \in \mathcal{G}$:

$$D^{1'}_{\alpha jk, \alpha' j' k'}(y) = \delta_{\alpha\alpha'}\delta_{kk'}D^{\alpha}_{jj'}(y),$$
$$\mathbf{y}\mathbf{e}^{1'}_{\alpha jk,000}\mathbf{y}^{-1} = \sum_{j'} D^{\alpha}_{j'j}(y)\mathbf{e}^{1'}_{\alpha j'k,000}. \qquad (3.26)$$

4. COMPACT LIE GROUPS

A. The universal enveloping algebra

If $\mathcal{G}$ is a compact n-dimensional Lie group, the results of Sec. 2 may be slightly modified. The modifications arise from considering the Lie algebra instead of the group and embedding the group algebra in the universal enveloping algebra. We introduce these concepts only to such an extent that our considerations can be related to similar results of other authors.

For a compact *n-dimensional Lie group* it is possible to express the elements $\mathbf{y} \in \mathfrak{U}(\mathcal{G})$ as

$$\mathbf{y}(\eta_1, \cdots, \eta_n) = \exp[i(\eta_1 \mathbf{1}_1 + \cdots + \eta_n \mathbf{1}_n)], \qquad (4.1)$$

where the η's are real parameters and the $\mathbf{1}$'s, the *generators*, are self-adjoint operators in $L^2(\mathcal{G})$. The real n-dimensional vector space spanned by the generators may be identified with the *Lie algebra* $\mathfrak{L}(\mathcal{G})$ if the Lie bracket is defined by the commutator. Since the generators are unbounded operators their domain of definition are only subsets of $L^2(\mathcal{G})$. The functions $D^{\alpha*}_{jk}(x)$ belong to the domains of all generators:

$$\mathbf{1}_i D^{\alpha*}_{jk}(x) = \sum_l C^{\alpha}_{lj}(i) D^{\alpha*}_{lk}(x), \quad i = 1, 2, \ldots, n \qquad (4.2)$$

$$\begin{aligned}\Lambda &= \{C^{\alpha}_{jk}(i): i = 1, \ldots, n; \alpha \in A; j, k = 0, 1, \ldots, n_{\alpha} - 1\} \\ &= \text{a complete set of symmetric } [C^{\alpha}(i) = C^{\alpha+}(i)] \\ &\quad \text{irreducible matrix representations of } \mathfrak{L}(\mathcal{G}). \qquad (4.3)\end{aligned}$$

Δ and Λ are related by

$$D^{\alpha}(\eta_1, \cdots, \eta_n) = \exp\{i[\eta_1 C^{\alpha}(1) + \cdots + \eta_n C^{\alpha}(n)]\}. \qquad (4.4)$$

Because of Eqs. (4.1) and (4.4) a *second definition of an ITS* equivalent to the first one is obtained if Eq. (2.26) is replaced by

$$[\mathbf{1}_i, \mathbf{z}_{\beta r}] = \sum_s C^{\beta}_{sr}(i)\mathbf{z}_{\beta s}, \quad C^{\beta} \in \Lambda. \qquad (4.5)$$

Further modifications are suggested by the following reasoning: The elements $\mathbf{a} \in \mathfrak{A}(\mathcal{G})$ are "linear combinations" of the elements $\mathbf{x} \in \mathfrak{U}(\mathcal{G})$ and these in turn power series in the elements $\mathbf{1}_i \in \mathfrak{L}(\mathcal{G})$. Therefore it must be possible to express also the elements of $\mathfrak{A}(\mathcal{G})$ as power series in the generators. But considering polynomials in the generators and their linear combinations, one embeds $\mathfrak{A}(\mathcal{G})$ in a somewhat more general construction: the *universal enveloping algebra*[30,31] $\mathcal{E}(\mathcal{G})$. As was already done for the Lie algebra $\mathfrak{L}(\mathcal{G})$ we identify $\mathcal{E}(\mathcal{G})$ with a set of operators in $L^2(\mathcal{G})$. Every operator $\mathbf{p} \in \mathcal{E}(\mathcal{G})$ leaves a subspace irreducible with respect to $\mathfrak{A}(\mathcal{G})$ invariant and defines there an operator belonging to $\mathfrak{A}(\mathcal{G})$. For this we write symbolically

$$\mathbf{p} = \sum_{\alpha} \mathbf{p}^{\alpha}, \quad \mathbf{p} \in \mathcal{E}(\mathcal{G}), \mathbf{p}^{\alpha} \in \mathfrak{A}(\mathcal{G}). \qquad (4.6)$$

Like $\mathfrak{A}(\mathcal{G})$ the algebra $\mathcal{E}(\mathcal{G})$ is an associative ring and a linear space. It also admits a group of automorphisms isomorphic to $\mathcal{G}/\mathfrak{z}[\mathcal{G}]$ which is known as the *adjoint group*.[31] It is therefore possible to extend the definition of ITS's substituting the condition $\mathbf{z}_{\beta r} \in \mathfrak{A}(\mathcal{G})$ by $\mathbf{z}_{\beta r} \in \mathcal{E}(\mathcal{G})$. But every such ITS in $\mathcal{E}(\mathcal{G})$ defines by Eq. (4.6) elements of $\mathfrak{A}(\mathcal{G})$ which are ITS's of the same type because of Eq. (2.15). From there it follows together with Theorem 3 (Sec. 2D) that also polynomials in the generators, being components of ITS's ("multipole operators"[20]), can be used to define coupling or CG-coefficients. The best known example are the generators themselves which are usually chosen to be components of ITS's.[32]

B. Special results and explicit constructions

Theorem 9: In the group algebra $\mathfrak{A}(SU(n))$ ITS's of type β exist if and only if D^{β} is contained in a Kronecker product $D \times \cdots \times D^*$ of n_1 D's and n_2 D^*'s with $n_1 \equiv n_2$ modulo n, where D is the n-dimensional unirrep used to define $SU(n)$.

Proof: (a) Only if: D^{β} must be a unirrep of $SU(n)/\mathfrak{z}[SU(n)]$ (Theorem 1). $\mathfrak{z}[SU(n)] = \mathfrak{z}_n$ is a cyclic group of order n, represented in D by matrices $\{\nu^i E: i = 1, \ldots, n\}$, ν = primitive nth root of 1, $E = n \times n$ 1-matrix. The necessary and sufficient condition for a Kronecker product of n_1 D's and n_2 D^*'s to be a representation of $SU(n)/\mathfrak{z}_n$ is therefore $n_1 \equiv n_2$ modulo n.

(b) If: The above mentioned Kronecker products contain all unirreps of $SU(n)/\mathfrak{z}_n$ since these are also unirreps of $SU(n)$ and every such one is contained in a Kronecker product $D \times \cdots \times D^*$. Since D is faithful, there must be ITS's for every unirrep of $SU(n)/\mathfrak{z}_n$ (Theorem 2).

Note that in Theorem 9 $\mathfrak{A}(SU(n))$ may be replaced by $\mathcal{E}(SU(n))$ because of Eq. (4.6).

Theorem 9 says in particular that in $\mathfrak{A}(SU(2))$ ITS's of type j = integer (duality = 0 [33]) exist, and only these. This is also seen if the tensor basis (2.29) is constructed explicitly. Since $SU(2)$ is multiplicity-free ($m_{j_1 j_2 j_3} \leq 1$), the elements of a convenient tensor basis are determined up to phase factors already by their transformation properties and normalization. If unirreps are chosen the elements $D^j_{mm'}(x)$ of which are expressed by Wigner's formula[34] as polynomials in the matrix elements $D^{1/2}_{mm'}(x)$, then Condition 3 is satisfied because the matrices U^j ($\bar{j} = j$) and the CG-coefficients $(jmjm'|JM)$ are then known[35]:

$$\begin{aligned}\mathbf{z}^j_{JM} &= \sum_{mm'} [jmjm' \mid JM]\mathbf{e}^j_{mm'} \\ &= \sum_m i^{2m}(j\ m + M\ j - m\ |JM)\mathbf{e}^j_{m+M,m}. \qquad (4.7)\end{aligned}$$

Since the coupling coefficients are the matrix elements of the $\mathbf{z}$'s in a symmetry adapted basis, Eq. (4.7) may be interpreted as a definition of a tensor basis by means of irreducible matrix representations. This, however, was already done a long time ago by Racah[4] who was also interested in the inverse transformation of (4.7) since he needed the $\mathbf{e}$'s for the construction of higher-dimensional Lie algebras.

To introduce parameters, it suffices to parametrize $D^{1/2}(x)$, possible in several ways. The Eulerian angles[10] $\alpha\beta\gamma$ are best known; equally useful are the class-parameter ϕ ("angle of rotation") and the in-class parameters ϑ, φ ("axis of rotation").[27,36] The matrix elements of $D^{1/2}(x)$ are then linear combinations of exponential functions of the parameters and fulfill therefore Condition 2. Condition 1 is also satisfied because of

$$M[f] = \frac{1}{16\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} \sin\beta\, d\beta \int_0^{4\pi} d\gamma f(x(\alpha\beta\gamma))$$
$$= \frac{1}{16\pi^2}\int_0^{4\pi} (1-\cos\phi) d\phi \int_0^{\pi} \sin\vartheta\, d\vartheta \int_0^{2\pi} d\varphi f(x(\phi\vartheta\varphi)). \quad (4.8)$$

Therefore, for instance,

$$\mathbf{e}^j_{mm'} = \frac{2j+1}{16\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} \sin\beta\, d\beta \int_0^{4\pi} d\gamma D^{j*}_{mm'}(\alpha\beta\gamma)\mathbf{x}(\alpha\beta\gamma). \quad (4.9)$$

There exist, however, other expressions for the units exploiting the fact that $SU(2)$ is a Lie group. If we use the symbols J_i for the generators, one of these reads

$M \geqslant 0,$

$$\mathbf{e}^j_{m\pm M,m} = \left(\frac{(j\pm m)!(j\mp m - M)!}{(j\mp m)!(j\pm m+M)!}\right)^{1/2} J^M_{\pm} \frac{P^{j\pm}_{Mm}(J_0)}{P^{j\pm}_{Mm}(m)}\mathbf{e}^j, \quad (4.10)$$

$$J_{\pm} = J_1 \pm iJ_2, \qquad J_0 = J_3, \quad (4.11)$$

$$P^{j\pm}_{Mm}(t) = (t-m)^{-1}\prod_{n=-j}^{j-M}(t\mp n), \quad (4.12)$$

$$\mathbf{e}^j = \sum_m \mathbf{e}^j_{mm} = \frac{2j+1}{8\pi^2}\int_0^{\pi}\sin\vartheta\, d\vartheta \times \int_0^{2\pi} d\varphi \int_0^{4\pi} d\phi\, \sin\tfrac{1}{2}\phi\, \sin(j+\tfrac{1}{2})\phi\mathbf{x}(\phi\vartheta\varphi). \quad (4.13)$$

To obtain Eq. (4.10), we used the usual matrix representations $M^j(J_i)$ [37] and the fact that

$$\frac{P^{j\pm}_{Mm}(J_0)}{P^{j\pm}_{Mm}(m)}\mathbf{e}^j = \mathbf{e}^j_{mm} + \sum_{m'=\pm(j-M+1)}^{\pm j} \gamma^{\pm}_{jMmm'}\mathbf{e}^j_{m'm'}. \quad (4.14)$$

The coefficients $\gamma^{\pm}_{jMmm'}$ are chosen in such a way that the contributions of the powers J_0^n cancel out for $n > 2j - M$ if the expressions

$$\mathbf{e}^j_{mm} = [P^{j\pm}_{0m}(J_0)/P^{j\pm}_{0m}(m)]\mathbf{e}^j \quad (4.15)$$

are inserted into Eq. (4.14). From Eqs. (4.7) and (4.10) follows

$M \geqslant 0,$

$$\mathbf{z}^j_{J\pm M} = J^M_{\pm} Q^{j\pm}_{JM}(J_0)\mathbf{e}^j, \quad (4.16)$$

$$Q^{j\pm}_{JM}(t) = \sum_m i^{2m}(j\, m \pm M\, j\, -m \mid JM) \times \left(\frac{(j\pm m)!(j\mp m-M)!}{(j\mp m)!(j\pm m+M)!}\right)^{1/2} \frac{P^{j\pm}_{Mm}(t)}{P^{j\pm}_{Mm}(m)}. \quad (4.17)$$

$Q^{j\pm}_{JM}$ is a polynomial of degree J. For

$$\mathbf{z}^j_{JJ} = J^J_{+}(-1)^{j-J}\left(\frac{(2J+1)!(2j-J)!}{(2j+J+1)!(J!)^2}\right)^{1/2}\mathbf{e}^j, \quad (4.18)$$

$$[J_{\pm}, \mathbf{z}^j_{JM}] = [(J\mp M)(J\pm M+1)]^{1/2}\mathbf{z}^j_{JM\pm 1}, \quad (4.19)$$

[cf. Eq. (4.5)], and the commutation relations of the J_i's imply

$$[J_i, \text{polynomial in } J_k \text{ of degree } n] = \text{polynomial in } J_k \text{ of degree } n. \quad (4.20)$$

The polynomials $J^M_{\pm}Q^{j\pm}_{JM}(J_0)$ appearing in Eq. (4.16) coincide (up to phase factors) with those obtained by Corio.[5] He used matrix representations $J_i \to M^j(J_i)$ and orthonormalized the $(2j+1)^2$ linearly independent matrices $\{M^j(J^r_{\pm}J^s_0): r = 0, \ldots, 2j; s = 0, \ldots, 2j - r\}$.

As a further possibility we finally note that the units may be introduced in Eq. (4.7) also in the form

$$\mathbf{e}^j_{mm'} = \frac{(2j+1)!}{(2j)!}\left(\frac{(j+m)!(j+m')!}{(j-m)!(j-m')!}\right)^{1/2}\sum_r \frac{(-1)^r}{r!(2j+1+r)!} \times J^{r+j-m}_{+}J^{r+j-m'}_{-} \quad (4.21)$$

given by Shapiro[38] and clearly reflecting the embedding $\mathfrak{A}(SU(2)) \subset \mathcal{E}(SU(2))$.

In principle Conditions 1-3 are also satisfied for $SU(3)$. However, to obtain similar expressions as for $SU(2)$, first the different definitions scattered in the literature have to be fitted together. We do not deal with this question here but limit ourselves to the consequences of Theorem 9: In $\mathfrak{A}(SU(3))$ exist ITS's of type (p, q) if and only if $p \equiv q$ modulo 3 (triality = 0).[33]

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On analytic nonlocal potentials. II. Analyticity of the S matrix, for fixed l, its representations, and a dispersion relation for fixed t

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For a class of analytic short-ranged nonlocal potentials, we study the analyticity of the S matrix in the k plane, for fixed l, using Fredholm method for the Lippman–Schwinger equation for the partial scattering solution, and contour deformation in the analytic continuation of the S matrix, thereby extending a representation of the S matrix in terms of Fredholm determinants. We also obtain a representation of the S matrix in terms of Jost functions, for $l = 0$. For a subclass of this class of potentials, we obtain a dispersion relation for the full scattering amplitude, for fixed t in the range $0 \geq t > -4\gamma^2$, where γ is some parameter of the potential, using summation of the partial amplitude expansion of the full amplitude. Analyticity properties of the partial scattering solution, for all l, and of the regular and Jost solutions, for $l = 0$, are also discussed.

1. INTRODUCTION

In a previous article[1] we proposed a class of analytic short-ranged nonlocal potentials $V(\mathbf{x},\mathbf{x}')$ defined by the following conditions (A):

(A1) $V(\mathbf{x},\mathbf{x}')$ is real, $V(\mathbf{x},\mathbf{x}') = V(\mathbf{x}',\mathbf{x})$.

(A2) $V(\mathbf{x},\mathbf{x}')$ is rotationally invariant:

$$V(\mathbf{x},\mathbf{x}') = V(x,x',\cos\nu),$$
$$x = |\mathbf{x}| > 0, \quad x' = |\mathbf{x}'| > 0, \quad 1 \geqslant \cos\nu \geqslant -1,$$

where ν is the angle between $\mathbf{x}$ and $\mathbf{x}'$.

(A3) $$V(x,x',\cos\nu) = (e^{-\gamma x}/x^{\alpha})\, \tilde{V}(x,x',\cos\nu)(e^{-\gamma x'}/x'^{\alpha}),$$
$$\gamma > 0, \tfrac{3}{2} > \alpha \geqslant 0,$$

where $\tilde{V}(x,x',\cos\nu)$ is holomorphic in x and x', in $\operatorname{Re} x > 0$, $\operatorname{Re} x' > 0$, for $1 \geqslant \cos\nu \geqslant -1$, and continuous in all three variables in $\operatorname{Re} x > 0$, $\operatorname{Re} x' > 0$, $1 \geqslant \cos\nu \geqslant -1$, and

$$|V(x,x'\cos\nu)| \leqslant \text{const}, \quad \operatorname{Re} x > 0,\ \operatorname{Re} x' > 0,\ 1 \geqslant \cos\nu \geqslant 1.$$

We obtained a forward dispersion relation for potentials satisfying these conditions.

Here we first study the analyticity of the S matrix in the k plane, for fixed l, arriving at the holomorphy of the S matrix in the whole k plane cut from $i\gamma$ to $i\infty$ and from $-i\gamma$ to $-i\infty$, which we shall call Π, perhaps with the exception of poles at the nonreal zeroes of $\Delta_l(k)$, where $\Delta_l(k)$ is the Fredholm determinant of a certain integral operator. We extend the domain of validity of a representation of the S matrix in terms of Fredholm determinants introduced by Bertero *et al.*[2] to Π. The scattering solution $\psi_l(k;x)$, for fixed l, is shown to be holomorphic in k and x, for k in Π and $\operatorname{Re} x > 0$, perhaps with the exception of poles in Π at the zeroes of $\Delta_l(k)$.

We then show that, for $\alpha = \frac{1}{2}$, and $\tilde{V}(x,x',\cos\nu)$ a double Laplace transform of a suitable spectral function, the partial amplitude expansion of the full amplitude, valid for $k > 0$ and $\cos\theta$ in an ellipse with foci $-1, +1$, where θ is the scattering angle, can be summed for k in Π, and t in the range $0 \geqslant t > -4\gamma^2$, where t is the square of the momentum transfer, and that the resulting full amplitude is holomorphic in Π, perhaps with the exception of poles at the nonreal zeroes of $\Delta_l(k)$, where l is arbitrary, for $0 \geqslant t > 4\gamma^2$ if we assume that $\Delta_l(k=0) \neq 0$ for all l. We obtain a dispersion relation for the full amplitude, in the energy variable, for $0 \geqslant t > -4\gamma^2$.

Finally, for $l = 0$, we study the regular solution $\varphi(k;x)$, the Jost solutions $f^{\pm}(k;x)$, and the Jost functions $\mathcal{L}^{\pm}(k)$, for k in Π and $\operatorname{Re} x > 0$, and obtain a representation of the S matrix in terms of the Jost functions, for potentials satisfying Conditions (A). The Jost functions are meromorphic in Π, and the regular solutions and the Jost solutions are holomorphic in k and x, for k in Π and $\operatorname{Re} x > 0$, perhaps with the exception of poles in Π.

For $l \neq 0$, we may similarly define the regular solution, the Jost solutions, and the Jost functions, and obtain a representation of the S matrix in terms of the Jost functions, for potentials satisfying Conditions (A), if the lth partial potential $V_l(x,x')$ vanishes sufficiently rapidly as x and/or x' approach zero.

We remark that the results obtained in Ref. 1 and this article for potentials satisfying Conditions (A1)–(A3) can be immediately generalized in the case of potentials satisfying Conditions (A1), (A2), and the following Conditions (A3′):

$$V(x,x'\cos\nu) = \frac{e^{-\gamma x}(x+a)^m}{x^{\alpha}}\ \tilde{V}(x,x',\cos\nu)\, \frac{e^{-\gamma x'}(x'+a)^m}{x'^{\alpha}},$$
$$\gamma > 0, \quad a > 0, \quad m \geqslant 0, \quad \tfrac{3}{2} > \alpha \geqslant 0, \quad \text{(A3}')$$

where $\tilde{V}(x,x',\cos\nu)$ satisfies the same conditions as in (A3).

We also remark that an unsubtracted dispersion relation holds for the full scattering amplitude, for $0 \geqslant t > -4\gamma^2$, for potentials satisfying Conditions (A1), (A2), and (A3′), with m integral, $\alpha = \frac{1}{2}$, and $\tilde{V}(x,x',\cos\nu)$ belonging to the double Laplace Transform class mentioned above.

We note that a local Yukawian potential

$$V(x) = \int_{\mu}^{\infty} d\beta\, e^{-\beta x}\rho(\beta), \quad \mu > 0,\ x > 0,$$

with a continuous and absolutely integrable spectral function can be expressed as

$$V(x) = e^{-\mu x}\, \tilde{V}(x),$$

where $\tilde{V}(x)$ is holomorphic in $\operatorname{Re} x > 0$ and satisfies

$$|V(x)| \leqslant \text{const}, \quad \operatorname{Re} x > 0.$$

2. THE POTENTIAL, THE KERNEL, THE SCATTERING SOLUTION, AND THE PARTIAL SCATTERING AMPLITUDE

For potentials satisfying Conditions (A) the partial potentials $V_l(x,x')$, defined by

$$V_l(x,x') = (2\pi x x') \int_{-1}^{+1} d\cos\nu\, V(\mathbf{x},\mathbf{x}') P_l(\cos\nu)$$

satisfy the following conditions:

(1) $V_l(x,x')$ is real, $V_l(x,x') = V_l(x',x)$, $x>0, x'>0$

(2) $V_l(x,x') = (e^{-\gamma x}/x^\delta)\,\tilde{V}_l(x,x')(e^{-\gamma x'}/x'^\delta)$, $\frac{1}{2} > \delta \geq -1$

where

(i) $\tilde{V}_l(x,x')$ is holomorphic in $\mathrm{Re}\,x>0, \mathrm{Re}\,x'>0$.

(ii) $|\tilde{V}_l(x,x')| \leq \mathrm{const}/\sqrt{2l+1}$, $\mathrm{Re}\,x>0, \mathrm{Re}\,x'>0$.[3]

In the following, $V_l(x,x')$ is defined for $\mathrm{Re}\,x>0$, $\mathrm{Re}\,x'>0$, in terms of $\tilde{V}_l(x,x')$, by the above relation (2).

We introduce the function $K_l(k;x,x')$ defined by

$$K_l(k;x,x') = \left(\frac{k^{l+1}(kx)\,h_l^{(1)}(kx)}{ik}\right)\int_0^x \left(dx''\,\frac{(kx'')j_l(kx'')}{k^{l+1}}\right) V_l(x'',x') + \left(\frac{(kx)j_l(kx)}{k^l\cdot ik}\right)\int_x^\infty dx''[k^l(kx'')h_l^{(1)}(kx'')]\,V_l(x'',x'), \tag{2.1}$$

in $\mathrm{Im}k > -\gamma$, $\mathrm{Re}\,x>0$, $\mathrm{Re}\,x'>0$, and

$$K_l(k;x,x') = 0$$

in $\mathrm{Im}k>-\gamma$, $x=0$, $\mathrm{Re}\,x'>0$, i.e.,

$$K_l(k;x,x') = \int_0^\infty dx''\,G_l(k;x,x'')\,V_l(x'',x'),$$

$$G_l(k;x,x'') = [(kx_{\max})\,h_l^{(1)}(kx_{\max})(kx_{\min})j_l(kx_{\min})]/ik, \qquad k\neq 0,$$

$$G_l(k;x,x'') = [-1/(2l+1)](x_{\min}^{l+1}/x_{\max}^l).$$

The functions $zj_l(z)$, $zh_l^{(1)}(z)$, and their derivatives satisfy the following inequalities, for all z in the first and the third and for all $z\neq 0$ in the second and the last:

$$|zj_l(z)| \leq De^{|\mathrm{Im}z|}\left(\frac{|z|}{1+|z|}\right)^{l+1}, \tag{2.2a}$$

$$|zh_l^{(1)}(z)| \leq De^{-\mathrm{Im}z}\left(\frac{|z|}{1+|z|}\right)^{-l}, \tag{2.2b}$$

$$\left|\frac{d}{dz}(zj_l(z))\right| \leq De^{|\mathrm{Im}z|}\left(\frac{|z|}{1+|z|}\right)^{l}, \tag{2.2c}$$

$$\left|\frac{d}{dz}(zh_l^{(1)}(z))\right| \leq De^{-\mathrm{Im}z}\left(\frac{|z|}{1+|z|}\right)^{-(l+1)}, \tag{2.2d}$$

where D is a constant for fixed l.[5]

The function $K_l(k;x,x')$ is holomorphic in k, x, and x' in $\mathrm{Im}k>-\gamma$, $\mathrm{Re}\,x>0$, and $\mathrm{Re}\,x'>0$, and we find the following inequalities, for $\mathrm{Im}k \geq -(\gamma-\epsilon)$, $\gamma\geq\epsilon>0$, $x\geq 0$, $\mathrm{Re}\,x'>0$:

$$|K_l(k;x,x')| \leq N(\epsilon)\,xe^{(\gamma-\epsilon)x}\,|e^{-\gamma x'}/x'^\delta|, \tag{2.3a}$$

$$|K_l(k;x,x')| \leq N(\epsilon)\,|k|^{-1}e^{(\gamma-\epsilon)x}\,|e^{-\gamma x'}/x'^\delta|, \tag{2.3b}$$

where $N(\epsilon)$ depends on ϵ only for fixed l.

From Fredholm theory[7] and the inequality (2.3a) we find that, for $k>0$, the equation

$$\psi_l(k;x) = (kx)j_l(kx) + \int_0^\infty dx'\,K_l(k;x,x')\,\psi_l(k;x'), \quad x>0. \tag{2.4}$$

has a bounded continuous solution, the scattering solution, given explicitly by the formula

$$\psi_l(k;x) = (kx)j_l(kx) + \int_0^\infty dx'\,\frac{\Delta_l(k;x,x')}{\Delta_l(k)}\,(kx')j_l(kx'), \tag{2.5}$$

when $\Delta_l(k)\neq 0$, where $\Delta_l(k)$ and $\Delta_l(k;x,x')$ are the Fredholm determinant and the Fredholm minor of the integral operator $K_l(k)$ on the space of bounded measurable functions, with kernel $K_l(k;x,x')$, $k>0$, $x>0$, $x'>0$, and are given by

$$\Delta_l(k) = \sum_{n=0}^\infty [(-1)^n/n!]\,\Delta_{l,n}(k), \qquad \Delta_{l,0}(k) = 1, \tag{2.6}$$

$$\Delta_{l,n}(k) = \int_0^\infty\cdots\int_0^\infty dx_1\cdots dx_n \begin{vmatrix} K_l(k;x_1,x_1) & \cdots & K_l(k;x_1,x_n) \\ \vdots & & \vdots \\ K_l(k;x_n,x_1) & \cdots & K_l(k;x_n,x_n)\end{vmatrix}, \quad n\geq 1, \tag{2.7}$$

$$\Delta_l(k;x,x') = \sum_{n=0}^\infty [(-1)^n/n!]\,\Delta_{l,n}(k;x,x'), \tag{2.8}$$

$$\Delta_{l,0}(k;x,x') = K_l(k;x,x'),$$

$$\Delta_{l,n}(k;x,x') = \int_0^\infty\cdots\int_0^\infty dx_1\cdots dx_n \begin{vmatrix} K_l(k;x,x') & K_l(k;x,x_1)\cdots K_l(k;x,x_n) \\ K_l(k;x_1,x') & K_l(k;x_1,x_1)\cdots K_l(k;x_1,x_n) \\ \vdots & \vdots \\ K_l(k;x_n,x') & K_l(k;x_n,x_1)\cdots K_l(k;x_n,x_n)\end{vmatrix}, \quad n\geq 1. \tag{2.9}$$

This solution $\psi_l(k;x)$ is unique in the space of bounded measurable functions and is seen to belong to $C^\infty(0,\infty)$ from the following relationship:

$$\psi_l(k;x) = (kx)j_l(kx) + \int_0^\infty dx''\,G_l(k;x,x'') \times \int_0^\infty dx'\,V_l(x'',x')\,\psi_l(k;x'), \tag{2.10}$$

where $\int_0^\infty dx'\,V_l(x'',x')\,\psi_l(k;x')$ is holomorphic in x'', for $\mathrm{Re}\,x''>0$.

From (2.10) we also find that $\psi_l(k;x)$ satisfies the following partial wave integrodifferential equation:

$$\left(\frac{d^2}{dx^2} + k^2 - \frac{l(l+1)}{x^2}\right)y(z) = \int_0^\infty dx'\,V_l(x,x')\,y(x'), \quad x>0. \tag{2.11}$$

Conversely, we may show that any solution of (2.11) with absolutely continuous first derivative[8] and vanishing at the origin necessarily satisfies (2.10)[9] and consequently is given by (2.5) if it is bounded and if $\Delta_l(k)\neq 0$.

For $k>0$, $\Delta_l(k)\neq 0$, the solution (2.5) has the following behavior as $x\to 0$:

$$\psi_l(k;x) \underset{x\to 0}{=} O(x), \qquad l=0,$$

$$\psi_l(k;x) \underset{x\to 0}{=} \begin{cases} O(x^2\ln x), & l=1,\ \delta=0, \\ O(x^{2-\delta}), & l=1,\ \delta\neq 0, \end{cases} \tag{2.12}$$

$$\psi_l(k;x) \underset{x\to 0}{=} O(x^{2-\delta}), \qquad l\geq 2,$$

and the following asymptotic behavior:

$$\psi_l(k;x) \underset{x\to\infty}{\simeq} \sin[kx-(l\pi/2)] + e^{i[kx-(l\pi/2)]}\,T_l(k),$$

where

$$T_l(k) = (-1/k)\int_0^\infty dx(kx)j_l(kx)\int_0^\infty dx'\,V_l(x,x')\psi_l(k;x') \quad (2.13)$$

and is the partial scattering amplitude.

Using (2.2a) to (2.2d) we have

$$\psi_l'(k;x) \underset{x\to 0}{=} O(1)$$

hence we have

$$\psi_l(k;x)^*\psi_l'(k;x) - \psi_l(k;x)\psi_l'(k;x)^* \underset{x\to\infty}{\longrightarrow} 0.$$

We may then show that

$$T_l(k) = e^{i\delta_l(k)}\sin\delta_l(k), \quad (2.14)$$

where $\delta_l(k)$ is real.[10] $\delta_l(k)$ is the phase shift. The asymptotic form of $\psi_l(k;x)$ then becomes

$$\psi_l(k;x) \underset{x\to\infty}{\simeq} e^{i\delta_l(k)}\sin[kx-(l\pi/2)+\delta_l(k)]. \quad (2.15)$$

If we define the S matrix $S_l(k)$ as

$$S_l(k) = 1 + 2iT_l(k), \quad (2.16)$$

then we have

$$S_l(k) = e^{2i\delta_l(k)}. \quad (2.17)$$

Using (2.5), we have the following explicit form for $T_l(k)$:

$$T_l(k) = T_l^{(1)}(k) + [T_l^{(2)}(k)/\Delta_l(k)], \quad (2.18)$$

$$T_l^{(1)}(k) = (-1/k)\int_0^\infty dx(kx)j_l(kx) \times \int_0^\infty dx'\,V_l(x,x')(kx')j_l(kx'), \quad (2.19)$$

$$T_l^{(2)}(k) = (-1/k)\int_0^\infty dx(kx)j_l(kx)\int_0^\infty dx'\,V_l(x,x') \times \int_0^\infty dx''\Delta_l(k;x',x'')(kx'')j_l(kx''). \quad (2.20)$$

From a result of Ref. 2 for $l=0$ and its generalization to arbitrary l, we have the following representation for the S matrix:

$$S_l(k) = F_l(k)/F_l(-k),$$

where $F_l(-k)$ is the Fredholm determinant of $L_l(k)$, $L_l(k)$ being a Hilbert–Schmidt operator in a certain Hilbert space with kernel

$$L_l(k;x,x') = \int_0^\infty dx''\,V_l(x,x'')G_l(k;x'',x').$$

We have[2]

$$F_l(-k) = e^{-\sigma_{l,1}(k)}\lambda_l(k),$$

$$\sigma_{l,1}(k) = \int_0^\infty dx\,L_l(k;x,x),$$

$$\lambda_l(k) = \sum_{n=0}^{\infty}\lambda_{l,n}(k),$$

$$\lambda_{l,0}(k) = 1, \quad \lambda_{l,1}(k) = 0,$$

$$\lambda_{l,n}(k) = \frac{(-1)^n}{n!}\begin{vmatrix} 0 & n-1 & 0 & \cdots & 0 & 0 \\ \sigma_{l,2}(k) & 0 & n-2 & & 0 & 0 \\ \sigma_{l,3}(k) & \sigma_{l,2}(k) & 0 & & 0 & 0 \\ \cdot & & & & & \cdot \\ \cdot & & & & & \cdot \\ \cdot & & & & & \cdot \\ \sigma_{l,n}(k) & \sigma_{l,n-1}(k) & \sigma_{l,n-2}(k) & \cdots & \sigma_{l,2}(k) & 0 \end{vmatrix}, \quad n \geq 2$$

$$\sigma_{l,n}(k) = \int L_l(k)^n(x,x)\,dx, \quad n\geq 2.$$

Using the relationship

$$\int_0^\infty K_l(k)^n(x,x)\,dx = \sigma_{l,n}, \quad n\geq 1,$$

we find that[12]

$$\Delta_l(k) = F_l(-k), \quad \Delta_l(-k) = F_l(k).$$

Hence we have

$$S_l(k) = \Delta_l(-k)/\Delta_l(k). \quad (2.21)$$

We shall find in the following section that the zeroes of $\Delta_l(k)$, for $k>0$, are finite in number, and that $T_l(k)$ can be extended to a function holomorphic in a neighborhood of the positive real axis of k.

In Secs. 3, 4, 5, we shall consider analytic extensions of $\Delta_l(k)$, $T_l(k)$, and $S_l(k)$, in the k plane, for fixed l. We shall consider also an analytic extension of $\psi_l(k;x)$ in the k and x planes, for fixed l.

3. ZEROES OF $\Delta_l(k)$ AND BOUND STATES

Using the inequality (2.3a), we may extend the definitions (2.7) and (2.6) of $\Delta_{l,n}(k)$ and $\Delta_l(k)$ to the region $\mathrm{Im}k>-\gamma$. We may show that so defined, $\Delta_l(k)$ is holomorphic in $\mathrm{Im}k>-\gamma$. Also, from (2.36), we have[15]

$$|\Delta_{l,n}(k)| \leq (1/|k|^n)\,N(\epsilon)^n M(\epsilon)^n n^{n/2}, \quad n\geq 1$$

$$M(\epsilon) = \int_0^\infty dx\,x^{(1-\delta)}e^{-\epsilon x},$$

$$\mathrm{Im}k \geq -(\gamma-\epsilon), \ \gamma\geq\epsilon>0, \ k\neq 0.$$

Hence we have

$$\Delta_l(k) \underset{|k|\to\infty}{\to} 1, \quad \mathrm{Im}k\geq-(\gamma-\epsilon), \ \gamma\geq\epsilon>0 \quad (3.1)$$

for fixed l. Hence the number of zeroes of $\Delta_l(k)$, for fixed l, in $\mathrm{Im}k\geq-(\gamma-\epsilon)$, $\gamma\geq\epsilon>0$, is finite.

We have

$$K_l(-k^*;x,x') = K_l(k;x,x')^*, \quad \mathrm{Im}k>-\gamma, \ x\geq 0, \ x'>0.$$

Hence we obtain:

$$\Delta_l(-k^*) = \Delta_l(k)^*, \quad \mathrm{Im}k>-\gamma. \quad (3.2)$$

Using the inequality (2.3a), we may also extend the definitions (2.9) and (2.8) of $\Delta_{l,n}(k;x,x')$ and $\Delta_l(k;x,x')$ to the region $\mathrm{Im}k>-\gamma$, for $x\geq 0$, $\mathrm{Re}x'>0$. We find that $\Delta_l(k;x,x')$, so defined, is holomorphic in k and x' in $\mathrm{Im}k>-\gamma$, $\mathrm{Re}x'>0$, for $x\geq 0$, and continuous in x and x' in $x\geq 0$, $\mathrm{Re}x'>0$, for $\mathrm{Im}k>-\gamma$. Furthermore, we have

$$| \Delta_{l,n}(k;x,x') | \leq x\, e^{(\gamma-\epsilon)x} | e^{-\gamma x'}/x'^{\delta} | N(\epsilon)^{n+1} M(\epsilon)^n (n+1)^{(n+1)/2},$$

$$| \Delta_l(k;x,x') | \leq \text{const} \cdot x e^{(\gamma-\epsilon)x} | e^{-\gamma x'}/x'^{\delta} |, \tag{3.3}$$

$$\text{Im}k \geq -(\gamma-\epsilon), \quad \gamma \geq \epsilon > 0, \quad x \geq 0, \quad \text{Re}x' > 0.$$

The partial scattering amplitude $T_l(k)$ may now be defined for $|\text{Im}k| < \gamma$, $\Delta_l(k) \neq 0$, by

$$T_l(k) = T_l^{(1)}(k) + [T_l^{(2)}(k)/\Delta_l(k)], \tag{3.4}$$

where $T_l^{(1)}(k)$ and $T_l^{(2)}(k)$ are given by (2.19) and (2.20), now extended to $|\text{Im}k| < \gamma$. We find that $T_l^{(1)}(k)$ and $T_l^{(2)}(k)$ are holomorphic in $|\text{Im}k| < \gamma$. Hence, from the holomorphy of $\Delta_l(k)$ in $\text{Im}k > -\gamma$ and the boundedness of $T_l(k)$ for $k > 0$, $\Delta_l(k) \neq 0$, we find that $T_l(k)$ is holomorphic in a neighborhood of the positive real axis of k.

We now relate the zeroes of $\Delta_l(k)$ in $\text{Im}k \geq 0$ to solutions $\chi_l(k;x)$ of (2.11) with absolutely continuous first derivative satisfying

$$\chi_l(k;x) \underset{x\to 0}{=} O(x), \qquad \int_0^\infty dx\, |\chi_l(k;x)|^2 < \infty. \tag{3.5}$$

We shall find that any solution $\chi_l(k;x)$, $k \neq 0$, satisfying the above condition also satifies:

$$\chi_l'(k;x) \underset{x\to 0}{=} O(1), \qquad \chi_l(k;x) \underset{x\to\infty}{=} O(e^{-\gamma x}/x^{\delta}), \qquad \chi_l'(k;x) \underset{x\to\infty}{=} O(e^{-\gamma x}/x^{\delta}). \tag{3.6}$$

We suppose that (3.6) is valid. Since we have

$$\frac{d}{dx}[\chi_l(k;x)^* \chi_l'(k;x) - \chi_l(k;x)\chi_l'(k;x)^*] - \chi_l(k;x)^* \times \int_0^\infty dx'\, V_l(x,x')\chi_l(k;x') + \chi_l(k;x) \times \int_0^\infty dx'\, V_l(x,x')\chi_l(k;x')^* = -2i\,\text{Im}k^2\,|\chi_l(k;x)|,$$

we obtain

$$\int_0^\infty dx \frac{d}{dx}[\chi_l(k;x)^* \chi_l'(k;x) - \chi_l(k;x)\chi_l(k;x')^*] = -2i\,\text{Im}k^2 \int_0^\infty dx\,|\chi_l(k;x)|^2.$$

Hence from (3.5) and (3.6) we obtain

$$\text{Im}k^2 \int_0^\infty dx\,|\chi_l(k;x)|^2 = 0,$$

$$\therefore \text{Im}k^2 = 2\,\text{Im}k \cdot \text{Re}k = 0, \quad \text{i.e. } k^2 \text{ is real,}$$

$$\therefore \text{Im}k = 0 \quad \text{or} \quad \text{Re}k = 0. \tag{3.7}$$

We now suppose that $\Delta_l(k) = 0$, $\text{Im}k = 0$. Then the equation

$$\chi_l(k;x) = \int_0^\infty dx'\, K_l(k;x,x')\chi_l(k;x') \tag{3.8}$$

has a finite number of bounded measurable solutions.[7] For each such bounded solution we may write (3.8) as

$$\chi_l(k;x) = \int_0^\infty dx''\, G_l(k;x,x'') \int_0^\infty dx'\, V_l(x'',x')\chi_l(k;x'). \tag{3.9}$$

We may demonstrate using (3.9) that $\chi_l(k;x)$ belongs to $C^\infty(0,\infty)$ and that it satisfies (2.11). We may also demonstrate

$$\chi_l(k;x) \underset{x\to 0}{=} O(x), \qquad \chi_l'(k;x) \underset{x\to 0}{=} O(1)$$

using (2.2a) to (2.2d).

We may write (3.9), for $k \neq 0$, in the following form:

$$\chi_l(k;x) = \frac{(kx)h_l^{(1)}(kx)}{ik} I_l^{(1)}(k) + I_l^{(2)}(k),$$

with

$$I_l^{(1)}(k) = \int_0^\infty dx''(kx'')j_l(kx'') \int_0^\infty dx'\, V_l(x'',x')\chi_l(k;x').$$

We have

$$\chi_l(k;x)^* \chi_l'(k;x) - \chi_l(k;x)\chi_l'(k;x)^* \underset{x\to\infty}{\longrightarrow} 0.$$

Hence we may show

$$I_l^{(1)}(k) = 0,$$

$$I_l^{(2)}(k;x) \underset{x\to\infty}{=} O(e^{-\gamma x}/x^{\delta}),$$

$$I_l^{(2)\prime}(k;x) \underset{x\to\infty}{=} O(e^{-\gamma x}/x^{\delta}),$$

using (2.2a) to (2.2d). Hence $\int_0^\infty dx\,|\chi_l(k;x)|^2 < \infty$ and (3.6) holds.

For $k = 0$, we find immediately that $\chi_l(k=0;x)$ belongs to $C^\infty(0,\infty)$ and satisfies (3.5).

For $\Delta_l(k) = 0$, $\text{Im}k > 0$, again (3.8) has a finite number of bounded measurable solutions[7] which may be shown to belong to $C^\infty(0,\infty)$ and to satisfy (2.11). And again we may demonstrate that such bounded solutions satisfy (3.5) and (3.6).

We thus find that the zeroes of $\Delta_l(k)$ in $\text{Im}k \geq 0$ can only lie on the real axis or the upper imaginary axis, and placed symmetrically about the origin, from (3.2).

Suppose now that $\chi_l(k;x)$ has absolutely continuous first derivative and satisfies (2.11) and the condition (3.5), with $\text{Im}k \geq 0$. Then we have

$$\left|\int_0^\infty dx'\, V_l(x,x')\chi_l(k;x')\right| \leq \left[\int_0^\infty dx'\,|V_l(x,x')|^2\right]^{1/2} \times \left[\int_0^\infty dx'\,|\chi_l(k;x')^2\right]^{1/2} \leq \text{const} \cdot (e^{-\gamma x}/x^{\delta}).$$

Hence, using the condition (3.5), we find that [16] $\chi_l(k;x)$ must satisfy (3.9) with

$$\int_0^\infty dx(kx)j_l(kx)\int_0^\infty dx'\, V_l(x,x')\chi_l(k;x') = 0.$$

Hence $\chi_l(k;x)$ vanishes exponentially as $x \to \infty$. Hence we may change the order of integrations in (3.9) and obtain (3.8). Consequently $\Delta_l(k) = 0$.[7]

We may demonstrate that the function $\chi(k;\mathbf{x}) = [\chi_l(k;x)/x]Y_{lm}(\theta,\varphi)$, where θ and φ are the polar angles of $\mathbf{x}$ and $\chi_l(k;x)$, is any bounded $C^\infty(0,\infty)$ solution of (3.8), and where k is a zero of $\Delta_l(k)$, with $\text{Im}k \geq 0$, $m = l, l-1, \cdots, -l$, belongs[17] to $W^{2,2}$ and consequently are bound state solutions of the system of angular momentum quantum numbers l and m. It also follows from this and the self-adjointness of the Hamiltonian operator of the system that the zeroes of $\Delta_l(k)$ in $\text{Im}k \geq 0$ must lie on the real axis or the upper imaginary axis.

We suppose now that $\text{Im}k \geq 0$ and that

$$\chi(k;\mathbf{x}) = \sum_{m=-l}^{l} [\chi_{lm}(k;x)/x]\, Y_{lm}(\theta,\varphi)$$

is a bound state solution of the system of angular momentum quantum number l, where θ and φ are the polar angles of $\mathbf{x}$. Then $\chi(k;\mathbf{x})$ satisfies the following equation:

$$\chi(k;\mathbf{x}) = (-1/4\pi)\int d\mathbf{x}'\,[\exp(ik|\mathbf{x}-\mathbf{x}'|)/\mathbf{x}-\mathbf{x}'|]\times\int d\mathbf{x}''\,V(\mathbf{x}',\mathbf{x}'')\,\chi(k;\mathbf{x}'').$$

Hence using the expansion

$$\exp(ik\,|\,\mathbf{x}-\mathbf{x}')/|\mathbf{x}-\mathbf{x}'| = ik\sum_{l=0}^{\infty}(2l+1)\,h_l^{(1)}(kx_{\max})\,j_l(kx_{\min})\,P_l(\hat{\mathbf{x}}\cdot\hat{\mathbf{x}}),$$

$$\mathbf{x} = |\mathbf{x}|\,\hat{x} = x\hat{x},\ \mathbf{x}' = |\hat{\mathbf{x}}'|\,\hat{x}' = x'\hat{x}', \qquad |\mathbf{x}| \neq |\mathbf{x}'|,$$

we find that there is at least one function $\chi_{lm}(k;x)$ which is not identically zero and which satisfies (3.9) and is a bounded $C^\infty(0,\infty)$ solution of (3.8). Hence $\Delta_l(k) = 0$.

Further, using a result of Ref. 18, we find that no zeroes of $\Delta_l(k)$ can occur in $\mathrm{Im}k \geq 0$, for l sufficiently large. Hence the total number of zeroes of $\Delta_l(k)$, for all l, in $\mathrm{Im}k \geq 0$, is finite.

4. ANALYTIC CONTINUATION OF THE PARTIAL SCATTERING AMPLITUDE

In Sec. 2 we defined the partial scattering amplitude $T_l(k)$, for $|\mathrm{Im}k| < \gamma$, with the exception of nonreal zeroes of $\Delta_l(k)$, by (3.4). It is holomorphic in this region. We now consider an analytic continuation of $T_l(k)$, by contour rotation.

We consider, for $k = i\kappa$, $\gamma > \kappa > -\gamma$, the function

$$h_l(k;x) = \int_0^\infty dx'\,\tilde{V}_l(x,x')\,\frac{e^{-\gamma x'}}{x'^{\delta}}\,(kx')j_l(kx').$$

We have

$$h_l(i\kappa;x) = \lim_{\epsilon\to 0+}\ \lim_{R\to\infty}\int_\epsilon^R dx'\,\tilde{V}_l(x,x')\,\frac{e^{-\gamma x'}}{x'^{\delta}}\,(i\kappa x')j_l(i\kappa x').$$

The integrand is holomorphic in x' in $\mathrm{Re}x' > 0$. We may write

$$h_l(i\kappa;x) = \lim_{\epsilon\to 0+}\ \lim_{R\to\infty}\left(\int_{C_1}+\int_{C_2}-\int_{C_3}\right)dx' \times \tilde{V}_l(x,x')\,(e^{-\gamma x'}/x'^{\delta})\,(i\kappa x')j_l(i\kappa x'), \quad \text{(see Fig. 1)}$$

where C_1 and C_3 are circular arcs of angle ω, $\pi/2 > \omega > -\pi/2$.

Using the bound

$$|(i\kappa x')j_l(i\kappa x')| \leq De^{|\kappa||x'|\cos\varphi}\left(\frac{|\kappa||x'|}{1+|\kappa||x'|}\right)^{l+1},$$

for $x' = |x'|\,e^{i\varphi}$, $\omega \geq \varphi > 0$, obtainable from (2.2a), we find that

$$\lim_{\epsilon\to 0+}\int_{C_1} dx'\,\tilde{V}_l(x,x')\,(e^{-\gamma x'}/x'^{\delta})\,(i\kappa x')j_l(i\kappa x') = 0,$$

$$\lim_{R\to\infty}\int_{C_3} dx'\,\tilde{V}_l(x,x')\,(e^{-\gamma x'}/x'^{\delta})\,(i\kappa x')j_l(i\kappa x') = 0.$$

Hence

$$h_l(i\kappa;x) = \int_0^\infty d|x'|\,e^{i\omega}\,\tilde{V}(x,|x'|e^{i\omega})\,(e^{-\gamma|x'|e^{i\omega}}/|x'|^{\delta}e^{i\delta\omega}) \times (i\kappa|x'|e^{i\omega})j_l(i\kappa|x'|e^{i\omega}).$$

For $\gamma > \kappa > -\gamma$, $h_l(i\kappa;x)$ is holomorphic in x in $\mathrm{Re}x > 0$ and is bounded there. Hence we may apply the same change of contour of integration to the integral

$$\int_0^\infty dx(i\kappa x)\,j_l(i\kappa x)(e^{-\gamma x}/x^{\delta})\,h_l(i\kappa;x)$$

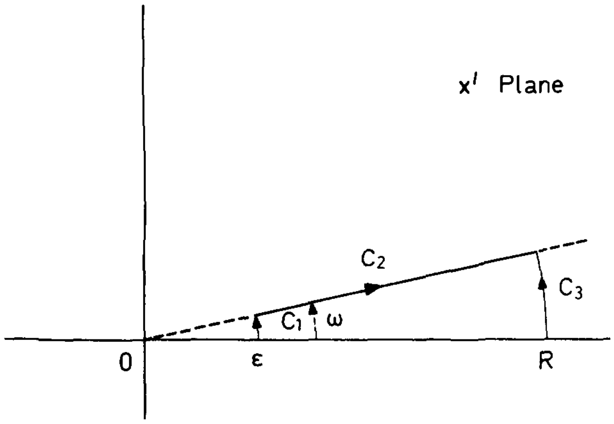

FIG. 1.

and obtain

$$T_l^{(1)}(i\kappa) = T_l^{(1)\omega}(i\kappa),$$

where

$$T_l^{(1)\omega}(k) = \frac{-1}{k}\int_0^\infty d|x|e^{i\omega}(k|x|e^{i\omega})j_l(k|x|e^{i\omega}) \times (e^{-\gamma|x|e^{i\omega}}/|x|^{\delta}e^{i\delta\omega})\int_0^\infty d|x'|e^{i\omega}\,\tilde{V}(|x|e^{i\omega},|x'|e^{i\omega}) \times (e^{-\gamma|x'|e^{i\omega}}/|x'|^{\delta}e^{i\delta\omega})\,(k|x'|e^{i\omega})j_l(k|x'|e^{i\omega})$$

is defined in the strip $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$, which is the strip $|\mathrm{Im}k| < \gamma\cos\omega$ rotated through ω in the clockwise direction about the origin (Fig. 2). Further $T^{(1)\omega}(k)$ is holomorphic in the strip $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$. Hence we have continued $T_l^{(1)}(k)$ to a function holomorphic in $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$, for every ω in the range $\pi/2 > \omega > -\pi/2$, and hence to a function holomorphic in Π.

Using the holomorphy of $\Delta_l(k;x,x')$ in k and x', in $\mathrm{Im}k > -\gamma$, $\mathrm{Re}x' > 0$, for $x \geq 0$, and the bound (3.3), we find that $T_l^{(2)}(k)$ can be continued to a function holomorphic in $\mathrm{Im}k > -\gamma$, cut from $i\gamma$ to $i\infty$. Hence $T_l(k)$ has been continued to a function holomorphic in $\mathrm{Im}k > -\gamma$, cut from $i\gamma$ to $i\infty$, perhaps with isolated poles at the nonreal zeroes of $\Delta_l(k)$. We have, in this region of holomorphy

$$T_l(k) = T_l^{(1)}(k) + [T_l^{(2)}(k)/\Delta_l(k)], \tag{4.2}$$

$$T_l^{(1)}(k) = T_l^{(1)\omega}(k), \qquad |\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega, \tag{4.3}$$

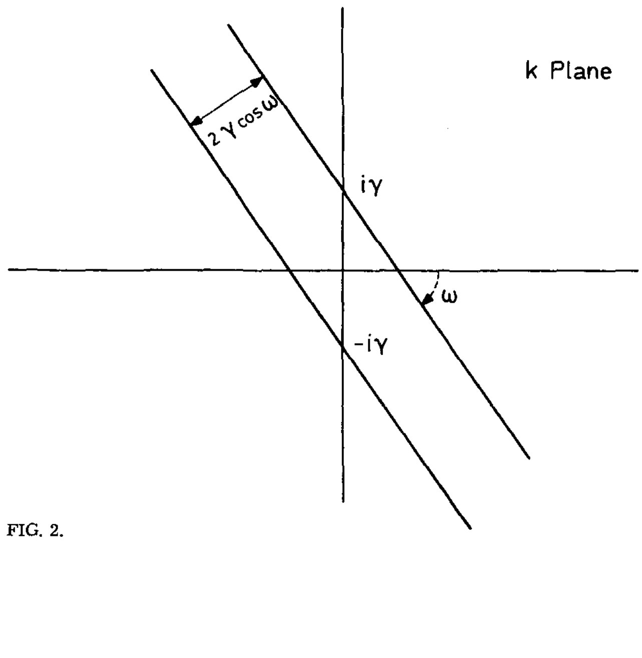

FIG. 2.

$$T_l^{(2)}(k) = -1/k \int_0^\infty d|x| e^{i\omega}(k|x|e^{i\omega}) j_l(k|x|e^{i\omega}) \times (e^{-\gamma |x| e^{i\omega}}/|x|^\delta e^{i\delta\omega}) \times \int_0^\infty dx' \tilde{V}_l(|x|e^{i\omega}, x')(e^{-\gamma x'}/x'^\delta) \times \int_0^\infty d|x''| e^{i\omega} \Delta_l(k; x', |x''|e^{i\omega})(k|x''|e^{i\omega}) \times j_l(k|x''|e^{i\omega}), \quad |\mathrm{Im} k e^{i\omega}| < \gamma \cos\omega. \tag{4.4}$$

Similarly, we may use (2.5) to define a function $\psi_l(k;x)$ in $|\mathrm{Im} k| < \gamma$, $\Delta_l(k) \neq 0$, $x \geq 0$, which is holomorphic in k in $|\mathrm{Im} k| < \gamma$, $\Delta_l(k) \neq 0$, for fixed $x \geq 0$, and which is a solution of (2.11)[19] with the behavior near the origin $x = 0$ given by (2.12), for $|\mathrm{Im} k| < \gamma$, $\Delta_l(k) \neq 0$, and to continue it to a function holomorphic in k in $\mathrm{Im} k > -\gamma$, $\Delta_l(k) \neq 0$, and cut from $i\gamma$ to $i\infty$, for fixed $x \geq 0$, and having the behavior near the origin given by (2.12), for fixed k in $\mathrm{Im} k > -\gamma$, $\Delta_l(k) \neq 0$, and not on the cut. For $\mathrm{Im} k \geq \gamma$, the function $\psi_l(k;x)$ need not be a solution of (2.11).

5. FURTHER ANALYTIC CONTINUATION

The Fredholm determinant $\Delta_l(k)$ was defined in Sec. 2 for $|\mathrm{Im} k| < \gamma$ by (2.6) and is holomorphic there. We now continue $\Delta_l(k)$ to a function holomorphic in the whole k plane cut from $-i\gamma$ to $-i\infty$.

We consider $k = i\kappa$, $\gamma > \kappa > -\gamma$. From the holomorphy of $K_l(k;x,x')$ in x and x' in $\mathrm{Re} x > 0$, $\mathrm{Re} x' > 0$, the inequalities (2.2a) and (2.2b), and using the method of contour rotation similar to what we did in Sec. 4, and also using induction and the relationships

$$\Delta_{l,n}(i\kappa) = \int_0^\infty dx\, \Delta_{l,n-1}(k;x,x),$$

$$\Delta_{l,n}(i\kappa;x,x') = -n \int_0^\infty dx''\, \Delta_{l,n-1}(i\kappa;x,x'') K_l(i\kappa;x'',x') + \Delta_{l,n}(i\kappa) K_l(i\kappa;x,x'),$$

we may show that $\Delta_{l,n}(i\kappa)$ and $\Delta_{l,n}(i\kappa;x,x')$ satisfy

$$\Delta_{l,0}(i\kappa) = 1,$$

$$\Delta_{l,n}(i\kappa) = \int_0^\infty \cdots \int_0^\infty d|x_1| \cdots d|x_n| e^{in\omega} \frac{e^{-\gamma|x_1|e^{i\omega}}}{|x_1|^\delta e^{i\delta\omega}} \cdots \frac{e^{-\gamma|x_n|e^{i\omega}}}{|x_n|^\delta e^{i\delta\omega}} \times \begin{vmatrix} A_l(i\kappa;|x_1|e^{i\omega},|x_1|e^{i\omega}) \cdots A_l(i\kappa;|x_1|e^{i\omega},|x_n|e^{i\omega}) \\ \vdots \\ A_l(i\kappa;|x_n|e^{i\omega},|x_1|e^{i\omega}) \cdots A_l(i\kappa;|x_n|e^{i\omega},|x_n|e^{i\omega}) \end{vmatrix}, \quad n \geq 1,$$

$$\Delta_{l,0}(i\kappa;x,x') = K_l(i\kappa;x,x'), \tag{5.1}$$

$$\Delta_{l,n}(i\kappa;x,x') = \int_0^\infty \cdots \int_0^\infty d|x_1| \cdots d|x_n| e^{in\omega} \frac{e^{-\gamma x'}}{x'^\delta} \frac{e^{-\gamma|x_1|e^{i\omega}}}{|x_1|^\delta e^{i\delta\omega}} \cdots \frac{e^{-\gamma|x_n|e^{i\omega}}}{|x_n|^\delta e^{i\delta\omega}} \times \begin{vmatrix} A_l(i\kappa;x,x') & A_l(i\kappa;x,|x_1|e^{i\omega}) \cdots A_l(i\kappa;x,|x_n|e^{i\omega}) \\ A_l(i\kappa;|x_1|e^{i\omega},x') & \\ \vdots & \vdots \\ A_l(i\kappa;|x_n|e^{i\omega},x') & \cdots \quad A_l(i\kappa;|x_n|e^{i\omega},|x_n|e^{i\omega} \end{vmatrix}, \quad n \geq 1, \quad x \geq 0, \quad \mathrm{Re} x' > 0,$$

where $\pi/2 > \omega > -\pi/2$ and

$$A_l(i\kappa;x,x') = \left(\frac{(i\kappa)^{l+1}(i\kappa x)h_l^{(1)}(i\kappa x)}{-\kappa}\right) \int_0^\infty dx'' \left(\frac{(i\kappa x'')j_l(i\kappa x'')}{(i\kappa)^{l+1}}\right) \frac{e^{-\gamma x''}}{x''^\delta} \tilde{V}_l(x'',x') + \left(\frac{(i\kappa x)j_l(i\kappa x)}{(i\kappa)^l(-\kappa)}\right) \times \int_x^\infty dx''[(i\kappa)^l(i\kappa x'')h_l^{(1)}(i\kappa x'')] \frac{e^{-\gamma x''}}{x''^\delta} \tilde{V}_l(x'',x'), \quad \mathrm{Re} x > 0, \quad \mathrm{Re} x' > 0.$$

Hence we have

$$\Delta_{l,n}(i\kappa) = \Delta_{l,n}^\omega(i\kappa),$$

where $\Delta_{l,n}^\omega(k)$ is defined, using (2.2a) and (2.2b), in the strip $|\mathrm{Im} k e^{i\omega}| < \gamma \cos\omega$, $\pi/2 > \omega > -\pi/2$, by

$$\Delta_{l,0}^\omega(k) = 1,$$

$$\Delta_{l,n}^\omega(k) = \int_0^\infty \cdots \int_0^\infty d|x_1| \cdots d|x_n| e^{in\omega} \frac{e^{-\gamma|x_1|e^{i\omega}}}{|x_1|^\delta e^{i\delta\omega}} \cdots \frac{e^{-\gamma|x_n|e^{i\omega}}}{|x_n|^\delta e^{i\delta\omega}} \times \begin{vmatrix} A_l(k;|x_1|e^{i\omega},|x_1|e^{i\omega}) \cdots A_l(k;|x_1|e^{i\omega},|x_n|e^{i\omega}) \\ \vdots \\ A_l(k;|x_n|e^{i\omega},|x_1|e^{i\omega}) \cdots A_l(k;|x_n|e^{i\omega},|x_n|e^{i\omega}) \end{vmatrix}, \quad n \geq 1, \tag{5.2}$$

where $A_l(k;|x|e^{i\omega},|x'|e^{i\omega})$ is given by

$$A_l(k; |x|e^{i\omega}, |x'|e^{i\omega}) = \left(\frac{k^{l+1}(k|x|e^{i\omega})\, h_l^{(1)}(k|x|e^{i\omega})}{ik}\right) \times \int_0^{|x|} d|x''|e^{i\omega}\left(\frac{(k|x''|e^{i\omega})\, j_l(k|x''|e^{i\omega})}{k^{l+1}}\right)\frac{e^{-\gamma|x''|e^{i\omega}}}{|x''|^\delta e^{i\delta\omega}} \times \tilde{V}_l(|x''|e^{i\omega}, |x'|e^{i\omega}) + \left(\frac{(k|x|e^{i\omega})\, j_l(k|x|e^{i\omega})}{k^l\cdot ik}\right) \times \int_{|x|}^{\infty} d|x''|e^{i\omega}[k^l(k|x''|e^{i\omega})\, h_l^{(1)}(k|x''|e^{i\omega})] \times \frac{e^{-\gamma|x''|e^{i\omega}}}{|x''|^\delta e^{i\delta\omega}}\, \tilde{V}_l(|x''|e^{i\omega}, |x'|e^{i\omega}), \tag{5.3}$$

$$|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega, \quad \pi/2 > \omega > -\pi/2, \quad |x| > 0, \quad |x'| > 0.$$

Since $A_l(k; |x|e^{i\omega}, |x'|e^{i\omega})$ is holomorphic in k in $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$, for $|x| > 0$, $|x'| > 0$, we find, using (2.2a) and (2.2b), that $\Delta_{l,n}^{\omega}(k)$ is holomorphic in $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$. And using

$$|A_l(k; |x|e^{i\omega}, |x'|e^{i\omega})| \leqslant \text{const}\cdot |x|\, e^{|\mathrm{Im}ke^{i\omega}||x|}, \tag{5.4}$$

for $|\mathrm{Im}ke^{i\omega}| \leqslant \gamma\cos\omega - \epsilon$, $\gamma\cos\omega \geqslant \epsilon > 0$, $\pi/2 > \omega > -\pi/2$, we find that the series

$$\sum_{h=0}^{\infty} \frac{(-1)^n}{n!}\, \Delta_{l,n}^{\omega}(k)$$

is convergent and the sum is holomorphic in $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$. Hence $\Delta_l(k)$ has been continued to a function holomorphic in $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$, and hence to a function holomorphic in the whole k plane cut from $-i\gamma$ to $-i\infty$, if we use a previous result. We denote this function by $\Delta_l(k)$ also. For k in $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$, we have

$$\Delta_l(k) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\, \Delta_{l,n}^{\omega}(k). \tag{5.5}$$

Further, using the relation

$$|A_l(k; |x|e^{i\omega}, |x'|e^{i\omega})| \leqslant \frac{\text{const}}{|k|\cos^2\omega},$$

$$k \neq 0, \quad k = \pm|k|e^{i\omega}, \quad \pi/2 > \omega > -\pi/2 \tag{5.6}$$

for fixed l, and (3.1), we find that

$$\Delta_l(k) \xrightarrow[|k|\to\infty]{} 1, \tag{5.7}$$

for fixed l, uniformly in $(3\pi/2) - \epsilon \geqslant \arg k \geqslant -(\pi/2 - \epsilon)$, for any fixed ϵ in the range $\pi/2 > \epsilon > 0$. Hence from (2.21), we find that the S matrix $S_l(k)$ is holomorphic in Π, perhaps with the exception of isolated poles which are finite in number in the regions $(3\pi/2) - \epsilon \geqslant \arg k \geqslant -((\pi/2) - \epsilon)$, $\pi/2 > \epsilon > 0$, and $|\mathrm{Im}k| \leqslant \gamma - \epsilon$, $\gamma > \epsilon > 0$, at the nonreal zeroes of $\Delta_l(k)$, and that we have the representation

$$S_l(k) = \Delta_l(-k)/\Delta_l(k), \tag{5.8}$$

for k in Π.

Using

$$h_l^{(1)}(-z^*) = (-1)^l h_l(z)^*, \qquad j_l(-z^*) = (-1)^l j_l(z)^*,$$

and

$$V_l(x^*, x'^*) = V_l(x, x')^*,$$

which follows from Schwartz reflection principle,[20,21] we get

$$\Delta_l(-k^*) = \Delta_l(k)^*. \tag{5.9}$$

Consequently, we have

$$S_l(-k^*) = S_l(k^*)^{-1} = S_l(k)^*. \tag{5.10}$$

From (5.7), we also have

$$S_l(k) \xrightarrow[|k|\to\infty]{} 1 \tag{5.11}$$

for fixed l, uniformly in $(\pi/2) - \epsilon \geqslant \omega \geqslant -(\pi/2 - \epsilon)$, $\pi/2 \geqslant \epsilon > 0$, for $\omega = -\arg(\pm k)$.

The partial scattering amplitude $T_l(k)$ is therefore continued to a function holomorphic in Π, perhaps with poles at the nonreal zeroes of $\Delta_l(k)$, via the relationship

$$S_l(k) = 1 + 2iT_l(k). \tag{5.12}$$

Using (5.1), and the bounds (2.2a) and (2.2b), and using contour rotation, we obtain the following representation for $T_l(k)$ in $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$:

$$T_l(k) = T_l^{(1)}(k) + [T_l^{(2)}(k)/\Delta_l(k)] \tag{5.13}$$

where

$$T_l^{(1)}(k) = \frac{-1}{k}\int_0^{\infty} d|x|e^{i\omega}(k|x|e^{i\omega})\, j_l(k|x|e^{i\omega})\, \frac{e^{-\gamma|x|e^{i\omega}}}{|x|^\delta e^{i\delta\omega}} \times \int_0^{\infty} d|x'|e^{i\omega}\, \tilde{V}_l(|x|e^{i\omega}, |x'|e^{i\omega})\, \frac{e^{-\gamma|x'|e^{i\omega}}}{|x'|^\delta e^{i\delta\omega}} \times (k|x'|e^{i\omega})\, j_l(k|x'|e^{i\omega}), \tag{5.14}$$

$$T_l^{(2)}(k) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\, B_{l,n}(k), \tag{5.15}$$

$$B_{l,0}(k) = \frac{-1}{k}\int_0^{\infty} d|x|e^{i\omega}(k|x|e^{i\omega})\, j_l(k|x|e^{i\omega})\, \frac{e^{-\gamma|x|e^{i\omega}}}{|x|^\delta e^{i\delta\omega}} \int_0^{\infty} d|x'|e^{i\omega}\, \tilde{V}_l(|x|e^{i\omega}, |x'|e^{i\omega})\, \frac{e^{-\gamma|x'|e^{i\omega}}}{|x'|^\delta e^{i\delta\omega}} \times \int_0^{\infty} d|x''|e^{i\omega} A_l(k; |x'|e^{i\omega}, |x''|e^{i\omega})\, \frac{e^{-\gamma|x''|e^{i\omega}}}{|x''|^\delta e^{i\delta\omega}}\, (k|x''|e^{i\omega})\, j_l(k|x''|e^{i\omega}),$$

$$B_{l,n}(k) = \frac{-1}{k}\int_0^{\infty} d|x|e^{i\omega}(k|x|e^{i\omega})\, j_l(k|x|e^{i\omega})\, \frac{e^{-\gamma|x|e^{i\omega}}}{|x|^\delta e^{i\delta\omega}} \int_0^{\infty} d|x'|e^{i\omega}\, \tilde{V}(|x|e^{i\omega}, |x'|e^{i\omega})\, \frac{e^{-\gamma|x'|e^{i\omega}}}{|x'|^\delta e^{i\delta\omega}} \tag{5.16}$$

$$\times \int_0^{\infty} d|x''|e^{i\omega}(k|x''|e^{i\omega})\, j_l(k|x''|e^{i\omega})\, \frac{e^{-\gamma|x''|e^{i\omega}}}{|x''|^\delta e^{i\delta\omega}} \int_0^{\infty}\cdots\int_0^{\infty} d|x_1|\cdots d|x_n|\, e^{in\omega}\, \frac{e^{-\gamma|x_1|e^{i\omega}}}{|x_1|^\delta e^{i\delta\omega}}\cdots\frac{e^{-\gamma|x_n|e^{i\omega}}}{|x_n|^\delta e^{i\delta\omega}}$$

$$\times \begin{vmatrix} A_l(k; |x'|e^{i\omega}, |x''|e^{i\omega}) & A_l(k; |x'|e^{i\omega}, |x_1|e^{i\omega}) \cdots & A_l(k; |x'|e^{i\omega}, |x_n|e^{i\omega}) \\ A_l(k; |x_1|e^{i\omega}, |x''|e^{i\omega}) & & \\ \vdots & & \vdots \\ A_l(k; |x_n|e^{i\omega}, |x''|e^{i\omega}) & \cdots & A_l(k; |x_n|e^{i\omega}, |x_n|e^{i\omega}) \end{vmatrix}, \quad n \geqslant 1.$$

From (5. 10), (5. 11), and (5. 12), we have

$$T_l(-k^*) = T_l(k)^*, \quad (5.17)$$

$$T_l(k) \xrightarrow[|k|\to 0]{} 0 \quad (5.18)$$

for fixed l, uniformly in $\pi/2 - \epsilon \geqslant \arg(\pm k) \geqslant -(\pi/2-\epsilon)$, $\pi/2 \geqslant \epsilon > 0$.

Further, the scattering solution $\psi_l(k;x)$ admits an extension to a function holomorphic in k and x, for k in Π, perhaps with the exception of isolated poles at the zeroes of $\Delta_l(k)$, and Re$x > 0$, if we use contour deformation. We call this extended function $\psi_l(k;x)$ also. For k in $|\mathrm{Im} ke^{i\omega}| < \gamma \cos\omega$, $\pi/2 > \omega > -\pi/2$, it has the following representation:

$$\psi_l(k;x) = (kx) j_l(kx) + \frac{1}{\Delta_l(k)} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \psi_{l,n}^{\omega}(k;x),$$

$$\Delta_l(k) \neq 0, \quad \mathrm{Re}x > 0 \quad (5.19)$$

with

$$\psi_{l,0}^{\omega}(k;x) = \int_0^\infty d|x'|e^{i\omega}(k|x'|e^{i\omega}) j_l(k|x'|e^{i\omega}) \frac{e^{-\gamma|x'|e^{i\omega}}}{|x'|^{\delta} e^{i\delta\omega}} A_l(k;x,|x'|e^{i\omega}),$$

$$\psi_{l,n}^{\omega}(k;x) = \int_0^\infty d|x'|e^{i\omega}(k|x'|e^{i\omega}) j_l(k|x'|e^{i\omega}) \frac{e^{-\gamma|x'|e^{i\omega}}}{|x'|^{\delta} e^{i\delta\omega}}$$
$$\times \int_0^\infty \cdots \int_0^\infty d|x_1| \cdots d|x_n| e^{in\omega} \frac{e^{-\gamma|x_1|e^{i\omega}}}{|x_1|^{\delta} e^{i\delta\omega}} \cdots \frac{e^{-\gamma|x_n|e^{i\omega}}}{|x_n|^{\delta} e^{i\delta\omega}}$$
$$\times \begin{vmatrix} A_l^s(k;x,|x'|e^{i\omega}) & A_l^s(k;x,|x_1|e^{i\omega}) \cdots A_l^s(k;x_1|x_n|e^{i\omega}) \\ A_l^s(k;|x_1|e^{i\omega},|x'|e^{i\omega}) & \\ \vdots & \vdots \\ A_l^s(k;|x_n|e^{i\omega},|x'|e^{i\omega}) & \cdots \quad A_l^s(k;|x_n|e^{i\omega},|x_n|e^{i\omega}) \end{vmatrix}, \quad n \geqslant 1 \quad (5.20)$$

where $A_l^s(k;x,|x'|e^{i\omega})$, is defined, for $|\mathrm{Im} ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$, Re$x > 0$, $|x'| > 0$, by

$$A_l^s(k;x,|x'|e^{i\omega})$$
$$= \left(\frac{k^{l+1}(kx)h_l^{(1)}(kx)}{ik}\right)\int_0^x dx'' \left(\frac{(kx'')j_l(kx'')}{k^{l+1}}\right)$$
$$\times \frac{e^{-\gamma x''}}{x''^{\delta}} \tilde{V}(x'',|x'|e^{i\omega}) + \left(\frac{(kx)j_l(kx)}{k^l \cdot ik}\right)$$
$$\times \left(\int_{|x|}^\infty d|x''|e^{i\omega}[k^l(k|x''|e^{i\omega})h_l^{(1)}(k|x''|e^{i\omega})]\right.$$
$$\times \frac{e^{-\gamma|x''|e^{i\omega}}}{|x''|^{\delta}e^{i\delta\omega}} \tilde{V}(|x''|e^{i\omega},|x'|e^{i\omega})$$
$$\left. + \int_C dx''\{k^l(kx'')h_l^{(1)}(kx'')\} \frac{e^{-\gamma x''}}{x''^{\delta}} \tilde{V}(x'',|x'|e^{i\omega})\right) \quad (5.21)$$

where C is an arc from x to $|x|e^{i\omega}$, and

$$A_l^s(k;x,|x'|e^{i\omega}) = 0, \quad x = 0. \quad (5.22)$$

The function $\psi_l(k;x)$ in the above domain of definition in the k plane has the behavior near the origin $x = 0$ given by (2. 12), and for $|\mathrm{Im}k| > \gamma$, $x > 0$, it need not be a solution of (2. 11).

We have, for $k \in \Pi$,

$$\psi_l(-k^*;x) = (-1)^{l+1}\psi_l(k;x)^*, \quad x \geqslant 0. \quad (5.23)$$

6. ANALYTICITY OF THE SCATTERING AMPLITUDE IN THE t PLANE AND A DISPERSION RELATION FOR FIXED t

We here consider a class of potentials satisfying Conditions (A) for $\alpha = \frac{1}{2}$, and also the following condition:

$$\tilde{V}(x,x',\cos\nu) = \int_0^\infty \int_0^\infty d\beta d\beta' e^{-\beta x} e^{-\beta' x'} \sigma(\beta,\beta',\cos\nu),$$

where $\sigma(\beta,\beta',\cos\nu)$ satisfies

(i) $\sigma(\beta,\beta',\cos\nu)$ is real, $\sigma(\beta,\beta',\cos\nu) = \sigma(\beta',\beta,\cos\nu)$;

(ii) $\sigma(\beta,\beta',\cos\nu)$ is continuous in $\infty > \beta > 0$, $\infty > \beta' > 0$, and $1 \geqslant \cos\nu \geqslant -1$, and in this region

$$|\sigma(\beta,\beta',\cos\nu)| \leqslant \Sigma(\beta,\beta'),$$

$$\Sigma(\beta,\beta') = \Sigma(\beta',\beta),$$

$$\int_0^\infty \int_0^\infty d\beta\, d\beta'\, \Sigma(\beta,\beta') < \infty,$$

where $\Sigma(\beta,\beta')$ is continuous in $\infty > \beta > 0$, $\infty > \beta' > 0$.

For such a potential, the partial potentials satisfy

$$V_l(x,x') = x^{1/2} e^{-\gamma x} \tilde{V}_l(x,x') x'^{1/2} e^{-\gamma x'},$$

$$\tilde{V}_l(x,x') = \int_0^\infty \int_0^\infty d\beta\, d\beta' e^{-\beta x} e^{-\beta' x'} \sigma_l(\beta,\beta'),$$

where

$$\sigma_l(\beta,\beta') = 2\pi \int_{-1}^{+1} d\cos\nu\, \sigma(\beta,\beta',\cos\nu) P_l(\cos\nu)$$

and

(i) $\sigma_l(\beta,\beta')$ is real, $\sigma_l(\beta,\beta') = \sigma_l(\beta',\beta)$;

(ii) $\sigma_l(\beta,\beta')$ is continuous in $\infty > \beta > 0$, $\infty > \beta' > 0$, and in this region

$$|\sigma_l(\beta,\beta')| \leqslant \mathrm{const}[\Sigma(\beta,\beta')/\sqrt{2l+1}].$$

The partial scattering amplitude $T_l(k)$, for $k > 0$, has the following form

$$T_l(k) = T_l^{(1)}(k) + [T_l^{(2)}(k)/\Delta_l(k)], \quad (6.1)$$

where $T_l^{(1)}(k)$ and $T_l^{(2)}(k)$ are, from (2. 19) and (2. 20), given by

$$T_l^{(1)}(k) = (-1/k) \int_0^\infty \int_0^\infty d\beta\, d\beta'\, \sigma_l(\beta,\beta')$$
$$\times \int_0^\infty dx (kx) j_l(kx) x^{1/2} e^{-(\gamma+\beta)x}$$
$$\times \int_0^\infty dx' (kx') j_l(kx') x'^{1/2} e^{-(\gamma+\beta')x'}, \quad (6.2)$$

$$T_l^{(2)}(k) = (-1/k)\int_0^\infty\int_0^\infty\int_0^\infty d\beta\, d\beta'\, d\beta''\, \sigma_l(\beta,\beta') \times \int_0^\infty dx'\, x'^{1/2} e^{-(\gamma+\beta')x'} \rho_l(k;x',\beta'') \times \int_0^\infty dx(kx) j_l(kx)\, x^{1/2} e^{-(\gamma+\beta)x} \times \int_0^\infty dx''(kx'') j_l(kx'')\, x''^{1/2} e^{-(\gamma+\beta'')x''}, \quad (6.3)$$

where we have used the following relationship[22]

$$\Delta_l(k;x',x'') = x''^{1/2} e^{-\gamma x''} \int_0^\infty d\beta''\, e^{-\beta'' x''} \rho_l(k;x',\beta''), \quad (6.4)$$

with $\rho_l(k;x',\beta'')$ continuous in $\infty > x' \geq 0$, $\infty > \beta'' > 0$, for $k > 0$, and[22]

$$|\rho_l(k;x',\beta'')| \leq (D_1/\sqrt{2l+1}) \int_0^\infty d\beta'\, \Sigma(\beta',\beta''), \quad (6.5)$$

where D_1 is a constant.

We now show that, for $k > 0$, and $\Delta_l(k) \neq 0$ for all l, the series

$$(1/k) \sum_{l=0} (2l+1) T_l(k) P_l(\cos\theta)$$

is convergent inside an ellipse in the $\cos\theta$ plane with foci at $-1, +1$, and semimajor axis equal to $1 + (2\gamma^2/k^2)$. We denote the sum by $F(k;\cos\theta)$. If we introduce $t = 2k^2(1-\cos\theta)$, then $\mathfrak{F}(k;t) = F(k;\cos\theta)$ is holomorphic inside an ellipse in the t plane which includes the interval $0 \geq t > -4\gamma^2$.

Using the bound[23]

$$|G_l(k;x,x')| \leq \sqrt{\pi/(2l+1)}\, x_{\min}$$

for k real, we find that

$$|K_l(k;x,x')| \leq (D_2/\sqrt{2l+1})\, x'^{1/2} e^{-\gamma x'}, \quad (6.6)$$

where D_2 is a constant. Hence using Hadamard's theorem,[14] we have, from (2.7),

$$|\Delta_{l,n}(k)| \leq (1/(2l+1))^{n/2} D_2^n M^n n^{n/2}, \quad n \geq 1, \qquad M = \int_0^\infty dx\, x^{1/2} e^{-\gamma x}. \quad (6.7)$$

Hence we have

$$\Delta_l(k) \xrightarrow[l\to\infty]{} 1$$

uniformly in $k > 0$.

We consider the behavior of $T_l^{(1)}(k)$ and $T_l^{(2)}(k)$ as $l \to \infty$. We have[24]

$$\int_0^\infty dx(kx) j_l(kx)\, x^{1/2} e^{-(\gamma+\beta)x} = \sqrt{(\pi k/2)} \cdot [k^2 + (\gamma+\beta)^2]^{-3/2} \cdot [(l+\tfrac{1}{2})\sqrt{k^2+(\gamma+\beta)^2} + (\gamma+\beta)]\{k/[\sqrt{k^2+(\gamma+\beta)^2} + (\gamma+\beta)]\}^{l+1/2}. \quad (6.8)$$

Hence we obtain

$$\left|\int_0^\infty dx(kx) j_l(kx)\, x^{1/2} e^{-(\gamma+\beta)x}\right| \leq \sqrt{\pi k/2}\, [(l+\tfrac{3}{2})/(k^2+\gamma^2)]\, e^{-\lambda l},$$

where

$$\lambda = \ln[(\sqrt{k^2+\gamma^2} + \gamma)/k], \quad k > 0.$$

Hence we obtain

$$|T_l^{(1)}(k)| \leq \frac{1}{k} \int_0^\infty\int_0^\infty d\beta\, d\beta' \frac{\Sigma(\beta,\beta')}{\sqrt{2l+1}} \cdot \frac{\pi k}{2} \cdot \frac{(l+\frac{3}{2})^2}{(k^2+\gamma^2)^2} e^{-2\lambda l}, \quad (6.9)$$

$$|T_l^{(2)}(k)| \leq \frac{1}{k} \frac{D_1 M}{\sqrt{2l+1}} \left(\int_0^\infty\int_0^\infty d\beta\, d\beta' \frac{\Sigma(\beta,\beta')}{\sqrt{2l+1}}\right)^2 \times \frac{\pi k}{2} \cdot \frac{(l+\frac{3}{2})^2}{(k^2+\gamma^2)^2} e^{-2\lambda l}. \quad (6.9)$$

Therefore, using the inequality[25]

$$|P_l(\cos\theta)| \leq \text{const} \cdot [e^{(l+1/2)|\text{Im}\,\theta|} / |\sin\theta|^{1/2} (l+\tfrac{1}{2})^{1/2}], \quad (6.10)$$

we find that the series

$$(1/k) \sum_{l=0}^{\infty} (2l+1) T_l(k) P_l(\cos\theta)$$

converges, for $k > 0$, and $\Delta_l(k) \neq 0$, for all l, when $|\text{Im}\,\theta| < 2\lambda$, which is the interior of an ellipse in the $\cos\theta$ plane with foci at $-1, +1$, and semimajor axis equal to $\cosh 2\lambda$, which is $1 + 2\gamma^2/k^2$. Further, the sum $F(k;\cos\theta)$ is holomorphic in $\cos\theta$ inside this ellipse. Hence, we have demonstrated our previous statement.

We now consider the analyticity of $\mathfrak{F}(k;t)$ in the k plane for fixed t in the range $0 \geq t > -4\gamma^2$. We have seen that $T_l(k)$ is holomorphic in II, perhaps with the exception of poles at the nonreal zeroes of $\Delta_l(k)$, which are finite in number in the regions $(3\pi/2) - \epsilon \geq \arg k \geq -(\pi/2 - \epsilon)$, $\pi/2 \geq \epsilon > 0$, and $|\text{Im}\,k| \leq \gamma - \epsilon$, $\gamma \geq \epsilon > 0$. We examine the convergence of the series defining $\mathfrak{F}(k;t)$, for $\text{Im}\,k > -\gamma$.

Using the bound

$$|G_l(k;x,x')| \leq (\text{const}/\sqrt{2l+1})\, x_{\min}, \quad \text{Im}\,k \geq 0,$$

which may be derived by

$$|G_l(k;x,x')| = |(kx_{\max}) h_l^{(1)}(kx_{\max}) \cdot x_{\min} j_l(kx_{\min})| = \left|\frac{xx'}{2}\int_{-1}^{+1} d\cos\theta \cdot \frac{\exp(ik|\mathbf{x}-\mathbf{x}'|)}{|\mathbf{x}-\mathbf{x}'|} P_l(\cos\theta)\right|$$
$$\leq \frac{\text{const}}{\sqrt{2l+1}}\, x_{\min} \int_{-1}^{+1} d\cos\theta \frac{1}{(\sin\theta)^{1/2}} \times \frac{1}{\sqrt{1+\alpha^2 - 2\alpha\cos\theta}}, \quad \alpha = \frac{x_{\min}}{x_{\max}},$$
$$\leq (\text{const}/\sqrt{2l+1})\, x_{\min},$$

$$|\mathbf{x}| = x, \quad |\mathbf{x}'| = x', \quad \mathbf{x}\cdot\mathbf{x}' = xx'\cos\theta,$$

and the bound

$$|G_l(k;x,x')| \leq (\text{const}/\sqrt{2l+1})\, x_{\min}\, e^{|\text{Im}\,k|(x+x')}, \quad \text{Im}\,k < 0,$$

which may be similarly derived, we obtain

$$|K_l(k;x,x')| \leq (\text{const}/\sqrt{2l+1})\, x'^{1/2} e^{-\gamma x'}, \quad \text{Im}\,k \geq 0,$$
$$|K_l(k;x,x')| \leq (\text{const}/\sqrt{2l+1})\, e^{|\text{Im}\,k|x} x'^{1/2} e^{-\gamma x'},$$
$$\text{Im}\,k \geq -(\gamma-\epsilon), \quad \gamma \geq \epsilon > 0,$$

for fixed l. Consequently we obtain

$$\Delta_l(k) \xrightarrow[l\to\infty]{} 1 \quad (6.11)$$

uniformly in k in $\text{Im}\,k \geq -(\gamma-\epsilon)$, $\gamma \geq \epsilon > 0$.

Equation (6.8) holds for $|\text{Im}\,k| < \gamma + \beta$, and the right side is the analytic continuation of the left side in II. If we denote the right side of (6.8) by $g_l(k;\beta)$, then we have, from (2.19) and (2.20), the following representation for $T_l^{(1)}(k)$ and $T_l^{(2)}(k)$:

$$T_l^{(1)}(k) = (-1/k) \int_0^\infty \int_0^\infty d\beta d\beta' \sigma_l(\beta,\beta') g_l(k;\beta) g_l(k;\beta'),$$

$$T_l^{(2)}(k) = (-1/k) \int_0^\infty \int_0^\infty \int_0^\infty d\beta d\beta' d\beta'' \sigma_l(\beta,\beta') \times \int_0^\infty dx' x'^{1/2} e^{-(\gamma+\beta')x'} \rho_l(k;x',\beta'') g_l(k;\beta) g_l(k;\beta''), \tag{6.12}$$

in $\text{Im}k > -(\gamma - \epsilon)$, $\gamma \geq \epsilon > 0$, cut from $i\gamma$ to $i\infty$, where $\rho_l(k;x',\beta'')$[26] is holomorphic in k in this region for $\infty > x' \geq 0$, $\infty > \beta'' > 0$, and continuous in x' and β'' in $\infty > x' \geq 0$, $\infty > \beta'' > 0$, for k in the above region, and (6. 5) holds for k in this extended region, for x' and β'' in the above region. We have

$$|T_l^{(1)}(k)| \leq \frac{\text{const}}{|k|} \int_0^\infty \int_0^\infty d\beta d\beta' \frac{\Sigma(\beta,\beta')}{\sqrt{2l+1}} |g_l(k;\beta) g_l(k;\beta')|,$$

$$|T_l^{(2)}(k)| \leq \frac{\text{const}}{|k|} \cdot D_1 M \left(\int_0^\infty \int_0^\infty d\beta d\beta' \frac{\Sigma(\beta,\beta')}{\sqrt{2l+1}} |g_l(k;\beta)|\right)^2. \tag{6.13}$$

Since

$$|\sqrt{k^2 + (\gamma+\beta)^2} + (\gamma+\beta)| \geq |\sqrt{k^2+\gamma^2} + \gamma|, \quad \infty > \beta > 0,$$

for k in Π, as may be demonstrated using the inequalities[27]

$$\text{Re}\sqrt{k^2 + (\gamma+\beta)^2} \geq \text{Re}\sqrt{k^2+\gamma^2}, \quad \infty > \beta > 0,$$

$$|k^2 + (\gamma+\beta)^2| + \beta^2 + 2\beta\gamma > |k^2 + \gamma^2|, \quad \infty > \beta > 0,$$

we find

$$|g_l(k;\beta)| \leq \sqrt{\frac{\pi|k|}{2}} \cdot \frac{|k|^{1/2}}{|k^2 + (\gamma+\beta)|^{1/2}} \times \left(\frac{|l-\frac{1}{2}|}{\sqrt{k^2+\gamma^2}+\gamma} + \frac{1}{|k^2+(\gamma+\beta)^2|^{1/2}}\right) e^{-\lambda l} \tag{6.14}$$

for k in Π, where λ is given by

$$\lambda = \ln|(\sqrt{k^2+\gamma^2} + \gamma)/k|$$

and

$$\cosh 2\lambda = (1/|k|^2)(|k^2+\gamma^2| + \gamma^2).$$

We consider, for each k in $\text{Im}k > -(\gamma - \epsilon)$, $\gamma \geq \epsilon > 0$, cut from $i\gamma$ to $i\infty$, the ellipse in the t plane which is the map of the region $|\text{Im}\theta| < 2\lambda$ in the θ plane. The intercept of this ellipse with the negative t axis is given by

$$t = -2|k|^2 \cdot \frac{\cosh^2(2\lambda) - 1}{\cosh 2\lambda + \cos 2\varphi} = -4\gamma^2, \quad k = |k|e^{i\varphi}. \tag{6.15}$$

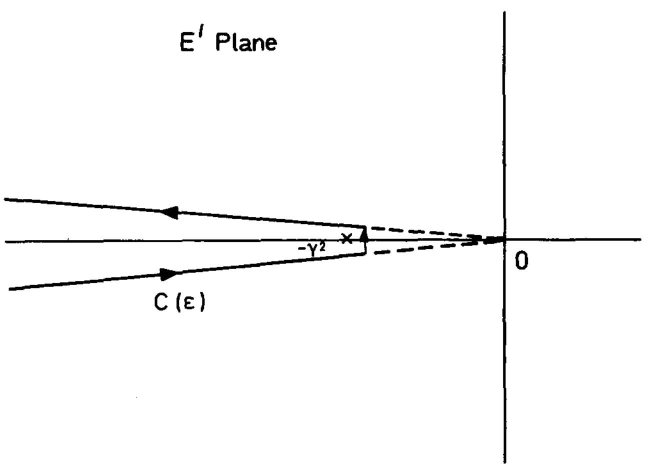

FIG. 3.

Hence the interval $0 \geq t > -4\gamma^2$ is included in every ellipse in the t plane which is the map of the region $|\text{Im}\theta| < 2\lambda$ in the θ plane, for every such k. Hence, using (6. 10), (6. 11), (6. 13), and (6. 14), we find that for each t in $0 \geq t > -4\gamma^2$ the series

$$\frac{1}{k} \sum_{l=0}^{\infty} (2l+1) T_l(k) P_l \left(1 - \frac{t}{2k^2}\right)$$

is convergent, uniformly with respect to k, in $\text{Im}k > -(\gamma-\epsilon)$, $\gamma \geq \epsilon > 0$, cut from $i\gamma$ to $i\infty$, with $k \neq 0$, and k not equal to any nonreal zero of $\Delta_l(k)$, for all l, and its sum $\mathfrak{F}(k;t)$ is holomorphic in k in $\text{Im}k > -\gamma$, cut from $i\gamma$ to $i\infty$, with $k \neq 0$ and k not equal to any nonreal zero of $\Delta_l(k)$, for all l. And from (6. 12) we find that, if $\Delta_l(k=0) \neq 0$ for all l, then, for each t in $0 \geq t > -4\gamma^2$, the series $(1/k)T_l(k)P_l[1-(t/2k^2)]$ is holomorphic in k in a neighborhood of $k=0$, and we may similarly demonstrate that the sum $\mathfrak{F}(k;t)$ of the series

$$(1/k) \sum_{l=0}^{\infty} (2l+1) T_l(k) P_l[1-(t/2k^2)]$$

is holomorphic in a neighborhood of $k=0$ under the same assumptions on $\Delta_l(k=0)$.

From (5. 17), we obtain

$$\mathfrak{F}(-k^*;t) = \mathfrak{F}(k;t)^*. \tag{6.16}$$

We note that for $k = i\kappa$, $\gamma > \kappa > 0$, the intercept of the above ellipse in the t plane with the positive t axis approaches zero as κ approaches γ.

We now discuss the asymptotic behavior of $\mathfrak{F}(k;t)$. We have, from (3. 1) and (6. 11),

$$|\Delta_l(k)| > \tfrac{1}{2}, \quad |k| > R, \quad \text{Im}k > -(\gamma-\epsilon), \quad \gamma \geq \epsilon > 0 \tag{6.17}$$

for all l, where R is a constant. We also have, for $k = |k|e^{i\varphi}$, $\pi \geq \varphi > \pi/2$, $\pi/2 > \varphi \geq 0$, and $|k| \gg \gamma$, that

$$\lambda = (\gamma/|k|)|\cos\varphi| + O(\gamma^2/k^2),$$

$$|\text{Im}\theta| = (\sqrt{|t|}/|k|)|\cos\varphi|[1 + O(\gamma^2/k^2)],$$

where the approach to the asymptotic limit is uniform in $\cos\phi$. Hence, from (6. 10) and (6. 13), we obtain

$$|\mathfrak{F}(k;t)| \leq \text{const}/|k|, \tag{6.18}$$

for $\pi \geq \arg k > (\pi/2) + \epsilon$, $(\pi/2) - \epsilon > \arg k \geq 0$, $\pi/2 \geq \epsilon > 0$, $|k| \gg \gamma$, for fixed t in the range $0 \geq t > -4\gamma^2$. Consequently, we have the following unsubtracted dispersion relation[28] for $f(E;t) = \mathfrak{F}(k;t)$:

$$f(E;t) = \sum_{i=1}^{I} \sum_{j=1}^{J_i} \frac{d_{ij}(t)}{(E-E_i)^j} + \frac{1}{\pi} \int_0^\infty dE' \frac{\text{Im} f(E';t)}{E'-E} - \frac{1}{2\pi i} \int_{C(\epsilon)} dE' \frac{f(E';t)}{E'-E}, \tag{6.19}$$

(Fig. 3) where $E \neq E_i$, E is not on the cut from 0 to ∞ and is on the right of the contour $C(\epsilon)$, the E_i's are the negative bound state energies for the system in the lth angular momentum state, which are greater than $-\gamma^2$, for all l. ϵ may be taken arbitrarily small.

$C(\epsilon)$ is the curve consisting of parts of the two half-lines at an angle $\epsilon > 0$ with the negative real axis and on the left of the imaginary axis, and part of a straight line parallel to the imaginary axis and at a distance ϵ to the right of $E' = -\gamma^2$. ϵ is less than $\pi/2$ and γ^2 and is sufficiently small so that all E_i are on the right of $C(\epsilon)$.

7. THE REGULAR SOLUTION, THE JOST SOLUTIONS, THE JOST FUNCTIONS AND A REPRESENTATION OF THE S MATRIX, FOR $l = 0$

In this section we are concerned with solution of the s wave radial Schrödinger equation, the Jost functions, and a representation of the S matrix in terms of the Jost functions, for $l = 0$, for potentials satisfying Conditions (A).

A. The regular solution

We introduce the following integral equation, for $|\mathrm{Im}k| < \gamma$:

$$\varphi(k;x) = (\sin kx/k) + \int_0^\infty dx'\, K^{(1)}(k;x,x')\,\varphi(k;x'),\ x > 0, \tag{7.1}$$

where

$$K^{(1)}(k;x,x') = (1/k)\int_0^\infty dx''\,\sin k(x-x'')\,V_0(x'',x'). \tag{7.2}$$

$K^{(1)}(k;x,x')$ is holomorphic in all its variables in the whole k plane, $\mathrm{Re}x > 0$ and $\mathrm{Re}x' > 0$.

For $|\mathrm{Im}k| < \gamma - \epsilon$, $\gamma > \epsilon > 0$, $x \geq 0$, and $\mathrm{Re}x' > 0$, we have the following bound obtainable from (2.2a) and (2.2b):

$$|K^{(1)}(k;x,x')| \leq \text{const}\cdot x\, e^{|\mathrm{Im}k|x}\, |e^{-\gamma x'}/x'^{\delta}|. \tag{7.3}$$

We also have

$$|K^{(1)}(k;x,x')| \leq \mathcal{K}^{(1)}(k;x)\,|e^{-\gamma x'}/x'^{\delta}|, \tag{7.4}$$

for $|\mathrm{Im}k| < \gamma$, $\mathrm{Re}x > 0$, $\mathrm{Re}x' > 0$, where $\mathcal{K}^{(1)}(k;x)$ is continuous in $|\mathrm{Im}k| < \gamma$, $\mathrm{Re}x > 0$.

For $k > 0$, (7.1) has a unique bounded continuous solution given by[7]

$$\varphi(k;x) = \frac{\sin kx}{k} + \int_0^\infty dx'\,\frac{\Delta^{(1)}(k;x,x')}{\Delta^{(1)}(k)}\cdot\frac{\sin kx'}{k}, \tag{7.5}$$

when $\Delta^{(1)}(k) \neq 0$, where $\Delta^{(1)}(k)$ and $\Delta^{(1)}(k;x,x,x')$ are the Fredholm determinant and the Fredholm minor, respectively, of the kernel $K^{(1)}(k;x,x')$. This solution belongs to $C^\infty(0,\infty)$, is a solution of (2.11) for $l = 0$, and satisfies the following relationships at the origin:

$$\varphi(k;x=0) = 0,\qquad \frac{d}{dx}\varphi(k;x=0) = 1. \tag{7.6}$$

Using (7.3) and (7.4), we may define the Fredholm determinant and the Fredholm minor, $\Delta^{(1)}(k)$ and $\Delta^{(1)}(k;x,x')$, in $|\mathrm{Im}k| < \gamma$, $\mathrm{Re}x > 0$, $\mathrm{Re}x' > 0$, by Fredholm series, and so defined, $\Delta^{(1)}(k)$ is holomorphic in $|\mathrm{Im}k| < \gamma$, and $\Delta^{(1)}(k;x,x')$ is holomorphic in k, x, and x', in $|\mathrm{Im}k| < \gamma$, $\mathrm{Re}x > 0$, and $\mathrm{Re}x' > 0$. And for $|\mathrm{Im}k| < \gamma - \epsilon$, $\gamma > \epsilon > 0$, $x \geq 0$, $\mathrm{Re}x' > 0$, we have

$$|\Delta^{(1)}(k;x,x')| \leq \text{const}\cdot x\cdot e^{|\mathrm{Im}k|x}\,|e^{-\gamma x'}/x'^{\delta}|. \tag{7.7}$$

For $|\mathrm{Im}k| < \gamma$, (7.5) defines a function $\varphi(k;x), x \geq 0$, which is a $C^\infty(0,\infty)$ solution of (7.1) (see Ref. 7) and of (2.11) for $l = 0$, and which satisfies (7.6). We call this solution the regular solution. Further, the function $\varphi(k;x)$ can be extended, via (7.5), to a function holomorphic in k and x, in $|\mathrm{Im}k| < \gamma$ and $\mathrm{Re}x > 0$.

As in Sec. 5, we may continue $\Delta^{(1)}(k)$ to a function holomorphic in Π. If we call this function by $\Delta^{(1)}(k)$ also, then in the strip $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$, we have a representation of $\Delta^{(1)}(k)$ given by (5.5) and (5.2) with $\Delta_l(k)$ replaced by $\Delta^{(1)}(k)$, $\Delta^{\omega}_{l,n}(k)$ replaced by $\Delta^{(1)\,\omega}_n(k)$, and $A_l(k;|x|e^{i\omega},|x'|e^{i\omega})$ replaced by

$$A^{(1)}(k;|x|e^{i\omega},|x'|e^{i\omega}) = \frac{1}{k}\int_0^{|x|} d|x''|\,e^{i\omega}\sin[k(|x|-|x''|)e^{i\omega}] \times \frac{e^{-\gamma|x''|e^{i\omega}}}{|x''|^{\delta}e^{i\delta\omega}}\,\tilde V_0(|x''|e^{i\omega},|x'|e^{i\omega}), \tag{7.8}$$

where we have used the inequality

$$|A^{(1)}(k;|x|e^{i\omega},|x'|e^{i\omega})| \leq \text{const}\cdot|x|\,e^{|\mathrm{Im}ke^{i\omega}||x|} \tag{7.9}$$

for $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega - \epsilon$, $\gamma\cos\omega > \epsilon > 0$, and ω fixed.

We may also extend the function

$$g^{(1)}(k;x) = \int_0^\infty dx'\,\Delta^{(1)}(k;x,x')(\sin kx'/k) \tag{7.10}$$

to a function holomorphic in k and x, for k in Π and $\mathrm{Re}x > 0$, which we shall also call $g^{(1)}(k;x)$. Hence $\varphi(k;x)$ has been extended to a function holomorphic in k and x, for k in Π, perhaps with the exception of poles at the zeroes of $\Delta^{(1)}(k)$, and $\mathrm{Re}x > 0$, via

$$\varphi(k;x) = (\sin kx/k) + g^{(1)}(k;x) \tag{7.11}$$

which we shall also call $\varphi(k;x)$. For k in the strip $|\mathrm{Im}ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$, and for $\mathrm{Re}x > 0$, $\varphi(k;x)$ has a representation given by (5.19) and (5.20) with $\psi_l(k;x)$ replaced by $\varphi(k;x)$, $\psi^{\omega}_{l,n}(k;x)$ replaced by $\varphi^{\omega}_n(k;x)$, $(k|x'|e^{i\omega})\cdot j_l(k|x'|e^{i\omega})$ replaced by $\sin(k|x'|e^{i\omega})/k$, and $A_l(k;x,|x'|e^{i\omega})$, $A_l(k;|x_1|e^{i\omega},|x'|e^{i\omega})$, etc., replaced by $A^{(1)}(k;x,|x'|e^{i\omega})$, $A^{(1)}(k;|x_1|e^{i\omega},|x'|e^{i\omega})$, etc., with

$$A^{(1)}(k;x,|x'|e^{i\omega}) = (1/k)\int_0^x dx''\,\sin k(x-x'')(e^{-\gamma x''}/x''^{\delta}) \times \tilde V_0(x'',|x'|e^{i\omega}).$$

For $k > 0$, $\Delta_0(k) \neq 0$, $\Delta^{(1)}(k) \neq 0$, we have

$$\psi_0(k;x) = G(k)\,\varphi(k;x),\qquad G(k) \neq 0, \tag{7.12}$$

since then (2.11) has a unique bounded solution with absolutely continuous first derivative and vanishing at the origin, for $l = 0$. The function $G(k)$ is sectionally continuous.

We have the following symmetry properties, for k in Π:

$$\Delta^{(1)}(-k) = \Delta^{(1)}(k),\qquad \Delta^{(1)}(k^*) = \Delta^{(1)}(k)^*, \tag{7.13}$$

$$\varphi(-k;x) = \varphi(k;x),\quad \mathrm{Re}x > 0,\qquad \varphi(k^*;x) = \varphi(k;x)^*,\quad x \geq 0. \tag{7.14}$$

Using

$$|A^{(1)}(k;|x|e^{i\omega},|x'|e^{i\omega})| \leq \text{const}/|k|\cos^2\omega,\qquad k \neq 0, \tag{7.15}$$

for $k = \pm|k|e^{i\omega}$, all ω in $\pi/2 > \omega > -\pi/2$, we obtain

$$\Delta^{(1)}(k) \xrightarrow[|k|\to\infty]{} 1 \tag{7.16}$$

uniformly in the region $(\pi/2) - \epsilon \geq |\arg(\pm k)| \geq 0$, $\pi/2 > \epsilon > 0$. Hence the zeroes of $\Delta^{(1)}(k)$ in the region $(\pi/2) - \epsilon \geq |\arg(\pm k)| \geq 0$, $\pi/2 > \epsilon > 0$, and also in the region $|\mathrm{Im}k| \leq \gamma - \epsilon$, $\gamma > \epsilon > 0$, are finite in number.

We may define $\Delta_0(k)H(k)$ in π via

$$H(k) = k + (1/i)\int_0^\infty dx'\,e^{ikx'}\int_0^\infty dx''\,V_0(x',x'')\psi_0(k;x''). \tag{7.17}$$

Then $\Delta_0(k)H(k)$ is holomorphic in Π. Also we know that $\Delta_0(k)\psi_0(k;x)$ is holomorphic in k and x, for k in Π and $\text{Re}x > 0$. Further, $\psi_0(k;x)/H(k)$ is defined and is holomorphic in k and x, for k in Π, perhaps except at the zeroes of $\Delta_0(k)H(k)$, where there may be poles, and $\text{Re}x > 0$, is a solution of (2.11) for $|\text{Im}k| < \gamma$, $l = 0$, and satisfies (7.6) with $\varphi(k;x)$ replaced by $\psi_0(k;x)/H(k)$. Hence $\psi_0(k;x)/H(k)$, for k in Π and $\text{Re}x > 0$, belongs to the same analytic function as $\varphi(k;x)$. Hence we have obtained another representation for $\varphi(k;x)$.

B. The Jost solutions

We introduce the following integral equations, for $|\text{Im}k| < \gamma$:

$$f^{\pm}(k;x) = e^{\pm ikx} + \int_0^\infty dx'\, K^{(\text{II})}(k;x,x') f^{\pm}(k;x'), \qquad x > 0, \tag{7.18}$$

where

$$K^{(\text{II})}(k;x,x') = (1/k)\int_x^\infty dx'' \sin k(x-x'')\, V_0(x'',x'). \tag{7.19}$$

$K^{(\text{II})}(k;x,x')$ is holomorphic in all its variables in $|\text{Im}k| < \gamma$, $\text{Re}x > 0$, and $\text{Re}x' > 0$. We have

$$|K^{(\text{II})}(k;x,x')| \leqslant \frac{\text{const}}{|k|}\frac{e^{-\gamma x}}{x^\delta}\left|\frac{e^{-\gamma x'}}{x'^\delta}\right|\frac{1}{\gamma-|\text{Im}k|}, \tag{7.20}$$

for $|\text{Im}k| < \gamma$, $k \neq 0$, $x > 0$, $\text{Re}x' > 0$. We also have

$$|K^{(\text{II})}(k;x,x')| \leqslant \text{const}\cdot e^{|\text{Im}k|x}\left|\frac{e^{-\gamma x'}}{x'^\delta}\right|\frac{1}{\gamma-|\text{Im}k|}, \tag{7.21}$$

for $|\text{Im}k| < \gamma$, $x \geqslant 0$, $\text{Re}x' > 0$, using (2.2a) and (2.2b). We therefore obtain

$$|K^{(\text{II})}(k;x,x')| \leqslant \frac{\text{const}}{1+|k|}\, e^{-\gamma x}\left|\frac{e^{-\gamma x'}}{x'^\delta}\right|\frac{1}{\gamma-|\text{Im}k|}, \tag{7.22}$$

for $|\text{Im}k| < \gamma$, $x \geqslant 0$, $\text{Re}x' > 0$.

Further, we have

$$|K^{(\text{II})}(k;x,x')| \leqslant \mathcal{K}^{(\text{II})}(k;x)\,|e^{-\gamma x'}/x'^\delta|, \tag{7.23}$$

for $|\text{Im}k| < \gamma$, $\text{Re}x > 0$, $\text{Re}x' > 0$, where $\mathcal{K}^{(\text{II})}(k;x)$ is continuous in $|\text{Im}k| < \gamma$, $\text{Re}x > 0$.

For $k > 0$, each of the integral equations of (7.18) has a unique bounded continuous solution $f^{\pm}(k;x)$, respectively, given by[7]

$$f^{\pm}(k;x) = e^{\pm ikx} + \int_0^\infty dx'\, \frac{\Delta^{(\text{II})}(k;x,x')}{\Delta^{(\text{II})}(k)}\, e^{\pm ikx'}, \tag{7.24}$$

when $\Delta^{(\text{II})}(k) \neq 0$, where $\Delta^{(\text{II})}(k)$ and $\Delta^{(\text{II})}(k;x,x')$ are the Fredholm determinant and the Fredholm minor, respectively, of the kernel $K^{(\text{II})}(k;x,x')$. Each of the solutions belongs to $C^\infty(0,\infty)$, is a solution of (2.11) for $l = 0$, and satisfies the following behavior at infinity, respectively:

$$f^{\pm}(k;x) \underset{x\to\infty}{\simeq} e^{\pm ikx}. \tag{7.25}$$

Using (7.22) and (7.23), we may define the Fredholm determinant and the Fredholm minor, $\Delta^{(\text{II})}(k)$ and $\Delta^{(\text{II})}(k;x,x')$, in $|\text{Im}k| < \gamma$, $\text{Re}x > 0$, $\text{Re}x' > 0$, by Fredholm series, and so defined, $\Delta^{(\text{II})}(k)$ is holomorphic in $|\text{Im}k| < \gamma$, and $\Delta^{(\text{II})}(k;x,x')$ is holomorphic in k, x, and x', in $|\text{Im}k| < \gamma$, $\text{Re}x > 0$, $\text{Re}x' > 0$. And for $|\text{Im}k| < \gamma - \epsilon$, $\gamma > \epsilon > 0$, $x \geqslant 0$, $\text{Re}x' > 0$, we have

$$|\Delta^{(\text{II})}(k;x,x')| \leqslant [\text{const}/(1+|k|)]\, e^{-\gamma x}\, |e^{-\gamma x'}/x'^\delta|. \tag{7.26}$$

For $|\text{Im}k| < \gamma$, (7.24) defines functions $f^{\pm}(k;x)$, $x \geqslant 0$, which are $C^\infty(0,\infty)$ solutions of (2.11) for $l = 0$, and which satisfy (7.25). We call these solutions the Jost solutions. Further, the functions $f^{\pm}(k;x)$ can be extended, via (7.24), to functions holomorphic in k and x, in $|\text{Im}k| < \gamma$, $\text{Re}x > 0$.

Again, as in Sec. 5 we may continue $\Delta^{(\text{II})}(k)$ to a function holomorphic in Π. If we call this function $\Delta^{(\text{II})}(k)$ also, then in the strip $|\text{Im}ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$, we have a representation of $\Delta^{(\text{II})}(k)$ given by (5.5) and (5.2) with $\Delta_l(k)$ replaced by $\Delta^{(\text{II})}(k)$, $\Delta^{\omega}_{l,n}(k)$ replaced by $\Delta^{(\text{II})\,\omega}_n(k)$, and $A_l(k;|x|e^{i\omega},|x'|e^{i\omega})$ replaced by

$$\begin{aligned} A^{(\text{II})}&(k;|x|e^{i\omega},|x'|e^{i\omega}) \\ &= (1/k)\int_{|x|}^\infty d|x''|e^{i\omega} \\ &\times \sin[k(|x|-|x''|)e^{i\omega}]\,(e^{-\gamma|x''|e^{i\omega}}/|x''|^\delta e^{i\delta\omega}) \\ &\times \tilde V_0(|x''|e^{i\omega},|x'|e^{i\omega}), \end{aligned} \tag{7.27}$$

where we have used the inequality

$$|A^{(\text{II})}(k;|x|e^{i\omega},|x'|e^{i\omega})| \leqslant \frac{\text{const}}{1+|k|}\cdot\frac{e^{-\gamma|x|\cos\omega}}{\gamma\cos\omega-|\text{Im}ke^{i\omega}|} \tag{7.28}$$

for fixed ω.

We may also extend the functions

$$g^{(\text{II})\pm}(k;x) = \int_0^\infty dx'\, \Delta^{(\text{II})}(k;x,x')\, e^{\pm ikx'} \tag{7.29}$$

to functions holomorphic in k and x, for k in Π and $\text{Re}x > 0$, which we shall call $g^{(\text{II})\pm}(k;x)$ also. Hence $f^{\pm}(k;x)$ have been extended to functions holomorphic in k and x, for k in Π, perhaps with the exception of poles at the zeroes of $\Delta^{(\text{II})}(k)$, and $\text{Re}x > 0$, which we shall call $f^{\pm}(k;x)$ also, via

$$f^{\pm}(k;x) = e^{\pm ikx} + [g^{(\text{II})\pm}(k;x)/\Delta^{(\text{II})}(k)]. \tag{7.30}$$

For k in the strip $|\text{Im}ke^{i\omega}| < \gamma\cos\omega$, $\pi/2 > \omega > -\pi/2$, and for $\text{Re}x > 0$, $f^{\pm}(k;x)$ have representations given by (5.19) and (5.20), with $\psi_l(k;x)$ replaced by $f^{\pm}(k;x)$, $\psi^{\omega}_{l,n}(k;x)$ replaced by $f^{\pm\,\omega}_n(k;x)$, $(k|x'|e^{i\omega})j_l(k|x'|e^{i\omega})$ replaced by $e^{\pm ik|x'|e^{i\omega}}$, and $A_l(k;x,|x'|e^{i\omega})$, $A_l(k;|x_1|e^{i\omega}, |x'|e^{i\omega})$etc., replaced by $A^{(\text{II})}(k;x,|x'|e^{i\omega})$, $A^{(\text{II})}(k;|x_1|e^{i\omega},|x'|e^{i\omega})$, etc., respectively, with

$$\begin{aligned} A^{(\text{II})}&(k;x,|x'|e^{i\omega}) \\ &= (1/k)\int_{|x|}^\infty d|x''|e^{i\omega}\sin[k(x-|x''|e^{i\omega})] \\ &\quad\times(e^{-\gamma|x''|e^{i\omega}}/|x''|^\delta e^{i\delta\omega})\,\tilde V_0(|x''|e^{i\omega},|x'|e^{i\omega}) \\ &\quad+ (1/k)\int_C dx''\sin k(x-x'')\,(e^{-\gamma x''}/x''^\delta)\,\tilde V_0(x'',|x'|e^{i\omega}), \end{aligned} \tag{7.31}$$

where C is an arc from x to $|x|e^{i\omega}$.

We have the following symmetry properties:

$$\begin{aligned} \Delta^{(\text{II})}(-k) &= \Delta^{(\text{II})}(k), \\ \Delta^{(\text{II})}(k^*) &= \Delta^{(\text{II})}(k)^*, \end{aligned} \tag{7.32}$$

$$\begin{aligned} f^-(-k;x) &= f^+(k;x), && k \text{ real}, \text{Re}x > 0, \\ f^{\pm}(-k^*;x) &= f^{\pm}(k;x)^*, && x \geqslant 0, \\ f^-(k^*;x) &= f^+(k;x)^*, && x \geqslant 0. \end{aligned} \tag{7.33}$$

Using

$$|A^{(\text{II})}(k;|x|e^{i\omega},|x'|e^{i\omega})| \leqslant \text{const}/|k|\cos^2\omega, \quad k \neq 0, \tag{7.34}$$

for $k = \pm|k|e^{i\omega}$, all ω in $\pi/2 > \omega > -\pi/2$, we obtain

$$\Delta^{(\text{II})}(k) \xrightarrow[|k|\to\infty]{} 1 \tag{7.35}$$

uniformly in the region $(\pi/2) - \epsilon \geq |\arg(\pm k)| \geq 0$, $\pi/2 > \epsilon > 0$. Hence the number of zeroes of $\Delta^{(II)}(k)$ in this region, and also in the region $|\mathrm{Im}k| \leq \gamma - \epsilon$, $\gamma > \epsilon > 0$, is finite.

We note that the functions $f^{\pm}(k; x = 0)$ are holomorphic in Π, perhaps with the exception of poles at the zeroes of $\Delta^{(II)}(k)$.

If we consider the following integral equations, for $|\mathrm{Im}k| < \gamma$,

$$v^{\pm}(k;x) = e^{\pm ikx} + \int_0^{\infty} dx' K_0(\pm k, x, x')v^{\pm}(k;x'), x > 0, \tag{7.36}$$

then we find, following the arguments concerning $\psi_l(k;x)$, that:

(i) For $k > 0$, each of the equations of (7.36) has a unique bounded continuous solution given explicitly by

$$v^{\pm}(k;x) = e^{\pm ikx} + \int_0^{\infty} dx'[\Delta_0(\pm k; x, x')/\Delta_0(\pm k)]e^{\pm ikx'}, \tag{7.37}$$

when $\Delta_0(\pm k) \neq 0$. The solutions belong to $C^{\infty}(0, \infty)$, satisfy (2.11) for $l = 0$, and have the following asymptotic behavior:

$$v^{\pm}(k;x) \underset{x\to\infty}{=} H^{\pm}(k)e^{\pm ikx} + O(1), \tag{7.38}$$

where

$$H^{\pm}(k) = 1 - \frac{1}{k}\int_0^{\infty} dx' \sin kx' \int_0^{\infty} dx'' \, V_0(x', x'')v^{\pm}(k;x''). \tag{7.39}$$

(ii) For $|\mathrm{Im}k| < \gamma$, the functions defined by (7.37) are $C^{\infty}(0, \infty)$ solutions of (7.36) and of (2.11) for $l = 0$, and satisfy

$$v^{\pm}(k;x) \underset{x\to\infty}{=} H^{\pm}(k)e^{\pm ikx} + o(e^{\pm ikx}) \tag{7.40}$$

with $H^{\pm}(k)$ defined by (7.39) now extended to $|\mathrm{Im}k| < \gamma$.

(iii) The functions $v^{\pm}(k;x)$ can be extended to functions holomorphic in k and x, for k in Π, perhaps with poles at the zeroes of $\Delta_0(\pm k)$, and $\mathrm{Re}x > 0$. We call the extended functions $v^{\pm}(k;x)$ also. For k in the strip $|\mathrm{Im}ke^{i\omega}| < \gamma \cos\omega$, $\pi/2 > \omega > -\pi/2$, they are given by (5.19) and (5.20) with $\psi_l(k;x)$ replaced by $v^{\pm}(k;x)$, $\psi_{l,n}^{\omega}(k;x)$ replaced by $v_n^{\pm\omega}(k;x)$, $(k|x'|e^{i\omega})j_l(k|x'|e^{i\omega})$ replaced by $e^{\pm ik|x'|e^{i\omega}}$ and $A_l(k;x,|x'|e^{i\omega}), A_l(k;|x|e^{i\omega}, |x'|e^{i\omega})$, etc., replaced by $A_0(\pm k;x,|x'|e^{i\omega}), A_0(\pm k; |x|e^{i\omega}, |x'|e^{i\omega})$, etc.

(iv) The functions $v^{\pm}(k;x)$ are continuous at $x = 0$, from $\mathrm{Re}x > 0$, for k in Π and $\Delta_0(\pm k) \neq 0$.

We may define $\Delta_0(\pm k)H^{\pm}(k)$ in Π via (7.39) and using contour rotation. Then $\Delta_0(\pm k)H^{\pm}(k)$ is holomorphic in Π. Also we know that $\Delta_0(\pm k)v^{\pm}(k;x)$ are holomorphic in k and x, for k in Π and $\mathrm{Re}x > 0$. Further, $v^{\pm}(k;x)/H^{\pm}(k)$ are defined and are holomorphic in k and x, for k in Π, perhaps except at the zeroes of $\Delta_0(\pm k)H^{\pm}(k)$, where there may be poles, and $\mathrm{Re}x > 0$, are solutions of (2.11) for $|\mathrm{Im}k| < \gamma$, $l = 0$, and satisfy (7.25) with $v^{\pm}(k;x)/H^{\pm}(k)$ in place of $f^{\pm}(k;x)$. Hence $v^{\pm}(k;x)/H^{\pm}(k)$, for k in Π and $\mathrm{Re}x > 0$, belong to the same analytic functions as $f^{\pm}(k;x)$, respectively. Hence we have obtained further representations for $f^{\pm}(k;x)$. We have $\Delta_0(-k^*)H^-(k^*) = \Delta_0(k)^* \times H^+(k)^*$.

We note that from their behavior as $x \to \infty$, we find that $f^{\pm}(k,x)$ are linearly independent when they are both defined, and when $|\mathrm{Im}k| < \gamma$, $k \neq 0$.

We also note that from the representations $v^{\pm}(k;x)/H^{\pm}(k)$ of $f^{\pm}(k;x)$, the functions $f^{\pm}(k;x)$ are holomorphic in k and x, for k in Π, perhaps with the exception of poles where both $\Delta^{(II)}(k)$ and $\Delta_0(\pm k)H^{\pm}(k)$ are zero, and $\mathrm{Re}x > 0$. A similar remark applied to the function $\varphi(k;x)$.

C. The Jost functions and a representation of the *S* matrix

We consider first $k > 0$, and $\Delta_0(k) \neq 0$, $\Delta^{(I)}(k) \neq 0$, $\Delta^{(II)}(k) \neq 0$. Then we know that the functions $f^{\pm}(k;x)$ are linearly independent solutions of (2.11) for $l = 0$, and that any bounded solution of (2.11) for $l = 0$, and that any bounded solution of (2.11) for $l = 0$, and with absolutely continuous first derivative is a linear combination of $f^{\pm}(k;x)$. Further, one and only one bounded solution of (2.11) exists, for $l = 0$, and with absolutely continuous first derivative, which vanishes at the origin. Hence we have

$$\psi_0(k;x) = G(k)\varphi(k;x), \qquad G(k) \neq 0, \tag{7.41}$$

$$\varphi(k;x) = (1/2ik)[\mathcal{L}^-(k)f^+(k;x) - \mathcal{L}^+(k)f^-(k;x)], \tag{7.42}$$

for $x \geq 0$ and $\mathrm{Re}x > 0$, where $\mathcal{L}^+(k)$ and $\mathcal{L}^-(k)$ are not both zero.

Taking the Wronskian of both sides of (7.42) with $f^+(k;x)$, we obtain

$$\mathcal{L}^+(k) = -2ik \frac{W[f^+(k;x), \varphi(k;x)]_{x=\infty}}{W[f^+(k;x), f^-(k;x)]_{x=\infty}}. \tag{7.43}$$

From the behaviors as $x \to \infty$ of $f^{\pm}(k;x)$ and their derivatives, we obtain

$$W[f^+(k;x), f^-(k;x)] = -2ik. \tag{7.44}$$

Further, since both $f^+(k;x)$ and $\varphi(k;x)$ satisfy (2.11) for $l = 0$, we have

$$W[f^+(k;x), \varphi(k;x)]_{x=\infty} = W[f^+(k;x), \varphi(k;x)]_{x=0}. \tag{7.45}$$

Consequently, from (7.6) we obtain

$$W[f^+(k;x), \varphi(k;x)]_{x=\infty} = f^+(k;x=0). \tag{7.46}$$

Hence

$$\mathcal{L}^+(k) = f^+(k;x=0). \tag{7.47}$$

Similarly, we obtain

$$\mathcal{L}^-(k) = f^-(k;x=0). \tag{7.48}$$

From (7.25), (7.41), and (7.42), we have

$$\psi_0(k;x) \underset{x\to\infty}{\simeq} [G(k)/2ik][\mathcal{L}^-(k)e^{ikx} - \mathcal{L}^+(k)e^{-ikx}]. \tag{7.49}$$

From Sec. 2 we have

$$\psi_0(k;x) \underset{x\to\infty}{\simeq} e^{i\delta_0(k)} \sin[kx + \delta_0(k)] \tag{7.50}$$

where $\delta_0(k)$ is the s-wave phase shift. Hence we obtain

$$\mathcal{L}^+(k) = k/G(k), \tag{7.51}$$

$$\mathcal{L}^-(k) = [k/G(k)]e^{2i\delta_0(k)} = [k/G(k)]S_0(k). \tag{7.52}$$

Hence the s-wave S matrix has the following representation:

$$S_0(k) = \mathcal{L}^-(k)/\mathcal{L}^+(k). \tag{7.53}$$

We also have

$$\psi_0(k;x) = [k/\mathcal{L}^+(k)]\varphi(k;x). \tag{7.54}$$

If we define $\mathcal{L}^{\pm}(k)$ by (7.47) and (7.48) whenever $f^{\pm}(k; x=0)$ are defined in the k plane, then $\mathcal{L}^{\pm}(k)$ are holomorphic in Π, perhaps with the exception of poles where both $\Delta^{\text{II}}(k)$ and $\Delta_0(\pm k) H^{\pm}(k)$ are zero. Consequently, the representation (7.53) can be extended to Π. We call $\mathcal{L}^{\pm}(k)$ Jost functions. We have, from (7.33),

$$\mathcal{L}^{-}(k^*) = \mathcal{L}^{+}(k)^*. \qquad (7.55)$$

The relationships (7.42) and (7.54) may be similarly extended.

A REMARK

We remark that it can be shown[29] that all bound state poles corresponding to energies E_i with $0 > E_i > -\gamma^2$ in the dispersion relation (6.19) and the dispersion relations in Ref. 1 are necessarily simple.

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[1] T. H. Yao, J. Math. Phys. **14**, 1141 (1973).

[2] M. Bertero, G. Talenti, and G. A. Viano, Nucl. Phys. A **113**, 625 (1968).

[3] We use (Ref. 4, p. 100) $|P_l(\cos\theta)| \leqslant \text{const} \cdot \exp[(l+\frac{1}{2})|\text{Im}\theta|]/[(\sin\theta)^{1/2}(l+\frac{1}{2})^{1/2}]$.

[4] V. De Alfaro and T. Regge, *Potential Scattering* (North-Holland, Amsterdam, 1965).

[5] Equations (2.2a) and (2.2b) appear in Ref. 6. Equations (2.2c) and (2.2d) follow from (2.2a) and (2.2b) by using recursion relations for $j_l(z)$ and $h_l^{(1)}(z)$.

[6] R. G. Newton: J. Math. Phys. 1, 319 (1960).

[7] W. V. Lovitt, *Linear Integral Equations* (Dover, New York, 1950). The discussions in this reference are concerned with real continuous functions on a bounded interval. However, the arguments and the results remain valid in all cases discussed in this paper where this reference is quoted.

[8] We mean, here and afterwards, absolute continuity in the open interval $\infty > x > 0$.

[9] We use the method of variation of constants: cf. Ref. 4, Appendix B.

[10] Here we follow Ref. 11.

[11] M. Bertero, G. Talenti, and G. A. Viano, Comm. Math. Phys. **6**, 128 (1967).

[12] See Refs. 13 and 14. Here $\Delta_l(-k)$ is defined, for $k > 0$, by (2.6) and (2.7).

[13] R. G. Newton, *Scattering Theory of Particles and Waves* (McGraw-Hill, New York, 1966).

[14] F. Smithies, *Integral Equations* (Cambridge U. P., Cambridge, 1958).

[15] We use Hadamard's theorem. See Ref. 14.

[16] Again, we use the method of variation of constants. See Ref. 4, Appendix B.

[17] M. Bertero, G. Talenti, and G. A. Viano, Nuovo Cimento **62**, 27 (1969); and K. Yosida, *Functional Analysis* (Springer, Berlin, 1968). $W^{2,2}(R^3)$, a Sobolev space, is the domain of definition of our Hamiltonian operator of the system.

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[19] From Ref. 7, $\psi_l(k; x)$ satisfies (2.4) and consequently (2.11).

[20] E. C. Titchmarsh, *The Theory of Functions* (Oxford U. P., London 1950).

[21] We use the Principle extended to the case of two complex variables.

[22] This may be obtained using a method similar to that in Appendix 3 of Ref. 1.

[23] A. Martin, Nuovo Cimento 23, 641 (1962).

[24] *Bateman Manuscript. Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. 1.

[25] See Ref. 4, p. 100. Using Cauchy's integral formula, we may show from this inequality, that for any $\epsilon > 0$, there is an $\epsilon_1 > 0$ such that $|P_l(\cos\theta)| \leqslant \text{constant} \cdot \exp[(l+\frac{1}{2})\epsilon]/(l+\frac{1}{2})$, for $\epsilon_1 > |\cos\theta - 1| \geqslant 0$;

[26] For a proof of what follow concerning $\rho_l(k; x', \beta'')$, see Ref. 22.

[27] To prove the first inequality to follow, we have: $(d/d\xi)\,\text{Re}\,(k^2+\xi^2)^{1/2} = \xi[\text{Re}(k^2+\xi^2)^{1/2}/|k^2+\xi^2|]$.

[28] See REMARK at the end of this paper

[29] T. H. Yao, J.Math.Phys. 15,(1974), next article.

On analytic nonlocal potentials. III. Local correlations

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We give examples of "analytic nonlocal potentials" which show local correlations for a finite range of the distance, bounded below and above.

1. INTRODUCTION

Any potential between two nucleons is nonlocal at small distances and becomes approximately local at large distances. Recently, studies have been made on a class A of analytic nonlocal potentials, and a subclass C of it, and dispersion relations have been obtained.[1,2] In this article we show, by explicit construction, that there exist potentials within these classes which show local correlations in a finite range of the distance, for distances neither too small nor too large. These examples suggest that the classes A and C might be sufficiently wide to include potentials having the properties mentioned in the beginning of this paragraph.

2. LOCAL CORRELATIONS

We first consider the class A of analytic nonlocal potentials $V(\mathbf{x},\mathbf{x}')$ defined by the following conditions (A):

(A1) $V(\mathbf{x},\mathbf{x}')$ is real, $V(\mathbf{x},\mathbf{x}')=V(\mathbf{x}',\mathbf{x})$

(A2) $V(\mathbf{x},\mathbf{x}')$ is rotationally invariant:

$$V(\mathbf{x},\mathbf{x}')=V(x,x',\cos\nu)$$

$$x=|\mathbf{x}|>0,\quad x'=|\mathbf{x}'|>0,\quad 1\geqslant\cos\nu\geqslant-1,$$

where ν is the angle between $\mathbf{x}$ and $\mathbf{x}'$.

(A3) $$V(x,x',\cos\nu)=\frac{\exp(-\gamma x)(x+a)^m}{x^\alpha}\tilde{V}(x,x',\cos\nu)\times\frac{\exp(-\gamma x')(x'+a)^m}{x'^\alpha},\quad\gamma>0,\quad a>0,$$

$$m\geqslant0,\quad\tfrac{3}{2}>\alpha\geqslant0,$$

where $\tilde{V}(x,x',\cos\nu)$ is holomorphic in x and x', in $\mathrm{Re}x>0$, $\mathrm{Re}x'>0$, for $1\geqslant\cos\nu\geqslant-1$, and continuous in all these variables in $\mathrm{Re}x>0$, $\mathrm{Re}x'>0$, $1\geqslant\cos\nu\geqslant-1$, and

$$|\tilde{V}(x,x',\cos\nu)|\leqslant\text{const.}$$

for $\mathrm{Re}x>0$, $\mathrm{Re}x'>0$, $1\geqslant\cos\nu\geqslant-1$.

The following potential $V_1(\mathbf{x},\mathbf{x}')$ belongs to this class:

$$V_1(\mathbf{x},\mathbf{x}')=\exp(-\gamma x)\tilde{V}_1(x,x',\cos\nu)\exp(-\gamma x'),$$

where

$$\tilde{V}_1(x,x',\cos\nu)=g\exp\left\{-\tau_1\left(\frac{x}{x+b}\right)^{1/2}\left[\ln\left(\frac{x+c}{x'+c}\right)\right]^2\right\}\times\exp\left\{-\tau_1\left(\frac{x'}{x'+b}\right)^{1/2}\left[\ln\left(\frac{x+c}{x'+c}\right)\right]^2\right\}\cdot\exp[-\tau_2(xx')^{1/2}u]$$

with g real, $\tau_1>0$, $\tau_2>0$, $b>0$, $c>0$, and $u=1-\cos\nu$.

The function $\tilde{V}_1(x,x',\cos\nu)$ is bounded in $\mathrm{Re}x>0$, $\mathrm{Re}x'>0$, $1\geqslant\cos\nu\geqslant-1$, since $\mathrm{Re}(xx')^{1/2}u\geqslant0$ for these values of x, x', and $\cos\nu$, and since the functions

$$f_1(x,x')=\left(\frac{x}{x+b}\right)^{1/2}\left[\ln\left(\frac{x+c}{x'+c}\right)\right]^2,$$

$$f_2(x,x')=\left(\frac{x'}{x'+b}\right)^{1/2}\left[\ln\left(\frac{x+c}{x'+c}\right)\right]^2,$$

map the region $\mathrm{Re}x>0$, $\mathrm{Re}x'>0$ onto a region in the complex z plane which lies to the right of $\mathrm{Re}z=p$, for some $p<0$.

We next consider a subclass C of A, namely the class of $V(\mathbf{x},\mathbf{x}')$ satisfying Conditions (A) with $\tilde{V}(x,x',\cos\nu)$ satisfying the following Condition (C)[3]:

(C) $$\tilde{V}(x,x',\cos\nu)=\int_0^\infty\int_0^\infty d\beta\,d\beta'\exp(-\beta x)\times\exp(-\beta'x')\sigma(\beta,\beta',\cos\nu).$$

where $\sigma(\beta,\beta',\cos\nu)$ satisfies

(i) $\sigma(\beta,\beta',\cos\nu)$ is real, $\sigma(\beta,\beta',\cos\nu)=\sigma(\beta',\beta,\cos\nu)$;

(ii) $\sigma(\beta,\beta',\cos\nu)$ is continuous in β, β', and $\cos\nu$ in $\infty>\beta>0$, $\infty>\beta'>0$, $1\geqslant\cos\nu\geqslant-1$, and in this region

$$|\sigma(\beta,\beta',\cos\nu)|\leqslant\Sigma(\beta,\beta'),$$

$$\Sigma(\beta,\beta')=\Sigma(\beta',\beta),$$

$$\int_0^\infty\int_0^\infty d\beta\,d\beta'\,\Sigma(\beta,\beta')<\infty,$$

where $\Sigma(\beta,\beta')$ is continuous in β and β', in $\infty>\beta>0$, $\infty>\beta'>0$.

The following potential $V_2(\mathbf{x},\mathbf{x}')$ belongs to C:

$$V_2(\mathbf{x},\mathbf{x}')=\exp(-\gamma x)(x+a)^s\tilde{V}_2(\mathbf{x},\mathbf{x}',\cos\nu)\times\exp(-\gamma x')(x'+a)^s,$$

where

$$\tilde{V}_2(x,x',\cos\nu)=\frac{\gamma^2x^2}{(x+a)^s}\tilde{V}_1(x,x',\cos\nu)\frac{\gamma^2x'^2}{(x'+a)^s}$$

satisfies Condition (C) for some integer $s>0$. This follows from a slight extension of a result on a set of sufficient conditions for a function of two complex variables to be a double Laplace transform of a continuous, bounded, symmetric, and absolutely integrable spectral function $\sigma(\beta,\beta')$ satisfying[4]:

$$|(1+\beta)^2\sigma(\beta,\beta')(1+\beta')^2|\leqslant\text{const.},\quad\infty>\beta\geqslant0,\quad\infty>\beta'\geqslant0.$$

We now consider local correlations for the potential $V_1(\mathbf{x},\mathbf{x}')$. We have

$$V_1(\mathbf{x},\mathbf{x}')=g\exp(-\gamma x)f(x,x')f(x',x)\exp[-\tau_2(xx')^{1/2}u]\times\exp(-\gamma x'),$$

$$f(x,x')=\exp[-\tau_1f_1(x,x')],$$

$V_1(\mathbf{x},\mathbf{x}) = g\exp[-2\gamma x],$

$|V_1(\mathbf{x},\mathbf{x}')| \leq |g|\exp[-\gamma x]W(x,x')$

with

$$W(x,x') = f(x,x')\exp(-\gamma x').$$

We consider, for fixed $x>0$, values of x' satisfying

$$|x'-x| \geq x/10 \tag{2.1}$$

For these values of x', we have

$$|V_1(\mathbf{x},\mathbf{x}')| \leq D|V_1(\mathbf{x},\mathbf{x})|,$$

where $D \ll 1$, if

$$\tau_1\left(\frac{x}{x+b}\right)^{1/2}\left(\frac{x}{x+c}\right)^2 \geq 100(\gamma x + A) \tag{2.2}$$

where we have put $D=\exp(-A)$. For suitable values of τ_1, b, c, and A, this inequality is satisfied if and only if x lies in some interval $[d_1, d_2]$, $d_2 > d_1 > 0$. Hence for these values of x, $|V_1(\mathbf{x},\mathbf{x}')|$ is very small compared with $|V_1(\mathbf{x},\mathbf{x})| = |g|\exp(-2\gamma x)$ for values of x' satisfying (2.1).

We have the following example of choices of τ_1, b, c, A and approximate values of d_1 and d_2:

$\tau_1 = 10^4$, $b=10/\gamma$, $c=5/\gamma$, $A=10$, $d_1 \approx 2/\gamma$, $d_2 \approx 100/\gamma$

For values of x' satisfying

$$|x'-x| \leq x/10$$

and for $x\in[d_1,d_2]$ with suitable choice of τ_1, b, c, and A, we may choose τ_2 large enough so that

$$\exp[-\tau_2(xx')^{1/2}u] \ll 1$$

for u outside some interval $[0,\rho]$, where ρ satisfying $2>\rho>0$ may be initially chosen arbitrarily small. Hence we have shown that with suitable choice of τ_1, τ_2, b, c, we have

$$|V_1(\mathbf{x},\mathbf{x}')| \leq D|V_1(\mathbf{x},\mathbf{x})| = D|g|\exp(-2\gamma x) \tag{2.3}$$

with $D\ll 1$, for $x\in[d_1,d_2]$ and for $\mathbf{x}'$ outside the region $|x'-x|\leq x/10$, $1\geq \cos\nu \geq 1-\rho$, $1\gg\rho>0$. Hence the potential $V_1(\mathbf{x},\mathbf{x}')$ shows local correlations for $x\in[d_1,d_2]$, with suitable choice of τ_1, τ_2, b, c, and A. For x sufficiently small or sufficiently large, there is no local correlation.

Similarly, for values of x' satisfying (2.1), we have

$$|V_2(\mathbf{x},\mathbf{x}')| \leq D|V_2(\mathbf{x},\mathbf{x})|$$

with $D\ll 1$, if

$$\tau_1\left(\frac{x}{x+b}\right)^{1/2}\left(\frac{x}{x+c}\right)^2 \geq 100(\gamma x + A), \quad \gamma x \geq 1, \tag{2.4a}$$

$$\tau_1\left(\frac{x}{x+b}\right)^{1/2}\left(\frac{x}{x+c}\right)^2 \geq 100(\gamma x + A - \ln(\gamma x)^2), \quad \gamma x < 1 \tag{2.4b}$$

Again, for suitable values of τ_1, b, c, and A, (2.4a) or both (2.4a) and (2.4b) are satisfied if and only if x lies in some interval $[d_1', d_2']$, $d_2' > d_1' > 0$. For these values of x, $|V_2(\mathbf{x},\mathbf{x}')|$ is very small compared with $|V_2(\mathbf{x},\mathbf{x})| = |g|(\gamma x)^4\exp(-2\gamma x)$ for values of x' satisfying (2.1). For a choice of τ_1, b, c, and A which is the same as the example given for $V_1(\mathbf{x},\mathbf{x}')$, we obtain $d_1' \approx 2/\gamma$, $d_2' \approx 100/\gamma$.

Again, by choosing τ_2 sufficiently large, $|V_2(\mathbf{x},\mathbf{x}')|$ is very small compared with $|V_2(\mathbf{x},\mathbf{x})|$, i.e.,

$$|V_2(\mathbf{x},\mathbf{x}')| \leq D|V_2(\mathbf{x},\mathbf{x})| = D|g|(\gamma x)^4\exp(-2\gamma x) \tag{2.5}$$

with $D\ll 1$, for $x\in[d_1',d_2']$ and for $\mathbf{x}'$ outside the region $|x'-x|\leq x/10$, $1\geq\cos\nu\geq 1-\rho$, $1\gg\rho>0$. Hence the potential $V_2(\mathbf{x},\mathbf{x}')$ shows local correlations for $x\in[d_1',d_2']$ with suitable choice of τ_1, τ_2, b, c, and A. For x sufficiently small or sufficiently large, there is no local correlation.

Remark: After this article was completed, we found, in Ref. 5, an investigation on the analyticity in k of the S matrix for real and complex angular momentum for examples of nonseparable nonlocal potentials.

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[1]T. H. Yao, J. Math. Phys. 14, 1141 (1973).
[2]T. H. Yao, J. Math. Phys. 15, 1211 (1974).
[3]In Ref. 2 we considered the case m integral and $\alpha = \frac{1}{2}$. See also Ref. 1 for a similar class with $m=0$, $\alpha = 0, \frac{1}{2}, 1$.
[4]See Ref. 1, Appendix B.
[5]L. S. Chou and Y. B. Dai, Scientia Sinica 4, 695 (1965).

The T operator and an inverse problem for nonlocal potentials

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For a class of short-ranged nonlocal potentials, the T operator $T(k)$ is studied in the region $\text{Im}k > -\gamma$, where $\gamma > 0$ is some parameter of the potential. Inversion formulas are obtained which determine the potential from $t(E) = T(\sqrt{E})$ for any real E, for which $t(E)$ is defined, perhaps with the exception of a countable set of points.

1. INTRODUCTION

The two-particle T operator $t(E)$, where E is real, defined by

$$t(E) = V + \lim_{\epsilon\to 0+} V \frac{1}{E + i\epsilon - H} V,$$

where this limit exists,[1] and where V is the interparticle potential and H the internal Hamiltonian, occurs in the theory of three-particle systems[2] with local pair interactions. It is of interest to study the T operator for nonlocal potentials.

In this article we first study the two-particle T operator $T(k)$ in $\text{Im}k > -\gamma$, where $\gamma > 0$ is some parameter of the potential, for a class of rotationally invariant hermitian short-ranged purely nonlocal potentials. We find that $T(k)$ is a Hilbert–Schmidt operator in $L^2(R^3)$ holomorphic in $\text{Im}k > -\gamma$, with the exception of a finite number of simple poles at $\sqrt{E_i^-}$, $i = 1, 2, \cdots, N^-$, on the upper imaginery axis, for all the negative energy eigenvalues $E_i^- < 0$, a finite number of simple poles at $\pm\sqrt{E_i^+}$, $i = 1, 2, \cdots, N^+$, on the real axis, for all the positive energy eigenvalues $E_i^+ > 0$, and perhaps with the exception of a double pole at $k = 0$ and poles in $0 > \text{Im}k > -\gamma$. The function $t(z) = T(\sqrt{z})$ is analytic in $\text{Im}\sqrt{z} > -\gamma$ in the two-sheeted z plane with a branch point at $z = 0$, whose only singularities in the first sheet $2\pi > \arg z \geqslant 0, z \neq 0$, are simple poles at $z = E_i^-$ and $z = E_i^+$. We then show that for any real E, for which the operator $t(E)$ is defined, perhaps with the exception of a countable set of points, the potential can be expressed in terms of the kernel of the integral operator $t(E)$ by Fredholm series. The coordinate space is used in these considerations.

Results on the pole structure of the scattering amplitude $F(k; \cos\theta)$ in $\text{Im}k > 0$, for physical scattering angle, i.e., for $1 \geqslant \cos\theta \geqslant -1$, are obtained as a corollary.

The problem of determining a two-particle T operator $t(E)$, for some real E for which it is defined, from properties of a three-particle system, is interesting.

The class of potentials $V(\mathbf{x}, \mathbf{x}')$ which we study here are defined by the following conditions[3-4]

(1) $V(\mathbf{x}, \mathbf{x}')$ is real, $V(\mathbf{x}, \mathbf{x}') = V(\mathbf{x}', \mathbf{x})$;

(2) $V(\mathbf{x}, \mathbf{x}')$ is rotationally invariant:

$$V(\mathbf{x}, \mathbf{x}') = V(x, x', \cos\nu), \quad x = |\mathbf{x}| > 0, \quad x' = |\mathbf{x}'| > 0, \quad 1 \geqslant \cos\nu \geqslant -1,$$

where ν is the angle between $\mathbf{x}$ and $\mathbf{x}'$;

(3) $$V(x, x', \cos\nu) = \frac{e^{-\gamma x}(x + a)^m}{x^\alpha} \tilde{V}(x, x', \cos\nu) \frac{e^{-\gamma x'}(x' + a)^m}{x'^\alpha},$$

$$\gamma > 0, \quad a > 0, \quad m \geqslant 0, \quad \tfrac{3}{2} > \alpha \geqslant 0,$$

where $\tilde{V}(x, x', \cos\nu)$ is continuous in x, x', and $\cos\nu$ in $\infty > x > 0$, $\infty > x' > 0$, $1 \geqslant \cos\nu \geqslant -1$, and in this region of the variables x, x', and $\cos\nu$, we have

$$|\tilde{V}(x, x', \cos\nu)| \leqslant \text{const.}$$

The potential operator V with kernel $V(\mathbf{x}, \mathbf{x}')$ is of the Hilbert–Schmidt class.

2. THE RESOLVENT

For any potential satisfying conditions (1)–(3), the spectrum $\text{sp}(H)$ of the Hamiltonian operator H consists of a sectionally continuous part from 0 to ∞ with a finite number of discontinuities at the positive eigenvalues and a finite number of real nonpositive eigenvalues.[3,5] For $z \notin \text{sp}(H)$, the resolvent operator $g(z)$ is defined by

$$g(z) = \frac{1}{z - H} = \frac{1}{z - (H_0 + V)}, \tag{2.1}$$

where H_0 is the free part of H and V the potential operator. We introduce the operator $G(k)$, defined by $G(k) = g(z = k^2)$, for $\text{Im}k > 0$ and $k^2 \notin \text{sp}(H)$. $G(k)$ is a bounded operator for k in this region of the k plane and holomorphic there. And following Ref. 6, we find the following for $\text{Im}k > 0$, $k^2 \notin \text{sp}(H)$:

(i) $G(k)$ is an integral operator of Carleman type satisfying the following resolvent equation:

$$G(k) = G_0(k) + G_0(k)VG(k), \tag{2.2}$$

where $G_0(k) = 1/(k^2 - H_0)$ is a bounded integral operator of Carleman type with kernel $G_0(k; \mathbf{x}, \mathbf{x}')$:

$$G_0(k; \mathbf{x}, \mathbf{x}') = \frac{-1}{4\pi} \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|}. \tag{2.3}$$

(ii) The kernel $G(k; \mathbf{x}, \mathbf{x}')$ of $G(k)$ is symmetric:

$$G(k; \mathbf{x}, \mathbf{x}') = G(k; \mathbf{x}', \mathbf{x}) \tag{2.4}$$

almost everywhere in $R^3 \times R^3$, and satisfies the followin kernel equation:

$$G(k; \mathbf{x}, \mathbf{x}') = G_0(k; \mathbf{x}, \mathbf{x}') + \int d\mathbf{x}'' K(k; \mathbf{x}, \mathbf{x}'') G(k; \mathbf{x}'', \mathbf{x}') \tag{2.5}$$

as a function of $\mathbf{x}$ almost everywhere in R^3 for almost every $\mathbf{x}'$ in R^3, where

$$K(k; \mathbf{x}, \mathbf{x}'') = \int d\mathbf{x}''' G_0(k; \mathbf{x}, \mathbf{x}''') V(\mathbf{x}''', \mathbf{x}''). \tag{2.6}$$

(iii) Any solution $L(k; \mathbf{x}, \mathbf{x}')$ of (2.5) such that $L(k; \cdot, \mathbf{x}') \in L^2(R^3)$ for each $\mathbf{x}'$ is the kernel $G(k; \mathbf{x}, \mathbf{x}')$ for almost every $\mathbf{x}$ and $\mathbf{x}'$ in $R^3 \times R^3$.

We now solve (2.5) for $G(k;\mathbf{x},\mathbf{x}')$ using iteration and Fredholm method.

Putting

$$G(k;\mathbf{x},\mathbf{x}') = G_0(k;\mathbf{x},\mathbf{x}') + G^{(1)}(k;\mathbf{x},\mathbf{x}'), \quad (2.7)$$

we obtain an equation equivalent to (2.5):

$$G^{(1)}(k;\mathbf{x},\mathbf{x}') = G_0^{(1)}(k;\mathbf{x},\mathbf{x}') + \int d\mathbf{x}'' K(k;\mathbf{x},\mathbf{x}'')G^{(1)}(k;\mathbf{x}'',\mathbf{x}'), \quad (2.8)$$

where

$$G_0^{(1)}(k;\mathbf{x},\mathbf{x}') = \int d\mathbf{x}'' K(k;\mathbf{x},\mathbf{x}'')G_0(k;\mathbf{x}'',\mathbf{x}'). \quad (2.9)$$

The inhomogeneous term is continuous and bounded in $\mathbf{x}$ in R^3, for $\mathbf{x}'$ in R^3, and (2.8) has a unique continuous and bounded solution given by the Fredholm series, for each[7] $\mathbf{x}'$:

$$G^{(1)}(k;\mathbf{x},\mathbf{x}') = G_0^{(1)}(k;\mathbf{x},\mathbf{x}') + \int d\mathbf{x}'' \frac{\Delta(k;\mathbf{x},\mathbf{x}'')}{\Delta(k)} G_0^{(1)}(k;\mathbf{x}'',\mathbf{x}'), \quad (2.10)$$

where $\Delta(k)$ and $\Delta(k;\mathbf{x},\mathbf{x}'')$ are respectively the Fredholm determinant[8] and the Fredholm minor of the kernel $K(k;\mathbf{x},\mathbf{x}'')$, and are holomorphic in k in $\mathrm{Im}k > -\gamma$, for $\mathbf{x}$ and $\mathbf{x}''$ in $R^3 \times R^3$.[3]

For $\mathrm{Im}k > 0$, $k^2 \notin \mathrm{sp}(H)$, $\Delta(k)$ is never zero,[3] the solution $G^{(1)}(k;\mathbf{x},\mathbf{x}')$ is continuous in $\mathbf{x}$ and $\mathbf{x}'$ in $R^3 \times R^3$, and $G^{(1)}(k;\cdot,\mathbf{x}')$ belongs to $L^2(R^3)$ for each $\mathbf{x}'$. Hence we have obtained the resolvent kernel, via (2.7).

Using (2.10), we can define a function $G^{(1)}(k;\mathbf{x},\mathbf{x}')$ for k in $\mathrm{Im}k > -\gamma$, $\Delta(k) \neq 0$, and for $\mathbf{x}$ and $\mathbf{x}'$ in $R^3 \times R^3$:

$$G^{(1)}(k;\mathbf{x},\mathbf{x}') = \tilde{G}^{(1)}(k;\mathbf{x},\mathbf{x}')/\Delta(k), \quad (2.11)$$

where $\tilde{G}^{(1)}(k;\mathbf{x},\mathbf{x}')$ is continuous in $\mathbf{x}$ and $\mathbf{x}'$ in $R^3 \times R^3$, for $\mathrm{Im}k > -\gamma$, and holomorphic in k in $\mathrm{Im}k > -\gamma$, for $\mathbf{x}$ and $\mathbf{x}'$ in $R^3 \times R^3$. Further, $\tilde{G}^{(1)}(k;\mathbf{x},\mathbf{x}')$ is symmetric and rotationally invariant,

$$\tilde{G}^{(1)}(k;\mathbf{x},\mathbf{x}') = \tilde{G}^{(1)}(k;\mathbf{x}',\mathbf{x}), \quad (2.12)$$

$$\tilde{G}^{(1)}(k;\mathbf{x},\mathbf{x}') = \tilde{G}^{(1)}(k;x,x',\cos\nu),$$

$$x = |\mathbf{x}| \geq 0,\ x' = |\mathbf{x}'| \geq 0,\ 1 \geq \cos\nu \geq -1, \quad (2.13)$$

where ν is the angle between $\vec{x}$ and $\vec{x}'$, and satisfies

$$|\tilde{G}^{(1)}(k;\mathbf{x},\mathbf{x}')| \leq \begin{cases} \text{const}, & \mathrm{Im}k \geq 0, \\ \text{const}\cdot e^{|\mathrm{Im}k|x} e^{|\mathrm{Im}k|x'}, & 0 \geq \mathrm{Im}k \geq -(\gamma-\epsilon),\ \gamma \geq \epsilon > 0. \end{cases} \quad (2.14)$$

We define a function $G(k;\mathbf{x},\mathbf{x}')$ for $\mathrm{Im}k > -\gamma$, $\Delta(k) \neq 0$, which is the resolvent kernel for $\mathrm{Im}k > 0$, $k^2 \notin \mathrm{sp}(H)$, by

$$G(k;\mathbf{x},\mathbf{x}') = G_0(k;\mathbf{x},\mathbf{x}') + G^{(1)}(k;\mathbf{x},\mathbf{x}'), \quad (2.15)$$

where $G_0(k;\mathbf{x},\mathbf{x}')$ is now defined by (2.3) for $\mathrm{Im}k > -\gamma$.

We now introduce the "eigenfunction expansion" of the resolvent kernel $G(k;\mathbf{x},\mathbf{x}')$, for $\mathrm{Im}k > 0$, $k^2 \notin \mathrm{sp}(H)$. Using the formula

$$G(k) = \int_{-\infty}^{+\infty} \frac{dE(\lambda)}{k^2-\lambda}, \quad (2.16)$$

where $E(\lambda)$ is the spectral family of H, we obtain, for any[9] f and $g \in L^2(R^3)$

$$(f, G(k)g) = \sum_{i=1}^{N^-} \frac{f_i^{-*}g_i^-}{k^2-k_i^{-2}} + \sum_{i=1}^{N^+} \frac{f_i^{+*}g_i^+}{k^2-k_i^{+2}} + \sum_{i=1}^{N^0} \frac{f_i^{0*}g_i^0}{k^2} + \int d\boldsymbol{\xi} \frac{1}{k^2-\xi^2} (\mathfrak{F}f)(\boldsymbol{\xi})^*(\mathfrak{F}g)(\boldsymbol{\xi}), \quad \xi = |\boldsymbol{\xi}| \quad (2.17)$$

with

$$\begin{aligned} f_i^{\pm,0} &= \int d\mathbf{x}\, \psi_i^{\pm,0}(\mathbf{x})^* f(\mathbf{x}), \\ g_i^{\pm,0} &= \int d\mathbf{x}\, \psi_i^{\pm,0}(\mathbf{x})^* g(\mathbf{x}), \\ (\mathfrak{F}f)(\boldsymbol{\xi}) &= \text{l.i.m.} \frac{1}{(2\pi)^{3/2}} \int d\mathbf{x}\, \psi(\boldsymbol{\xi};\mathbf{x})^* f(\mathbf{x}), \\ (\mathfrak{F}g)(\boldsymbol{\xi}) &= \text{l.i.m.} \frac{1}{(2\pi)^{3/2}} \int d\mathbf{x}\, \psi(\boldsymbol{\xi};\mathbf{x})^* g(\mathbf{x}), \end{aligned} \quad (2.18)$$

where l.i.m. denotes limit in mean; $\psi_i^+(\mathbf{x})$, $i = 1, 2, \cdots, N^+$, are the orthonormalized eigenfunctions of H with positive eigenvalue $E_i^+ = k_i^{+2}$, $k_i^+ > 0$, and $\psi_i^-(\mathbf{x})$, $i = 1, 2, \cdots, N^-$, are the orthonormalized eigenfunctions of H with negative eigenvalues $E_i^- = k_i^{-2}$, $\mathrm{Im}k_i^- > 0$, where E_i^+ and E_i^- are repeated according to the respective multiplicities; $\psi_i^0(\mathbf{x})$, $i = 1, 2, \cdots, N^0$, are the orthonormalized eigenfunctions of H with eigenvalue zero if zero is an eigenvalue of H, and $\psi_i^0(\mathbf{x}) = 0$ otherwise; and $\psi(\boldsymbol{\xi};\mathbf{x})$ are the scattering solutions defined by[3]

$$\psi(\boldsymbol{\xi};\mathbf{x}) = e^{i\boldsymbol{\xi}\cdot\mathbf{x}} + \int d\mathbf{x}' \frac{\Delta(\xi;\mathbf{x},\mathbf{x}')}{\Delta(\xi)} e^{i\boldsymbol{\xi}\cdot\mathbf{x}'};$$

$$\boldsymbol{\xi} \in R^3, \quad \xi = |\boldsymbol{\xi}|, \quad \Delta(\xi) \neq 0, \quad (2.19)$$

and

$$\psi(\boldsymbol{\xi} = \xi_0\hat{\xi};\mathbf{x}) = \lim_{\xi\to\xi_0} \psi(\boldsymbol{\xi} = \xi\hat{\xi};\mathbf{x}), \quad \Delta(\xi_0) = 0, \quad \xi_0 > 0, \quad (2.20)$$

where $\hat{\xi}$ is any unit vector. The existence of the above (limit) will be shown in the Appendix.

We shall also show in the Appendix that $\xi\psi(\boldsymbol{\xi} = \xi\hat{\xi};\mathbf{x})$ is continuous in ξ, μ, χ, and $\mathbf{x}$, in $\xi \in D$, $\pi \geq \mu \geq 0$, $2\pi \geq \chi \geq 0$, $\mathbf{x} \in R^3$, where D is a sufficiently small neighborhood of the interval $(0,\infty)$, and μ and χ are the polar angles of $\hat{\xi}$, is holomorphic in ξ in D, for $\pi \geq \mu \geq 0$, $2\pi \geq \chi \geq 0$, $\mathbf{x} \in R^3$, and satisfies

$$|\psi(\boldsymbol{\xi} = \xi\hat{\xi};\mathbf{x})| \leq \text{const}\,[(\xi+b)/\xi]\cdot e^{\gamma x/2}, \ x = |\mathbf{x}| \geq 0,\ b > 0 \quad (2.21)$$

for $\xi \in D$ and μ, χ, and $\mathbf{x}$ in the above region. Here we suppose that D is inside $|\mathrm{Im}\xi| < \gamma/2$.

We state, as a corollary, that $\frac{\partial}{\partial\xi}\{\xi\psi(\boldsymbol{\xi} = \xi\hat{\xi};\mathbf{x})\}$ is continuous in $\xi, \mu, \chi, \mathbf{x}$ in $\xi \in D$, $\pi \geq \mu \geq 0$, $2\pi \geq \chi \geq 0$, $\mathbf{x} \in R^3$, with:

$$\left|\frac{\partial}{\partial\xi}\psi(\boldsymbol{\xi} = \xi\hat{\xi};\mathbf{x})\right| \leq \text{const}\,[(\xi+b)/\xi]^2 e^{\gamma x/2},\ x = |\mathbf{x}| \geq 0,\ b > 0 \quad (2.22)$$

for ξ belonging to a sufficiently small neighborhood of the interval $(0,\infty)$ contained in D, and μ, χ, and $\mathbf{x}$ in the above region. These results follow from those of the preceding paragraph with the use of the relation:

$$\frac{\partial}{\partial\xi}\{\xi\psi(\boldsymbol{\xi} = \xi\hat{\xi};\mathbf{x})\} = \frac{1}{2\pi i} \oint d\xi' \frac{\xi'\psi(\boldsymbol{\xi}' = \xi'\hat{\xi};\mathbf{x})}{(\xi'-\xi)^2}$$

3. THE T OPERATOR

The T operator $T(k)$, for $\mathrm{Im}k > 0$, $k^2 \notin \mathrm{sp}(H)$, is defined by

$$T(k) = V + VG(k)V. \quad (3.1)$$

Since V is a Hilbert–Schmidt operator and $G(k)$ is a bounded operator, $T(k)$ is a Hilbert–Schmidt operator.

The kernel $T(k;\mathbf{x},\mathbf{x}')$ of the operator $T(k)$ is given by

$$T(k;\mathbf{x},\mathbf{x}') = V(\mathbf{x},\mathbf{x}') + \int\int d\mathbf{x}''d\mathbf{x}'''V(\mathbf{x},\mathbf{x}'')G(k;\mathbf{x}'',\mathbf{x}''')V(\mathbf{x}''',\mathbf{x}'). \quad (3.2)$$

This relation enables us to extend the domain of definition of the function $T(k;\mathbf{x},\mathbf{x}')$ to $\mathrm{Im}k > -\gamma$, $\Delta(k) \neq 0$, $\mathbf{x}$ and $\mathbf{x}'$ in $R^3 \times R^3$. For k in $\mathrm{Im}k > -\gamma$, $\Delta(k) \neq 0$, $T(k;\mathbf{x},\mathbf{x}')$ is continuous in $\mathbf{x}$ and $\mathbf{x}'$ in $R^3 \times R^3$, and satisfies

$$\int\int d\mathbf{x}d\mathbf{x}' |T(k;\mathbf{x},\mathbf{x}')|^2 < \infty \quad (3.3)$$

and hence is the kernel of an operator $T(k)$ of Hilbert–Schmidt class. From the bound

$$\left|\frac{\partial}{\partial k}\tilde{G}^{(1)}(k;\mathbf{x},\mathbf{x}')\right| \leqslant \begin{cases}\text{const}, & \mathrm{Im}k \geqslant 0,\\ \text{const}\cdot e^{|\mathrm{Im}k|x}e^{|\mathrm{Im}k|x'}, & 0 \geqslant \mathrm{Im}k \geqslant -(\gamma-\epsilon),\end{cases} \quad \gamma \geqslant \epsilon > 0 \quad (3.4)$$

and the holomorphy of $\Delta(k)$ in $\mathrm{Im}k > -\gamma$, we find that $T(k)$ is holomorphic in $\mathrm{Im}k > -\gamma$, perhaps with the exception of poles at the zeroes of $\Delta(k)$. We have the following results for the kernel $T(k;\mathbf{x},\mathbf{x}')$:

(i) $T(k;\mathbf{x},\mathbf{x}')$ is symmetric:

$$T(k;\mathbf{x},\mathbf{x}') = T(k;\mathbf{x}',\mathbf{x}). \quad (3.5)$$

(ii) $T(k;\vec{x},\vec{x}')$ is rotationally invariant:

$$T(k;\mathbf{x},\mathbf{x}') = T(k;x,x',\cos\nu),$$

$$x = |\mathbf{x}| > 0,$$

$$x' = |\mathbf{x}'| > 0,\ 1 \geqslant \cos\nu \geqslant -1 \quad (3.6)$$

where ν is the angle between $\mathbf{x}$ and $\mathbf{x}'$.

(iii)

$$T(k;x,x',\cos\nu) = \frac{e^{-\gamma x}(x+a)^m}{x^\alpha}\,\frac{\tilde{T}(k;x,x',\cos\nu)}{\Delta(k)} \times \frac{e^{-\gamma x}(x'+a)^m}{x'^\alpha}, \quad (3.7)$$

where $\tilde{T}(k;x,x',\cos\nu)$ is continuous in x, x', and $\cos\nu$ in $\infty > x > 0$, $\infty > x' > 0$, $1 \geqslant \cos\nu \geqslant -1$, for $\mathrm{Im}k > -\gamma$, and holomorphic in k in $\mathrm{Im}k > -\gamma$, for $\infty > x > 0$, $\infty > x' > 0$, $1 \geqslant \cos\nu \geqslant -1$, and satisfies

$$|\tilde{T}(k;x,x',\cos\nu| \leqslant \text{const} \quad (3.8)$$

for $\mathrm{Im}k \geqslant -(\gamma-\epsilon)$, $\gamma \geqslant \epsilon > 0$, and x, x', and $\cos\nu$ in the above region.

The kernel of the operator $T(k)$ in momentum space, for $\mathrm{Im}k > -\gamma, \Delta(k) \neq 0$, denoted by $\mathcal{T}(k;\mathbf{p},\mathbf{p}')$, satisfies the following:

$\mathcal{T}(k;\mathbf{p},\mathbf{p}')$ is symmetric:

$$\mathcal{T}(k;\mathbf{p},\mathbf{p}') = \mathcal{T}(k;\mathbf{p}',\mathbf{p}). \quad (3.9)$$

(ii) $\mathcal{T}(k;\mathbf{p},\mathbf{p}')$ is rotationally invariant:

$$\mathcal{T}(k;\mathbf{p},\mathbf{p}') = \mathcal{T}(k;p,p',\cos\omega), \qquad p = |\mathbf{p}| \geqslant 0,$$

$$p' = |\mathbf{p}'| \geqslant 0, \quad 1 \geqslant \cos\omega \geqslant -1, \quad (3.10)$$

where ω is the angle between $\mathbf{p}$ and $\mathbf{p}'$.

(iii) $$\mathcal{T}(k;p,p',\cos\omega) = \tilde{\mathcal{T}}(k;p,p',\cos\omega)/\Delta(k), \quad (3.11)$$

where $\tilde{\mathcal{T}}(k;p,p',\cos\omega)$ is continuous in p, p', and $\cos\omega$ in $\infty > p \geqslant 0$, $\infty > p' \geqslant 0$, $1 \geqslant \cos\omega \geqslant 1$, for $\mathrm{Im}k > -\gamma$, and holomorphic in k, p, and p' in $\mathrm{Im}k > -\gamma$, $|\mathrm{Im}p| < \gamma$, $|\mathrm{Im}p'| < \gamma$, for $1 \geqslant \cos\omega \geqslant -1$. Further, we have

$$\tilde{\mathcal{T}}(k;p,p',\cos\omega) \underset{p\to\infty}{\longrightarrow} 0 \quad (3.12)$$

uniformly for k, p', and $\cos\omega$ in $\mathrm{Im}k \geqslant -(\gamma-\epsilon)$, $\gamma \geqslant \epsilon > 0$, $\infty > p' \geqslant 0$, $1 \geqslant \cos\omega \geqslant -1$.

We now assert that $T(k)$ has simple poles at the zeroes of $\Delta(k)$, i.e., $k = k_i^-$, $i = 1, 2, \cdots, N^-$, and $k = \pm k_i^+$, $i = 1, 2, \cdots, N^+$, in $\mathrm{Im}k \geqslant 0$, $k \neq 0$. This follows from (3.1), (2.17), the continuity of $\psi(\xi = \xi\hat{\xi};\mathbf{x})$ and of $\frac{\partial}{\partial\xi}\psi(\xi = \xi\hat{\xi};\mathbf{x})$ in $\xi \in (0,\infty)$, $\pi \geqslant \mu \geqslant 0$, $2\pi \geqslant \chi \geqslant 0$, $\mathbf{x} \in R^3$, and the bounds (2.21) and (2.22).[10] Further, $T(k)$ has a double pole at $k = 0$, if zero is an eigenvalue of H.

We also have

$$T(-k^*) = T(k)^*, \quad \mathrm{Im}k > -\gamma,\ \Delta(k) \neq 0. \quad (3.13)$$

We remark that the poles of the scattering amplitude $F(k;\cos\theta)$:

$$F(k;\cos\theta) = \mathcal{T}(k;k\hat{p},k\hat{p}'),$$

$\hat{p}$ and $\hat{p}'$ being unit vectors with $\hat{p}\cdot\hat{p}' = \cos\theta$, in the interval $k = iK$, $\gamma > K > 0$, are necessarily simple.[3] From this it follows that the poles of the partial scattering amplitude[11] $T_l(k)$ in this interval for any l, are also simple.[12] Further, for $V(x,x',\cos\nu)$ of the following form[13]:

$$\tilde{V}(x,x',\cos\nu) = \sum_{l=0}^{L} P_l(\cos\nu)(xx')^l \sum_{p,g=0}^{N_l} C_{lpq}\, e^{-p\lambda x}\, e^{-q\lambda x}$$

$$\lambda > 0,\ C_{lpq}\ \text{real},\ C_{lpq} = C_{lqp}$$

any bound state pole of the scattering amplitude $F(k;\cos\theta)$ on the upper imaginery axis must also necessarily be simple, if $-(\gamma + p\lambda)^2$, $p = 1, 2, \ldots, \max N_l$ are all distinct from the negative energy eigenvalues.[12]

We now turn to a Lippman–Schwinger equation satisfied by $T(k)$, for $\mathrm{Im}k > -\gamma$, $\Delta(k) \neq 0$.

We have, from (2.2) and (3.1), the following equation for $T(k)$, for $\mathrm{Im}k > 0$, $k^2 \notin \mathrm{sp}(H)$:

$$T(k) = V + T(k)G_0(k)V. \quad (3.14)$$

For $\mathrm{Im}k > -\gamma, \Delta(k) \neq 0$, we have the following equation for the kernel $T(k;\mathbf{x},\mathbf{x}')$ of the operator $T(k)$:

$$T(k;\mathbf{x},\mathbf{x}') = V(\mathbf{x},\mathbf{x}') + \int\int d\mathbf{x}''d\mathbf{x}'''T(k;\mathbf{x},\mathbf{x}'')G_0(k;\mathbf{x}'',\mathbf{x}''')V(\mathbf{x}''',\mathbf{x}'). \quad (3.15)$$

In particular, for E real and $\delta(E) = \Delta(\sqrt{E}) \neq 0$, we have the following equation for $t(E;\mathbf{x},\mathbf{x}') = T(\sqrt{E};\mathbf{x},\mathbf{x}')$:

$$t(E;\mathbf{x},\mathbf{x}') = V(\mathbf{x},\mathbf{x}') + \int\int d\mathbf{x}''d\mathbf{x}'''t(E;\mathbf{x},\mathbf{x}'')g_0(E;\mathbf{x}'',\mathbf{x}''')V(\mathbf{x}''',\mathbf{x}') \quad (3.16)$$

$$g_0(E;\vec{x}'',\vec{x}''') = G_0(\sqrt{E};\vec{x}'',\vec{x}''') \quad (3.17)$$

4. THE INVERSION METHOD

We study the following problem: Find values of E, where E is real and such that the operator $t(E) = T(\sqrt{E})$ is defined, for which one can determine the potential

$V(\mathbf{x},\mathbf{x}')$ from $t(E)$, and determine $V(\mathbf{x},\mathbf{x}')$ from $t(E)$ for any such E. We consider the cases $E < 0$ and $E \geqslant 0$.

(i) $E < 0$: In this case we have $\mathrm{Im}\sqrt{E} > 0$, and we have, from (3.14)

$$t(E) = V + t(E)g_0(E)V \tag{4.1}$$

for any E for which $t(E)$ is defined, where

$$g_0(E) = 1/(E - H_0). \tag{4.2}$$

We have, from (4.1),

$$\{1 + t(E)g_0(E)\}V = t(E). \tag{4.3}$$

Hence we have

$$V = \{1/[1 + t(E)g_0(E)]\}t(E) \tag{4.4}$$

if E is not a zero of $d(E) = \det\{1 + t(E)g_0(E)\}$. Here $t(E)$ and $t(E)g_0(E)$ are Hilbert–Schmidt operators, and $\{1/[1 + t(E)g_0(E)]\} - 1$ is also a Hilbert–Schmidt operator if $d(E) \neq 0$. The kernel of $\{1/[1 + t(E)g_0(E)]\} - 1$, for $d(E) \neq 0$, can be given by a Fredholm series. (4.4) determines the potential uniquely.

The Fredholm determinant $D(k) = \det\{1 + T(k)G_0(k)\}$ can be shown to be holomorphic in $\mathrm{Im}k > 0$, $k^2 \notin \mathrm{sp}(H)$. Hence $d(E)$ can have at most a countable number of zeroes in $E < 0$, $E \notin \mathrm{sp}(H)$.

(ii) $E \geqslant 0$: In this case we write (3.16) as

$$V(\mathbf{x},\mathbf{x}') = t(E;\mathbf{x},\mathbf{x}') + \int d\mathbf{x}''\, h(E;\mathbf{x},\mathbf{x}'')\, V(\mathbf{x}'',\mathbf{x}'), \tag{4.5}$$

where

$$h(E;\mathbf{x},\mathbf{x}'') = \int d\mathbf{x}'''\, t(E;\mathbf{x},\mathbf{x}''')g_0(E;\mathbf{x}''',\mathbf{x}''). \tag{4.6}$$

We obtain the following equation for $\tilde{V}(\mathbf{x},\mathbf{x}')$:

$$\tilde{V}(\mathbf{x},\mathbf{x}') = \frac{\tilde{t}(E;\mathbf{x},\mathbf{x}')}{\delta(E)} + \int d\mathbf{x}''\, \tilde{h}(E;\mathbf{x},\mathbf{x}'')\tilde{V}(\mathbf{x}'',\mathbf{x}'), \tag{4.7}$$

where

$$\tilde{V}(\mathbf{x},\mathbf{x}') = \tilde{V}(x,x',\cos\nu),$$
$$\tilde{t}(E;\mathbf{x},\mathbf{x}') = \tilde{T}(\sqrt{E};x,x',\cos\nu), \tag{4.8}$$
$$x = |\mathbf{x}| > 0, \quad x' = |\mathbf{x}'| > 0, \quad 1 \geqslant \cos\nu \geqslant -1,$$

ν being the angle between $\mathbf{x}$ and $\mathbf{x}'$, and

$$\delta(E) = \Delta(\sqrt{E}),$$
$$\tilde{h}(E;\mathbf{x},\mathbf{x}'') = \int d\mathbf{x}'''\, \frac{\tilde{t}(E;\mathbf{x},\mathbf{x}''')}{\delta(E)}\, \tilde{g}_0(E;\mathbf{x}''',\mathbf{x}'') \tag{4.9}$$

with

$$\tilde{g}_0(E;\mathbf{x}''',\mathbf{x}'') = \frac{e^{-\gamma x'''}(x''' + a)^m}{x'''^{\alpha}}\, g_0(E;\mathbf{x}''',\mathbf{x}'')\frac{e^{-\gamma x''}(x'' + a)^m}{x''^{\alpha}} \tag{4.10}$$
$$x''' = |\mathbf{x}'''| > 0, \quad x'' = |\mathbf{x}''| > 0.$$

For each $\mathbf{x}'$ in R^3 which is nonzero, (4.7) has a unique continuous bounded solution given by Ref. 7:

$$\tilde{V}(\mathbf{x},\mathbf{x}'') = \frac{\tilde{t}(E;\mathbf{x},\mathbf{x}'')}{\delta(E)} + \int d\mathbf{x}''\, \frac{\tilde{d}(E;\mathbf{x},\mathbf{x}'')}{\tilde{d}(E)}\, \frac{\tilde{t}(E;\mathbf{x}'',\mathbf{x}')}{\delta(E)} \tag{4.11}$$

if E is not a zero of $\tilde{d}(E)$, where $\tilde{d}(E)$ and $\tilde{d}(E;\mathbf{x},\mathbf{x}'')$ are the Fredholm determinant and the Fredholm minor of the kernel $\tilde{h}(E;\mathbf{x},\mathbf{x}'')$. Hence for such values of E, the potential is uniquely determined.

We can show that $\tilde{D}(k) = \tilde{d}(k^2)$ can be extended to a function holomorphic in $\mathrm{Im}k > -\gamma, \Delta(k) \neq 0$. Hence the number of zeroes of $\tilde{d}(E)$ in $E \geqslant 0$, $\delta(E) \neq 0$, is countable.

APPENDIX

We now prove our assertions concerning the scattering solution $\psi(\xi = \xi\hat{\xi};\mathbf{x})$.

First we mention, without going into the details here, that we can establish[14] that $\psi(\xi\hat{\xi};\mathbf{x})$ is continuous in ξ, μ, χ, and $\mathbf{x}$, in $\xi \in D_{\epsilon,\rho}$, $\pi \geqslant \mu \geqslant 0$, $2\pi \geqslant \chi \geqslant 0$, $\mathbf{x} \in R^3$, where $D_{\epsilon,\rho}$ consists of all points at a distance less than some ϵ, $\epsilon > 0$, from the interval $(0,\infty)$ and at a distance greater than ρ from the zeroes of $\Delta(\xi)$, i.e., $\xi = k_i^+$, $i = 1, 2, \cdots, N^+$, and possibly $\xi = 0$ in the interval $[0,\infty)$, ρ being any positive number less than ϵ. Then we establish that the limit (2.20) exists and that $\xi\psi(\xi = \xi\hat{\xi};\mathbf{x})$ is continuous in ξ, μ, χ, and $\mathbf{x}$, in $\xi \in D_\tau$, $\pi \geqslant \mu \geqslant 0$, $2\pi \geqslant \chi \geqslant 0$, $\mathbf{x} \in R^3$, where D_τ consists of open discs of radii τ, $\tau > 0$, with centers at the zeros of $\Delta(\xi)$ in the interval $[0,\infty)$, with τ sufficiently small. To show these, we proceed as follows.

Let ξ_0 be any zero of $\Delta(\xi)$ in the interval $(0,\infty)$. Then the limit[15]

$$\lim_{\epsilon\to 0+} \int_{c \geq |\boldsymbol{\xi}| > \xi_0+\epsilon} d\boldsymbol{\xi}\, |(\mathfrak{F}f)(\boldsymbol{\xi})|^2$$

exists, where c is any positive number such that no zero of $\Delta(\xi)$ lie in the interval $(\xi_0, c]$ and where $(\mathfrak{F}f)(\boldsymbol{\xi})$ is defined by (2.18) for any $f \in L^2(R^3)$.

In particular, the above limit exists if $f(\mathbf{x})$ is any of a set of measurable functions $\phi_i(\mathbf{x})$, $i = 1, 2, \ldots$, which are zero in $|\mathbf{x}| > r$ and which together form a complete orthonormal set in $L^2(S_r)$, S_r being the sphere $r \geqslant |\mathbf{x}| \geqslant 0$ and r being an arbitrary positive number. We thus have the existence of the limit

$$\lim_{\epsilon\to 0+} \int_{\xi_0+\epsilon}^{c} d\xi\, \xi^2 \int d\Omega(\hat{\xi}) \left| \int_{S_r} d\mathbf{x}\, \frac{\tilde{\psi}(\xi = \xi\hat{\xi};\mathbf{x})\varphi_i(\mathbf{x})}{\Delta(\xi)} \right|^2 \tag{A1}$$

for any i, where we have put

$$\psi(\xi = \xi\hat{\xi};\mathbf{x}) = \tilde{\psi}(\xi = \xi\hat{\xi};\mathbf{x})/\Delta(\xi). \tag{A2}$$

The holomorphy of $\Delta(\xi)$ in $\mathrm{Im}\xi > -\gamma$ enables us to write

$$1/\Delta(\xi) = J(\xi)/(\xi - \xi_0)^n \tag{A3}$$

for $\xi \neq \xi_0$ and ξ in a sufficiently small neighborhood of ξ_0, where n is the order of the zero of $\Delta(\xi)$ at ξ_0 and $J(\xi)$ is holomorphic in the same neighborhood of ξ_0 with $J(\xi_0) \neq 0$.

The holomorphy of $\tilde{\psi}(\xi = \xi\hat{\xi};\mathbf{x})$ in ξ in $\mathrm{Im}\xi > -\gamma$ enables us to have a Taylor expansion of $\tilde{\psi}(\xi = \xi\hat{\xi};\mathbf{x})$ in ξ about ξ_0, for ξ in a sufficiently small neighborhood of ξ_0:

$$\tilde{\psi}(\xi = \xi\hat{\xi};\mathbf{x}) = C_0(\hat{\xi};\mathbf{x}) + C_1(\hat{\xi};\mathbf{x})(\xi - \xi_0) + C_2(\hat{\xi};\vec{x})(\xi - \xi_0)^2 + \cdots, \tag{A4}$$
$$\pi \geqslant \mu \geqslant 0, \quad 2\pi \geqslant \chi \geqslant 0, \quad \mathbf{x} \in R^3,$$

$$C_j(\hat{\xi};\mathbf{x}) = \frac{1}{2\pi i} \oint d\xi\, \frac{\tilde{\psi}(\xi = \xi\hat{\xi};\mathbf{x})}{(\xi - \xi_0)^{j+1}}, \tag{A5}$$

where $C_j(\hat{\xi};\mathbf{x})$, $j = 0, 1, 2, \cdots$, are continous functions of μ, χ, and $\mathbf{x}$. The existence of the limit (A1) for any i and arbitrary $r > 0$ then leads to

$$C_0(\hat{\xi};\mathbf{x}) = C_1(\hat{\xi};\mathbf{x}) = \ldots = C_{n-1}(\hat{\xi};\mathbf{x}) = 0 \quad \text{(A6)}$$

for μ, χ, and $\mathbf{x}$ in the above region.

Consequently, we have

$$\psi(\xi = \xi\hat{\xi};\mathbf{x}) = J(\xi)\{C_n(\hat{\xi};\mathbf{x}) + C_{n+1}(\hat{\xi};\mathbf{x})(\xi - \xi_0) + \cdots\} \quad \text{(A7)}$$

for ξ in a sufficiently small neighborhood U of ξ_0. Hence the limit (2.20) exist. Using (A5), we find that the above series converges uniformly in ξ, μ, χ, and $\mathbf{x}$, $\xi \in U, \pi \geqslant \mu \geqslant 0, 2\pi \geqslant \chi \geqslant 0, \mathbf{x} \in R^3$, and is therefore continuous in these variables in this region.

Similarly, we find that $\xi\psi(\xi = \xi\hat{\xi};\mathbf{x})$ is continuous in ξ, μ, χ, and $\mathbf{x}$ in $\xi \in W, \pi \geqslant \mu \geqslant 0, 2\pi \geqslant \chi \geqslant 0, \mathbf{x} \in R^3$, where W is a sufficiently small neighborhood of zero.

This analysis also clearly shows that $\psi(\xi = \xi\hat{\xi};\mathbf{x})$ is holomorphic in ξ in a sufficiently small neighborhood of any zero of $\Delta(\xi)$ which lies in the interval $[0, \infty)$, and consequently is holomorphic in ξ in a sufficiently small neighborhood D of the interval $(0, \infty)$, for $\pi \geqslant \mu \geqslant 0$, $2\pi \geqslant \chi \geqslant 0$, $\mathbf{x} \in R^3$.

The inequality (2.21) follows from (2.19) and the above discussions.

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[1]The underlying space for the operators $t(E)$, V, H, and the operators $g(z)$, H_0, $G(k)$, $T(k)$, introduced below, is $L^2(R^3)$.

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[8]We remark here the following asymptotic behavior:

$$\Delta(k) \underset{|k| \to \infty}{\to} 1, \quad \mathrm{Im}\,k \geqslant -(\gamma - \epsilon), \quad \gamma \geqslant \epsilon > 0.$$

From this and the holomorphy of $\Delta(k)$, we conclude that the number of zeroes of $\Delta(k)$ in $\mathrm{Im}k \geqslant -(\gamma - \epsilon)$, $\gamma \geqslant \epsilon > 0$, is finite.

[9]Cf. Ref. 5.

[10]The integral in (2.17) approaches a finite limit as k approaches the points $\pm k_i^+$, $i = 1, 2, \ldots, N^+$, from the upper k-plane $Im\,k > 0$. See N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff, Groningen, 1953).

[11]The expansion

$$F(k;\cos\theta) = \frac{1}{k} \sum_{l=0} (2l+1)\, T_l(k) P_l(\cos\theta)$$

converges for $k > 0$, with

$$T_l(k) = \frac{k}{2} \int_{-1}^{+1} d\cos\theta\, F(k;\cos\theta)\, P_l(\cos\theta)$$

This is a consequence of a result of M. Bertero, G. Talenti, and G. A. Viano, Nucl. Phys. A 115, 395 (1968).

[12]We have not proven that $F(k;\cos\theta)$ has a pole at $k = k_i^-$, $i = 1, 2, \cdots, N^-$.

[13]The only singularities of the resulting scattering amplitude $F(k;\cos\theta)$ in $Im k \geqslant 0$ are poles on the upper imaginery axis.

[14]We first establish the relevant continuity property of $K(\zeta; x, x')$. See Ref. 5, Theorem 3.2.

[15]See Ref. 5.

Representations of the Jost solutions and the S matrix for a class of analytic nonlocal potentials

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We derive representations of the Jost solutions, the Jost functions, and the S matrix, for analytic nonlocal potentials belonging to a double Laplace transform class, for the s-wave case, in terms of the spectral function for the potential.

I. INTRODUCTION

We have studied a class of analytic nonlocal potentials[1,2] and we have obtained results including forward dispersion relation, the analyticity properties of the scattering, the regular, and the Jost solutions, and the analyticity property of the S matrix and its representations in terms of Fredholm determinants and in terms of Jost functions. This class includes potentials $V(\mathbf{x},\mathbf{x}')$ of a double Laplace transform class defined by

$$V(\mathbf{x},\mathbf{x}') = V(x,x',\cos\nu), \quad x = |\mathbf{x}| > 0, \quad x' = |\mathbf{x}'| > 0, \quad 1 \geqslant \cos\nu \geqslant -1,$$

where ν is the angle between $\mathbf{x}$ and $\mathbf{x}'$, with

$$V(x,x',\cos\nu) = \frac{e^{-\gamma x}(x+a)^m}{x^\alpha}\tilde{V}(x,x',\cos\nu)\frac{e^{-\gamma x'}(x'+a)^m}{x'^\alpha}$$

$$\gamma > 0, a > 0, m \geqslant 0, \tfrac{3}{2} > \alpha \geqslant 0,$$

and

$$\tilde{V}(x,x',\cos\nu) = \int_0^\infty\int_0^\infty d\beta\, d\beta' e^{-\beta x}e^{-\beta' x'}\sigma(\beta,\beta',\cos\nu),$$

where $\sigma(\beta,\beta',\cos\nu)$ is continuous in β,β', and $\cos\nu$ in $\infty > \beta \geqslant 0, \infty > \beta' \geqslant 0, 1 \geqslant \cos\nu \geqslant -1$, and satisfies

(i) $\sigma(\beta,\beta',\cos\nu)$ is real, $\sigma(\beta,\beta',\cos\nu) = \sigma(\beta',\beta,\cos\nu)$ for β,β', and $\cos\nu$ in the above region, and

(ii) $\int_0^\infty\int_0^\infty d\beta\, d\beta' |\sigma(\beta,\beta',\cos\nu)| < \text{const}, 1 \geqslant \cos\nu \geqslant -1.$

For $m = 0$, $\alpha = \frac{1}{2}$, and for $\sigma(\beta,\beta',\cos\nu)$ satisfying a slightly more detailed condition, we have obtained a fixed t dispersion relation,[2] for t in $0 \geqslant t > -4\gamma^2$, where t is the square of the momentum transfer.

We also note that there exist potentials belonging to this double Laplace transform class which show local correlations for x in some finite interval $[c_1, c_2]$, $c_2 > c_1 > 0$.[3]

In this article we derive representations of the Jost solutions, the Jost functions, and the S matrix, in the k plane, for the s-wave case, for any potential belonging to the above double Laplace transform class with $m = 0$ and $\alpha = 1$, and with $\sigma(\beta,\beta',\cos\nu)$ satisfying:

$$|\sigma(\beta,\beta',\cos\nu)| \leqslant \frac{\text{const}}{(\beta+\beta_0)^{1+\lambda}(\beta'+\beta_0)^{1+\lambda}}$$

$$\infty > \beta \geqslant 0, \infty > \beta' \geqslant 0, 1 \geqslant \cos\nu \geqslant -1, \quad \text{for some } \beta_0 > 0, \ \lambda > 0. \tag{1.1}$$

II. THE REPRESENTATIONS (S WAVE)

We now obtain the above-mentioned representations for any potential belonging to the double Laplace transform class with $m = 0$, $\alpha = 1$ and $\sigma(\beta,\beta',\cos\nu)$ satisfying condition (1.1), for k in the k plane cut from $i\gamma$ to $i\infty$ and from $-i\gamma$ to $-i\infty$.

For such a potential, the s-wave partial potential $V_0(x,x')$, defined by

$$V_0(x,x') = 2\pi(xx')\int_{-1}^{+1} V(x,x',\cos\nu)\, d\cos\nu \tag{2.1}$$

has the following representation:

$$V_0(x,x') = \int_\gamma^\infty\int_\gamma^\infty d\beta\, d\beta'\, e^{-\beta x}e^{-\beta' x'}s(\beta,\beta'), \tag{2.2}$$

where $s(\beta,\beta')$ satisfies

(i) $s(\beta,\beta')$ is real, $s(\beta,\beta') = s(\beta',\beta)$;

(ii) $s(\beta,\beta')$ is continuous in β and β' in $\infty > \beta \geqslant \gamma, \infty > \beta' \geqslant \gamma$, and in this region:

$$|s(\beta,\beta')| \leqslant \text{const}/\beta^{(1+\lambda)}\beta'^{(1+\lambda)}.$$

We have, for $k > 0$, and $\Delta^{(\mathrm{II})}(k) \neq 0$,[4] and $\infty > x \geqslant 0$:

$$f^\pm(k;x) = e^{\pm ikx} + \frac{1}{k}\int_x^\infty dx' \sin k(x-x')\int_0^\infty dx''\, V_0(x'x'')f^\pm(k;x''), \tag{2.3}$$

where $\Delta^{(\mathrm{II})}(k)$ is the Fredholm determinant of the kernel $K^{(\mathrm{II})}(k;x,x')$:

$$K^{(\mathrm{II})}(k;x,x') = \frac{1}{k}\int_x^\infty dx''\, \sin k(x-x'')V_0(x'',x')$$

and $f^\pm(k;x)$ are the Jost solutions.[2] $\Delta^{(\mathrm{II})}(k)$ is holomorphic in the doubly cut k plane.

Since the functions $f^\pm(k;x)$ are bounded in $\infty > x \geqslant 0$,[2] we obtain

$$f^\pm(k;x) = e^{\pm ikx} + \int_\gamma^\infty d\beta\, e^{-\beta x}[\xi^\pm(k;\beta)/(k^2+\beta^2)], \tag{2.4}$$

where

$$\xi^\pm(k;\beta) = -\int_\gamma^\infty d\beta'\, s(\beta,\beta')\int_0^\infty dx'\, e^{-\beta' x'}f^\pm(k;x'), \tag{2.5}$$

and

$$|\xi^\pm(k;\beta)| \leqslant \text{const}/\beta^{(1+\lambda)}, \tag{2.6}$$

for fixed k. Hence $\xi^\pm(k;\beta)$ belong to both $L^1(\gamma,\infty)$ and $L^2(\gamma,\infty)$.

From the following radial Schrödinger equation for $f^\pm(k;x)$:

$$\left(\frac{d}{dx^2} + k^2\right)f^\pm(k;x) = \int_0^\infty dx'\, V_0(x,x')f^\pm(k;x') \tag{2.7}$$

and using (2.4) and the identity theorem in Laplace transform theory,[5] we obtain the following integral equations for $\xi^\pm(k;\beta)$:

$$\xi^\pm(k;\beta) = \xi^{\pm(0)}(k;\beta) + \int_\gamma^\infty d\beta'\, J(k;\beta,\beta')\xi^\pm(k;\beta'), \tag{2.8}$$

with

$$\xi^{\pm(0)}(k;\beta) = \int_\gamma^\infty d\beta'\, \frac{s(\beta,\beta')}{\beta' \mp ik}, \tag{2.9}$$

$$J(k;\beta,\beta') = \frac{1}{k^2+\beta^2}\int_\gamma^\infty d\beta''\, \frac{s(\beta,\beta'')}{\beta'+\beta''}. \tag{2.10}$$

We consider the integral equations of (2.8) for k in $B(\epsilon)$, where $B(\epsilon)$ is the domain in the k plane consisting of all points at a distance more than ϵ from the cuts from $i\gamma$ to $i\infty$ and from $-i\gamma$ to $-i\infty$, where $\gamma > \epsilon > 0$. Then the inhomogeneous terms and the kernel are square integrable in $\infty > \beta \geq \gamma$ and in $\infty > \beta \geq \gamma, \infty > \beta' \geq \gamma$, respectively. Hence we may apply the method of Smithies.[7,8] We find that when the Fredholm determinant $D(k)$ of the kernel $J(k;\beta,\beta')$ is not zero, each of the equations (2.8) has a unique square integrable solution given by

$$\xi^{\pm}(k;\beta) = \xi^{\pm(0)}(k;\beta) + \int_\gamma^\infty d\beta' \frac{D(k;\beta,\beta')}{D(k)} \xi^{\pm(0)}(k;\beta'), \quad (2.11)$$

with

$$D(k) = e^{-\tau_1(k)} \delta(k), \quad (2.12)$$

$$\delta(k) = \sum_{n=0}^{\infty} \delta_n(k), \quad \delta_0(k) = 1, \quad \delta_1(k) = 0, \quad (2.13)$$

$$\delta_n(k) = \frac{(-1)^n}{n!} \begin{vmatrix} 0 & n-1 & 0\ldots & 0 & 0 \\ \tau_2(k) & 0 & n-2 & 0 & 0 \\ \tau_3(k) & \tau_2(k) & 0 & 0 & 0 \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \tau_n(k) & \tau_{n-1}(k) & \tau_{n-2}(k)\ldots & \tau_2(k) & 0 \end{vmatrix}, \quad n \geq 2, \quad (2.14)$$

$$D(k;\beta,\beta') = e^{-\tau_1(k)} \delta(k;\beta,\beta'), \quad (2.15)$$

$$\delta(k;\beta,\beta') = \sum_{n=0}^{\infty} \delta_n(k;\beta,\beta'),$$
$$\delta_0(k;\beta,\beta') = J(k;\beta,\beta'), \ \delta_1(k;\beta,\beta') = J^2(k;\beta,\beta'). \quad (2.16)$$

$$\delta_n(k;\beta,\beta') = \frac{(-1)^n}{n!} \begin{vmatrix} J(k;\beta,\beta') & n & 0\ldots & 0 & 0 \\ J^2(k;\beta,\beta') & 0 & n-1 & 0 & 0 \\ J^3(k;\beta,\beta') & \tau_2(k) & 0 & 0 & 0 \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ \cdot & & & & \cdot \\ J^{n+1}(k;\beta,\beta') & \tau_n(k) & \tau_{n-1}(k)\ldots & \tau_2(k) & 0 \end{vmatrix}, \quad n \geq 2, \quad (2.17)$$

where

$$\tau_n(k) = \mathrm{Tr} J^n(k), \quad (2.18)$$

$J(k)$ being the Hilbert–Schmidt operator in $L^2(\gamma,\infty)$ with kernel $J(k;\beta,\beta')$.

Using the holomorphy of $J(k;\beta,\beta')$ and the bound

$$|J(k;\beta,\beta')| \leq \mathrm{const}/\beta^{(1+\lambda)}(\beta' + \gamma), \quad (2.19)$$

for k in $B(\epsilon)$, we find that $\delta_n(k)$ is holomorphic in $B(\epsilon)$. And using the inequality[9]:

$$|\delta_n(k)| \leq e^{n/2} \|J(k)\|^n / n^{n/2}, \quad n \geq 2, \quad (2.20)$$

and

$$\|J(k)\| \leq \mathrm{const}, \quad (2.21)$$

for k in $B(\epsilon)$, we find that $\delta(k)$ is holomorphic in $B(\epsilon)$, for each ϵ in $\gamma > \epsilon > 0$. Hence $\delta(k)$ is holomorphic in the doubly cut k plane. Consequently $D(k)$ is also holomorphic in the doubly cut k plane.

Similarly, $\delta_n(k;\beta,\beta')$ is holomorphic in k in $B(\epsilon)$, for $\infty > \beta \geq \gamma, \infty > \beta' \geq \gamma$, and using (2.19) and

$$|J^2(k;\beta,\beta')| \leq \mathrm{const}/\beta^{(1+\lambda)}(\beta' + \gamma), \quad (2.22)$$

for k in $B(\epsilon)$, we have[10]

$$|\delta_n(k;\beta,\beta')| \leq \frac{\mathrm{const}}{\beta^{(1+\lambda)}(\beta' + \gamma)} \frac{e^{(n-1)/2}\|J(k)\|^{n-1}}{n^{(n-2)/2}}, \quad n \geq 2. \quad (2.23)$$

Hence $\delta(k;\beta,\beta')$ is holomorphic in k in $B(\epsilon)$, and consequently in the doubly cut k plane, for $\infty > \beta \geq \gamma, \infty > \beta' \geq \gamma$. Also, we establish

$$|\delta(k;\beta,\beta')| \leq \mathrm{const}/\beta^{(1+\lambda)}(\beta' + \gamma), \quad (2.24)$$

for k in $B(\epsilon)$.

Hence, using

$$|\xi^{\pm(0)}(k;\beta)| \leq \mathrm{const}/\beta^{(1+\lambda)}, \quad (2.25)$$

for k in $B(\epsilon)$, we find that $\int_\gamma^\infty d\beta' \delta(k;\beta,\beta')\xi^{\pm(0)}(k;\beta')$ and consequently $\int_\gamma^\infty d\beta' D(k;\beta,\beta')\xi^{\pm(0)}(k;\beta')$ are holomorphic in k in $B(\epsilon)$, and hence in the doubly cut k plane, for $\infty > \beta \geq \gamma$. Hence we have demonstrated that, for k in the doubly cut k plane, and for $D(k) \neq 0$, the equations of (2.8) have unique square integrable solutions $\xi^{\pm}(k;\beta)$ respectively, which are holomorphic in k in the doubly cut k plane, perhaps with the exception of poles where $D(k) = 0$. And we have

$$|\xi^{\pm}(k;\beta)| \leq \mathrm{const}/\beta^{(1+\lambda)}, \quad (2.26)$$

for k in $B(\epsilon)$. Hence $\xi^{\pm}(k;\beta)$ belong to both $L^1(\gamma,\infty)$ and $L^2(\gamma,\infty)$. Further, $\xi^{\pm}(k;\beta)$ are continuous in β in $\infty > \beta \geq \gamma$.

The right side of (2.4) are therefore functions holomorphic in k and x in the doubly cut k plane, perhaps with the exception of poles where $D(k) = 0$, and $\mathrm{Re}\, x > 0$. These functions, for k in the doubly cut k plane, and for $\Delta^{(\mathrm{II})}(k) \neq 0, D(k) \neq 0$, are just the Jost solutions $f^{\pm}(k;x)$ defined in Ref. 2. Hence we have obtained representations for the Jost solutions in terms of the spectral function $\sigma(\beta,\beta', \cos\nu)$.

We now show

$$\Delta^{(\mathrm{II})}(k) = D(k)$$

in the doubly cut k plane.

We first consider $k > 0$. Then the integral operators $K^{(\mathrm{II})}(k)$ and $J(k)$ defined on $L^2(0,\infty)$ and $L^2(\gamma,\infty)$, respectively, with kernels $K^{(\mathrm{II})}(k;x,x')$ and $J(k;\beta,\beta')$, are Hilbert–Schmidt operators. We have

$$K^{(\mathrm{II})}(k;x,x') = \int_\gamma^\infty \int_\gamma^\infty d\beta \, d\beta' \, e^{-\beta x} e^{-\beta' x'} \frac{s(\beta,\beta')}{k^2 + \beta^2}. \quad (2.27)$$

Hence, we have

$$K^{(\mathrm{II})^n}(k;x,x') = \int_\gamma^\infty \ldots \int_\gamma^\infty d\beta \, d\beta_1 \ldots d\beta_n \frac{e^{-\beta x}}{k^2 + \beta^2} \prod_{i=1}^{n-1} \frac{1}{k^2 + \beta_i^2}$$
$$\times \int_\gamma^\infty \ldots \int_\gamma^\infty d\beta' d\beta_1' \ldots d\beta_n' e^{-\beta' x'} \prod_{i=1}^{n-1} \frac{1}{\beta_i + \beta_i'}$$
$$\times s(\beta,\beta_1') \prod_{i=1}^{n-2} s(\beta_i,\beta_{i+1}') s(\beta_{n-1},\beta'). \quad (2.28)$$

Consequently, we have

$$\mathrm{Tr} K^{(\mathrm{II})^n}(k) = \int_\gamma^\infty \ldots \int_\gamma^\infty d\beta_1 \ldots d\beta_n \prod_{i=1}^{n} \frac{1}{k^2 + \beta_i^2}$$
$$\times \int_\gamma^\infty \ldots \int_\gamma^\infty d\beta_1' \ldots d\beta_n' \prod_{i=1}^{n} \frac{1}{\beta_i + \beta_i'} \prod_{i=1}^{n} s(\beta_i,\beta_{i+1}'), \quad (2.29)$$

with $\beta'_{n+1} = \beta'_1$, which is just $\tau_n(k), n \geq 1$.

Hence, we have

$$\Delta^{(II)}(k) = D(k), \tag{2.30}$$

for $k > 0$, and consequently as a result of holomorphy, in the doubly cut k plane.

The Jost functions have the following representations for k in the doubly cut k plane:

$$\mathcal{L}^{\pm}(k) = 1 + \int_{\gamma}^{\infty} d\beta\,[\xi^{\pm}(k;\beta)/(k^2 + \beta^2)]. \tag{2.31}$$

The S matrix has the following representation for k in the same region:

$$S(k) = \frac{1 + \int_{\gamma}^{\infty} d\beta[\xi^{-}(k;\beta)/(k^2 + \beta^2)]}{1 + \int_{\gamma}^{\infty} d\beta[\xi^{+}(k;\beta)/(k^2 + \beta^2)]}. \tag{2.32}$$

We remark that the representations (2.4), (2.31), and (2.32) allow us to discuss the analytic continuation in k, of $f^{\pm}(k;x)$, for fixed x, and $\mathcal{L}^{\pm}(k)$, $S(k)$, across the intervals $k = \pm i\kappa$, $\kappa \in (\gamma, \infty)$, for analytic partial spectral functions $s(\beta, \beta')$, by contour deformation. The possibility of such analytic continuations would, of course, convey information on the limiting behaviors of these functions as k approaches the above intervals from the doubly cut plane.

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[3]We may use a result of Ref. 1, Appendix B.
[4]Here and in the following, we follow the notations of Ref. 2.
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[9]See Ref. 7, Eq. (7) of Sec. 6.4. Here $\|\ \|$ is the Hilbert-Schmidt norm.
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An approximate interior solution in Brans–Dicke theory

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An approximate interior solution of the field equations of Brans–Dicke theory is obtained for a static spherically symmetric metric which can be considered to be an analog of Schwarzschild's interior solution in Einstein's theory.

I. INTRODUCTION

In previous papers[1,2] we have obtained approximate solution of the static spherically symmetric metric for the vacuum case and for a point charged mass in the Brans–Dicke[3] theory of gravitation starting from the usual variational principle

$$\delta\int\left[\phi R+\frac{16\pi L}{c^4}-\frac{\omega\phi_{,i}\phi^{,i}}{\phi}\right](-g)^{1/2}d^4x=0, \tag{1}$$

where R is the scalar curvature, L the Langrangian, ω the dimensionless constant, and ϕ the scalar playing the role of G^{-1}, following a technique used first by Weyl[4] and then by Pauli.[5] A similar solution for the static spherically symmetric metric for a fluid sphere is well worth consideration.

In this paper we obtain an approximate interior solution of the field equations of the Brans–Dicke theory of gravitation for a static spherically symmetric metric following the same technique. The solution is then compared with the interior solution in Einstein's theory.

II. FIELD EQUATIONS

We consider the line element for the static spherically symmetric metric case in the form[5]

$$ds^2=(dx^1)^2+(dx^2)^2+(dx^3)^2+l(x^1dx^1+x^2dx^2+x^3dx^3)^2+g_{44}(dx^4)^2. \tag{2}$$

The scalar curvature R has been calculated to be[1,5]

$$R=-\frac{1}{r^2\Delta}\frac{d}{dr}\left(\frac{r^2g'_{44}}{\Delta}\right)+\frac{2}{r}\frac{\Delta'}{\Delta^3}g_{44}-\frac{2}{r^2\Delta}\frac{d}{dr}\left(\frac{rg_{44}}{\Delta}\right)-\frac{2}{r^2}, \tag{3}$$

at $x^1=r$, $x^2=0$, $x^3=0$ where dashes denote differentiation with respect to r and

$$g_{11}=h^2=1+lr^2,\quad \Delta=(-g)^{1/2}=h(-g_{44})^{1/2}. \tag{4}$$

The energy tensor of a homogeneous incompressible fluid is given by

$$T_{ik}=(\mu_0+p)u_iu_k+pg_{ik}. \tag{5}$$

We set the Lagrangian as[4]

$$L=\mu_0-(v_iv^i)^{1/2}, \tag{6}$$

where the scalar p denotes the pressure, μ_0 is the constant, density and

$$(\mu_0+p)u_i=v_i. \tag{7}$$

Also $v^1=v^2=v^3=0$ for static case.

Consequently, the variational principle (1) in this case can be written as

$$\delta\int\{\phi R+16\pi[\mu_0-(vh/\Delta)]-(\omega/h^2)(\phi'/\phi)^2\}r^2\Delta\,dr=0, \tag{8}$$

where

$$d^4x=d^4x^4d\Omega\,dr r^2$$

($d\Omega$ is an element of solid angle at the origin),

$$\phi_{,i}\phi^{,i}=g^{11}(\phi'^2/\phi)=(1/h^2)(\phi'^2/\phi).$$

R is given by (3) and the velocity of light is taken to be unity.

Now variation with respect to ϕ, Δ, and h in (8), respectively, leads to the following field equations;

$$-\frac{d}{dr}\left(\frac{r^2g'_{44}}{\Delta}\right)-\frac{2r\Delta'}{h^2}-\frac{2d}{dr}\left(\frac{rg_{44}}{\Delta}\right)-2\Delta=-\frac{\omega r^2\Delta}{h^2}\frac{\phi'^2}{\phi^2}-2\omega\frac{d}{dr}\left(\frac{r^2\Delta}{h^2}\frac{\phi'}{\phi}\right), \tag{9}$$

$$\frac{d}{dr}\frac{2r}{h^2}-2=\frac{\omega r^2}{h^2}\frac{\phi'^2}{\phi^2}-16\pi r^2\mu_0\phi^{-1}, \tag{10}$$

$$\frac{2r\Delta'}{h^3}=-\frac{\omega r^2\Delta}{h^3}\frac{\phi'^2}{\phi^2}+8\pi r^2v\phi^{-1}. \tag{11}$$

Also, since, in a connected space filled with fluid, v has a constant value we have[4]

$$v=(\mu_0+p)(-g_{44})^{1/2}=\mu_0/h_0=(\mu_0+p)\Delta/h. \tag{12}$$

Using (4) the above field equations can be written as

$$-\frac{d}{dr}\left(\frac{r^2g'_{44}}{\Delta}\right)+\frac{2rg_{44}\Delta'}{\Delta^2}-2\frac{d}{dr}\left(\frac{rg_{44}}{\Delta}\right)-2\Delta=\frac{\omega r^2g_{44}}{\Delta}\frac{\phi'^2}{\phi^2}+2\omega\frac{d}{dr}\left(\frac{r^2g_{44}}{\Delta}\frac{\phi'}{\phi}\right), \tag{9'}$$

$$-\frac{2rg'_{44}}{\Delta}-\frac{2g_{44}}{\Delta}+\frac{4rg_{44}\Delta'}{\Delta^2}-2\Delta=-\frac{\omega r^2g_{44}}{\Delta}\frac{\phi'^2}{\phi^2}-\frac{16\pi r^2\mu_0\Delta}{\phi}, \tag{10'}$$

$$-\frac{2rg_{44}\Delta'}{\Delta^2}=\frac{\omega r^2g_{44}}{\Delta}\frac{\phi'^2}{\phi^2}+8\pi r^2vh\phi^{-1}. \tag{11'}$$

III. SOLUTION OF THE FIELD EQUATIONS

We consider the equation (9′) which can be written [using (3)] as

$$Rr^2\Delta=\frac{\omega r^2g_{44}}{\Delta}\frac{\phi'^2}{\phi^2}+2\omega\frac{d}{dr}\left(\frac{r^2g_{44}}{\Delta}\frac{\phi'}{\phi}\right). \tag{13}$$

Also we have[3]

$$Rr^2\Delta=\frac{\omega r^2g_{44}}{\Delta}\frac{\phi'^2}{\phi^2}+8\pi T\phi^{-1}r^2\Delta\left(\frac{2\omega}{3+2\omega}\right). \tag{14}$$

From (13) and (14) we have

$$\frac{d}{dr}\left(\frac{r^2g_{44}}{\Delta}\frac{\phi'}{\phi}\right)=8\pi T\phi^{-1}r^2\Delta(3+2\omega)^{-1}, \tag{15}$$

where $T=3p-\mu_0$ from (5).

And so using (12) and (15), the field equations (9′)–(11′) become

$$-\frac{d}{dr}\left(\frac{r^2g_{44}'}{\Delta}\right)+\frac{2rg_{44}\Delta'}{\Delta^2}-2\frac{d}{dr}\left(\frac{rg_{44}}{\Delta}\right)-2\Delta=\frac{\omega r^2g_{44}}{\Delta}\frac{\phi'^2}{\phi^2}+8\pi\phi^{-1}(3p-\mu_0)r^2\Delta\left(\frac{2\omega}{3+2\omega}\right), \quad (9'')$$

$$-\frac{2rg_{44}'}{\Delta}-\frac{2g_{44}}{\Delta}+\frac{4rg_{44}\Delta'}{\Delta^2}-2\Delta=-\frac{\omega r^2g_{44}}{\Delta}\frac{\phi'^2}{\phi^2}-\frac{16\pi r^2\mu_0\Delta}{\phi}, \quad (10'')$$

$$-\frac{2rg_{44}\Delta'}{\Delta^2}=\frac{\omega r^2g_{44}}{\Delta}\frac{\phi'^2}{\phi^2}+\frac{8\pi r^2}{\phi}(\mu_0+p)\Delta. \quad (11'')$$

Equations (9″), (10″), and (11″) constitute only two independent equations which can be taken as

$$\frac{d}{dr}\left(\frac{rg_{44}}{\Delta}\right)=-\Delta\left[1+8\pi r^2\phi^{-1}\left(\frac{p-\mu_0}{2}\right)\right],$$
$$\frac{d}{dr}\left(\frac{r^2g_{44}'}{\Delta}\right)=\Delta\left[\frac{4rg_{44}\Delta'}{\Delta^3}+8\pi r^2\phi^{-1}\mu_0\left(\frac{2\omega}{3+2\omega}\right)-\frac{8\pi r^2p}{\phi}\left(\frac{2\omega-6}{3+2\omega}\right)\right]. \quad (16)$$

Also we have

$$\frac{d}{dr}\left(\frac{r^2g_{44}}{\Delta}\frac{\phi'}{\phi}\right)=8\pi\phi^{-1}r^2\Delta(3p-\mu_0)(3+2\omega)^{-1},$$
$$v=(\mu_0+p)(-g_{44})^{1/2}=\mu_0/h_0=(\mu_0+p)(\Delta/h). \quad (17)$$

Now the problem reduces to finding Δ, g_{44}, ϕ, and p from (16) and (17).

Let us consider the field equations (9), (10), (11), and (12). When $\phi=\text{const}=\phi_0$ (which is to be calculated to the second order in ϕ_0^{-1}) we get the general relativity interior solution

$$\Delta=(3h-h_0)/2h_0, \quad (-g_{44})^{1/2}=(3h-h_0)/2hh_0;$$
$$p=\mu_0[(h_0-h)/(3h-h_0)], \quad 1/h^2=1-r^2/R^2, \quad (18)$$

where

$$R^2=3/8\pi\mu_0\phi_0^{-1}$$

and h_0 is the value of h on the surface of the sphere. Also when $\phi=\text{constant}=\phi_0$, $\mu_0=0$, and $p=0$ we get the Schwarzschild's exterior solution. In view of the difficulty in finding an exact solution of the equations (16) and (17), we find an approximate solution correct up to the second order in r/R by using the method of successive approximation.[1]

Let us consider the equations (16) and (17). Now, when $\phi=\text{constant}=\phi_0$ substituting the values from (18) in the right-hand side of Eqs. (16) and integrating with respect to r and keeping the terms up to the second order in r/R in the expansion of resulting expression (since r^3/R^3 and higher terms contains ϕ_0^{-3} and higher terms), we get

$$rg_{44}/\Delta\approx-r+\tfrac{3}{4}(rr_0^2/R^2)+(r^3/4R^2)+A, \quad A=\text{const}, \quad (19)$$

$$r^2g_{44}'/\Delta\approx-(2r^3/R^2)[(\omega+3)/(3+2\omega)]+B, \quad B=\text{const}. \quad (20)$$

Since our solution is to be regular as $r\to 0$, the constants of integration in (19) and (20) must be put equal to zero. Hence we get

$$g_{44}/\Delta\approx-1+\tfrac{3}{4}(r_0^2/R^2)+(r^2/4R^2),$$
$$g_{44}'/\Delta\approx-(2r/R^2)[(\omega+3)/(3+2\omega)], \quad (21)$$

where

$$R^2=\tfrac{3}{8}\pi\mu_0\phi_0^{-1}.$$

Eliminating Δ in (21), integrating with respect to r and keeping the terms upto the second order in r/R in the expansion of the resulting expression for g_{44}, we get

$$g_{44}\approx C\{1+(r^2/R^2)[(\omega+3)/(3+2\omega)]\}, \quad C=\text{const}.$$

Since our solution should go over to the Brans–Dicke[3] exterior solution in this approximation, on the surface of the sphere, i.e., at $r=r_0$, viz.,

$$g_{44}\approx-1+\frac{2M\phi_0^{-1}}{r^0}\left(\frac{4+2\omega}{3+2\omega}\right)=-1+\frac{r_0^2}{R^2}\left(\frac{4+2\omega}{3+2\omega}\right),$$

where

$$M=4\pi r_0^3\mu_0/3$$

we must have

$$C\approx-\{1-(r_0^2/R^2)[(3\omega+7)/(3+2\omega)]\}$$

so that

$$g_{44}\approx-1+\frac{r_0^2}{R^2}\left(\frac{3\omega+7}{3+2\omega}\right)-\frac{r^2}{R^2}\left(\frac{\omega+3}{3+2\omega}\right). \quad (22)$$

Using (22) in (21), we have

$$\Delta\approx1-\frac{r_0^2}{4R^2}\left(\frac{6\omega+19}{3+2\omega}\right)+\frac{r^2}{4R^2}\left(\frac{6\omega+15}{3+2\omega}\right). \quad (23)$$

Again from (17) we have [using (18)]

$$(g_{44}/\Delta)(\phi'/\phi)\approx-(r/R^2)(3+2\omega)^{-1},$$
$$(\mu_0+p)(-g_{44})^{1/2}\approx\mu_0[1-(r_0^2/2R^2)]. \quad (24)$$

Now using (22) and (21) in (24) and making the same approximations as the above, we obtain

$$\phi\approx D[1+(r^2/2R^2)(3+2\omega)^{-1}], \quad D=\text{const}, \quad (25)$$

$$p\approx\mu_0\left[\frac{r_0^2}{2R^2}\left(\frac{\omega+3}{3+2\omega}\right)-\frac{r^2}{2R^2}\left(\frac{\omega+3}{3+2\omega}\right)\right]. \quad (26)$$

Again to evaluate the integration constant D in (25) we invoke the condition that our solution should go over to the Brans–Dicke[3] exterior solution at $r=r_0$ in this approximation, viz.,

$$\phi\approx\phi_0\{1+[2M\phi_0^{-1}/r_0(3+2\omega)]\}, \quad M=4\pi r_0^3\mu_0/3$$
$$=\phi_0[1+(r_0^2/R^2)(3+2\omega)^{-1}],$$

so that

$$D\approx\phi_0[1+(r_0^2/2R^2)(3+2\omega)^{-1}].$$

So we have

$$\phi\approx\phi_0[1+(r_0^2/2R^2)(3+2\omega)^{-1}+(r^2/2R^2)(3+2\omega)^{-1}]. \quad (27)$$

Now considering (22), (23), (26), and (27) we can write down the approximate interior solution for the metric (2) in the Brans–Dicke's theory as

$$g_{44} \approx -1 + \frac{r_0^2}{R^2}\left(\frac{3\omega+7}{3+2\omega}\right) - \frac{r^2}{R^2}\left(\frac{\omega+3}{3+2\omega}\right),$$

$$\Delta \approx 1 - \frac{r_0^2}{4R^2}\left(\frac{6\omega+19}{3+2\omega}\right) + \frac{r^2}{4R^2}\left(\frac{6\omega+15}{3+2\omega}\right), \tag{28}$$

$$p \approx \mu_0\left[\frac{r_0^2}{2R^2}\left(\frac{\omega+3}{3+2\omega}\right) - \frac{r^2}{2R^2}\left(\frac{\omega+3}{3+2\omega}\right)\right],$$

$$\phi \approx \phi_0[1 + (r_0^2/2R^2)(3+2\omega)^{-1} + (r^2/2R^2)(3+2\omega)^{-1}].$$

Thus, we see that the solution (28) is an analog of the Schwarzschild's interior solution in Einstein's theory. It is interesting to note that when $\omega \to \infty$ the solution (28) exactly agrees with the general relativity interior solution in the same approximation. And when $r = r_0$, i.e., on the surface of the sphere the solution goes over to the Brans–Dicke exterior solution in the same approximation. It can be, also, seen that there are no singularities at $r=0$, i.e., at the center of the sphere.

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On the transport properties of van der Waals fluids.* II. Explicit calculations

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Starting from the formal expansion of an arbitrary transport coefficient X in series of the inverse range γ of a van der Waals potential, we establish the explicit form of the first γ correction to X; we show that it can be expressed solely in terms of the Fourier transform V_y^L of the long-range interaction and in terms of the equilibrium and transport properties of the short-range reference system. A comparison with previous work on related problems is also given.

I. INTRODUCTION

In a preceding paper, two of the authors (J.P. and P.R.), have performed a formal analysis of the transport coefficients of a three-dimensional van der Waals fluid[1] (this reference is hereafter referred to as I). Such a fluid is characterized by an interaction potential $V(r)$ which can be decomposed according to

$$V(r) = V^S(r) + \gamma^3 V^L(\gamma r), \tag{I.1}$$

where $V^S(r)$ is the short-range part while $\gamma^3 V^L(\gamma r)$ describes the long-range tail of the total potential: the motivation of the splitting (I.1) is that the inverse range γ is supposed to be small and furnishes thus an expansion parameter for the calculation of equilibrium and transport properties.

Starting from the Green—Kubo expression for an arbitrary transport coefficient X, our main result, obtained through a detailed many-body analysis, is the following expansion:

$$X = X^S + \sum_{n=1}^{\infty} \gamma^n X^{(n)}(\gamma), \tag{I.2}$$

where X^S denotes the pure hard-core contribution while the coefficients $X^{(n)}(\gamma)$, which are still (possibly nonanalytic) functions of γ, are such that

$$\lim_{\gamma\to 0} X^{(n)}(\gamma) = \text{finite const.} \tag{I.3}$$

More precisely, Eq. (I.2) is an immediate consequence of a similar property for the various operators[2] Ψ_0^l, $\mathcal{C}_{k0}^l$, $\mathcal{D}_0^l$ and $\mathcal{G}_k^l$ which appear in the microscopic analysis of X. For example, we have shown that the linearized collision operator Ψ_0^l, which plays a central role in the theory, can be expanded according to

$$\Psi_0^l(v_1 \,|\, \gamma) = \Psi_0^{l,S}(v_1) + \sum_{n=1}^{\infty} \gamma^n \Psi_0^{l(n)}(v_1 \,|\, \gamma). \tag{I.4}$$

Let us stress the nontrivial nature of the expansion (I.4); indeed, the naive but straightforward perturbation expansion of Ψ_0^l, which expresses this operator as a functional of the free-particle propagator G_k^0,

$$\Psi_0^l(v_1 \,|\, \gamma) = \Psi_0^l(v_1 \,|\, \gamma \,|\, \{G_k^0\}), \tag{I.5}$$

$$G_k^0(v_1; z) = 1/(z - kv_1), \tag{I.6}$$

does not lend itself naturally to an expansion of the type (I.4). Rather, we first have to renormalize the one-particle propagator, taking into account the interaction of the propagating particle with the rest of the fluid. We write thus first

$$\Psi_0^l(v_1 \,|\, \gamma) = \Psi_0^l(v_1 \,|\, \gamma \,|\, \{G_k\}), \tag{I.7}$$

$$G_k(v_1; z) = 1/[z - kv_1 + \Psi_k^l(v_1; z)], \tag{I.8}$$

where G_k is the exact propagator while Ψ_k^l describes the collision of particle 1 with the remaining $(N-1)$ particles of the fluid.

A crucial observation in our analysis is that, because of the long-range character of the potential V^L, the dominant contributions to Ψ_0^l due to V^L come, in (I.7), from small values of k ($k \lesssim \gamma$) and z ($z \lesssim \gamma$). In this limit, we are able to get an exact expression for the dominant contributions to the operator G_k. We have indeed

$$\lim_{\gamma} G_k(v_1; z) = \sum_{\alpha=1}^{5} |\bar{f}_\alpha^{1k}(y)\rangle [z - i\Lambda_\alpha^k(y)]^{-1} \langle f_\alpha^{1k}(y)|, \tag{I.9}$$

where $\lim_\gamma$ is an abbreviation for the following limiting procedure:

$$\gamma \to 0, \quad k/\gamma = y \text{ finite}, \quad z/\gamma = w \text{ finite}. \tag{I.10}$$

The eigenvalues $\Lambda_\alpha^k(y)$ and the corresponding eigenfunctions were already explicitly displayed in I for k oriented along the x axis; we give them here for an arbitrary orientation of k. We have

$$\Lambda_{1,2}^k(y) = \pm ic(y)k - \Gamma(y)k^2, \tag{I.11a}$$

$$|f_{1,2}^{1k}(y)\rangle = \frac{1}{\sqrt{2}} \left[\frac{\sqrt{k_B T}}{c(y)} \,|1\rangle \pm |2^{1k}\rangle + \frac{1}{nc(y)C_v^S} \left(\frac{3k_B T}{2}\right)^{1/2} \times \left(\frac{\partial p}{\partial T}\right)_n^S |5\rangle \right], \tag{I.11b}$$

$$\langle \bar{f}_{1,2}^{1k}(y)| = \frac{1}{\sqrt{2}} \left[\frac{1}{c(y)\sqrt{k_B T}} \frac{1}{n\chi_T(y)} \langle 1| \pm \langle 2^{1k}| + \left(\frac{2k_B T}{3}\right)^{1/2} \frac{1}{c(y)nk_B} \left(\frac{\partial p}{\partial T}\right)_n^S \langle \bar{\chi}_S| \right], \tag{I.11c}$$

$$\Lambda_{3,4}^k(y) = -\eta^S k^2/n, \tag{I.12a}$$

$$|f_{3,4}^{1k}(y)\rangle = |3^{1k}, 4^{1k}\rangle, \tag{I.12b}$$

$$\langle \bar{f}_{3,4}^{1k}(y)| = \langle 3^{1k}, 4^{1k}|, \tag{I.12c}$$

$$\Lambda_5^k(y) = -\kappa^S k^2/nC_p(y), \tag{I.13a}$$

$$|f_5^{1k}(y)\rangle = \frac{1}{c^2(y)} \left[-\left(\frac{3}{2}\right)^{1/2} \frac{T}{n}\left(\frac{\partial p}{\partial T}\right)_n^S |1\rangle + \frac{1}{n\chi_T(y)} |5\rangle \right], \tag{I.13b}$$

$$\langle \bar{f}_5^{1k}(y)| = \left[-\frac{1}{nC_v^S}\left(\frac{2}{3}\right)^{1/2} \left(\frac{\partial p}{\partial T}\right)_n^S \langle 1| + \langle \bar{\chi}_5| \right]. \tag{I.13c}$$

Here $|i^{1k}\rangle$ $(i = 2, 3, 4)$, respectively, denote the longitudinal and the two orthogonal components of the velocity field; they have the following velocity space representation:

$$\langle v|2^{1k}\rangle = \langle 2^{1k}|v\rangle = \varphi^{eq}(v)(v_x 1_{k_x} + v_y 1_{k_y} + v_z 1_{k_z})/\sqrt{k_B T},$$

$$\langle v|3^{1_k}\rangle=\langle 3^{1_k}|v\rangle=\varphi^{\rm eq}(v)(-v_x 1_{k_x}1_{k_y}+v_y(1_{k_x}^2+1_{k_z}^2)$$
$$\varphi^{\rm eq}(v)-v_z 1_{k_z}1_{k_y})/\sqrt{k_BT(1_{k_z}^2+1_{k_x}^2)}, \qquad \text{(I. 14)}$$
$$\langle v|4^{1_k}\rangle=\langle 4^{1_k}|v\rangle=(v_z 1_{k_x}-v_x 1_{k_z})/\sqrt{k_BT(1_{k_z}^2+1_{k_y}^2)},$$

where $1_k=\mathbf{k}/|\mathbf{k}|$. All other symbols appearing in (I. 12) have been defined in I: Let us simply recall here that $c(y)$, $C_p(y)$, $\chi_T(y)$, respectively, are finite y-generalizations of the adiabatic sound velocity, specific heat at constant pressure, and isothermal compressibility of the van der Waals fluid. Equations (I. 11–13) thus give the hydrodynamical eigenvalues and eigenfunctions of this van der Waals fluid, suitably generalized to finite y.

We shall not reproduce here the calculations leading to these expressions for an arbitrary vector 1_k; let us simply remark that for $1_k=1_x$, they exactly reduce to Eqs. (I. V. 27–29); moreover, the vectors $|i^{1_k}\rangle$ are orthonormal with our definition (I. A. 9) of the scalar product.

With this renormalized from (I. 5), we have been able not only to establish the expansion (I. 4) but also to obtain the explicit form of the first few corrections $\Psi_0^{l(n)}$ $(n=1,2,3)$ in terms of the Prigogine–Balescu diagram technique (suitably adapted to the present problem). For example, the first correction, $\Psi_0^{l(1)}$, is given by the graph depicted in Fig. 1. Here again, we refer the reader to I for the detailed meaning of this diagram: Roughly speaking, it represents, to dominant order in γ, an arbitrary pure hard-core process (the dashed bubble) from which two particles emerge with wavenumbers k and $-k$; these particles then propagate hydrodynamically in the presence of the van der Waals forces (the two heavy lines) and then again interact through an arbitrary hard-core process; finally, in order to get the correct result, we should subtract from this graph the corresponding pure hard-core term, obtained by formally setting $V^L\equiv 0$ in the hydrodynamical lines of this same graph.

The corresponding corrections for the quantities $\mathcal{C}_{k0}^l$, $\mathcal{D}_0^l$, $\mathcal{P}_k^l$ are given in I, Table III.

The aim of the present paper is to go beyond these formal results and to give an explicit evaluation of the first correction $X^{(1)}(\gamma=0)$ for the various transport coefficients. However, whenever it will be necessary to specify the explicit nature of X, we shall perform the detailed calculation for the thermal conductivity $(X=T\kappa)$ only, in order to avoid undue lengthiness. For the shear and bulk viscosities, we shall merely quote the results.

In Sec. II, we establish a fundamental property of the dashed bubble of Fig. 1: Indeed, we show that, in the $k\to 0$ limit, this quantity, when acting on a product of two hydrodynamical eigenfunctions, can be reduced to the pure hard-core *linearized* collision operator $\Psi_0^{l,S}$, which also appears as the leading term of (I. 4).

In Sec. III, this property is explicitly used in order to calculate $X^{(1)}(\gamma=0)$ and leads to the remarkable result that this correction can be cast in a form which only involves equilibrium fluctuations and hydrodynamical eigenvalues: In particular, the collision operator $\Psi_0^{l,S}$, entirely disappears from our formulas, which can then be calculated *independently of any specific model of*

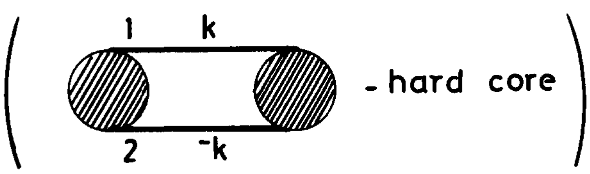

FIG. 1. The first correction $\Psi_0^{l(1)}$ (v_1/γ).

the hard-core dynamics. We then give an explicit calculation of the above-mentioned equilibrium fluctuations and we get an expression for $X^{(1)}(\gamma=0)$ which has the following form:

$$X^{(1)}(\gamma=0)=\int_0^\infty dy\, f^X(V_y^L,\{X^S\},\{Y^S\}), \qquad \text{(I. 15)}$$

where $\{X^S\}$ and $\{Y^S\}$, respectively, denote the transport coefficients and the thermodynamic properties of the pure hard-core reference system; moreover, f^X is a simple algebraic function of the Fourier transform of the long-range potential, denoted by V_y^L.

The simplicity of this results makes it *a posteriori* plausible that this result can also be obtained using semimacroscopic arguments, similar to those used in the mode–mode coupling analysis.[3] That this is indeed the case is shown in Sec. IV.

Finally some remarks of general interest, including the connection of our results with the recently discovered long-time behavior of the Green–Kubo integrands,[4] are presented in Sec. V.

Many mathematical developments have been relegated in Appendices.

II. A REDUCTION FORMULA FOR $\gamma\Psi_0^{l(1)}$, $\gamma\mathcal{C}_{k_0}^{l(1)}$, $\gamma\mathcal{D}_0^{l(1)}$, and $\gamma\mathcal{G}_k^{l(1)}$

A straightforward application of the rules given in I (see Table I of that paper), leads to the following formal expression for the correction $\gamma\Psi_0^{l(1)}(\gamma)$ depicted in Fig. 1 [compare also with Eq. (I. III. 8)]:

$$\gamma\Psi_0^{l(1)}(v_1|\gamma)=\left(\frac{\Omega}{8\pi^3}\frac{1}{2!}\int dk\int dv\left\{\Psi_{\{0\};k_1,-k_2,\{0\}'}(v_1,v_2;i\epsilon)\right.\right.$$
$$\times\left[\lim_{t\to\infty} i\int_0^t d\tau\, X_k(v_1;\tau)X_{-k}(v_2;\tau)\right]$$
$$\left.\left.\times\hat{\Psi}_{k_1,k_2,\{0\}';\{0\}}(v_1,v_2;i\epsilon)-\text{hard core}\right\}\right), \qquad \text{(II. 1)}$$

where the propagator $X_k(v_1;\tau)$ is defined by (I. III. 5, 9), while $\Psi_{\{0\};k_1,-k_2,\{0\}'}$ and $\hat{\Psi}_{k_1,-k_2,\{0\}';\{0\}}$ are *two*-particle operators, representing the bubbles of Fig. 1. More precisely $\Psi_{\{0\};k_1,-k_2,\{0\}'}$ is an operator which acts on an arbitrary two-particle function $\Phi_2(v_1,v_2)$ in the following way:

$$\Psi_{\{0\};k_1,-k_2,\{0\}'}(v_1,v_2;z)\Phi_2(v_1,v_2)$$
$$=\left(\sum_{u\neq t=1}^{N}\int dv^{N-2}[\tilde{\Psi}^S_{\{0\};k_u,-k_t,\{0\}'}(\{v\};z)]_{u,t}\right.$$
$$\left.\times\Phi_2(v_u,v_t)/\varphi^{\rm eq}(v_u)\varphi^{\rm eq}(v_t)\right)+O(\gamma), \qquad \text{(II. 2)}$$

where we have

$$[\tilde{\Psi}^S_{\{0\};k_u,-k_t,\{0\}'}(\{v\};z)]_{u,t}$$

$$= \sum_{n=1}^{\infty} \Big((\{0\}|_1\{(-\delta L^S)[(L_0 - z)^{-1}Q_k^2(-\delta L^S)]^n\}_{u \text{ or } t}^{\text{F.C}} \times |k_u, -k_t, \{0\}) \prod_{i=1}^{N} \varphi^{\text{eq}}(v_i) + \sum_{\substack{\{k'\}\neq 0 \\ k'_u = k'_t = 0}} (\{0\}|_1\{(-\delta L^S) \times [(L_0 - z)^{-1}Q_k^2(-\delta L^S)]^n\}_{u \text{ or } t}^{\text{F.C}} |k_u, -k_t, \{k'\}) \times (\{k'\}|\Omega^N \rho^{\text{eq}}|\{0\}) \Big); \tag{II.3}$$

in the following, we shall also need the same operator for $u=t$ [see (II.12)]. It is obtained by setting $k_u = k_t = 0$ and $u \equiv t$ into (II.3). In this equation, we have introduced the projector

$$Q_k^2 = 1 - |\{0\})(\{0\}| - \sum_{a\neq b=1}^{n} |\{0\}', k_a, -k_b)(k_a, -k_b, \{0\}'| \tag{II.4}$$

which eliminates not only the "vacuum component" $|\{0\})$ (as is usual in the definition of a collision operator) but also all intermediate states with a single pair of lines (a, b) with wave vectors $k_a = k_u = k$ and $k_b = k_t = -k$; this supplementary restriction is necessary because such states are already included in the propagators $X_k(v_1; \tau)$ and $X_{-k}(v_2; \tau)$ of Eq. (II.1). Note, however, that, in the $k \to 0$ limit of Eq. (II.3), the projector Q_k^2 reduces to

$$Q \equiv 1 - |\{0\})(\{0\}|. \tag{II.5}$$

Similarly, $\hat{\Psi}_{k_1, -k_2, \{0\}'; \{0\}}$ acts on any one-particle function in such a way that

$$\hat{\Psi}_{k_1, -k_2, \{0\}'; \{0\}}(v_1, v_2; z)\Phi(v_1) = \sum_{t=1}^{N} \int dv^{N-2} \tilde{\Psi}'^S_{k_1, -k_2, \{0\}'; \{0\}}(\{v\}; z)\Phi(v_t)/\varphi^{\text{eq}}(v_t), \tag{II.6}$$

where now

$$\tilde{\Psi}'^S_{k_1, -k_2, \{0\}'; \{0\}} = \sum_{n=1}^{\infty} \Big((k_1, -k_2, \{0\}'|_{1 \text{ or } 2}\{(-\delta L^S)[(L - z)^{-1}Q_k^2 \times (-\delta L^S)]^n\}_t^{\text{F.C}} |\{0\}) \prod_{i=1}^{N} \varphi_1^{\text{eq}}(v_i) + \sum_{\substack{\{k'\}\neq 0 \\ k'_t = 0}} (k_1, -k_2, \{0\}'|_{1 \text{ or } 2}\{(-\delta L^S)[(L_0 - z)^{-1}Q_k^2 \times (-\delta L^S)]^n\}_t^{\text{F.C}} |\{k'\})(\{k'\}|\Omega^N \rho^{\text{eq}}|\{0\}) \Big). \tag{II.7}$$

Although the most difficult problem in "translating" Fig. 1 into these analytical expressions is clearly a question of notation (which can be best understood by working out explicitly a few simple examples), the following remarks can be helpful in the understanding of these equations (II.1, 4):

(1) If we had followed strictly the rules given in I, Table I, we should have expressed all contributions in terms of renormalized vertices. However, to avoid a complicated notation, we found it more convenient to apply backward the theorem on propagation of equilibrium correlations [see I, Eq. (II.31) and following]; by this trick, we can lump together all these equilibrium factors at the right of the operator $\tilde{\Psi}^S$—the reader will easily convince himself that this is indeed a legitimate procedure.

(2) Both in Eqs. (II.2) and (II.6), we have neglected terms of order γ. Indeed, we should take there the complete contributions of type II segments (see I, Sec. III) which generally involve long range vertices; the dominant contributions are however of pure short-range nature, as indicated by the superscript S in Eqs. (II.3) and (II.7).

(3) Let us still point out the factor $(2!)^{-1}$ in Eq. (II.1); indeed, when we interchange the label of the particles respectively carrying wave number k and $-k$ in Fig. 1, we do not generate a distinct graph while the two corresponding contributions have both been retained in the bracketed term of Eq. (II.2): This overcounting is corrected for by dividing by $2!$.

Let us now insert into Eq. (II.1) the expansion (I.III.10) for the propagators; more precisely, we use the following representation for the operator $X_k(v; \tau)$ acting on an arbitrary function $\Phi(v)$:

$$X_k(v; \tau)\Phi(v) = \sum_{\alpha=1}^{5} \exp[\Lambda_\alpha^k(\gamma)\tau] f_\alpha^k(v|\gamma)\langle \bar{f}_\alpha^k(\gamma)|\Phi\rangle + [X_k(v; \tau)\Phi(v)]_{\text{nonhyd}}, \tag{II.8}$$

where the subscript "nonhyd" denotes the nonhydrodynamical contributions, which generally have a complicated time behavior; moreover, $f_\alpha^k(v|\gamma)$ is the velocity space representation of the eigenfunction $|f_\alpha^k(\gamma)\rangle$ and the scalar product $\langle f|g\rangle$ is defined by

$$\langle f|g\rangle = \int dv[\varphi^{\text{eq}}(v)]^{-1} f(v) g(v). \tag{II.9}$$

We then assume that the nonhydrodynamical part of $X_k(v; \tau)$ gives a finite contribution to the time integral appearing in (II.1) when $\gamma \to 0$; taking into account that the k-integral in (II.1) is restricted to $|k| \lesssim \gamma$, we get then

$$\gamma\Psi_0^{l(1)}(v_1|\gamma) = \Big(\frac{\Omega}{8\pi^3}\frac{1}{2!}\sum_{\alpha,\beta}\int dk \int dv_2 \Big\{ \Psi_{\{0\};\{0\}}(v_1, v_2; i\epsilon) \times f_\alpha^{1k}(v_1|y) f_\beta^{-1k}(v_2|y)[i(\Lambda_\alpha^k(y) + \Lambda_\beta^{-k}(y))]^{-1} \times \int dv'_1 dv'_2 [\varphi^{\text{eq}}(v'_1)\varphi^{\text{eq}}(v'_2)]^{-1} \bar{f}_\alpha^{1k}(v'_1|y) \times \bar{f}_\beta^{-1k}(v'_2|y)\hat{\Psi}_{\{0\};\{0\}}(v'_1, v'_2; i\epsilon) - \text{hard core}\Big\}\Big) \times [1 + O(\gamma^{\min(\mu,1)})]. \tag{II.10}$$

A word of comment is required here to explain our estimate of the terms neglected in going from (II.1) to (II.10). Besides the γ^1 correction involved in (II.2) and (II.6), we first have dropped the nonhydrodynamical part of $X_k(v; \tau)$: following our remark after (II.8), this correction is only of order γ^2 compared to the leading term retained in (II.10). Second, we have replaced $\Psi_{\{0\}; k_1, -k_2, \{0\}'}$ by $\Psi_{\{0\},\{0\}}$ which, for $k \leq \gamma$, should lead to an error not larger than $O(\gamma)$. Similarly, the replacement of the exact eigenfunctions $|f_\alpha^k(\gamma)\rangle$ by their leading contribution $|f_\alpha^{1k}(y)\rangle$ [see (I.11, 13)] is also expected to involve errors of $O(\gamma)$ for $k \lesssim \gamma$. Finally, we have replaced the exact eigenvalues $\Lambda_\alpha^k(\gamma)$ by their dominant part $\Lambda_\alpha^k(y)$ [see again (I.11, 13)]. Here the situation seems less favorable; indeed, we have now indications that the slow decay of the Green–Kubo integrands for long times[4] has a counterpart on the k-behavior of transport eigenvalues Λ_α^k, even for a pure short-range system. On the basis of semimacroscopic arguments, one expects[5]

$$\Lambda_\alpha^k = (\Lambda_\alpha^k)_{\rm hyd}[1 + O(k^\mu)], \qquad (\text{II}.11)$$

where $(\Lambda_\alpha^k)_{\rm hyd}$ denotes the usual hydrodynamical eigenvalues; the exponent μ is expected to be $\frac{1}{2}$. As we are interested here in a microscopic theory while we only have semimacroscopic arguments to support (II.11), we shall be a little more careful and we shall take min(1, μ) as our estimate of the neglected terms, leaving μ as an unknown parameter.

As it stands in (II.10), our expression for $\gamma\Psi_0^{l(1)}$ is still very formal because it involves the two-particle operators $\Psi_{\{0\};\{0\}}$ and $\hat{\Psi}_{\{0\};\{0\}}$ which cannot be written in a compact form.

However, a cruicial simplification occurs when we realize that these operators, when acting on a product of two hydrodynamical modes [see (II.10)] can be reduced to the one-particle short-range operator $\Psi_0^{l,S}$ [see (I.4)]. We present here a formal proof of this result; moreover, due to the key role played by this remarkable property in the present analysis, we also prove it explicitly in Appendix E for the dilute gas; in this latter case the same result was already implicitly used by Dorfman and Cohen.[6]

We first notice that the operators $\tilde{\Psi}^S_{\{0\};\{0\}}(\{v\}; i\epsilon)$ and $\tilde{\Psi}'^S_{\{0\};\{0\}}(\{v\}; i\epsilon)$, from which $\Psi_{\{0\};\{0\}}$ and $\hat{\Psi}_{\{0\};\{0\}}$ are built [see (II.2) and (II.6)], conserve the collision invariants; we have, for example,

$$\sum_{t=1}^{N} [[\tilde{\Psi}_{\{0\};\{0\}}(\{v\}; i\epsilon)]_{u,t}, i_\alpha(v_t)] = 0, \qquad (\text{II}.12)$$

where $i_\alpha(v)$ is any of the five collision normalized invariants $[i_1 = 1, i_{2,3,4} = (v_1)_{x,y,z}/\sqrt{k_B T}; i_5 = \sqrt{2/3}(v^2/2k_B T - 3/2)]$. The commutation relation (II.12) is trivial to prove for i_1 (particle conservation) and $i_{2,3,4}$ (momentum conservation); for the kinetic energy invariant i_5, the proof is more involved but has been given previously in a different context[7]; we shall not reproduce it here. Let us also mention another important property of $[\tilde{\Psi}^S_{\{0\};\{0\}}]_{u,t}$: It gives zero when acting on a constant

$$[\tilde{\Psi}^S_{\{0\};\{0\}}(\{v\}; i\epsilon)]_{u,t} C^t = 0. \qquad (\text{II}.13)$$

This latter property merely reflects the fact the Maxwellian distribution is a stationary solution of the generalized Boltzmann equation [see (II.3)].

If we now take into account that the eigenfunctions $f_\alpha^{1k}(v|y)$ are linear combinations of these invariants, we can simplify (II.10) in a decisive manner. We have indeed

$$f_\alpha^{1k}(v|y)/\varphi^{\rm eq}(v) \equiv I_\alpha^{1k}(v|y) = \sum_{\beta=1}^{5} c_{\alpha\beta}^{1k}(y) i_\beta(v), \qquad (\text{II}.14)$$

where the $c_{\alpha\beta}^{1k}$ are v_1-independent coefficients which are readily calculated from (I.11, I.13). Using twice Eq. (II.12) and then Eq. (II.13), we get in succession

$$\begin{aligned}
&\sum_{t\neq u} [\tilde{\Psi}^S_{\{0\};\{0\}}]_{u,t} I_\alpha^{1k}(v_t|y) I_\beta^{-1k}(v_u|y) \\
&= \sum_{\text{all } t,u} [\tilde{\Psi}^S_{\{0\};\{0\}}]_{u,t} I_\alpha^{1k}(v_t|y) I_\beta^{-1k}(v_u|y) \\
&\quad - \sum_t [\tilde{\Psi}^S_{\{0\};\{0\}}]_{t,t} I_\alpha^{1k}(v_t|y) I_\beta^{-1k}(v_t|y) \\
&= \sum_{\text{all } t,u} I_\alpha^{1k}(v_t|y) [\tilde{\Psi}^S_{\{0\};\{0\}}]_{u,t} I_\beta^{-1k}(v_u|y) \\
&\quad - \sum_t [\tilde{\Psi}^S_{\{0\};\{0\}}]_{t,t} I_\alpha^{1k}(v_t|y) I_\beta^{-1k}(v_t|y) \\
&= \sum_{\text{all } t,u} I_\alpha^{1k}(v_t|y) I_\beta^{-1k}(v_u|y) [\tilde{\Psi}^S_{\{0\};\{0\}}]_{u,t} 1 \\
&\quad - \sum_t [\tilde{\Psi}^S_{\{0\};\{0\}}]_{t,t} I_\alpha^{1k}(v_t|y) I_\beta^{-1k}(v_t|y) \\
&= -\sum_t [\tilde{\Psi}^S_{\{0\};\{0\}}]_{t,t} I_\alpha^{1k}(v_t|y) I_\beta^{-1k}(v_t|y).
\end{aligned} \qquad (\text{II}.15)$$

The remarkable feature of this equation is that in the initial form—at the extreme left-hand side of (II.15)—$\tilde{\Psi}^S_{\{0\};\{0\}}$ acts on a function of two variables v_t and v_u, while at the extreme right-hand side it only operates on a function of one variable!

Inserting this result into (II.2)—taken at $k_1 = -k_2 = 0$ and $z = i\epsilon$—we obtain after integration over v_2

$$\begin{aligned}
&\int dv_2 \Psi_{\{0\};\{0\}}(v_1, v_2; i\epsilon) f_\alpha^{1k}(v_1|y) f_\beta^{-1k}(v_2|y) \\
&= -\sum_{t=1}^{N} \int dv^{N-1} [\tilde{\Psi}^S_{\{0\};\{0\}}(\{v\}; i\epsilon)]_{t,t} I_\alpha^{1k}(v_t|y) I_\beta^{-1k}(v_t|y) + O(\gamma) \\
&= -\Psi_0^{l,S}(v_1) I_\alpha^{1k}(v_1|y) I_\beta^{-1k}(v_1|y) \varphi^{\rm eq}(v_1) + O(\gamma),
\end{aligned} \qquad (\text{II}.16)$$

where $\Psi_0^{l,S}(v_1)$ denotes the purely short range *linearized* collision operator, obtained from (I.II.24) by setting $z = i\epsilon$ and putting everywhere the superscript S; this operator is precisely the leading term of the expansion (I.4).

Notice that in going from the second to the third member of Eq. (II.16), we have made the nontrival identification

$$\Psi_0^{l,S}(v_1)\Phi(v_1) = \sum_{t=1}^{N} \int dv^{N-1} [\tilde{\Psi}^S_{\{0\};\{0\}}(\{v\}; i\epsilon)]_{t,t} \Phi(v_t)/\varphi^{\rm eq}(v_t), \qquad (\text{II}.17)$$

which is justified by the remark after (II.3).

From (II.10), we see that we also have to transform the quantity

$$A = \int dv_1' dv_2' \bar{I}_\alpha^{1k}(v_1'|y) \bar{I}_\beta^{-1k}(v_2'|y) \hat{\Psi}_{\{0\};\{0\}}(v_1', v_2'; i\epsilon) \Phi(v_1'). \qquad (\text{II}.18)$$

We shall not present this calculation here because, except for numerical factors, A is essentially the conjugate of the left-hand side of (II.15) and can be handled by the same method.

The result is

$$A = -\frac{1}{N} \int dv_1' \bar{I}_\alpha^{1k}(v_1'|y) \bar{I}_\beta^{-1k}(v_1'|y) \Psi_0^{l,S}(v_1') \Phi(v_2') + O(\gamma). \qquad (\text{II}.19)$$

Combining (II.10), (II.16), and (II.18), we get finally

$$\begin{aligned}
&\gamma \Psi_0^{l(1)}(v_1|\gamma)\Phi(v_1) \\
&= \Psi_0^{l,S}(v_1) \left[\frac{1}{8\pi^3 n} \frac{1}{2!} \sum_{\alpha,\beta} \int d^3k \left(I_\alpha^{1k}(v_1|y) I_\beta^{-1k}(v_1|y) \varphi^{\rm eq}(v_1) \right.\right. \\
&\quad \times \frac{1}{i[\Lambda_\alpha^k(y) + \Lambda_\beta^{-k}(y)]} \int dv_1' \bar{I}_\alpha^{1k}(v_1'|y) \bar{I}_\beta^{-1k}(v_1'|y) \\
&\quad \left.\left. \times \Psi_0^{l,S}(v_1')\Phi(v_1') - \text{hard core} \right) \right] + O(\gamma^{1+\min(1,\mu)}).
\end{aligned} \qquad (\text{II}.20)$$

Thus, the only operator which appears in this equation is the hard-core linearized collision operator $\Psi_0^{l,S}$; this property is a generalization to arbitrary density and interaction of a result previously established by Dorfman and Cohen for dilute hard speres,[6] in the context of the $t^{-3/2}$ decay law for the Green-Kubo integrands.

As we shall see later, this linearized collision operator itself will disappear from the final formulas when computing the γ^1 correction to the transport coefficient X. However, before we can show this, we first have to derive the analog of (II. 20) for the other quantities which appear in the calculation of $X^{(1)}$, namely for $\mathcal{D}_0^{l(1)}(\gamma)$, $\mathcal{C}_{k0}^{l(1)}(\gamma)$, $\mathcal{P}_k^{l(1)}(\gamma)$. As this analysis follows the same line as the previous one, we shall be very brief, stressing mainly the few points where new features appear.

Consider for example the case of $\mathcal{D}_0^{l(1)}(\gamma)$; from I, Table III, we obtain, in analogy with (II. 1),

$$\gamma\mathcal{D}_0^{l(1)}(v_1; i\epsilon) = \left\{\frac{\Omega}{8\pi^3}\frac{1}{2!}\int dk\left[\int dv_2\Psi_{\{0\};k_1,-k_2,\{0\}'}(v_1,v_2;i\epsilon)\right.\right. \times\left(\lim_{t\to\infty} i\int_0^t d\tau\, X_k(v_1;\tau)X_{-k}(v_2;\tau)\right)\int dv^{N-2} \times\Big((k_1,-k_2|[J^x-\delta J^x]\Omega^N\rho^{\text{eq}}|0) + \sum_{k\neq 0}\tilde{\mathcal{D}}^S_{k_1,-k_2,\{0\}';\{k'\}} \times(\{v\};i\epsilon)(\{k'\}|[J^x-\delta J^x]\Omega^N\rho^{\text{eq}}|0)\Big) - \text{hard core}\Big]\Big\}, \quad (\text{II. }21)$$

where we have put

$$\tilde{\mathcal{D}}^S_{k_1,-k_2,\{0\}';\{k'\}}(\{v\};z) = \sum_{n=1}^{\infty}(k_1,-k_2|\{[-\delta L^S Q_k^2(L_0-z)^{-1}]^n\}^{\text{F.C.}}|\{k'\}) + O(\gamma). \quad (\text{II. }22)$$

Inserting the representation (II. 8) into (II. 21) and using (II. 15), we get after some straightforward manipulations

$$\gamma\mathcal{D}_0^{l(1)}(v_1; i\epsilon) = \Psi_0^{l,S}(v_1)\left(\frac{-1}{8\pi^3 n}\frac{1}{2!}\sum_{\alpha,\beta}\int dk(I_\alpha^{1k}(v_1|y)I_\beta^{-1k}(v_1|y) \times\{i[\Lambda_\alpha^k(y)+\Lambda_\beta^{-k}(y)]\}^{-1}\hat{\Phi}'^x_{\alpha\beta}(1_k,y) - \text{hard core})\right) + O(\gamma^{1+\min(\mu,1)}). \quad (\text{II. }23)$$

Here we have introduced the velocity-independent quantity $\hat{\Phi}'^x_{\alpha\beta}(1_k,y)$:

$$\hat{\Phi}'^x_{\alpha\beta}(1_k,y) = \lim_\gamma \frac{1}{N}\sum_{a\neq b=1}^{N}\int dv^N \bar{I}_\alpha^{1k}(v_a|y)\bar{I}_\beta^{-1k}(v_b|y) \times\Big((k_a,-k_b|(J^x-\delta J^x)\Omega^N\rho^{\text{eq}}|0) + \sum_{\{k'\}\neq 0}\tilde{\mathcal{D}}^S_{k_a,-k_b,\{0\}';\{k'\}}(\{v\};i\epsilon)(\{k'\}|(J^x-\delta J^x) \times\Omega^N\rho^{\text{eq}}|0)\Big) + O(\gamma) \quad (\text{II. }24)$$

and we have used the definition (I. 10) taken for $w=0$.

Let us stress that, in this latter formula, the limit $k\to 0$, $y=k/\gamma$ finite, has to be taken with great care and is *not* obtained by merely setting $k_a=-k_b=0$. Indeed (as was pointed out in Ref. 1 Sec. IV), the flow term $(\{k'\}|(J^x-\delta J^x)\Omega^N\rho^{\text{eq}}|0)$ involves long-range contributions which remain finite when $\gamma\to 0$: In other words, Eq. (II. 24) is not purely short range (although the operator $\tilde{\mathcal{D}}^S$ is!) and we thus have to keep y finite when going to the $k\to 0$ limit.

The bracket of (II. 24) involves equilibrium correlations which have a nonanalytical behavior at $k\to 0$ in the canonical esemble used here; for example, we have

$$\lim_{k\to 0}(k_a,-k_b|(J^x-\delta J^x)\Omega^N\rho^{\text{eq}}|0) \neq (0|(J^x-\delta J^x)\Omega^N\rho^{\text{eq}}|0), \quad (\text{II. }25)$$

even for purely short-range terms! The situation here is completely analogous to the well-known case of the pair correlation function $\tilde{g}_2(k)$, where

$$\lim_{k\to 0} N\int dv^N \rho^{\text{eq}}_{k_1,-k_2,\{0\}'}(\{v\}) = \lim_{k\to 0} n^{-1}\tilde{g}_2(k) = k_B T\left(\frac{\partial n}{\partial p}\right)_T - 1 \neq N\int dv^N\rho_0^{\text{eq}}(\{v\}] = N! \quad (\text{II. }26)$$

Due to these difficulties, we shall provisionally maintain $\hat{\Phi}'^x_{\alpha\beta}$ as it is defined in (II. 24), leaving for later the proof that it can be reduced to purely *equilibrium fluctuations*, which can then be computed according to standard methods.

The so-called creation operator $\mathcal{C}_{k0}^{l(1)}(v_1|\gamma)$ can be similarly transformed; we get

$$\gamma\sum_{\{k'\}\neq 0}(0|(J_1^x-\delta\tilde{J}_1^x)|\{k'\})\mathcal{C}^{l(1)}_{\{k'\};0}(v_1|\gamma)\Phi(v_1) = \frac{-1}{8\pi^3 n}\frac{1}{2!}\sum_{\alpha,\beta}\int dk(\Phi'^x_{\alpha\beta}(1_k,y)\{i[\Lambda_\alpha^k(y)+\Lambda_\beta^{-k}(y)]\}^{-1} \times\int dv_1\bar{I}_\alpha^{1k}(v_1|y)\bar{I}_\beta^{-1k}(v_1|y)\Psi_0^{l,S}(v_1)\Phi(v_1) - \text{hard core} + O(\gamma^{1+\min(\mu,1)}). \quad (\text{II. }27)$$

Here the function $\Phi'^x_{\alpha\beta}(1_k,y)$ is defined by

$$\Phi'^x_{\alpha\beta}(1_k,y) = \lim_\gamma\sum_{a\neq b}\int dv^N[(0|(J_1^x-\delta\tilde{J}_1^x)|(k_a,-k_b) \times\prod_{i=1}^N\varphi^{\text{eq}}(v_i) + \sum_{k'\neq 0}(0|(J_1^x-\delta\tilde{J}_1^x)|\{k'\}) \times(\{k'\}|\tilde{\mathcal{C}}^S(\{v\};i\epsilon)|k_a,-k_b)]I_\alpha^{1k}(v_a|y)I_\beta^{-1k}(v_b|y), \quad (\text{II. }28)$$

with

$$(\{k'\}|\tilde{\mathcal{C}}^S(\{v\};z)|k_a,-k_b) = \sum_{n=1}^{\infty}\Big[(\{k'\}|\{[(L_0-z)^{-1}Q_k^2(-\delta L^S)]^n\}^{\text{F.C.}}_{a\text{ or }b}|k_a,-k_b)\prod_{i=1}^N\varphi^{\text{eq}}(v_i) + \sum_{\substack{\{k''\}\neq 0\\ k''_a=k''_b=0}}(\{k'\}|\{[(L_0-z)^{-1}Q_k^2(-\delta L^S)]^n\}^{\text{F.C.}}|\{k''\},k_a,-k_b)\Big] \times(\{k''\}|(\Omega^N\rho^{\text{eq}})^S|0). \quad (\text{II. }29)$$

Finally, for $\mathcal{P}_k^{l(1)}(v_1|\gamma)$ we find

$$\gamma\int dv_1\sum_{\{k'\}\neq 0}(0|(J_1^x-\delta\tilde{J}_1^x)|\{k'\})\mathcal{P}_{k'}^{l(1)}(v_1|\gamma)$$

$$= (8\pi^3 n)^{-1}(2!)^{-1}\sum_{\alpha\beta}\int dk(\Phi'^{x}_{\alpha\beta}(1_k, y)\{i[\Lambda^k_\alpha(y) + \Lambda^{-k}_\beta(y)]\}^{-1} \times\hat{\Phi}'^{x}_{\alpha\beta}(1_k, y) - \text{hard core}) + O(\gamma^{1+\min(\mu,1)}). \quad (\text{II}.30)$$

III. EXPLICIT CALCULATION OF THE FIRST CORRECTION $\chi^{(1)}$

With the important formulas (II.20), (II.23), (II.27), and (II.30), we have all the basic elements required for the calculation of the γ^1 correction to any transport coefficient X. Rather than giving immediately the detailed calculations for the general situation, we prefer to discuss first the simpler problem of the purely kinetic contributions to X. Indeed, in this case, the result can be obtained in a few lines and the salient features of the calculation are not obscured by technical aspects. In particular, we will see very clearly the way in which the linearized collision operator entirely disappears from the final equations. The general case, involving the potential part, will be considered later on.

From Eq. (I.II.38) and (I.II.39), it is obvious that we can split X into a kinetic part $X^{(K)}$ and a potential part $X^{(V)}$:

$$X^{(K)} = -\beta n \lim_{\epsilon\to 0}\int dv_1 (0|(J_1^{x(K)} - \delta\tilde{J}_1^{x(K)})|0) \times\{i[\Psi_0^l(v_1; i\epsilon) + i\epsilon]\}^{-1}\int dv^{N-1}(0|(J_1^{x(K)} - \delta J_1^{x(K)}) \times\rho^{\text{eq}}\Omega^N|0), \quad (\text{III}.1)$$

$$X^{(V)} = X' + X'' - X^{(K)}, \quad (\text{III}.2)$$

where $J_1^{x(K)}$, $\delta\tilde{J}_1^{x(K)}$, and $\delta J_1^{x(K)}$ denote the kinetic parts of the corresponding flow operators. For example, in the case of thermal conductivity, we have

$$J_1^{T\kappa(K)} = v_{1x}v^2/2,$$
$$\delta\tilde{J}_1^{T\kappa(K)} = \delta J_1^{T\kappa(K)} = \tfrac{1}{2}(5k_B T)v_{1x}. \quad (\text{III}.3)$$

The simplicity of (III.1) comes of course from the fact that it only involves the linearized collision operator Ψ_0^l; the other basic quantities of the theory, namely $\mathcal{C}^l_{k0}$, $\mathcal{D}^l_0$, $\mathcal{P}^l_k$ all appear in the potential part $X^{(V)}$ only.

From the expansions (I.2) and (I.4), we get immediately

$$\gamma X^{(K)(1)}(\gamma) = -\beta n \lim_{\epsilon\to 0}\int dv_1[J_1^{x(K)}(v_1) - \delta\tilde{J}_1^{x(K)}(v_1)] \times\{i[\Psi_0^{l,S}(v_1) + i\epsilon]\}^{-1}[-i\gamma\Psi_0^{(1)}(v_1|\gamma)] \times\{i[\Psi_0^{l,S}(v_1) + i\epsilon]\}^{-1}[J_1^{x(K)}(v_1) - \delta J_1^{x(K)}(v_1)]\varphi^{\text{eq}}(v_1), \quad (\text{III}.4)$$

where we have used the fact that the kinetic flow operators only depend on the velocity of one particle.

Inserting now (II.20) into this equation, we obtain

$$\gamma X^{(K)(1)}(\gamma) = -\frac{\beta}{8\pi^3}\frac{1}{2!}\sum_{\alpha,\beta=1}^{5}\int d^3k(f^x_{\alpha\beta}(1_k|y)\hat{f}^x_{\alpha\beta}(1_k|y) \times\{[\Lambda^k_\alpha(y) + \Lambda^{-k}_\beta(y)]\}^{-1} - \text{hard core}) + O(\gamma^{1+\min(\mu,1)}), \quad (\text{III}.5)$$

where we have introduced

$$f^x_{\alpha\beta}(1_k|y) = \int dv_1[J_1^{x(K)}(v_1) - \delta\tilde{J}_1^{x(K)}(v_1)] \times I^{1k}_\alpha(v_1|y)I^{-1k}_\beta(v_1|y)\varphi^{\text{eq}}(v_1) \quad (\text{III}.6\text{a})$$

and

$$\hat{f}^x_{\alpha\beta}(1_k|y) = \int dv_1[J_1^{x(K)}(v_1) - \delta J_1^{x(K)}(v_1)] \times\bar{I}^{1k}_\alpha(v_1|y)\bar{I}^{-1k}_\beta(v_1|y)\varphi^{\text{eq}}(v_1). \quad (\text{III}.6\text{b})$$

In the derivation of (III.5), a crucial role is played by the identities

$$\lim_{\epsilon\to 0}\langle\bar{\Phi}|\{i[\Psi_0^{l,S}(v_1) + i\epsilon]\}^{-1}i\Psi_0^{l,S}(v_1) = \langle\bar{\Phi}|, \quad (\text{III}.7\text{a})$$

and

$$\lim_{\epsilon\to 0}\{i[\Psi_0^{l,S}(v_1) + i\epsilon]\}^{-1}i\Psi_0^{l,S}(v_1)|\Phi\rangle = |\Phi\rangle \quad (\text{III}.7\text{b})$$

which are valid for any vector $|\Phi\rangle$ (and $\langle\bar{\Phi}|$) which is orthogonal to the null-space of $\Psi_0^{l,S}$. As discussed in Ref. I, the choice of δJ_1^x, and $\delta\tilde{J}_1^x$, is precisely such that this orthogonality property is satisfied.

Equation (III.5) essentially gives us the answer to our problem for $X^{(K)}$: Indeed, from (III.6) and (II.14), we can easily get an explicit form for $f^x_{\alpha\beta}(1_k|y)$ (in terms of the equilibrium properties of the reference system and of V_y^L) by performing the trivial velocity integration indicated in (III.6); notice that, in this operation, most of the $f^x_{\alpha\beta}$ will vanish for symmetry reasons: For example, in the case of thermal conductivity [see (III.3)] we will get a nonvanishing $f^{T\kappa}_{\alpha\beta}$ only if one of the $I^{1k}_{\alpha\beta}$ has a vector component along the x axis and if, simultaneously, the second one is a scalar quantity. The next steps are then to insert the eigenvalues (I.11a), (I.12a), (I.13a), into (III.5), to perform the integral over the angles of k and to make the change of variable $|k| = \gamma y$. We are then left with an expression which is precisely of the type (I.15). We shall, however, not perform these calculations explicitly here because $X^{(K)}$ is of little significance in a dense system; furthermore, a similar analysis will be performed later in the general case, including the potential part, which we consider presently.

We now have to start from the complete expression for X, given by Eq. (I.II38)-(II.39). Using again (I.4) and the analogous expansions for $\mathcal{C}^l_{k0}$, $\mathcal{D}^l_0$, and $\mathcal{P}^l_k$, a straightforward calculation, based on (II.20), (II.23), (II.27), (II.30), and (III.7), readily leads to

$$\gamma X^{(1)}(\gamma) = -\frac{\beta}{8\pi^3}\frac{1}{2!}\sum_{\alpha,\beta=1}^{5}\int d^3k(\Phi^x_{\alpha\beta}(1_k|y)\hat{\Phi}^x_{\alpha\beta}(1_k|y) \times\{[\Lambda^k_\alpha(y) + \Lambda^{-k}_\beta(y)]\}^{-1} - \text{hard core}) + O(\gamma^{1+\min(\mu,1)}). \quad (\text{III}.8)$$

Comparing with (III.5), we see that the structure of this γ^1-correction is similar to the one obtained in the kinetic case except that the simple factors $f^x_{\alpha\beta}$ and $\bar{f}^x_{\alpha\beta}$ are now replaced by the more elaborate expressions $\Phi^x_{\alpha\beta}$ and $\hat{\Phi}^x_{\alpha\beta}$. They are defined by the following formulas:

$$\Phi^x_{\alpha\beta}(1_k|y) = \Phi'^x_{\alpha\beta}(1_k|y) + \int dv_1\Big((0|(J_1^x - \delta\tilde{J}_1^x)|0) + \sum_{\{k'\}\neq 0}(0|(J_1^x - \delta\tilde{J}_1^x)|\{k'\})\mathcal{C}^{l,S}_{\{k'\};0}(v_1; i\epsilon)\Big) \times\varphi^{\text{eq}}(v_1)I^{1k}_\alpha(v_1|y)I^{-1k}_\beta(v_1|y) \quad (\text{III}.9)$$

and

$$\hat{\Phi}^x_{\alpha\beta}(1_k|y) = \hat{\Phi}'^x_{\alpha\beta}(1_k|y) + \int dv_1\{\bar{I}^{1k}_\alpha(v_1|y)\bar{I}^{-1k}_\beta(v_1|y)$$

$$\times [\int dv^{N-1}(0|(J_1^x - \delta J_1^x)\Omega^N \rho^{eq}|0) + \mathcal{D}_0^{l,S}(v_1; i\epsilon)]\}. \qquad \text{(III. 10)}$$

Here the quantities $\Phi'^x_{\alpha\beta}$ and $\hat{\Phi}'^x_{\alpha\beta}$ are given by Eqs. (II. 24), (II. 28) while $\mathcal{C}^{l,S}_{\{k'\};0}$ and $\mathcal{D}_0^{l,S}$ are the pure hard-core analogs of the quantities introduced in Eq. (I. II. 38).

We can expect, from our previous discussion of the kinetic case, that $\Phi^x_{\alpha\beta}$ and $\hat{\Phi}^x_{\alpha\beta}$, like $f^x_{\alpha\beta}$ and $\hat{f}^x_{\alpha\beta}$, can be reduced to purely equilibrium properties and that most of them will vanish for symmetry reasons. As we shall now indicate, this is indeed the case; yet, this proof is far from trivial and, in order not to interrupt our analysis by too many technical details, most of the calculations are relegated in Appendices.

First of all, let us notice that, because of (II. 14), the $\Phi^x_{\alpha\beta}$ (and $\hat{\Phi}^x_{\alpha\beta}$) are bilinear functionals of the invariants $i_\gamma(v_1)$ $(\gamma = 1\ldots 5)$. In order to get rid of awkward numerical factors, we write

$$\Phi^x_{\alpha\beta}(1_k|y) = \sum_{\gamma,\delta=1}^{5} d_{\alpha\beta,\gamma\delta}(1_k|y) m^x_{\gamma\delta}(1_k|y), \qquad \text{(III. 11)}$$

where we have put

$$d_{\alpha\beta,\gamma\delta}(1_k|y) = c^{1_k}_{\alpha\gamma}(y) c^{-1_k}_{\beta\delta}(y), \qquad \text{(III. 12)}$$

and a similar formula for $\hat{\Phi}^x_{\alpha\beta}$,

$$\hat{\Phi}^x_{\alpha\beta}(1_k|y) = \sum_{\gamma,\delta=1}^{5} \bar{d}_{\alpha\beta,\gamma\delta}(1_k|y) \overline{m}^x_{\gamma\delta}(1_k|y), \qquad \text{(III. 13)}$$

with

$$\bar{d}_{\alpha\beta,\gamma\delta}(1_k|y) = \bar{c}^{1_k}_{\alpha\gamma}(y) \bar{c}^{-1_k}_{\beta\delta}(y). \qquad \text{(III. 14)}$$

The definitions of $m^x_{\alpha\beta}(1_k|y)$ and $\overline{m}^x_{\alpha\beta}(1_k|y)$ are readily obtained from (III. 9) and (III. 10) by replacing $I^{1_k}_\alpha(v_1|y) \to i_\alpha(v_1)$ etc. They are explicitly evaluated in Appendix A and (B), respectively, where the following results are shown to hold in the particular case of thermal conductivity:

$$m^{T\kappa}_{12}(1_k|y) = m^{T\kappa}_{21}(1_k|y) = n\sqrt{k_B T}\left[\left(\frac{\partial h/n}{\partial n}\right)^S_T + V^L_y + \frac{1}{2} 1^2_{k_x} y \frac{\partial V^L_y}{\partial y}\right], \qquad \text{(III. 15a)}$$

$$m^{T\kappa}_{13}(1_k|y) = m^{T\kappa}_{31}(1_k|y) = n\sqrt{k_B T}\left(1_{kx} 1_{ky} y \frac{\partial V^L_y}{\partial y}\right), \qquad \text{(III. 15b)}$$

$$m^{T\kappa}_{14}(1_k|y) = m^{T\kappa}_{41}(1_k|y) = n\sqrt{k_B T}\left(1_{kx} 1_{kz} y \frac{\partial V^L_y}{\partial y}\right), \qquad \text{(III. 15c)}$$

$$m^{T\kappa}_{52}(1_k|y) = m^{T\kappa}_{25}(1_k|y) = \sqrt{\tfrac{2}{3}}\, \sqrt{k_B T}\, T\left(\frac{\partial h/n}{\partial T}\right)^S_n, \qquad \text{(III. 15d)}$$

while all the other $m^{T\kappa}_{\alpha\beta}$ vanish for symmetry reasons. Similarly, we have

$$\overline{m}^{T\kappa}_{1i}(1_k|y) = \overline{m}^{T\kappa}_{i1}(1_k|y) = m^{T\kappa}_{1i}[nk_B T\chi_T(y)] + O(\gamma) \quad (i = 2, 3, 4), \qquad \text{(III. 16a)}$$

$$\overline{m}^{T\kappa}_{5i}(1_k|y) = \overline{m}^{T\kappa}_{i5}(1_k|y) = m^{T\kappa}_{52}(1_k|y)\delta^{K_T}_{2,i} + m^{T\kappa}_{1i}\sqrt{\tfrac{2}{3}}\,\frac{1}{k_B T}[nk_B T\chi_T(y)] \times\left[\left(\frac{\partial e}{\partial n}\right)^S_T - \frac{3k_B T}{2} - nV^S_0\right] + O(\gamma); \qquad \text{(III. 16b)}$$

all other coefficients $\overline{m}^{T\kappa}_{\alpha\beta}$ vanish for symmetry reasons. For the other transport coefficients, the corresponding $m^x_{\alpha\beta}$ and $\overline{m}^x_{\alpha\beta}$ are listed respectively in Appendices A and B.

From these formulas, it is now a straightforward though tedious matter to express the first correction to X in the form suggested in (I. 15): In a first step, we use (III. 11) and (III. 13) to calculate the functions $\Phi^x_{\alpha\beta}(1_k|y)$ and $\hat{\Phi}^x_{\alpha\beta}(1_k|y)$; in doing this, we also need (III. 12), (III. 14), and (II. 14) where the coefficients $c^{1_k}_{\alpha\beta}(y)$ are obtained by comparison with (I. 11–14). We get, after considerable algebraic simplifications,

$$\Phi^{T\kappa}_{12}(1_k|y) = \Phi^{T\kappa}_{21}(1_k|y) = (k_B T)^{3/2} 1_{k_x} \mathcal{G}^{T\kappa}_{12}(y), \qquad \text{(III. 17a)}$$

$$\Phi^{T\kappa}_{35}(1_k|y) = \Phi^{T\kappa}_{53}(1_k|y) = (k_B T)^{3/2}\left(\frac{-1_{k_x}1_{k_y}}{(1^2_{k_x} + 1^2_{k_z})^{1/2}}\right)\mathcal{G}^{T\kappa}_{35}(y), \qquad \text{(III. 17b)}$$

$$\Phi^{T\kappa}_{45}(1_k|y) = -\Phi^{T\kappa}_{54}(1_k|y) = (k_B T)^{3/2}\,\frac{-1_{k_z}}{(1^2_{k_x} + 1^2_{k_z})^{1/2}}\,\mathcal{G}^{T\kappa}_{35}(y), \qquad \text{(III. 17c)}$$

where we have introduced the dimensionless constants

$$\mathcal{G}^{T\kappa}_{12}(y) = \frac{1}{c(y)\sqrt{k_B T}}\left[n\left(\frac{\partial h/n}{\partial n}\right)^S_T + \frac{(\partial p/\partial T)^S_n}{nC^S_v}\, T\left(\frac{\partial h/n}{\partial T}\right)^S_n + nV^L_y + \frac{n}{2} y\frac{\partial V^L_y}{\partial y}\right], \qquad \text{(III. 18a)}$$

and

$$\mathcal{G}^{T\kappa}_{35}(y) = \sqrt{\tfrac{2}{3}}\,\frac{T}{c^2(y)}\left\{\frac{1}{nk_B T\chi_T(y)}\left(\frac{\partial h/n}{\partial T}\right)^S_n - \frac{1}{k_B T}\left(\frac{\partial p}{\partial T}\right)^S_n\left[\left(\frac{\partial h/n}{\partial n}\right)^S_T + nV^L_y\right]\right\}. \qquad \text{(III. 18b)}$$

Similarly, we find

$$\hat{\Phi}^{T\kappa}_{12}(1_k|y) = \hat{\Phi}^{T\kappa}_{21}(1_k|y) = \Phi^{T\kappa}_{12}(1_k|y), \qquad \text{(III. 19a)}$$

$$\hat{\Phi}^{T\kappa}_{35}(1_k|y) = \hat{\Phi}^{T\kappa}_{53}(1_k|y) = (k_B T)^{3/2}[-1_{k_x}1_{k_y}/(1^2_{k_x} + 1^2_{k_z})^{1/2}] \times\{\tfrac{3}{2}[nk_B T\chi_T(y)][c^2(y)/k_B T]\}\mathcal{G}^{T\kappa}_{35}(y), \qquad \text{(III. 19b)}$$

$$\hat{\Phi}^{T\kappa}_{45}(1_k|y) = -\hat{\Phi}^{T\kappa}_{54}(1_k|y) = (k_B T)^{3/2}[-1_{k_z}/(1^2_{k_x} + 1^2_{k_z})^{1/2}] \times\{\tfrac{3}{2}[nk_B T\chi_T(y)][c^2(y)/k_B T]\}\mathcal{G}^{T\kappa}_{35}(y). \qquad \text{(III. 19c)}$$

The quantities $\Phi^{T\kappa}_{\alpha\beta}(1_k|y)$ and $\hat{\Phi}^{T\kappa}_{\alpha\beta}(1_k|y)$ which we have not written down explicitly here either vanish for symmetry reasons [as for example $\Phi^{T\kappa}_{55}(1_k|y)$] or only contribute to (III. 8) to higher order in γ {for example, the combination of one sound mode with any other mode, as in $\Phi^{T\kappa}_{15}(1_k|y)$, gives a contribution of order γ^2 to (III. 8) [see (I. 11a) and (I. 13a)]. The corresponding formulas for shear and bulk viscosity are displayed in Appendix C.

The next step is simply to introduce these results into (III. 8) and to perform the angular integration over k; in terms of the variable $y = |k|/\gamma$, we get then, after some elementary thermodynamic manipulations,

$$\kappa^{(1)}(\gamma)=\frac{k_B}{6\pi^2}\int_0^\infty dy\left\{\left[\left(1+\frac{n}{2c^2(y)}y\frac{\partial V_y^L}{\partial y}\right)^2\frac{c^2(y)}{2\Gamma(y)}-\frac{c^{S2}}{2\Gamma^S}\right]\right.$$
$$+2T\left(\frac{C_p(y)}{\eta^S/n+\kappa^S/nC_p(y)}\right.$$
$$\left.\left.-\frac{C_p^S}{\eta^S/n+\kappa^S/nC_p^S}\right)\right\}+O(\gamma^{\min(1,\mu)}). \qquad \text{(III. 20)}$$

The two terms in the integrand with the negative sign correspond to the purely hard-core part in Eq. (III. 8) and, as is readily checked, they are obtainable from the two terms with the positive sign by putting formally $V_y^L=0$. As we have assumed from the very beginning that $V_y^L\to 0$ for $y\gg 1$, we see thus that the integral involved in Eq. (III. 20) is improper but convergent.

Equation (III. 20) is our final result for thermal conductivity; without making an explicit assumption about the long-range potential V_y^L, the y integral cannot be performed in closed form. Yet, even in this form, we see the remarkable property of the van der Waals transport coefficients: The first correction can be computed by a simple quadrature provided we know the equilibrium and transport properties of the the short-range reference system, plus of course the Fourier transform V_y^L of the long-range potential.

Using the formulas of Appendix C, we have similarly shown that the first correction to the shear viscosity is

$$\eta^{(1)}(\gamma)=\frac{k_BT}{60\pi^2}\int_0^\infty dy\left[[n\chi_T(y)]^2\left(\frac{\gamma(y)-1}{\gamma(y)}\right)^2\left(ny\frac{\partial V_y^L}{\partial y}\right)^2\right.$$
$$\left.\times\frac{nC_p(y)}{2\kappa^S}+\left(1+\frac{n}{2c^2(y)}y\frac{\partial V_y^L}{\partial y}\right)^2\frac{1}{\Gamma(y)}-\frac{1}{\Gamma^S}\right]$$
$$+O(\gamma^{\min(1,\mu)}), \qquad \text{(III. 21)}$$

where we have used the notation

$$\gamma(y)=C_p(y)/C_v^S. \qquad \text{(III. 22)}$$

For the bulk viscosity, we have found

$$\zeta^{(1)}(\gamma)=\frac{k_BT}{4\pi^2}\int_0^\infty dy\left[\left(b_1(y)\frac{1}{2\kappa^S/nC_p(y)}-\text{hard core}\right)\right.$$
$$\left.+\left(b_2(y)\frac{1}{2\Gamma(y)}-\text{hard core}\right)\right]+O(\gamma^{\min(1,\mu)}), \qquad \text{(III. 23)}$$

where

$$b_1(y)=\frac{n^2}{T^2}\left(\frac{\partial T(y)}{\partial n}\right)_T^2[\gamma(y)-1]^2\left[\frac{T}{C_p(y)}\left(\frac{\partial C_p(y)}{\partial T}\right)_p\right.$$
$$-n^2\left(\frac{\partial C_p(y)}{\partial p}\right)_T\left(\frac{\partial T(y)}{\partial n}\right)_p+\frac{1}{c^2(y)}\frac{T}{n[\partial T(y)/\partial n]_p}$$
$$\left.\times\tfrac{1}{3}ny\frac{\partial V_y^L}{\partial y}\right]^2 \qquad \text{(III. 24a)}$$

and

$$b_2(y)=\left[\frac{1}{3}+\frac{1}{2}\left(\frac{\partial c^2(y)}{\partial T}\right)_n\frac{n}{[\partial p(y)/\partial T]_n}[1-1/\gamma(y)]\right.$$
$$\left.-\left(\frac{\partial p(y)}{\partial e}\right)_n+\left(\frac{n}{c(y)}\right)\frac{\partial c(y)}{\partial n}\,_T+\frac{1}{6c^2(y)}ny\frac{\partial V_y^L}{\partial y}\right]^2. \qquad \text{(III. 24b)}$$

In these formulas, we have used the notation

$$\left(\frac{\partial g(y)}{\partial\alpha}\right)_\beta=\left(\frac{\partial g(\alpha,\beta|y)}{\partial\alpha}\right)_\beta \qquad \text{(III. 25)}$$

and the "van der Waals" thermodynamic function $g(\alpha,\beta|y)$ is obtainable from the "free-energy density"

$$f(n,T|y)=f^S(n,T)+\tfrac{1}{2}n^2V_y^L \qquad \text{(III. 26)}$$

by the same standard thermodynamic formulas that allow to obtain the thermodynamic function $g(\alpha,\beta)$ from the usual free-energy density $f(n,T)$. This point is explained in detail in Appendix B.

IV. A MACROSCOPIC FORMULATION OF THE PROBLEM

The fact that our final expression for $X^{(1)}$ only involves the macroscopic properties of the hard-core fluid and the Fourier transform of the long-range potential is a strong indication that these results can also be established on a purely macroscopic basis. As a matter of fact, attempts in this direction were made previously by Zwanzig and co-workers[8] and by Kawasaki[9] in their discussion of critical properties of transport coefficients.

We shall show here that this type of macroscopic argument can indeed be used to reproduce our results; we shall also point out the difference between the present calculation and the above-mentioned papers.

To be as simple as possible, we limit ourselves to the case of shear viscosity. The Green–Kubo formula reads thus

$$\eta=\lim_{T\to\infty}\lim_{\Omega}\frac{\beta}{\Omega}\int_0^T dt\langle J^\eta(t)J^\eta(0)\rangle, \qquad \text{(IV. 1)}$$

where the momentum flow J^η is given by

$$J^\eta(t)=\sum_{i=1}^N v_{i,x}(t)v_{i,y}(t)-\frac{1}{2}\sum_{i\neq j=1}^N\frac{\partial V(t)}{\partial r_{ij,x}}r_{ij,y}(t). \qquad \text{(IV. 2)}$$

Before analyzing (IV. 1), let us first recall that, according to macroscopic fluctuation theory, the long-wavelength fluctuations are Gaussian.[10] Defining thus the Fourier transform of the density and velocity fluctuations by

$$\delta n_k=\Omega^{-1/2}\sum_{i=1}^N\exp(ikr_i), \qquad \text{(IV. 3)}$$

$$u_k=(\Omega)^{-1/2}n^{-1}\sum_{i=1}^N v_i\exp(ikr_i), \qquad \text{(IV. 4)}$$

these fluctuations are characterized, for a wavenumber k smaller than *any* inverse length of the problem, by the statistical weight

$$\exp-\tfrac{1}{2}\beta[n|u_k|^2+(|\delta n_k|^2/n^2\chi_T)]. \qquad \text{(IV. 5)}$$

As shown by Van Kampen,[11] such Gaussian fluctuations persist in the range $k\sim\gamma$ provided that, in (IV. 5), we replace χ_T by the wavenumber-dependent suceptibility

$$\chi_T\to\chi_T(k\gamma^{-1})=\left[n\left(\frac{\partial p}{\partial n}\right)_T^S+n^2V_{k\gamma^{-1}}^L\right]^{-1}. \qquad \text{(IV. 6)}$$

Due to this difference in weight, we see that the equilibrium fluctuations of the van der Waals fluid will differ from those of the hard-core system in the range $k\gamma^{-1}\lesssim 1$.

Moreover, in this long-wavelength regime, we shall assume that the motion of these fluctuations are governed by the equations of linearized hydrodynamics, suitably *modified* by an average field term due to the long-range van der Waals potential.[8,9] The linearized Stokes–Navier equation becomes thus

$$\partial_t u_k(t) + ik\frac{1}{n}\left(\frac{\partial p}{\partial n}\right)_T^S \delta n_k(t) + ikV^L_{k\gamma^{-1}}\delta n_k(t) + ik\frac{1}{n}\left(\frac{\partial p}{\partial T}\right)_n^S \delta T_k(t)$$
$$= -\left(\frac{\eta^S}{n}k^2 u_k(t) + \frac{1}{n}(\zeta^S + \tfrac{1}{3}\eta^S)k[ku_k(t)]\right), \qquad \text{(IV.7)}$$

while the continuity equation for $\delta u_k(t)$ and the temperature equation for $\delta T_k(t)$ keep their classical form. We find here a second reason for a different behavior of the van der Waals fluid compared to the reference one.

To lowest order in γ, we assume that these two effects are entirely responsible for the correction to the transport coefficient due to the long-range potential. To perform the calculation, we then replace in (IV.1) the equilibrium ensemble by a restricted ensemble where the only fluctuating quantities are the long-wavelength components of δn_k and u_k with $k < k_0$, k_0 being a small cutoff wavenumber such that $k_0 \gg \gamma$. In this ensemble, we can replace the flow J^η by $J^{\eta,L}$ defined by[12]

$$J^{\eta,L}(t) = \sum_{\substack{k\neq 0\\ k<k_0}}\left(nu_{k,x}(t)u_{-k,y}(t) + \tfrac{1}{2}y\frac{k_x k_y}{k^2}\frac{\partial V^L_y}{\partial y}\delta u_k(t)\delta u_{-k}(t)\right). \qquad \text{(IV.8)}$$

In order to obtain the time dependence of $\delta u_k(t)$ and $u_k(t)$, we can use the well-known decompositions

$$\delta n_k(t) = \exp - tk^2\Gamma(y)\left[\frac{1}{\gamma(y)}\delta n_k(0)\cos kc(y)t + \frac{in}{c(y)}\left(\frac{\mathbf{k}\cdot\mathbf{u}_k(0)}{k}\right)\sin kc(y)t\right] + \frac{\gamma(y)-1}{\gamma(y)}$$
$$\times \exp t\Lambda_5^k(y)\delta u_k(0) \qquad \text{(IV.9)}$$

and

$$u_{k,n}(t) = \exp - tk^2\Gamma(y)\left[k_x\left(\frac{\mathbf{k}\cdot\mathbf{u}_k(0)}{k^2}\right)\cos kc(y)t + \frac{ik_x c(y)}{k\gamma(y)}\frac{\delta u_k(0)}{n}\sin kc(y)t\right]$$
$$+ \exp t\Lambda_3^k\left[u_{k,n}(0) - k_x\left(\frac{\mathbf{k}\cdot\mathbf{u}_k(0)}{k^2}\right)\right]. \qquad \text{(IV.10)}$$

Note that, as a consequence of the mean field term in (IV.7), we have to introduce here y-dependent transport coefficients, as defined in the previous sections [see (I.11) and (III.22)].

Inserting these expressions into (III.8) and integrating over time, we obtain for the dominant contribution

$$\int_0^\infty dt J^{\eta,L}(t) = \frac{1}{2}\sum_{\substack{k\neq 0\\ k<k_0}}\frac{n}{2k^2\Gamma(y)}\left(\frac{c^2(y)}{n^2}\frac{|\delta n_k(0)|^2}{\gamma(y)^2} + \frac{|\mathbf{k}\cdot\mathbf{u}_k(0)|^2}{k^2}\right)\frac{k_x k_y}{k^2}\left(1 + \frac{1}{2}\frac{n}{c^2(y)}y\frac{\partial V^L_y}{\partial y}\right)$$
$$+ \frac{1}{2}\sum_{\substack{k\neq 0\\ k<k_0}}\frac{n}{2\Lambda_5^k(y)}\frac{k_x k_y}{k^2}y\frac{\partial V^L_y}{\partial y} \times |\delta n_k(0)|^2\left(\frac{\gamma(y)-1}{\gamma(y)}\right)^2$$
$$+ \text{(transverse velocity field contributions)}. \qquad \text{(IV.11)}$$

The transverse velocity field terms $[\alpha(\Lambda_3^k)^{-1}]$ have not been written down explicitly because they take the same form in the van der Waals fluid and in the reference fluid, and so they do not contribute to the final result (at least to lowest order in γ).

From (IV.1), (IV.8), and (IV.11), we obtain for the long-wavelength contribution to η

$$\eta^L = \frac{1}{\Omega kT}\int_0^\infty dt\langle J^{\eta,L}(t)J^{\eta,L}(0)\rangle$$
$$= \frac{1}{2\Omega kT}\sum_{\substack{k\neq 0\\ k<k_0}}\frac{n}{2k^2\Gamma(y)}\frac{k_n k_y}{k^2}\left(1 + \frac{1}{2}\frac{ny}{c^2(y)}\frac{\partial V^L_y}{\partial y}\right)$$
$$\times\left(n\left\langle u_{k,n}u_{-k,y}\frac{|\mathbf{k}\cdot\mathbf{u}_k|^2}{k^2}\right\rangle + \tfrac{1}{2}y\frac{\partial V^L_y}{\partial y}\frac{k_x k_y}{k^2}\left(\frac{c^2(y)}{\gamma^2(y)n^2}\right)\right.$$
$$\left.\times\langle|\delta u_k|^2[|\delta u_k|^2 - \langle|\delta u_k|^2\rangle]\rangle\right)$$
$$+ \frac{1}{2\Omega kT}\sum_{\substack{k\neq 0\\ k<k_0}}\frac{1}{2\Lambda_5^k(y)}\left(\frac{\gamma(y)-1}{\gamma(y)}\right)^2\frac{k_x^2 k_y^2}{k^2}\left(y\frac{\partial V^L_y}{\partial y}\right)^2$$
$$\times\langle|\delta n_k|^2[|\delta n_k|^2 - \langle|\delta n_k|^2\rangle]\rangle$$
$$+ \text{(transverse velocity field contributions)}. \qquad \text{(IV.12)}$$

In deriving this last expression, we have used the fact that fluctuations with different wavenumbers are uncorrelated. From the statistical weight given in (IV.5), we have

$$\left\langle u_{k,n}u_{-k,y}\frac{|\mathbf{k}\cdot\mathbf{u}_k|^2}{k^2}\right\rangle = \frac{k_x k_y}{k^2}\left(\frac{k_B T}{n}\right)^2, \qquad \text{(IV.13)}$$

$$\langle|\delta n_k|^2[|\delta n_k|^2 - \langle|\delta n_k|^2\rangle]\rangle = [n^2 k_B T\chi_T(y)]^2. \qquad \text{(IV.14)}$$

Inserting these fluctuation formulas into (IV.12), we then take the difference between the values of η^L for the van der Waals fluid and for the reference fluid [formally obtained from (IV.12) by setting $V^L_y = 0$]. We then replace the sum over k by an integral over $y = k\gamma^{-1}$ and perform the angular integration. We then recover (III.21) if we let $k_0/\gamma \to \infty$.

Although, strictly speaking, these authors only considered the critical region, the considerations of Zwanzig *et al.* and of Kawasaki are very similar to ours. However, they assumed from the start that the kinetic part (more generally, the short-range part) of the flow J^η is rapidly decaying and they thus only retained the long-range potential part of this flow. This kind of contribution, proportional to $(\partial V^L_y/\partial y)^2$, is identical to ours. Yet, in agreement with our microscopic calculation, we find supplementary terms connected to the short-range part of the flow. These terms should, however, be of no surprise: Indeed, it is now well-known that purely short-range flows have a slow decay for long times, due to the propagation of coupled hydrodynamical modes in the fluid.[4,5] As this propagation is different in the van der Waals fluid and in the reference fluid—due to the mean field term in Eq. (IV.7)—we expect indeed such supplementary corrections.

As a matter of fact, the reader can easily check that (IV.12) is nothing else than the time *integral* of the difference between the asymptotic behavior of the Green–Kubo integrand for, respectively, the van der Waals fluid and the reference fluid. If, in this latter case, an explicit $t^{-3/2}$ power law decay is easily obtained, it should however be pointed out that, with long range forces (and for times of the order $\sqrt{t} \sim \gamma^{-1}$), no such simple analytical expression exists because of the complicated wavenumber dependence introduced by $V^{L}_{k\gamma^{-1}}$.

A similar argument can be developed for the other transport coefficients but we will not present it here.

V. DISCUSSION

The present calculation essentially brings the van der Waals model to the same status as the other existing soluble models for fluids. Indeed, in much the same way as for the dilute gas (virial expansion, Boltzmann equation and its generalization to higher densities[13]), for the hot plasma (Debye–Hückel theory Balescu–Lenard–Gurnsey kinetic equation) or for the Brownian motion of a heavy particle (trivial Maxwell–Boltzmann distribution, Fokker–Planck equation), we now have available both the equilibrium and the transport properties. From this point of view, the weakness of the present work is that we do not have a complete kinetic description but only the transport coefficients.

Moreover, we have here the first example of a fully microscopic treatment of a mode mode coupling description in a dense fluid.[3]

It should be stressed that, although few calculations may pretend to be less mathematically rigorous than the one presented here, we nevertheless believe that our final results are *exact*. Indeed, no assumptions were made in the course of our proof except the validity of a series a formal manipulations (for example, infinite perturbation calculus, small wavenumber expensions, etc.) from which our final results, expressed in a compact form, appear to be completely independent. In this context, it is also worthwhile to point out once more the unusual character of the expansion (I.2): While each coefficient $X^{(n)}(\gamma)$ has a finite limit when $\gamma \to 0$, it is nevertheless highly probable that $X^{(n)}(\gamma)$ is a nonanalytic function of γ; this is a consequence of a similar property for the small wavenumber expansion of the hydrodynamical modes. Moreover, we should also again stress that (I.2) is not an expansion in power of V^L; as a matter of fact, it is amusing to notice that if one tries to perform such a naive expansion, the low-order terms converge but lead to corrections which are of higher order (γ^4) than the dominant contribution (γ^2) retained here; as explained in I, when such an expansion is systematically pursued, divergence difficulties appear which have been resolved here by the formal resummation presented in the first paper of this series.

In Sec. IV, we have already compared our results with previous work on the subject and we shall not comment on this question any further here. We just want to stress again the close connection between this van der Waals problem and the long-time behavior of the Green–Kubo integrands. In fact, using techniques very similar to the one followed here, it is possible to develop a kinetic theory, valid at *arbitrary* density, for this asymptotic time behavior. This point will be the object of forthcoming publications. In the same respect, it is also interesting to note that we have refrained from extending our calculation to two dimensions. Indeed, the present calculation is based on the very existence of transport coefficients (in particular for the reference system) and this property is presently very doubtful in two dimensions.

Finally, let us point out that, although we have not discussed this question in detail here, it is very simple to verify that, to order, γ, the first correction to the self-diffusion coefficient identically vanishes:

$$D^{(1)}(\gamma=0)=0. \qquad (V.1)$$

This can be obtained either by a slight extension of our microscopic method (by introducing the self-diffusive mode of a given particle) or by the macroscopic method of Sec. IV; in both cases, the physical reason for (V.1) is that the dominant mode–mode term involves the combination

$$\Lambda^k_{\eta}s + \Lambda^k_{D}s, \qquad (V.2)$$

where

$$\Lambda^k_{\eta}s = -\eta^S k^2/n, \qquad (V.3)$$

$$\Lambda^k_{D}s = -D^S k^2, \qquad (V.4)$$

which are both γ-independent. Thus their contribution is the same for the van der Waals fluid and for the reference system and it disappears in the final result. In this case, we have, however, the hope of being able to calculate the first nonvanishing correction which should be due (a) to more complicated mode–mode couplings, leading to γ^2 corrections and (b) to the fact that, to higher order in γ, we should replace $\Lambda^k_{\eta}s \to \Lambda^k_{\eta(\gamma)}$ where $\eta(\gamma)$ is given by an expansion of the type (I.2). The consistency of this procedure is, however, not easy to establish and will be discussed in a future publication.

APPENDIX A: CALCULATION OF $m^x_{\alpha\beta}(1_k|y_0)$

A. General discussion

From (III.11), (III.9), (II.28), and (II.14), we get the following expression for $m^x_{\alpha\beta}(1_k|y)$:

$$m^x_{\alpha\beta}(1_k|y)=\lim_{\gamma}\int \sum_{\text{all } a,b=1}^{N}\Big((0|(J_1^x-\delta\tilde{J}_1^x)|k_a,-k_b)\prod_{i=1}^{N}\varphi^{\text{eq}}(v_i) + \sum_{\{k'\}\neq 0}(0|(J_1^x-\delta\tilde{J}_1^x)|\{k'\}(\{k'\}|\tilde{C}^s(\{v\};i\epsilon) \times|k_a,-k_b)\Big)\, i_\alpha(v_a)i_\beta(v_b). \qquad (A1)$$

(For $a=b$, the quantities in the integral are obtained by formally setting $k_a=k_b=0$.)

Let us stress that we have here complete sums over all a and b, including the terms $a=b$. As a matter of fact, these terms can be shown to give a finite contribution to (A1), as also do the contributions $a\neq b$.

In the second term of the bracket in (A1), we can take immediately the limit $k=0$ because none of the difficulties mentioned after (II.24) occur here; in particular, there is no long-range contribution, as can be shown by using the method presented in I, Sec. III. In the first part of this bracket, there is, however, such a γ^0 contribution involving the long-range force, as was illustrated in I, Eq. (IV.3); there, we have thus to split

$(J_1^x - \delta\tilde{J}_1^x)$, according to

$$(0|(J_1^x - \delta\tilde{J}_1^x)|k_a, -k_b) = (0|(J_1^x - \delta\tilde{J}_1^x)^S|k_a, -k_b) + (0|(J_1^x - \delta\tilde{J}_1^x)^L|k_a, -k_b). \quad (A2)$$

For example, in the case of thermal conductivity, we find

$$\lim_\gamma (0|(J_1^{T\kappa} - \delta\tilde{J}_1^{T\kappa})^S|k_a, -k_b) = v_{1,x}[\tfrac{1}{2}v_1^2 - (h/n)]\delta_{a,b}^{K\gamma} + \Omega^{-1}v_{1,x}V_0^S(1-\delta_{a,b}^{K\gamma}) \times (\delta_{a,1}^{K\gamma} + \delta_{b,1}^{K\gamma}) \quad (A3)$$

and

$$\lim_\gamma (0|(J_1^{T\kappa} - \delta\tilde{J}_1^{T\kappa})^L|k_a, -k_b) = (2\Omega)^{-1}\left(v_{1,x}V_{k\gamma^{-1}}^L + \frac{\partial k V_{k\gamma^{-1}}^L}{\partial k_x} v_1\right)(1-\delta_{a,b}^{K\gamma})(\delta_{a,1}^{K\gamma} + \delta_{b,1}^{K\gamma}). \quad (A4)$$

In order to further simplify (A1), we also use in (II. 29) the property (II. 5) as well as the identity

$$(\{k\}|(\Omega^N\rho^{eq})^S|0) \equiv \hat{C}_{\{k\};0}(\{v\}; i\epsilon)\prod_{i=1}^N \varphi^{eq}(v_i), \quad (A5)$$

with

$$\hat{C}_{\{k\};0}(\{v\}; z) = \sum_{n=1}^\infty (\{k\}|[(L_0 - z)^{-1}Q(-\delta L^S)]^n|0); \quad (A6)$$

this important result was established in Ref. 7.

Putting all these remarks together we can split $m_{\alpha\beta}^x$ into two parts:

$$m_{\alpha\beta}^x(1_k|y) = [m_{\alpha\beta}^x(1_k|y)]^L + [m_{\alpha\beta}^x]^S. \quad (A7)$$

Here the long-range term $[m_{\alpha\beta}^x]^L$ is defined by

$$[m_{\alpha\beta}^x(1_k|y)]^L = \lim_\gamma \int dv^N \sum_{a\neq b}(0|(J_1^x - \delta\tilde{J}_1^x)^L|k_a, -k_b) \times \prod_{i=1}^N \varphi^{eq}(v_i) i_\alpha(v_a) i_\beta(v_b), \quad (A8)$$

while the short-range contribution $[m_{\alpha\beta}^x]^S$ can be written

$$[m_{\alpha\beta}^x]^S = \int dv^N \sum_G \sum_{a,b\in(G)} A_{(G)}^x(\{v\}) \prod_{i\in G}\varphi^{eq}(v_i) i_\alpha(v_a) i_\beta(v_b). \quad (A9)$$

In this latter equation, we have introduced the operator $A_{(G)}^x$ defined by

$$A_{(G)}^x = \left((0|(J_1^x - \delta\tilde{J}_1^x)^S|0) + \sum_{\{k_G\neq 0\}}(0|(J_1^x - \delta\tilde{J}_1^x)^S|\{k_G\}) \times \hat{C}_{\{k_G\};0}^S(\{v\}; i\epsilon)\right)_{(G)}, \quad (A10)$$

where the subscript (G) means that in the right-hand side of (A10) we only retain those contributions which explicitly involve G particles, including particle 1; in Eq. (A9), $[m_{\alpha\beta}^x]^S$ is thus given as a sum over all possible grouping of particles: This seemingly artificial decomposition will turn out to be very useful in the following.

B. Calculation of the long-range part $[m_{\alpha\beta}^x(1_k|y)]^L$

From (A4) and similar formulas for the other transport coefficients, it is easy to get an explicit expression for (A8) by performing the trivial velocity integration. Taking again the example of thermal conductivity, we get

$$(m_{12}^{T\kappa})^L = (m_{21}^{T\kappa})^L = n\sqrt{k_BT}\left(V_y^L + \frac{(1_{k_x})^2}{2} y\frac{\partial V_y^L}{\partial y}\right), \quad (A11)$$

$$(m_{13}^{T\kappa})^L = (m_{31}^{T\kappa})^L = \frac{n\sqrt{k_BT}}{2}\left(1_{k_x}1_{k_y} y\frac{\partial V_y^L}{\partial y}\right), \quad (A12)$$

$$(m_{14}^{T\kappa})^L = (m_{41}^{T\kappa})^L = \frac{n\sqrt{k_BT}}{2}\left|1_{k_x}1_{k_z} y\frac{\partial V_y^L}{\partial y}\right|, \quad (A13)$$

and all other coefficients $[m_{\alpha\beta}^{T\kappa}]^L$ vanish for symmetry reasons.

C. Calculation of the short-range part $[m_{\alpha\beta}^x]^S$

The explicit evaluation of (A9) is rather tricky but it can be done by the method developed in Ref. 14 in a similar context: we shall thus be rather brief.

Consider first in (A9) the case $\alpha = 1$, thus $i_\alpha(v) = 1$. If we notice that the sum of all the graphs involving G particles is of order n^{G-1} in the density, we can write formally

$$A_{(G)}\prod_{i\in(G)}\varphi^{eq}(v_i)\left(\sum_{a\in(G)}1\right)\left(\sum_{b\in(G)}i_\beta(v_b)\right) \times \propto n^{G-1}G \propto \frac{\partial}{\partial n} n\cdot n^{G-1} = \frac{\partial}{\partial n}\Big)_T nA_{(G)}\prod_{i\in(G)}\varphi^{eq}(v_i)\left(\sum_{b\in(G)}i_\beta(v_b)\right). \quad (A14)$$

Similarly by a simple differentiation, we get for $\alpha = 5$

$$A_{(G)}\prod_{i\in(G)}\varphi^{eq}(v_i)\left[\sum_{a\in(G)}\left(\frac{2}{3}\right)^{1/2}\left(\frac{v_a^2}{2k_BT} - \frac{3}{2}\right)\right]\left(\sum_{c\in(G)}i_\beta(v_c)\right) = \left(\frac{2}{3}\right)^{1/2} T\frac{\partial}{\partial T}\Big)_n A_{(G)}\prod_{i\in(G)}\varphi^{eq}(v_i)\left(\sum_{c\in(G)}i_\beta(v_c)\right), \quad (A15)$$

while for $\alpha = 2, 3, 4$, momentum conservation implies

$$A_{(G)}\prod_{i\in(G)}\varphi^{eq}(v_i)\left(\sum_{a\in(G)}\frac{v_{a,x}}{\sqrt{k_BT}}\right)\left(\sum_{b\in(G)}i_\beta(v_b)\right) = \sum_{a\in(G)}\frac{v_{a,x}}{\sqrt{k_BT}}A_{(G)}\prod_{i\in(G)}\varphi^{eq}(v_i)\left(\sum_{b\in(G)}i_\beta(v_b)\right). \quad (A16)$$

Note that in (A14) and (A15), the thermodynamic coefficients which appear in $A_{(G)}$ [through $\delta\tilde{J}_1^x$: see (A10) or in $i_\beta(v_b)$], have to be kept *constant* when taking the derivative with respect to n or T.

Applying then again the same type of formulas to eliminate $i_\beta(v_b)$, we can easily reduce (A9) to simple equilibrium properties of the hard-core system. Let us illustrate this point by discussing in detail the coefficient $[m_{12}^{T\kappa}]^S$.

From (A9) we have

$$[m_{12}^{T\kappa}]^S = \int dv^N\sum_{(G)}\left((0|(J_1^{T\kappa} - \delta\tilde{J}_1^{T\kappa})|0) + \sum_{\{k'\}}(0|(J_1^{T\kappa} - \delta\tilde{J}_1^{T\kappa})|\{k'\})\hat{C}_{\{k'\};0}^S\right)_{(G)} \times \prod_{i\in(G)}\varphi^{eq}(v_i)\left(\sum_{a\in(G)}1\right)\left(\sum_{b\in(G)}\frac{v_{bx}}{\sqrt{k_BT}}\right). \quad (A17)$$

We use (A14) and (A16) to get

$$[m_{12}^{T\kappa}]^S = \frac{\partial}{\partial n}\Big)_T n \int dv^N \sum_{(G)}\Big(\sum_{b\in(G)}\frac{v_{bx}}{\sqrt{k_BT}}\Big)\Big((0|(J_1^{T\kappa}-\delta J_1^{T\kappa})|0) + \sum_j\sum_{k\neq 0}(0|(J_1^{T\kappa}-\delta\tilde{J}_1^{T\kappa})|k_1,-k_j)\hat{C}^S_{k_1,-k_j;0}\Big)_{(G)} \times \prod_{i\in(G)}\varphi^{eq}(v_i). \quad (A18)$$

Now, with the help of (I. II. 7), a simple symmetry argument shows that the only nonvanishing contribution in (A18) corresponds to $b=1$. Then using (A5), we get

$$[m_{12}^{T\kappa}]^S = \Big(\frac{\partial}{\partial n}\Big)_T n\int dv^N \frac{v_{1x}^2}{\sqrt{k_BT}}\Big[\Big(\frac{v_1^2}{2}+\frac{1}{\Omega}\sum_{j=1}^N V_0^S\prod_i\varphi^{eq}(v_i) + \frac{1}{\Omega}\sum_{j=1}^N\sum_k\Big(\frac{1}{2\Omega}V_k^S+\frac{1}{2\Omega}\frac{\partial k_xV_k^S}{\partial k_x}\Big)\rho^{eq,S}_{k,-k} - \Big(\frac{\tilde{h}^S}{n}\Big)\times\prod_i\varphi^{eq}(v_i)\Big], \quad (A19)$$

where the tilde on the factor (h^S/n) indicates that it should *not* be differentiated with respect to n. The integral in the left-hand side of (A19) is directly related to the enthalpy per particle; we get

$$[m_{12}^{T\kappa}]^S = \sqrt{k_BT}\Big(\frac{n}{\partial n}\Big)_T n\Big[\frac{h^S}{n}-\Big(\frac{\tilde{h}^S}{n}\Big)\Big] = \sqrt{k_BT}\,n\Big(\frac{\partial h/n}{\partial n}\Big)_T^S. \quad (A20)$$

A similar calculation leads to

$$[m_{21}^{T\kappa}]^S = [m_{12}^{T\kappa}]^S, \quad (A21)$$

$$[m_{25}^{T\kappa}]^S = [m_{52}^{T\kappa}]^S = \sqrt{\tfrac{2}{3}}\sqrt{k_BT}\,T\Big(\frac{\partial h/n}{\partial T}\Big)_n^S, \quad (A22)$$

while, for symmetry reasons, all other $[m_{\alpha\beta}^{T\kappa}]^S$ vanish.

If we now combine (A11)–(A13) and (A20)–(A22), we recover Eqs. (III. 15a–d) of the text.

Similar calculations can be performed for the other transport coefficients; for completeness, we give here the final formulas. For the shear viscosity, the only nonvanishing coefficients are

$$m_{11}^{\eta}(1_k|y) = 1_{k_x}1_{k_y}ny\frac{\partial V_y^L}{\partial y}, \quad (A23a)$$

$$m_{23}^{\eta}(1_k|y) = m_{32}^{\eta}(1_k|y) = k_BT, \quad (A23b)$$

while for the combination $B=4\eta/3+\zeta$, we have

$$m_{11}^B(1_k|y) = n\Big\{\Big(\frac{\partial^2 p}{\partial n^2}\Big)_T^S + V_y^L - \Big(\frac{\partial p}{\partial e}\Big)_n^S\Big[\Big(\frac{\partial^2 e}{\partial n^2}\Big)_T^S + V_y^L\Big] + 1_{k_x}^2 y\frac{\partial V_y^L}{\partial y}\Big\}, \quad (A24a)$$

$$m_{15}^B(1_k|y) = m_{51}^B(1_k|y) = \sqrt{\tfrac{2}{3}}\Big[T\Big(\frac{\partial^2 p}{\partial n\partial T}\Big)^S - \Big(\frac{\partial p}{\partial e}\Big)_n^S\Big(\frac{\partial^2 e}{\partial n\partial T}\Big)^S\Big], \quad (A24b)$$

$$m_{55}^B(1_k|y) = \frac{2}{3}\frac{T^2}{n}\Big[\Big(\frac{\partial^2 p}{\partial T^2}\Big)_n^S - \Big(\frac{\partial p}{\partial e}\Big)_n^S\Big(\frac{\partial^2 e}{\partial T^2}\Big)_n^S\Big], \quad (A24c)$$

$$m_{22}^B(1_k|y) = k_BT\Big[2-\Big(\frac{\partial p}{\partial e}\Big)_n^S\Big], \quad (A24d)$$

$$m_{33}^B(1_k|y) = m_{44}^B(1_k|y) = -k_BT\Big(\frac{\partial p}{\partial e}\Big)_n^S. \quad (A24e)$$

APPENDIX B: CALCULATION OF $\overline{m}^x_{\alpha\beta}(1_k|y)$

A. General discussion

From Eqs. (II. 13), (III. 10), (II. 24), and (II. 14), we get the following expression for $\overline{m}^x_{\alpha\beta}(1_k|y)$:

$$\overline{m}^x_{\alpha\beta}(1_k|y) = \lim_{\gamma} N^{-1}\int dv^N\sum_{\text{all } a,b} i_\alpha(v_a)i_\beta(v_b)\Big((k_a,-k_b|(J^x-\delta J^x)\Omega^N\rho^{eq}|0) + \sum_{\{k'\}\neq 0}\tilde{D}^S_{k_a,-k_b,\{0\}';\{k'\}}(\{v\};i\epsilon)\times(\{k'\}|(J^x-\delta J^x)\Omega^N\rho^{eq}|0)\Big). \quad (B1)$$

Here again the terms $a=b$ are obtained by formally putting $k_a=-k_b=0$.

This expression can be reduced to purely equilibrium fluctuations. Indeed, consider first the case where α and $\beta\in 1,2\cdots 4$. It is then an easy matter to prove that

$$\int dv^N\sum_{\text{all } a,b} i_\alpha(v_a)i_\beta(v_b)\tilde{D}^S_{k_a,-k_b,\{0\}';\{k'\}},(\{v\};i\epsilon)\cdots = 0. \quad (B2)$$

This is an immediate consequence of both particle and momentum conservation. Analytically, (B2) is proved by first taking notice of the Liouville operator $\delta L^{ij}\alpha\partial/\partial v_{ij}$ [see (II. 22)]; an integration by parts on the right-hand side of (B2) then immediately leads to the required result.

Using the definition of the matrix elements given in (I. II. 9), we get thus for $\alpha,\beta\in 1\cdots 4$

$$\overline{m}^x_{\alpha\beta}(1_k|y) = \lim_{\gamma} N^{-1}\int dv^N dr^N\sum_{\text{all } a,b} i_\alpha(v_a)i_\beta(v_b)\times\exp[ik(r_a-r_b)](J^x-\delta J^x)\rho^{eq} \quad (\alpha,\beta\in 1\cdots 4) \quad (B3)$$

or

$$\overline{m}^x_{\alpha\beta}(1_k|y) = \lim_{\gamma} N^{-1}\int dr\,dr'\langle d_\alpha(r)d_\beta(r')(J^x-\delta J^x)\rangle\times\exp[ik(r-r')] \quad (\alpha,\beta\in 1\cdots 4). \quad (B4)$$

In this latter equation, we have used the traditional notation $\langle\cdots\rangle$ to represent the canonical average and we have introduced the density operators

$$d_\alpha(r) = \sum_{a=1}^N i_\alpha(v_a)\delta(r-r_a), \quad (B5)$$

which, up to a trivial constant, respectively represent the number density $n(r)$ and the momentum densities $v_i(r)$ $(i=x,y,z)$; indeed we have

$$d_1(r) = \sum_{a=1}^N \delta(r-r_a) = n(r), \quad (B6)$$

$$d_i(r) = (1/\sqrt{k_BT})\sum_a v_{a,i}\delta(r-r_i) = v_i(r)/\sqrt{k_BT}. \quad (B7)$$

Note that if we use the definition (B5) for $\alpha=5$, we get a quantity related to the kinetic energy density $\epsilon^K(r)$:

$$d_5(r) = \sum_{a=1}^N\sqrt{\tfrac{2}{3}}[(v_a^2/2k_BT)-\tfrac{3}{2}]\delta(r-r_a), = \sqrt{\tfrac{2}{3}}\{[\epsilon^K(r)/k_BT]-3n(r)/2\}. \quad (B8)$$

However, in the case α or (and) $\beta=5$, Eq. (B2) is no longer valid because the kinetic energy alone is not conserved by the Liouville operator and Eq. (B3) is thus *not* correct either.

A similar problem was already encountered in Ref. 15 where it was shown that the effect of $\tilde{\mathcal{D}}^S$ was essentially to replace the kinetic energy density in (B8) by the total energy density $[\epsilon(r) - nV_0^S]$. More precisely, let us consider the quantity

$$\sum_{\{k'\}\neq 0} \int dv^N \sum_{\text{all } a,b} i_\alpha(v_a) i_\beta(v_b) \tilde{\mathcal{D}}^S_{k_a,-k_b,\{0\}';\{k'\}}(\{v\}; i\epsilon)\cdots \quad \text{(B9)}$$

and let us use the fact that $\tilde{\mathcal{D}}^S$ has the following form [see (II.22)]:

$$\tilde{\mathcal{D}}^S \propto \sum_{i>j} (\delta L^{ij})^S (L_0 - z)^{-1}\Big(1 + \sum_{k>l} (\delta L^{kl})^S \cdots\Big). \quad \text{(B10)}$$

We then perform in (B9) successive integrations by parts over $(\delta L^{ij})^S \propto \partial/\partial v_{ij}$ and $(\delta L^{kl})^S \propto \partial/\partial v_{kl}$, considering separately the various cases $i =$ or $\neq$ from a, b, $j =$ or $\neq a, b$ etc. The result of this straightforward but tedious calculation is that, even for α or (and) $\beta = 5$, an equation similar to (B3) still holds, namely

$$\overline{m}^x_{\alpha\beta}(1_k|y) = \lim_\gamma N^{-1} \int dr\, dr' \langle \tilde{d}_\alpha(r)\tilde{d}_\beta(r')(J^x - \delta J^x)\rangle \times \exp[ik(r-r')], \quad \text{(B11)}$$

where

$$\tilde{d}_\alpha(r) = d_\alpha(r) \quad (\alpha \in 1\cdots 4),$$
$$\tilde{d}_5(r) = \sqrt{\tfrac{2}{3}}\{[\epsilon^S(r)/k_BT] - [\tfrac{3}{2} + (nV_0^S/k_BT)]n(r)\}. \quad \text{(B12)}$$

Note that only the hard-core energy density enters into Eq. (B12):

$$\epsilon^S(r) = \sum_{a=1}^N \tfrac{1}{2}v_a^2 + \tfrac{1}{2}\Big(\sum_{b\neq a=1}^N V^S(r_{ab})\Big)\delta(r - r_a). \quad \text{(B13)}$$

As was announced in Sec. III, $\overline{m}^x_{\alpha\beta}$ is thus indeed reduced to purely equilibrium quantities, from which we have to properly extract the leading γ^0-contribution.

B. Calculation of the equilibrium correlations

As is well-known,[16] for a purely hard-core system, the average appearing in (B11) can be reduced to purely thermodynamic fluctuations by going to the grand canonical ensemble (denoted by G.C.) and computing

$$\langle \Delta\tilde{d}_\alpha \Delta\tilde{d}_\beta (J^x - \delta J^x)\rangle_{\text{G.C.}} \quad \text{(B14)}$$

in terms of the grand canonical variables T and μ; here

$$\Delta\tilde{d}_\alpha = \int dr\, d_\alpha(r) - \langle \int dr\, d_\alpha(r)\rangle. \quad \text{(B15)}$$

Although this formula will turn out to be useful later on, it is not sufficient for our purpose: Indeed, we have to extract the $\lim_\gamma$ in (B11) by letting $k \to 0$ but keeping y finite [see (I.10)]. This will be achieved by using the method developed by Hemmer.[17]

Let us again consider the case of thermal conductivity:

$$\overline{m}^{T\kappa}_{\alpha\beta}(1_k|y) = \lim_\gamma \int dr\, dr' \Big\langle \tilde{d}_\alpha(r)\tilde{d}_\beta(r')\Big[\sum_i v_{ix}\Big(\frac{v_i^2}{2} + \frac{1}{2}\sum_{i\neq j} V(r_{ij}) - \frac{h}{n}\Big) - \frac{1}{2}\sum_{i\neq j} v_i \frac{\partial V}{\partial r_{ij}}(v_{ij})_x\Big]\Big\rangle, \quad \text{(B16)}$$

where we have followed the notation (I.1).

Simple invariance arguments show that the only nonvanishing coefficients in (B16) are $\overline{m}^{T\kappa}_{1i} = \overline{m}^{T\kappa}_{i1}$ and $\overline{m}^{T\kappa}_{5i} = \overline{m}^{T\kappa}_{i5}$ $(i = 2,3,4)$. Let us take the example of $\overline{m}^{T\kappa}_{52}$; we have

$$\overline{m}^{T\kappa}_{52}(1_k|y) = \lim_\gamma \frac{1}{N}\sqrt{\tfrac{2}{3}}\frac{1}{\sqrt{k_BT}}\sum_{\text{all } a,b}\int dr^N dv^N \exp(ikr_{ab}) \times\Big(\frac{v_a^2}{2k_BT} - \frac{3}{2} - \frac{nV_0^S}{k_BT} + \frac{1}{2}\sum_{S\neq a}\frac{V^S(r_{aS})}{k_BT}\Big) \times\Big[v^2_{x,b}\Big(\frac{v_b^2}{2} + \frac{1}{2}\sum_{t\neq b} V(r_{tb}) - \frac{1}{2}\sum_{t\neq b}\frac{\partial V}{\partial r_{tb}}(r_{tb})_x - \frac{h}{n}\Big)\Big]\rho^{\text{eq}}. \quad \text{(B17)}$$

We write this as

$$\overline{m}^{T\kappa}_{52}(1_k|y) = (\overline{m}^{T\kappa}_{52})^S + [\overline{m}^{T\kappa}_{52}(1_k|y)]^L, \quad \text{(B18)}$$

where the first term corresponds to the pure hard-core contribution (which is obviously y-independent) and the second term is the long-range correction.

For evaluating $(\overline{m}^{T\kappa}_{52})^S$, we can use (B14) by going to the grand canonical ensemble; we have [see I, Eq. (II.8)]

$$(\overline{m}^{T\kappa}_{52})^S = \frac{1}{N}\sqrt{\tfrac{2}{3}}\frac{1}{(k_BT)^{3/2}}\Big\langle\Big[\Delta\tilde{E} - \Big(\frac{3k_BT}{2} + nV_0^S\Big)\Delta\tilde{N}\Big] \times\sum_{b=1}^N v_{x,b}(J_b^{T\kappa,S} - \delta J_b^{T\kappa,S})\Big\rangle^S_{\text{G.C.}}. \quad \text{(B19)}$$

Using the well-known equivalence relations

$$\Delta\tilde{E} \to k_BT^2\frac{\partial}{\partial T}\Big)_{\mu/kT} \quad \text{(B20)}$$

and

$$\Delta\tilde{N} \to k_BT\frac{\partial}{\partial\mu}\Big)_T, \quad \text{(B21)}$$

we get

$$(\overline{m}^{T\kappa}_{52})^S = \frac{1}{N}\sqrt{\tfrac{2}{3}}\frac{1}{\sqrt{k_BT}}\Big[k_BT^2\frac{\partial}{\partial T}\Big)_{\mu/kT} - \Big(\frac{3k_BT}{2} + nV_0^S\Big)k_BT \times\frac{\partial}{\partial\mu}\Big)_T\Big]\Big[\Omega h(\mu,T) - \Big(\widetilde{\frac{h}{n}}\Big)N(\mu,T)\Big], \quad \text{(B22)}$$

where, as in (A19), the notation $(\widetilde{h/n})$ indicates that this quantity should not be differentiated. By simple thermodynamic transformations, Eq. (B22) can still be cast into the following form:

$$(\overline{m}^{\kappa T}_{52})^S = \sqrt{\tfrac{2}{3}}\sqrt{k_BT}\Big[T\Big(\frac{\partial h/n}{\partial T}\Big)^S + \Big[\Big(\frac{\partial e}{\partial n}\Big)^S - \Big(\frac{3k_BT}{2} + nV_0^S\Big)\Big] \times\Big(\frac{\partial h/n}{\partial n}\Big)^S_T n\Big(\frac{\partial n}{\partial p}\Big)^S_T\Big]. \quad \text{(B23)}$$

The calculation of $(m^{\kappa T}_{52}(1_k|y))^L$ is much more elaborate; first, it is readily checked that, to order γ^0, only the terms $a \neq b$ and $S \neq a, b$ contribute in (B18); we have thus

$$(m^{\kappa T}_{52}(1_k|y))^L = \lim_\gamma\Big(N\sqrt{\tfrac{2}{3}}\frac{1}{k_BT}\int dr^N dv^N \exp(ikr_{12}) \times\Big(-\frac{nV_0^S}{kT} + \frac{1}{2}\sum_{s\neq 1,2}\frac{V^S(r_{1s})}{k_BT}\Big)\Big\{v^2_{x,2}\Big[\frac{v_2^2}{2} + \frac{1}{2}\sum_{t\neq 2} V(r_{2t}) - \frac{1}{2}\sum_{t\neq 2}\Big(\frac{\partial V}{\partial r_{2t}}\Big)_x (r_{2t})_x - \frac{h}{n}\Big]\Big\}\rho^{\text{eq}}\Big)^L. \quad \text{(B24)}$$

After a trivial velocity integration, we find in (B24) three type of configurational averages:

(a) Those independent of the potential; they involve

$$I_1=\left(\lim_{\gamma} N\int dr^N \exp(ikr_{12})\rho_V^{eq}\right)^L, \quad \text{(B25)}$$

where

$$\rho_V^{eq}=\exp(-\beta V_N)/\int dr^N \exp(-\beta V_N). \quad \text{(B26)}$$

I_1 is simply related to the Fourier transform of the long-range part of the pair correlation function; it is known that[17]

$$I_1=\frac{1}{n}\tilde{g}_2^L(k)\equiv\frac{1}{n}\tilde{g}_{2,\gamma}^L=\frac{-k_BTn[(\partial n/\partial p)_T^S]^2V_\gamma^L}{1+n(\partial n/\partial p)_T^S V_\gamma^L}. \quad \text{(B27)}$$

(b) Those linear in the potential $V(r)$. Putting

$$\sigma_i(1,3)=V(r_{13}) \text{ or } \frac{\partial V}{\partial r_{13,x}}r_{13,x} \quad (i=1 \text{ or } 2),$$

$$\sigma_i^T(1,3)=\sigma_i^L(1,3)+\sigma_i^S(1,3), \quad \text{(B28)}$$

we find in (B23) a series of terms involving

$$I_2^{(T,S)}=\lim_{\gamma}[N^2\int dr^N\sigma_i^{(T,S)}(1,3)\exp(ikr_{12})\rho_V^{eq} +N\int dr^N\sigma_i^{(T,S)}(1,2)\exp(ikr_{12})\rho_V^{eq}]^L \quad \text{(B29)}$$

(we always work in the thermodynamic limit).

(c) Those quadratic in the potential $V(r)$:

$$I_3=\lim_{\gamma}\{N^3\int dr^N\sigma_j^S(1,3)\sigma_i^T(2,4)\exp(ikr_{12})\rho_V^{eq} +N^2\int dr^N\sigma_j^S(1,3)[\sigma_i^T(2,1)+\sigma_i^T(2,3)] \times\exp(ikr_{12})\rho_V^{eq}\}^L. \quad \text{(B30)}$$

Let us first learn how to deal with I_2^T; we have

$$I_2^T=I_{2,1}^T+I_{2,2}^T, \quad \text{(B31)}$$

where

$$I_{2,1}^T=\lim_{\gamma}[N^{-1}\int dr_1\,dr_2\,dr_3\sigma_i^T(1,3)\exp(ikr_{12})\bar{n}_3(1,2,3)]^L, \quad \text{(B32)}$$

$$I_{2,2}^T=\lim_{\gamma}[N\int dr^N\sigma_i^T(1,2)\exp(ikr_{12})\rho_V^{eq}]^L. \quad \text{(B33)}$$

Here we have introduced the three-particle distribution function $\bar{n}_3(1,2,3)$,

$$\bar{n}_3(1,2,3)=[N!/(N-3)!]\int dr^{N-3}\rho_V^{eq}. \quad \text{(B34)}$$

With the cluster decomposition

$$\bar{n}_3(1,2,3)=n^3+ng_2(1,2)+ng_2(1,3)+ng_2(2,3)+g(1,2,3), \quad \text{(B35)}$$

we immediately get

$$I_{2,1}^T=\lim_{\gamma}\left\{\tilde{g}_2(k)[\tilde{\sigma}_i^T(0)+\tilde{\sigma}_i^T(k)]+N^{-1}\int dr_1\,dr_2\,dr_3 \times\sigma_i(13)\exp(ikr_{12})g_3(1,2,3)\right\}^L, \quad \text{(B36)}$$

where have put

$$\tilde{g}_2(k)=\int dr\exp(ikr)g_2(2),$$

$$\tilde{\sigma}_i^T(k)=\int dr\exp(ikr)\sigma_i^T(2). \quad \text{(B37)}$$

The long-range part of the first term in Eq. (B36) is readily evaluated:

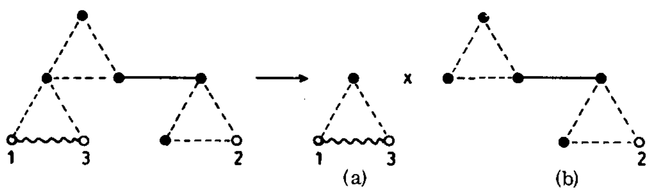

FIG. 2. A typical graph contributing to (B43) and its decomposition.

$$\lim_{\gamma}\{\tilde{g}_2(k)[\tilde{\sigma}_i^T(0)+\tilde{\sigma}_i^T(k)]\}^L=\tilde{g}_2^L(k)[2\tilde{\sigma}_i^S(0)+\tilde{\sigma}_i^L(k) +\tilde{\sigma}_i^L(0)]+\tilde{g}_2^S(0)\tilde{\sigma}_i^L(k). \quad \text{(B38)}$$

Here $\tilde{g}_2^L(k)$ is the long-range part (B27) of the pair correlation function, while of course

$$\tilde{g}_2^S(0)=n\left[k_BT\left(\frac{\partial n}{\partial p}\right)_T^S-1\right]. \quad \text{(B39)}$$

In order to deal with the second term of (B36), we follow the calculation of Hemmer[17] and we use his composite Mayer graph technique.

If we remember that

$$g_3(1,2,3)= \text{sum of all composite irreducible 3-graphs}, \quad \text{(B40)}$$

we see immediately that we may neglect

$$\lim_{\gamma}N^{-1}\int dr_1\,dr_2\,dr_3\sigma_i^L(1,3)g_3(1,2,3) \quad \text{(B41)}$$

because, already in the absence of $\sigma_i^L(1,3)$, we have a connected graph; it follows[17] that (B41) does not contribute in the $\lim_\gamma$. We are thus left with

$$\lim_{\gamma}N^{-1}\int dr_1\,dr_2\,dr_3\sigma_i^S(1,3)g_3(1,2,3). \quad \text{(B42)}$$

Denoting by a wiggly line the bond $\sigma_i^S(a,b)$ and following otherwise Hemmer's notation, a typical graph contributing to the long-range part of (B43) is shown in Fig. 2.

It can be divided into two disconnected parts: part (A) is a contribution to $\sigma_i^S(1,3)g_2^S(1,3)$ while part (B) contributes to $\tilde{g}_2^L(k)$. Noticing that part (B) can be attached to part A at any vertex of the latter, these vertices being in number equal to the order in the density, we arrive at

$$\lim_{\gamma}N^{-1}\int dr_1\,dr_2\,dr_3\sigma_i^S(1,3)g_3(1,2,3) =\frac{1}{n}\tilde{g}_2(k)\frac{\partial}{\partial n}\int dr\sigma_i^S(r)g_2^S(r). \quad \text{(B43)}$$

Finally, we find simply

$$I_{2,2}^T=n\tilde{\sigma}_i^L(k). \quad \text{(B44)}$$

Collecting these results, we obtain

$$I_2^T=\tilde{g}_2^L(k)[\tilde{\sigma}_i^L(k)+\tilde{\sigma}_i^L(0)]+[n+\tilde{g}_2^S(0)]\tilde{\sigma}^L(k) +\frac{1}{n}\tilde{g}_2^L(k)\frac{\partial}{\partial n}\left\{\int dr\sigma_i^S(r)[n^2+g_2^S(r)]\right\}. \quad \text{(B45)}$$

The modifications required to compute I_2^S are obvious, yielding

$$I_2^S=\frac{1}{n}\tilde{g}_2^L(k)\frac{\partial}{\partial n}\left\{\int dr\sigma_i^S(r)[n^2+g_2^S(r)]\right\}. \quad \text{(B46)}$$

It is interesting to point out that the difference between I_1 and I_2^S, namely the introduction of $\sum_a \sigma_i^S(1,a)$ in the canonical average, leads in the final result to the following multiplicative factor [see (B27)]:

$$I_2^S/I_1 = \frac{\partial}{\partial n}\int d^3r\sigma_i^S(r)[n^2 + g_2^S(r)]. \tag{B47}$$

The calculation of I_3 proceeds along the same way, but it is of course much more involved. To make a long story short, let us simply point out that we have proved a formula similar to (B47), namely,

$$I_3/I_2^T = \frac{\partial}{\partial n}\int dr\sigma_j^S(r)[g_2^S(r) + n^2], \tag{B48}$$

where I_2^T is given by (B40).

Combining all these results, together with the obvious formulas,

$$e^S - (3k_BT/2)n = \tfrac{1}{2}\int drV^S(r)[g_2^S(r) + n^2], \tag{B49}$$

$$h^S - \frac{5k_BT}{2}n = \frac{1}{2}\int dr\left(V^S(r) - r_x\frac{\partial V^S}{\partial r_x}\right)[g_2^S(r) + n^2], \tag{B50}$$

it is a matter of simple algebra to obtain the explicit form for $(\overline{m}_{52}^{T\kappa}(1_k|y))^L$. We get

$$(\overline{m}_{52}^{T\kappa}(1_k|y))^L = \sqrt{\tfrac{2}{3}}\,\sqrt{k_BT}\left[\left(\frac{\partial e}{\partial n}\right)_T^S - \frac{3k_BT}{2} - nV_0^S\right]\left\{(\tilde{g}_{2,y}^L/k_BT)\right.$$
$$\times\left[V_y^L + \tfrac{1}{2}1_{k_x}^2 y\frac{\partial V_y^L}{\partial y} + \left(\frac{\partial h/n}{\partial n}\right)_T^S\right] + n\left(\frac{\partial n}{\partial p}\right)_T^S$$
$$\left.\times\left(V_y^L + \tfrac{1}{2}1_{k_x}^2 y\frac{\partial V_y^L}{\partial y}\right)\right\}. \tag{B51}$$

When (B51) is added to (B23), we obtain the compact expression quoted in Eq. (III.16b) for $\overline{m}_{52}^{T\kappa}$. The other coefficients $\overline{m}_{\alpha\beta}^{\kappa T}$ are obtained by similar calculations as well as the $\overline{m}_{\alpha\beta}^{\eta}$ and $\overline{m}_{\alpha\beta}^{B}$ which are listed below.

C. List of the matrix elements $\overline{m}_{\alpha\beta}^{x}(1_k|y)$

For completeness, let us list here the $\overline{m}_{\alpha\beta}^{x}(1_k|y)$ corresponding to the other transport coefficients. For the shear viscosity, the nonvanishing coefficients are

$$\overline{m}_{11}^{\eta}(1_k|y) = m_{11}^{\eta}(1_k|y)[nk_BT\chi_T(y)]^2 + O(\gamma), \tag{B52a}$$

$$\overline{m}_{15}^{\eta}(1_k|y) = m_{11}^{\eta}(1_k|y)[nk_BT\chi_T(y)]^2\sqrt{\tfrac{2}{3}}\frac{1}{k_BT}$$
$$\times\left[\left(\frac{\partial e}{\partial n}\right)_T^S - \frac{3k_BT}{2} - nV_0^S\right] + O(\gamma) = \overline{m}_{51}^{\eta}(1_k|y), \tag{B52b}$$

$$\overline{m}_{55}^{\eta}(1_k|y) = m_{11}^{\eta}(1_k|y)[nk_BT\chi_T(y)]^2\frac{2}{3}\frac{1}{(k_BT)^2}$$
$$\times\left[\left(\frac{\partial e}{\partial n}\right)_T^S - \frac{3k_BT}{2} - nV_0^S\right]^2 + O(\gamma), \tag{B52c}$$

$$\overline{m}_{23}^{\eta}(1_k|y) = \overline{m}_{32}^{\eta}(1_k|y) = k_BT, \tag{B52d}$$

where we have used (A23); for $B = \frac{4}{3}\eta + \zeta$, we find

$$\overline{m}_{11}^{B}(1_k|y) = m_{11}^{B}(1_k|y)[nk_BT\chi_T(y)]^2 + O(\gamma), \tag{B53a}$$

$$\overline{m}_{15}^{B}(1_k|y) = \overline{m}_{51}^{B}(1_k|y)$$
$$= m_{15}^{B}(1_k|y)[nk_BT\chi_T(y)] + m_{11}^{B}(1_k|y)$$
$$\times[nkT\chi_T(y)]^2\sqrt{\tfrac{2}{3}}\frac{1}{k_BT}\left[\left(\frac{\partial e}{\partial n}\right)_T^S - \frac{3k_BT}{2}\right.$$
$$\left. - nV_0^S\right] + O(\gamma), \tag{B53b}$$

$$\overline{m}_{55}^{B}(1_k|y) = m_{55}^{B}(1_k|y) + 2m_{15}^{B}(1_k|y)[nk_BT\chi_T(y)]$$
$$\times\sqrt{\tfrac{2}{3}}\frac{1}{k_BT}\left[\left(\frac{\partial e}{\partial n}\right)_T^S - \frac{3k_BT}{2} - nV_0^S\right]$$
$$+ m_{11}^{B}[nk_BT\chi_T(y)]^2\frac{2}{3}\frac{1}{(k_BT)^2}\left[\left(\frac{\partial e}{\partial n}\right)_T^S\right.$$
$$\left. - \frac{3k_BT}{2} - nV_0^S\right]^2 + O(\gamma), \tag{B53c}$$

$$\overline{m}_{22}^{B}(1_k|y) = m_{22}^{B}(1_k|y) + O(\gamma), \tag{B53d}$$

$$\overline{m}_{33}^{B}(1_k|y) = \overline{m}_{44}^{B}(1_k|y) = m_{33}^{B}(1_k|y) + O(\gamma), \tag{B53e}$$

where we have used (A24).

APPENDIX C. THE FUNCTIONS $\Phi_{\alpha\beta}^{x}$ AND $\phi_{\alpha\beta}^{x}$

For completeness, we list here the relevant functions $\Phi_{\alpha\beta}^{x}$ and $\hat{\Phi}_{\alpha\beta}^{x}$ for the cases of shear viscosity and of bulk viscosity.

We have

$$\Phi_{12}^{\eta}(1_k|y) = \Phi_{21}^{\eta}(1_k|y) = k_BT1_{k_x}1_{k_y}\mathcal{G}_{12}^{\eta}(y), \tag{C1a}$$

$$\Phi_{33}^{\eta}(1_k|y) = -2k_BT1_{k_x}1_{k_y}, \tag{C1b}$$

$$\Phi_{34}^{\eta}(1_k|y) = -\Phi_{43}^{\eta}(1_k|y) = k_BT1_{k_z}, \tag{C1c}$$

$$\Phi_{55}^{\eta}(1_k|y) = k_BT1_{k_x}1_{k_y}\mathcal{G}_{55}^{\eta}(y), \tag{C1d}$$

where

$$\mathcal{G}_{12}^{\eta}(y) = 1 + \frac{1}{2c^2(y)}ny\frac{\partial V_y^L}{\partial y}, \tag{C2a}$$

$$\mathcal{G}_{55}^{\eta}(y) = \frac{1}{c^4(y)}\frac{2}{3}\frac{T}{n^2k_B}\left[\left(\frac{\partial p}{\partial T}\right)_n^S\right]^2 ny\frac{\partial V_y^L}{\partial y}, \tag{C2b}$$

and

$$\hat{\Phi}_{12}^{\eta}(1_k|y) = \hat{\Phi}_{21}^{\eta}(1_k|y) = \Phi_{12}^{\eta}(1_k|y), \tag{C3a}$$

$$\hat{\Phi}_{33}^{\eta}(1_k|y) = \Phi_{33}^{\eta}(1_k|y), \tag{C3b}$$

$$\hat{\Phi}_{34}^{\eta}(1_k|y) = -\hat{\Phi}_{43}^{\eta}(1_k|y) = \Phi_{34}^{\eta}(1_k|y), \tag{C3c}$$

$$\hat{\Phi}_{55}^{\eta}(1_k|y) = \left(\frac{9}{4}\frac{c^4(y)}{(C_v^ST)^2}(nk_BT\chi_T(y))^2\right)k_BT\mathcal{G}_{55}^{\eta}(y)1_{k_x}1_{k_y}. \tag{C3d}$$

Similarly, we have for $B = \frac{4}{3}\eta + \zeta$

$$\Phi_{12}^{B}(1_k|y) = \Phi_{21}^{B}(1_k|y) = k_BT[(1_{k_x}^2 - \tfrac{1}{3})\mathcal{G}_{12}^{\eta}(y) + \mathcal{G}_{12}^{\zeta}(y)], \tag{C4a}$$

$$\Phi_{33}^{B}(1_k|y) = k_BT\left\{\left(\frac{2(1_{k_x}^2 1_{k_y}^2)}{(1_{k_x}^2 + 1_{k_y}^2)} - \frac{2}{3}\right) + \left[\frac{2}{3} - \left(\frac{\partial p}{\partial e}\right)_n^S\right]\right\}, \tag{C4b}$$

$$\Phi_{34}^{B}(1_k|y) = -\Phi_{43}^{B}(1_k|y) = k_BT\; -2\frac{1_{k_x}1_{k_y}1_{k_z}}{(1_{k_x}^2 + 1_{k_z}^2)}, \tag{C4c}$$

$$\Phi_{44}^{B}(1_k|y) = k_BT\left\{\left(\frac{2(1_{k_z}^2)}{(1_{k_x}^2 + 1_{k_z}^2)} - \frac{2}{3}\right) + \left[\frac{2}{3} - \left(\frac{\partial p}{\partial e}\right)_n^S\right]\right\}, \tag{C4d}$$

$$\Phi_{55}^{B}(1_k|y) = k_BT[(1_{k_x}^2 - \tfrac{1}{3})\mathcal{G}_{55}^{\eta}(y) + \mathcal{G}_{55}^{\zeta}(y)], \tag{C4e}$$

where

$$\mathcal{G}_{12}^{\zeta}(y) = \frac{1}{2c^2(y)}n\left\{\left(\frac{\partial^2 p}{\partial n^2}\right)_T^S + V_y^L - \left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial n^2}\right)_T^S + V_y^L\right]$$
$$+ \frac{2(\partial p/\partial T)_n^S}{n^2C_v^S}T\left[\left(\frac{\partial^2 p}{\partial n\partial T}\right)^S - \left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial n\partial T}\right)^S\right]$$

$$+\frac{[(\partial p/\partial T)_n^S]^2}{n^2 C_v^{S2}}\frac{T^2}{n^2}\left[\left(\frac{\partial^2 p}{\partial T^2}\right)_n^S-\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial T^2}\right)_n^S\right]$$

$$+\tfrac{1}{3}y\frac{\partial V_y^L}{\partial y}+\frac{2c^2(y)}{3n}\Bigg\}, \tag{C5a}$$

$$\mathcal{G}_{55}^{\zeta}(y)=\frac{1}{c^4(y)}\frac{2}{3}\frac{T}{n^2k_B}\left(\left[\left(\frac{\partial p}{\partial T}\right)_n^S\right]^2\left\{n\left(\frac{\partial^2 p}{\partial n^2}\right)_T^S+nV_y^L\right.\right.$$
$$\left.-n\left(\frac{\partial p}{\partial e}\right)_n^S\left[\left(\frac{\partial^2 e}{\partial n^2}\right)_T^S+V_y^L\right]+\tfrac{1}{3}ny\frac{\partial V_y^L}{\partial y}\right\}-2\left(\frac{\partial p}{\partial T}\right)_n^S$$
$$\times\frac{1}{\chi_T(y)}\left[\left(\frac{\partial^2 p}{\partial n\partial T}\right)^S-\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial n\partial T}\right)_n^S\right]+\frac{1}{n\chi_T(y)^2}$$
$$\left.\times\left[\left(\frac{\partial^2 p}{\partial T^2}\right)_n^S-\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial T^2}\right)_n^S\right]\right), \tag{C5b}$$

and

$$\hat{\Phi}_{12}^B(1_k|y)=\hat{\Phi}_{21}^B(1_k|y)=\Phi_{12}^B(1_k|y), \tag{C6a}$$
$$\hat{\Phi}_{33}^B(1_k|y)=\Phi_{33}^B(1_k|y), \tag{C6b}$$
$$\hat{\Phi}_{34}^B(1_k|y)=-\hat{\Phi}_{43}^B(1_k|y)=\Phi_{34}^B(1_k|y), \tag{C6c}$$
$$\hat{\Phi}_{44}^B(1_k|y)=\Phi_{44}^B(1_k|y), \tag{C6d}$$
$$\Phi_{55}^B(1_k|y)=\{\tfrac{9}{4}[c^4(y)/(C_v^S T)^2](nk_B T\chi_T(y))^2\}k_B T\mathcal{G}_{55}^B(y). \tag{C6e}$$

Note that in these equations, we have separated $\Phi_{\alpha\beta}^B$ and $\hat{\Phi}_{\alpha\beta}^B$ into two parts:

$$\Phi_{\alpha\beta}^B(1_k|y)=\hat{\Phi}_{\alpha\beta}^{\eta}(1_k|y)+\hat{\Phi}_{\alpha\beta}^{\zeta}(1_k|y), \tag{C7}$$

which, respectively, correspond to the shear part, $\frac{4}{3}\eta$, and the bulk part, ζ, of the coefficient $B=\frac{4}{3}\eta+\zeta$. When the decomposition (C7) is inserted into (III.8), the integration over the angular part of k makes them mutually orthogonal.

APPENDIX D: CALCULATION OF $\zeta^{(1)}$

If we introduce (C4), (C6) into Eq. (III.8) and perform the integral over the angles, we obtain for $B^{(1)}$

$$B^{(1)}=\tfrac{4}{3}\eta^{(1)}+\zeta^{(1)}, \tag{D1}$$

where $\eta^{(1)}$ is precisely given by (III.21), while $\zeta^{(1)}$, which corresponds to bulk viscosity, is given by the following formula:

$$\zeta^{(1)}=\frac{kT}{4\pi^2}\int_0^\infty dy\left[\left(b_1(y)\frac{1}{2\kappa_S/nC_p(y)}-\text{hard core}\right)\right.$$
$$\left.+\left(b_2(y)\frac{1}{2\Gamma(y)}-\text{hard core}\right)\right]. \tag{D2}$$

Here b_1 and b_2 are, respectively, defined by

$$b_1(y)=[n\chi_T(y)]^2\left(\frac{\gamma(y)-1}{\gamma(y)}\right)^2\left(\frac{L(y)}{[(\partial p/\partial T)_n^S]^2}+\tfrac{1}{3}ny\frac{\partial V_y^L}{\partial y}\right)^2, \tag{D3}$$

$$b_2(y)=\left\{\frac{1}{2c^2(y)}K(y)+\left[\frac{1}{3}-\left(\frac{\partial p}{\partial e}\right)_n^S\right]+\frac{1}{6c^2(y)}ny\frac{\partial V_y^L}{\partial y}\right\}^2, \tag{D4}$$

with

$$L(y)=\left[\left(\frac{\partial p}{\partial T}\right)_n^S\right]^2\left[n\left(\frac{\partial^2 p(y)}{\partial n^2}\right)_T-n\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e(y)}{\partial n^2}\right)_T\right]$$
$$-2\left(\frac{\partial p}{\partial T}\right)_n^S\left(\frac{1}{\chi_T(y)}\right)\left[\left(\frac{\partial^2 p}{\partial n\partial T}\right)^S-\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial n\partial T}\right)^S\right]$$
$$+\frac{1}{n(\chi_T(y))^2}\left[\left(\frac{\partial^2 p}{\partial T^2}\right)_n^S-\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial T^2}\right)_n^S\right] \tag{D5}$$

and

$$K(y)=n\left[\left(\frac{\partial^2 p(y)}{\partial n^2}\right)_T-\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e(y)}{\partial n^2}\right)_T\right]$$
$$+2\left(\frac{\partial p}{\partial T}\right)_n^S\frac{T}{nC_v^S}\left[\left(\frac{\partial^2 p}{\partial n\partial T}\right)^S-\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial n\partial T}\right)^S\right]$$
$$+\left[\left(\frac{\partial p}{\partial T}\right)_n^S\right]^2\frac{T^2}{(nC_v^S)^2}\left[\left(\frac{\partial^2 p}{\partial T^2}\right)_n^S-\left(\frac{\partial p}{\partial e}\right)_n^S\left(\frac{\partial^2 e}{\partial T^2}\right)_n^S\right], \tag{D6}$$

where we have introduced

$$p(y)=p^S(n,T)+\tfrac{1}{2}n^2V_y^L, \tag{D7}$$
$$e(y)=e^S(n,T)+\tfrac{1}{2}n^2V_y^L. \tag{D8}$$

In order to bring $b_1(y)$ and $b_2(y)$ into the form given in Eq. (III.24), we use the following trick: Let us define *formally* a free energy density, function of y,

$$f(n,T|y)=f^S(n,T)+\tfrac{1}{2}n^2V_y^L. \tag{D9}$$

It can be interpreted as the free-energy density, taken in the van der Waals limit $\gamma\to 0$, of a *fictitious* fluid which has an attractive potential $\tilde{V}^L(r)$ such that[16]

$$V_y^L\equiv\int dr\tilde{V}^L(r). \tag{D10}$$

Now, it is easy to check that all the thermodynamic quantities which appear in Eqs. (D5)—(D6) are related to $f(n,T|y)$ by the usual thermodynamic formulas, *whether they are denoted with the superscript S or not.*

For example, the pressure associated with (D9) is

$$p(n,T|y)=-f(n,T|y)+n\left(\frac{\partial f(y)}{\partial n}\right)_T \tag{D11}$$
$$=p^S(n,T)+\tfrac{1}{2}n^2V_y^L, \tag{D12}$$

which is precisely (D7). Similarly, we get from (D12)

$$\left(\frac{\partial p(y)}{\partial T}\right)_n=\left(\frac{\partial p}{\partial T}\right)_n^S, \tag{D13}$$

which gives an example of the redundancy of the superscript S, etc.

We can thus rewrite (D5) as

$$L(y)=\left[\left(\frac{\partial p(y)}{\partial T}\right)_n\right]^2\left[n\left(\frac{\partial^2 p(y)}{\partial n^2}\right)_T-n\left(\frac{\partial p(y)}{\partial e}\right)_n\left(\frac{\partial^2 e(y)}{\partial n^2}\right)_T\right]$$
$$-2\left(\frac{\partial p(y)}{\partial T}\right)_n\frac{1}{\chi_T(y)}\left[\left(\frac{\partial^2 p(y)}{\partial n\partial T}\right)-\left(\frac{\partial p(y)}{\partial e}\right)_n\left(\frac{\partial^2 e(y)}{\partial n\partial T}\right)\right]$$
$$+\frac{1}{n[\chi_T(y)]^2}\left[\left(\frac{\partial^2 p(y)}{\partial T^2}\right)_n-\left(\frac{\partial p(y)}{\partial e}\right)_n\left(\frac{\partial^2 e(y)}{\partial T^2}\right)_n\right] \tag{D14}$$

and a similar formula for $K(y)$; here $p(n,T|y)$, $p(n,e|y)$, $e(n,T|y)$, etc. are thus all defined by the standard thermodynamic relations from the free energy $f(n,T|y)$.

Having established (D14), where y appears as a parameter, we can now transform this equation by standard manipulations, involving a judicious use of the classical relations of thermodynamics.[17] We then obtain Eq. (III.24) of the text, after considerable but elementary algebra, which will not be reproduced here.

APPENDIX E: THE REDUCTION FORMULA (II.15) IN THE DILUTE GAS CASE

Let us first recall that the linearized Boltzmann operator can be written

$$C^{lB}(v_1|f_1(v_1))=\int dv_2[C^B(v_1,v_2|f_1(v_1)\varphi^{eq}(v_2)) + C^B(v_1,v_2|\varphi^{eq}(v_1)f_1(v_2))], \quad \text{(E1)}$$

where the two-body operator $C^B(v_1, v_2|\ \ )$ is defined by

$$C^B(v_1,v_2|f_1(v_1)f_1'(v_2))=n\int d\Omega\sigma(\Omega|v_{12})|v_{12}| \times[f_1(v_1')f_1'(v_2')-f_1(v_1)f_1'(v_2)], \quad \text{(E2)}$$

for two arbitrary functions f_1 and f_1'. Here $\sigma(\Omega|v_{12})$ is the scattering cross section for angular deflection Ω and relative velocity $v_{12}=v_1-v_2$. Moreover, v_1' and v_2' denote the velocities of particle 1 and 2 after the collision process.

It is readily verified that, in the dilute gas limit, the operator $\Psi_{\{0\};\{0\}}(v_1,v_2;i\epsilon)$ precisely reduces to $C^B(v_1,v_2|\cdots)$ while $\Psi_0^{l,S}(v_1)$ becomes $C^{lB}(v_1|\cdots)$.[7] Let us prove explicitly Eq. (II.16) in this case.

As a consequence of particle, momentum, and energy conservation, we have obviously

$$C^B(v_1,v_2|(i_\alpha(v_1)+i_\alpha(v_2))f_1(v_1)f_1'(v_2)) =(i_\alpha(v_1)+i_\alpha(v_2))C^B(v_1,v_2|f_1(v_1)f_1'(v_2)), \quad \text{(E3)}$$

where $i_\alpha(v)$ is any of the five quantities

$$i_\alpha(v)\in 1, \mathbf{v}, v^2/2. \quad \text{(E4)}$$

We consider then [see (II.15)] the quantity defined by

$$J=\int dv_2 C^B(v_1,v_2|(i_\alpha(v_1)i_\beta(v_2)+i_\alpha(v_2)i_\beta(v_1))\varphi^{eq}(v_1)\varphi^{eq}(v_2)) \quad \text{(E5)}$$

and we transform it by adding and substracting the same term

$$J=\int dv_2 C^B(v_1,v_2|(i_\alpha(v_1)+i_\alpha(v_2))(i_\beta(v_1)+i_\beta(v_2))\varphi^{eq}(v_1)\varphi^{eq}(v_2)) - \int dv_2 C^B(v_1,v_2|(i_\alpha(v_1)i_\beta(v_1)+i_\alpha(v_2)i_\beta(v_2))\varphi^{eq}(v_1)\varphi^{eq}(v_2)). \quad \text{(E6)}$$

Using (E3) twice, together with the obvious property

$$C^B(v_1,v_2|\varphi^{eq}(v_1)\varphi^{eq}(v_2))=0, \quad \text{(E7)}$$

we see that the first term on the right-hand side of (E6) vanishes. From (E1), we get then

$$J=C^{lB}(v_1|i_\alpha(v_1)i_\beta(v_1)\varphi^{eq}(v_1)). \quad \text{(E8)}$$

Using the linear relationshio (II. 14) between the I_α^{1k} and the i_α, one readily verifies that (E8) is equivalent to (II. 16) in the dilute gas limit.

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Polynomial algebras. II. Commutation relations

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The present work completes the algorithm which Bhabha had prescribed so as to set up the commutation relations of spin algebras but could implement it only for spin one algebra using a third order permutation identity. Generally this work is concerned with the setting up of the commutation relations of derived polynomial algebras which are obtained by addition operation from a basic polynomial algebra. To obtain these commutation relations, a set of identities called Josthna identities are introduced among the permutations of a finite set of elements. With the help of these identities it is established that commutation relations for derived algebras can be set up directly. Applications to spin and parafield algebras are considered to obtain their commutation relations which make their deduction trivial.

1. INTRODUCTION

In a previous contribution[1] bearing the same title, hereafter referred to as I, a class of associative algebras called polynomial algebras $A[\alpha^1, \alpha^2, \ldots, \alpha^m]$ with $\{\alpha^i \mid i=1,2,\ldots m\}$ as generating elements, have been introduced and important properties studied. The bearing of the subject on theoretical physics was indicated by showing that through them a unified mathematical treatment of the class of algebras such as Clifford and Grassman algebras (ordinary and generalized) and spin and parafield algebras can be given. The possibility of this unified treatment strengthened our belief in the existance of a general procedure of obtaining the commutation relations of the derived algebras which are obtained by the addition process from a basic polynomial algebra.

In fact there exist a class of identities called here Josthna[2] identities, among the permutations on a finite set of elements, making use of commutator and anticommutator operations on permutations. We establish that these identities give us all the information required to set up the commutation relations of the derived polynomial algebras. In fact by making use of them one can trivially set up, for example, the commutation relations of spin and parafield algebras of arbitrary order and their generalizations.

In the second, third, and fourth sections, we introduce Josthna identities by setting them up through an inductive procedure. In the fifth section we establish the relevance of them in obtaining the commutation relations of polynomial algebras and in particular the nth order derived polynomial algebras obtained by an additive procedure from a basic polynomial algebra. We conclude this section and the paper by setting up the commutation relations of spin and parafield algebras.

2. NOTATION AND ELEMENTARY LEMMAS

As indicated in I the polynomial algebras are a particular case of simplicial algebras which are defined in terms of $\bar{\delta}$ and σ, the face (restriction) and degeneracy (substitution) operations. But, as is trivially seen, these operations coincide when applied to elements of sets. Hence, in what follows we shall be interested in face operations on sets of finite number of integers and in particular the set N of first n natural number and the permutations defined in these sets.

Generally, let $\bar{\delta}_{ij\cdots}N = N_{ij\cdots} = \{1,2,\ldots,\hat{i},\ldots,\hat{j},\ldots\}$ be the derived set obtained from N by deleting the elements $i, j, \cdots$. Note that $N_{12\cdots n} = \emptyset$, the null set. We also write $N_{ij\cdots}$ as $N^{12\cdots\hat{i}\cdots\hat{j}\cdots n}$ whenever it is convenient.

Let

$$p = \begin{pmatrix} 1\,2\cdots n \\ i_1, i_2, \ldots, i_n \end{pmatrix}$$

be a permutation on N. In what follows we fix the natural order $1\cdots n$ and write the permutation as $p=(i_1, i_2, \ldots, i_n)$ or simply as $i_1 i_2 \cdots i_n$. Further a permutation on $N_{ij\cdots}$ is written as $p_{ij\cdots}$. In particular, $\{p\}$, $\{p_i\}$, $\{p_{ij}\}$, $\cdots$ stand for the set of all permutations on N, N_i, N_{ij}, etc., respectively.

Now, let m and n be two positive integers such that $n \geq m$. Let $P=(i_1, \ldots, i_m)$ be a permutation on $(1, 2, \ldots, m)$ and $Q=(i_{m+1}, \ldots, i_n)$, a permutation on $(m+1, m+2, \ldots, n)$. Then by PQ and QP we mean the permutations $i_1 i_2 \cdots i_n$ and $i_{m+1} \cdots i_n i_1 \cdots i_n$ of N respectively. In general, if N is partitioned, then the products of permutations on these partitions of N have meaning as permutations on N.

Now, consider a sum $\sum$ of permutations from $\{P\}$ over N with natural integral coefficients $\mathcal{N}$. In fact all such sums define a group module of the nth order symmetric group over $\mathcal{N}$. Similar sums on $\{P_{ij\cdots}\}$ are written as $\sum_{ij\cdots}$. In particular let S stand for the symmetric sum of all the $n!$ permutations of N with unit coefficients. Extending this notation, we write $S_{ij\cdots}$ for a similar sum of all the (Card $N_{ij\cdots}$)! permutations on $N_{ij\cdots}$. Hence,

$$S = \sum_{\{p\}} 12\cdots n$$

and

$$S_{ij\cdots} = \sum_{\{p_{ij\cdots}\}} 12\cdots\hat{i}\cdots\hat{j}\cdots n.$$

In quantum mechanics the commutator and anticommutator operations on observables are of central importance. Now, let us define the following operations on permutations in analogy with these commutator and anticommutator operations:

$$[i, \textstyle\sum_i] = i\sum_i - \sum_i \qquad (2.1)$$

and

$$\{i, \textstyle\sum_i\} = i\sum_i + \sum_i\,, \qquad (2.2)$$

where $\sum_i$ is a sum of permutations over N_i.

From the definitions we have the following useful, though trivial, lemmas.

Lemma 1:

$$\sum_{\{P_{i_1}\}} \sum_{\{P_{i_1 i_2 \cdots i_{r+1}}\}} = (n-r)! \sum_{\{P_{i_1}\}} \tag{2.3}$$

Proof: This follows directly from the definitions of $\{P_{i_1 i_2 \cdots}\}$ by a simple enumeration.

Lemma 2:

$$2S = \sum_{i=1,2,\ldots,n} \{i, S_i\} \tag{2.4}$$

Proof: Obviously, $S = \sum iS_i = \sum S_i i$. Hence, the result by using (2). Hence,

$$2S = \{i, S_i\} + \sum_{j \in N_i} \{j, S_j\} \tag{2.5}$$

Lemma 3:

$$\sum_{\{P_i\}} \{j, S_j\} = (n-2)!\,(2S - \{i, S_i\}) \tag{2.6}$$

Proof: Obviously,

$$\sum_{\{P_i\}} \{j, S_j\} = (n-2)! \sum_{j \in N_i} \{j, S_j\},$$

which follows by a simple direct enumeration. Hence, (6) is obtained from (5).

Now let $K_n^i(n-2)$ be the set of all permutations of N which do not contain i either in first or the last place. We shall introduce in the fourth section $K_n^i(m)$ for n and m which are either both even or both odd. Now in terms of this notation we have

Lemma 4:

$$S = \{i, S_i\} + K_n^i(n-2) \tag{2.7}$$

Proof: Obviously, $K_n^i(n-2)$ is the sum of all the $(n-2)(n-1)!$ permutations of N which do not contain i either in the first or the last place. And $\{i, S_i\}$ contains from (2) all these permutations of N which contain i in the first or the last place. Hence, the result.

Now, let us introduce inductively on the order of permutations certain sums of permutations of the same order which play a central role in setting up the commutation relations of the derived algebras. For that let

$$C(i_1 i_2 i_3) = i_1 i_2 i_3 + i_3 i_2 i_1 \tag{2.8}$$

and inductively

$$C(i_1 i_2 \cdots i_n) = \{i_1,\ C(i_2 i_3 \cdots i_n)\} \tag{2.9}$$

A few typical C sums of permutations are $n(3, 6)$, dropping i,

$$\begin{aligned}
C(123) &= 123 + 321,\\
C(1234) &= 1234 + 1432 + 4321 + 2341,\\
C(12345) &= 12345 + 12543 + 15432 + 13452\\
&\quad + 54321 + 34521 + 23451 + 25431,\\
C(123456) &= 123456 + 123654 + 126543 + 124563\\
&\quad + 165432 + 145632 + 134562 + 136542\\
&\quad + 654321 + 456321 + 345621 + 365431\\
&\quad + 234561 + 236541 + 265431 + 245631.
\end{aligned} \tag{2.10}$$

Lemma 5: $C(i_1 \cdots i_n)$ has minimal symmetry.

Proof: With respect to i_{n-2}, i_n, the $C(i_1 \cdots i_n)$ remain invariant when the two elements are interchanged. Further, $C(i_1 \cdots i_n)$ contains 2^{n-2} permutations and the element i_{n-1} never occurs at the end of the permutations in $C(i_1 \cdots i_n)$. In fact we can enumerate very easily all the permutations in $C(i_1 \cdots i_n)$ which contain i_{n-1} in the pth place. Hence, we have the following:

Lemma 6: There occur $2_{n-3}C_{p-2}$ permutations in $C(i_1 \cdots i_n)$ which contain i_{n-1} in the pth place. (Note that ${}_nC_r = 0$ either if $r = 0$ or $n = 0$).

Proof: Note that the lemma is true when $n = 3$. Further from (9) we note that permutations in $C(i_1 \cdots i_n)$ with i_{n-1} in the pth position come from permutations in $C(i_2 i_3 \cdots i_n)$ which contain i_{n-1} in $(p^0 - 1)$th and pth positions only. Hence, assuming the result to be true for $(n-1)$th order C permutation sums and making use of the additive property of binomial coefficients, i.e., the structure of the Pascal triangle the result follows.

Now consider the number of permutations in C of order 3, 4, 5, and 6 in which 2, 3, 4, and 5 occur in different places. By the Lemma 6 we see that they can be arranged in the form of the Pascal triangle

$$\begin{matrix}
2\\
2\ 2\\
2\ 4\ 2\\
2\ 6\ 6\ 2\\
2\ 8\ 12\ 8\ 2\\
\cdot\ \cdot\ \cdot\ \cdot\ \cdot
\end{matrix} \tag{2.11}$$

which is nothing but the ordinary Pascal triangle in which each element is multiplyed by 2. Finally, we have

Lemma 7:

(i) $\sum_{\{p_{i_2}\}} C(i_1 i_2 i_3) = 2K_3^{i_2}(1)$

(ii) $\sum_{\{p_{i_3}\}} C(i_1 i_2 i_3 i_4) = 2K_4^{i_3}(2)$

Proof: This follows directly by the definition of C of order 3 and 4 and $K_3(1)$ and $K_4(2)$ and making use of the minimal symmetry of the C symbols.

3. JOSTHNA IDENTITIES OF SMALL ORDERS

To set up the identities, let us introduce a Lie type of permutation sums by making use of (2.2), namely

$$[i_1 i_2] = i_1 i_2 - i_2 i_1 \tag{3.1}$$

and inductively

$$[i_1 i_2 \cdots i_n] = [i_1 [i_2, \cdots, i_n]]. \tag{3.2}$$

Josthna identity of third order: From the definitions (2.8) and (3.2) it follows that

$$[jik] = C(jik) - C(ikj). \tag{3.3}$$

Considering the sum over $\{p_i\}$, we have

$$\begin{aligned}
\sum_{\{p_i\}} [jik] &= \sum_{\{p_i\}} C(jik) - C(ikj)\\
&= 2\,C(jik) - C(ikj) - C(kji),
\end{aligned}$$

by making use of the minimal symmetry property of

$C(jik)$. Hence, we have

$$3\,C(jik)=\sum_{\{p_i\}}[jik]+S, \tag{3.4}$$

where S is the sum of all permutations of $\{1,2,3\}$. (3.4) is the required identity.

In general we shall find an identity expressing some integral multiple of $C(i_1 i_2 \cdots i_n)$ in terms of

$$\sum_{\{p_{i_{n-1}}\}} i_1,\ldots,[i_{n-2}\, i_{n-1}\, i_n]$$

and

$$\sum_{\{p_{i_{n-1}}\}} i_1,\ldots,i_{(m-n)/2}\, C(j_1\cdots j_m)\, i'_1,\ldots,1'_{(m-n)/2}$$

and an integral multiple of S. This identity is called the Josthna identity of nth order. It is not obvious that such identities exist. However, we shall establish by the inductive procedure that not only Josthna identities exist but shall give also a procedure to set them up quickly.

To carry out the inductive procedure and to motivate the theory developed in the next section, we shall, in this section, set up Josthna identities of fourth and fifth orders which are quite typical, as a consequence of simple lemmas developed in the previous section.

Josthna identity of fourth order: Consider

$$3\{j, C(kil)\}=\sum_{\{p_{ij}\}}\{j,[kil]\}+\{j,S_j\}, \tag{3.5}$$

which follows from the third order identity by a trivial rearrangement of symbols. Now, sum over $\{p_i\}$ the above expression in analogy with what is done in the third order case. Hence,

$$3\sum_{\{p_i\}}\{j, C(kil)\}=\sum_{\{p_i\}}\sum_{\{p_{ij}\}}\{j,[kil]\}+\sum\{j,S_j\}. \tag{3.6}$$

Simplifying by using Lemmas 1 and 7, we get

$$6\,K_4^i(2)=2\sum_{\{p_i\}}\{j,[kil]\}+\sum_{\{p_i\}}\{j,S_j\}.$$

Now, using Lemmas 3 and 4, we have

$$3(S-\{i,S_i\})=\sum_{\{p_i\}}\{j,[kli]\}+2S-\{i,S_i\},$$

i.e.,

$$2\{i,S_i\}=\sum_{\{p_i\}}\{j,[kli]\}+S.$$

Using the third order Josthna identity in the form

$$S_i=3\,C(jkl)-\sum_{\{p_k\}}[jkl],$$

we obtain,

$$6\{i, C(jkl)\}=2\sum_{\{p_{ik}\}}\{i[jkl]\}+\sum_{\{p_i\}}\{j,[kli]\}+S,$$

or

$$6\,C(ijkl)=2\sum_{\{p_{ik}\}}\{i,[jkl]\}+\sum_{\{p_i\}}\{j,[kli]\}+S, \tag{3.7}$$

which is the fourth order identity.

It is interesting to note that all the known commutation relations of spin and parafield algebras of orders $\frac{1}{2}$, 1, $\frac{3}{2}$, and 2, 3, 4 respectively can be set up trivially with the help of the two identities (3.4) and (3.7).

Josthna identity of fifth order: Apart from the third and fourth order identities which are required for starting an inductive procedure, we want to set up the next identity also as it is typical and suggests a general method to obtain Josthna identities of all orders. To observe the new features that arise, we first refer to the Pascal triangle (2.11). It is obvious from it that the number of permutations in $C(12345)$ with 4 in different places are not the same. Hence, when we sum over different permutations as in (3.3) and (3.6), we get an unbalanced sum of permutations which can be put in the form (3.4) and (3.7) if only we make use of the third order identity. To establish this, consider

$$6\{j, C(klim)\}=\sum_{\{p_{ijk}\}}\{j\{k[lim]\}\}-\sum_{p_{jk}}\{j\{i[lkm]\}\}+\{j,S_j\}$$

which is obtained by finding the anticommutator of (3.7) by j after suitably relabelling the permutations. Further, note the preferred position for i when used in the above expression. Summing over $\{pi\}$, we have

$$6\sum_{\{p_i\}}\{j,C(klim)\}=\sum_{\{p_i\}}\{j,\ \Delta_4\}+\sum\{j,S_j\}, \tag{3.8}$$

where Δ_4 stands for all the mixed permutations in (3.7).

Now, we divide the permutations in $\{j, C(klim)\}$ into two classes $02220+00200$ where $0\alpha\beta\gamma0$ stands for a number of α, β, and γ permutations with i being in the second, third, and fourth, places respectively, such that each class has the minimal symmetry with respect to l and m. Considering now the pair $lC(jik)m$ of permutations that belong to 00200, their sum over $\{p_i\}$ gives

$$3\sum_{\{p_i\}} lC(jik)m=\sum_{\{p_i\}}\sum_{\{p_i lm\}} l[jik]m+\sum_{\{p_i\}} l\,S_{lm}\,m \tag{3.9}$$

by the third order identity. Carrying out the summation, using Lemma 1 and the minimal symmetry of C's, we have

$$3K_5^i(1)=\sum_{\{p_i\}} l\,[jik]\,m+K_5^i(3), \tag{3.10}$$

where $K_5^i(1)$ is the sum of all the fifth order permutations p with i in the middle position.

We also have, from the division $2(01210)=2(01110)+2(00100)$ of the third row in the Pascal triangle (2.11)

$$\sum_{\{p_i\}}\{j,C(klim)\}=2K_5^i(3)+2K_5^i(1). \tag{3.11}$$

Now, using (3.10) and (3.11), we obtain

$$3\sum_{\{p_i\}}\{j, C(klim)\}=8K_5^i(3)+2\sum_{\{p_i\}} l[jik]m. \tag{3.12}$$

Finally, eliminating $\sum_{\{p_i\}}\{j, C(klim)\}$ from (3.8) and (3.12), we have

$$16K_5^i(3)=\sum_{\{p_{i_1}\}}\{j,\Delta_4\}-4\sum_{\{p_i\}} l[jik]m+\sum_{\{p_{i_1}\}}\{j,S_j\} \tag{3.13}$$

or

$$8(S-\{i, S\hat{i}\})=-\tfrac{1}{2}\tilde{\Delta}_5+3(2S-\{i,S_i\})$$

by using Lemmas 3 and 4 and $\tilde{\Delta}_5$ for the mixed terms in (3.13). Note that by Lemma 1, each permutation in $\tilde{\Delta}_5$ is duplicated. Hence,

$$5\{i,S_i\}=\tfrac{1}{2}\tilde{\Delta}_5+2S. \tag{3.14}$$

Now, using the fourth order permutation identity in the form

$$6\,C(i_2 i_3 \cdots i_5) = \Delta_4^{i_2 i_3 i_4 i_5} + S_{i_1}$$

and substituting in (3.14), we get

$$30\,C(i_1 i_2 i_3 i_4 i_5) = -\tfrac{1}{2} \sum_{\{p_{i_1}\}} \{j, \Delta_4\} + 2 \sum_{\{p_{i_1}\}} l\,[jik]\,m - \{i_1,\ \Delta_4^{i_2 i_3 i_4 i_5}\} + 2S, \tag{3.15}$$

which is the fifth order Josthna identity.

4. JOSTHNA IDENTITIES OF ARBITRARY ORDER

A few more lemmas: First we generalize $K_3^i(n-2)$, $K_n^i(2)$ and $K_5^i(3)$, $K_5^i(1)$ by considering $K_n^i(n-2)$, $K_n^i(n-4)$, $\cdots$, etc. Note that $K_n^i(m)$ are such that either both n and m are even or both odd and $n > m$. Hence, $n-m$ is always even. Now let $K_n^i(m)$ stand for the sum of all those permutations which have i in the $[\frac{1}{2}(n-m)+1,\ \frac{1}{2}(n-m)+2,\ \cdots\ \frac{1}{2}(n+m)]$th places. When i is in these positions, it is said to be symmetrically situated. Note that $K_n^i(m)$ is not defined otherwise.

The simplest way to set up $K_n^i(m)$ is by considering the sum of all permutations of order m over a subset of integers from $\{12 \cdots n\}$ containing i and then pre- and postmultiplying them by $\frac{1}{2}(n-m)$ remaining integers in all possible ways. Hence, designating by $S^i(m)$ the sum of all permutations of m elements from N which contain i, we have the following:

Lemma 8:

$$(m-1)\,!\,K_n^i(m) = \sum_{\{p_i\}} i_1 i_2 \cdots i_{(n-m)/2}\, S^i(m)\, i_1' i_2' \cdots i'_{(n-m)/2}, \tag{4.1}$$

where i's and i''s are the distinct elements from N.

Proof: Obviously, all permutations on the right side are contained in the expression on the left and vice versa. Further, the order of $K_n^i(m)$ is $(n-1)!\,m$ and of the permutations on the right, $(n-1)!(m-1)!m$. Hence the result.

In Lemma 7, we established the relations between suitable sum's of C and K symbols which are of basic importance in setting up Josthna identities of orders 3, 4, and 5. We obtain generalizations of them that are used to set up all Josthna identities. To consider them, we introduce first of all what we call odd and even Pascal triangles. Let them be given by the figure shown below.

```
        1                        1  1
      1 2 1                    1  3  3  1
    1 4 6 4 1                1  5  10 10  5  1
 1 6 15 20 15 6 1         1 7 21 35 35 21 7 1
        ...                        ...
 Odd Pascal triangle      Even Pascal triangle
```

Now, consider characteristic vectors A_n^α, $\alpha = n$, $n-2$, $n-4$, $\cdots$, of order n with units in the place of entries in Pascal triangle as shown in the following figure for $n=7$ and 8 respectively, and zeros elsewhere, i.e., the units lie in the symmetrical places.

```
 0 0 0 x 0 0 0       0 0 0 x x 0 0 0
 0 0 x x x 0 0       0 0 x x x x 0 0
 0 x x x x x 0       0 x x x x x x 0
 x x x x x x x       x x x x x x x x
     n = 7               n = 8
```

Note that n and α are either even or odd together. Similarly, we write B_n^α for the vectors of order n with binomial coefficients as entries from a Pascal triangle which is either even or odd. In what follows, when convenient we shall drop the n's and assume that the Pascal triangle is bounded by an infinite sea of zeros. Now we have the important expansion of B_n^α in the basis of A_n given by

Lemma 9:

$$B^m = \sum A^m + ({}_mC_1 - {}_mC_0)A^{m-2} + ({}_mC_2 - {}_mC_1)A^{m-4} + \cdots + ({}_mC_{[(m-1)/2]} - {}_mC_{[(m-1)/2]-1})\ A^{m-2[(m-1)/2]}, \tag{4.2}$$

where ${}_mC_r$'s are the usual binomial coefficients and $[x]$ stands for the largest integral part of x.

Proof: Follows by a simple induction on binomial vectors B.

Note that $n-2\,[(n-1)/2]$ is 1 or 2 according as n is odd or even. We note a few consequences of Lemma 9.

Examples:

(01210) $=(01110)+(00100)$,

(14641) $=(11111)+3(01110)+2(00100)$,

$\cdots$ $\cdots$

(013310) $=(011110)+2(001100)$,

(15101051) $=(111111)+4(011110)+5(001100)$,

$\cdots$ $\cdots$

We further also have

Lemma 10:

$$(m-2) + ({}_{m-3}C_1 - {}_{m-3}C_0)(m-4) + ({}_{m-3}C_2 - {}_{m-3}C_1)(m-6) + \cdots + ({}_{m-3}C_{(m-1)/2} - {}_{m-3}C_{[(m-1)/2]-1})(m-2\,[(m-1)/2]) = 2^{m-3}. \tag{4.3}$$

Proof: This follows by rearranging the terms as

$$2({}_{m-3}C_0 + {}_{m-3}C_1 + \cdots + {}_{m-3}C_{[(m-1)/2]-1} + {}_{m-3}C_{[(m-1)/2]} \times (m-2\,[(m-2)/2]), \tag{4.4}$$

the last term being multiplied by 1 or 2 according as n is odd or even. Now making use of the symmetry ${}_mC_r = {}_mC_{m-r}$ of the binomial coefficients, and

$$\sum_{r=0}^{m-3} {}_{m-3}C_r = 2^{n-3},$$

the result follows.

Now, to generalize Lemma 7, let $C_\alpha^i(i_1 i_2 \cdots i_{m-1} i_m)$ stand for a set of $2({}_{m-3}C_\alpha - {}_{m-3}C_{\alpha-1})$ permutations of $C(i_1 i_2 \cdots i_m)$ which have the minimal symmetry with respect to i_{m-2} and i_m and are such that $i_{m-1} = i$ (say) is in the $[(m-\alpha)/2+1,\ (m-\alpha)/2+2,\ \ldots,\ (m+\alpha)/2]$th place when m and α are both odd or both even. Hence, by construction, we have

Lemma 11:

$$C(i_1 i_2 \cdots i_m) = \sum_{1 \text{ or } 2}^{m-2}{}' \quad C^i_\alpha(i_1 i_2 \cdots i_m), \tag{4.5}$$

where $\sum$ indicates that α should be increased or decreased by 2 in writing the terms of the summation.

Further, consider $i_1 i_2 \cdots i_{m-1} i_m$ as a subset of N containing $i = i_{n-1}$ in the $(m-1)$th place, i.e., $i_{m-1} = i_{n-1} = i$ (say) and pre- and postmultiplying (4.5) by $(n-m)/2$ of the remaining indices from N and taking the sum over $\{p_i\}$ of the identity (4.5), we have

Lemma 12:

$$\sum_{\{p_i\}} i'_2 \cdots i'_{(m-n)/2}\, C^i(i_1 i_2 \cdots i_{m-2}\, i\, i_m)\, i''_1\, i''_2 \cdots i''_{(m-n)/2} = 2 \sum_{1 \text{ or } 2}^{m-2} {}_{m-3}D_\alpha \;\; K^i_n(\alpha), \tag{4.6}$$

where

$$ {}_{m-3}D_\alpha = {}_{m-3}C_\alpha - {}_{m-3}C_{\alpha-1}. \tag{4.7}$$

Proof: The left side Lemma 11 is given to be

$$\sum_{2 \text{ or } 1}^{m-2} \sum_{\{p_i\}} i'_1\, i'_2 \cdots i'_{(m-n)/2} \;\; C^i_\alpha(i_1 i_2 \cdots i_m)\, i_1{}''\, i''_2 \;\cdots i''_{(m-n)/2}. \tag{4.8}$$

As C's have minimal symmetry, each term in the above summation is duplicated, and further as there is permutation over all symbols expecting i, there exists by Lemma 9 a further multiplicity of the permutations given by ${}_{n-3}C_\alpha - {}_{n-3}C_{\alpha-1}$ as C^i_α contains permutations with i lying in α central places. Hence, the contribution for (4.8) is $2\,{}_{n-3}D_\alpha\, K^i_n(\alpha)$, establishing the lemma. Further we have, similar to the above result,

Lemma 13:

$$\sum_{\{p_i\}} \{i_2, C(i_3 i_4 \cdots i\, i_{m+1})\} = 2 \sum_{\alpha=0}^{(n-1)/2} {}_{n-2}D_\alpha \;\; K(n - 2\alpha - 1). \tag{4.9}$$

Proof: This follows on the same lines as the previous lemma. However, note that the order of permutations on the left-hand side is $n+1$.

Induction hypothesis: We assume from the structure of Jasthna identities of order 3, 4 and 5, that it is possible to write the first $n-2$ identities as

$$a_n C(i_1 i_2 \cdots i_n) = \Delta_n + b_n S \tag{4.10}$$

where Δ_n are the terms which are contributed from commutation and anti-commutation operations of the form $\{j_1 j_2 \cdots [j_{n-2} j_{n-1} j_n]\}$ and $\{j_1 \cdots [ijk]\, j_p \cdots\}$; S is the sum of all $n!$ permutations on N; the constants a_n and b_n are functions of n only and $a_3 = 1$ and $a_4 = 6$ and $b_4 = 1$. Immediately we have the central

Lemma 14:

$$a_n\, 2^{n-2} = b_n n! \tag{4.11}$$

Proof: To prove this, we introduce an arithmetic function M on the set $\{\Sigma\}$ of the sums of permutations of N with integral coefficients. Let $\Sigma = \sum a_i(i_1 i_2 \cdots i_n)$, where $\mathbf{i} = i_1 i_2 \cdots i_n$ and $\Sigma = \Sigma'$ if $a_1 = a'_1$ for all the $n!$ permutations $\mathbf{i}$. Now, let

$$M(\Sigma) = \sum a_1.$$

It follows directly that

$$M(\Sigma_{\mu 1} + \Sigma_{\mu 2}) = M(\Sigma_{\mu 1}) + M(\Sigma_{\mu 2}).$$

Further, $M(\Delta_n) = 0$ as each term of Δ_n contains a triple commutator of the form $[ijk]$ according to the induction hypothesis. Now, to establish the lemma, evaluate the arithmetic function M on both sides of (4.11) and use the fact $M\,(C(i_1 i_2 \cdots i_n)) = 2^{n-2}$ and $M(S) = n!$

Another simple induction hypothesis and its proof: Consider integers m and n such that $n-m$ is an even positive integer. Let then

$$a_m C(i_1 i_2 \cdots i_m) = \Delta_m + b_m S^{i_1 i_2 \cdots i_m}. \tag{4.10$'$}$$

As C and S have minimal symmetry, Δ_m has also the same symmetry. Now pre- and postmultiply (4.10′) by $(n-m)/2$ elements from $N \cap \{i_1 \cdots i_m\}$, and summing over $\{p_i\}$ where $i = i_{m-1}$, we obtain

$$2\, a_m[K^i_n(m-2) + {}_{m-3}D_1 K^i_n(m-4) + \cdots + {}_{m-3}D_{[(m-1)/2]} K^i_n(m - 2\,[(m-1)/2])] = \sum_{\{p_i\}} i'_1 \cdots i'_{(n-m)/2}\;\; \Delta_m^{i_1 \cdots i_m}\; i''_1 \cdots i''_{(n-m)/2} + b_m \sum_{p_i} i'_1 \cdots \times S^{i_1 \cdots i_m} \cdots i''_{(n-m)/2}.$$

Using Lemmas 8 and 12, we obtain

$$a_m\,[K^i_n(m-2) + \cdots + {}_{m-3}D_{[(m-1)/2]-1}\;\; K^i_n(1 \text{ or } 2)] = \tfrac{1}{2}\Delta^i_n(m) + b_m\, \tfrac{1}{2}(m-1)!\;\; K^i_n(m). \tag{4.12}$$

Because of the minimal symmetry $\Delta^i_n(m)$ contains pairs of identical permutations. Hence, multiplication by a factor $\frac{1}{2}$ is meaningful.

The first few examples of (4.12) are

$$3K^i_n(1) = \tfrac{1}{2}\Delta^i_n(3) + K^i_n(3),$$
$$3.4\, K^i_n(2) = \tfrac{1}{2}\Delta^i_n(4) + 3.2K^i_n(4), \tag{4.13}$$

which follow from third and fourth order Josthna identities respectively.

Theorem 1:

$$A_{n-2}(n-2)K^i_n(n-2\alpha) = \Delta_{n-2\alpha,n-2} + A_{n-2}(n-2\alpha)K^i_n(n-2) \tag{4.14}$$

for $\alpha = 2, 3, \ldots, [(n-1)/2]$ with the constant A_{n-2} which is independent of α; and $\Delta_{n-2\alpha,n-2}$ is a sum of mixed permutations consisting of commutator and anticommutator operators on permutations.

Proof: By induction. First by using the arithmetic function M we obtain

$$(n-1)M(K^i_n(n-2\alpha+1)) = (n-2\alpha+1)M(K^i_n(n-1)).$$

As $M(K^i_n(m)) = (n-1)!\; m$ the above equation is consistant. Now obviously the theorem is true for $n = 3$ or 4 from the examples (4.13). On the basis of induction hypothesis we assume that the theorem is true for $(n-4)$ such that we have

$$A_{n-4}(n-4)K^i_n(n-2\alpha) = \Delta_{n-2\alpha,n-4} + (n-2\alpha)A_{n-4}K^i_n(n-4) \tag{4.15}$$

where $\alpha = 2, 3, 4, \ldots, [(n-1)/2]$ and A_{n-4} is independent of α and $n \geq 5$. Note that $\Delta_{n-4,n-4}=0$. From $m=n-2$, we have from (4.12) that

$$a_{n-2}[K_n^i(n-4)+{}_{n-5}D_1K_n^i(n-6)+\cdots+{}_{n-5}D_{[(n-3)/2]-1}\,K_n^i(n-2-2[(n-3)/2])]=\tfrac{1}{2}\Delta_n^i(n-2)+b_{n-2}\tfrac{1}{2}(n-3)!\,K_n^i(n-2).$$

Substituting for $K_n^i(n-2\alpha)$ from (4.15), we have

$$A_{n-4}a_{n-2}[(n-4)+{}_{n-5}D_1\,(n-6)+\cdots+{}_{n-5}D_{[(n-3)/2]-1}\,K_n^i(n-4)=\tfrac{1}{2}A_{n-4}\Delta_n^i(n-2)+A_{n-4}b_{n-2}\tfrac{1}{2}(n-3)!\,K_n^i(n-2)\times\sum_{\alpha=2}^{[(n-1)/2]-1}{}_{n-5}D_\alpha\,\Delta_{n-2\alpha,n-\alpha}.$$

Using Lemma 10 for $n-4$, we have

$$A_{n-4}\,[a_{n-2}/(n-4)]\,2^{n-5}\,K_n^i(n-4)=\tilde{\Delta}_n(n-2)+b_{n-2}A_{n-4}\times\tfrac{1}{2}(n-3)!\;K_n^i(n-2)$$

with obvious substitutions. Multiplying by $(n-2\alpha)$ and using again (4.15), we have

$$A_{n-4}a_{n-2}\;2^{n-5}\;K_n(n-2\alpha)=(n-2\alpha)\tilde{\Delta}_n(n-2)+[a_{n-2}/(n-4)]\,2^{n-5}\,\Delta_{n-2,n-4}+(n-2\alpha)\,b_{n-2}\;A_{n-4}\;\tfrac{1}{2}(n-3)!\;K_n^i(n-2).$$

This can be written as

$$(n-2)A_{n-2}\;K_n^i(n-2\alpha)=\Delta_{n-2\alpha,n-2}+(n-2\alpha)A'_{n-2}K_n(n-2)$$

for $\alpha=2,3,\ldots,[(n-1)/2]$, where

$$A_{n-2}=a_{n-2}\,[A_{n-4}/(n-2)]\;2^{n-5},$$

$$A'_{n-2}=b_{n-2}\;A_{n-4}\;\tfrac{1}{2}(n-3)!$$

and

$$\Delta_{n-2\alpha,n-2}=(n-2\alpha)\,\tilde{\Delta}_n(n-2)+[a_{n-2}/(n-4)]\,2^{n-5}\,\Delta_{n-2\alpha,n-4}. \tag{4.15'}$$

Now using Lemma 14, we have $A'_{n-2}=A_{n-2}$. By induction hypothesis A_{n-2} is also independent of α, since by assumption a_{n-2} and b_{n-2} are functions of n only. As the hypothesis is true for both $n=3$ and $n=4$ from (4.13), we have established the theorem.

Finally, we prove the main theorem of this paper by induction which establishes Josthna identities of all orders.

Theorem 2: In the above notation by induction it follows that

$$a_{n+1}=(n+1)!(n-2)!\cdots 2!\,1!/2^{n-1}, \tag{4.16}$$

$$b_{n+1}=(n-2)!\cdots 2!\,1!, \tag{4.17}$$

and

$$\Delta_{n+1}=\tfrac{1}{2}\sum_{\{p_i\}}\{i_2,\;\Delta_n^{i_3\cdots i_1 i_{n+1}}\}+(a_{n+1}b_n/a_n)\sum_{\alpha=2}^{[n/2]}\Delta_{n-2\alpha,n-\alpha}+\{i_1,\Delta_n^{i_2i_3\cdots i_{n+1}}\}. \tag{4.18}$$

Proof: Consider the following sum of anticommutators:

$$a_n\sum_{\{p_{i_1}\}}\{i_2,\,C(i_3i_4\cdots i_ni_1i_{n+1})\}=\sum_{\{p_{i_1}\}}\{i_2,\;\Delta_n^{i_3\cdots i_1i_{n+1}}\}+b_n\sum_{\{p_{i_1}\}}\{i_2,S_{i2}\},$$

which is obtained from (4.10) after carrying out suitable changes in the indices and $\{p_{i_1}\}$ is the set of all permutations of $\{1,2,\ldots,\hat{i}_1,\ldots,n+1\}$. Using Lemmas 4 and 11 and the minimal symmetry of C's, we have

$$2a_n\{K_{n+1}\,(n-1)+{}_{n-2}D_1K_{n+1}(n-3)+\cdots+{}_{n-2}D_{[n/2]}K_{n+1}(1\text{ or }2)\}=\sum_{\{p_{i_1}\}}\{i_2,\Delta_n\}+b_n(n-1)!\,(2S-\{i_1,\;Si_1\}).$$

Since Δ_n itself has the minimal symmetry a pair of permutations with identical coefficients are contributed from each term in $\sum_{\{p_{i_1}\}}\{i_2,\;\Delta_n\}$. Hence the above expression can be written as

$$a_n\{K_{n+1}(n-1)+{}_{n-2}D_1\;K_{n+1}(n-3)+\cdots+{}_{n-2}D_{n/2}K_{n+1}(1\text{ or }2)\}=\tfrac{1}{2}\sum_{\{p_{i_1}\}}\{i_2,\Delta_n\}+\tfrac{1}{2}b_n(n-1)!\;(2S-\{i_1,S_{i_1}\}). \tag{4.19}$$

Now, making use of (2.14) after changing $n\to n+1$ which depends only on the first $n-2$ Josthna identities, we obtain

$$[a_n/(n-1)]\;\{(n-1)+{}_{n-2}D_1\,(n-3)+\cdots+{}_{n-2}D_{[n/2]}\;(1\text{ or }2)\}\times K_{n+1}(n-1)=\tilde{\Delta}_{n+1}+\tfrac{1}{2}b_n(n-1)!\,(2S-\{i_1,S_{i_1}\},$$

by using the obvious substitution.

Now, by Lemma 10, we obtain

$$[a_n/(n-1)]\;2^{n-2}K_{n+1}(n-1)=\tilde{\Delta}_{n+1}+\tfrac{1}{2}b_n(n-1)!\,(2S-\{i_1,S\hat{i}_1\})$$

and then by Lemma 4 we have

$$[a_n/(n-1)]\;2^{n-2}(S-\{i_1,S_{i_1}\}),=\tilde{\Delta}_{n+1}+\tfrac{1}{2}b_n(n-1)!(2S-\{i_1,S_{i_1}\})$$

or

$$\{[a_n/(n-1)]2^{n-2}-b_n(n-1)!\}S=\tilde{\Delta}_{n+1}+\{[a_n/(n-1)]\;2^{n-2}-\tfrac{1}{2}b_n(n-1)!\}\;\{i_1,S_{i_1}\}.$$

Now, substituting (4.10), we have finally

$$a_{n+1}\;C(i_1i_2\cdots i_{n+1})=\Delta_{n+1}+b_{n+1}S,$$

where

$$a_{n+1}=\{[a_n/(n-1)]\;2^{n-2}-\tfrac{1}{2}b_n(n-1)!\}\;a_n/b_n, \tag{4.20}$$

$$b_{n+1}=\{[a_n/(n-1)]\;2^{n-2}-b_n(n-1)!\}, \tag{4.21}$$

and

$$\Delta_{n+1}=-\tilde{\Delta}_{n+1}+\{i_1,\;\Delta_n^{i_2\cdots i_{n+1}}\}\;\;a_{n+1}\times b_n/a_n,$$

which is equal to (4.18).

Note that a_{n+1}, b_{n+1} are purely functions of n only by induction hypothesis.

Now, using Lemma 14, we have

$$a_{n+1}=\tfrac{1}{2}(n-2)!\,(n+1)\,a_n\quad\text{and}\quad b_{n+1}=b_n(n-2)!.$$

Making use of the initial condition obtained from third and fourth order Josthna identities, we obtain (4.16) and (4.17) respectively. This establishes Theorem 2 and the fact that Josthna identities of all orders $n\geq 3$ exist. Finally we note that if $C(i_1i_2\cdots i_n)$ and $C(i'_1i'_2\cdots i'_n)$ are the C terms with two distinct permutations of i's and i's of N, then

$$a_nC(i_1i_2\cdots i_n)-\Delta_n(i_1\cdots i_n)=a_nC(i_1^1\cdots i_n^1)-\Delta_n(i_1^1\cdots i_n^1), \tag{4.22}$$

which follows directly from the nth order Josthna identity.

5. COMMUTATION RELATIONS OF POLYNOMIAL ALGEBRAS

Commutation relations of simplicial algebras

Suppose $A[\alpha', \ldots, \alpha^m]$ is an algebra not necessarily associative with a finite basis over an infinite field F. Let

$$L(x) = x_1\alpha^1 + x_2\alpha^2 + \cdots + x_m\alpha^m \tag{5.1}$$

be a general element of A in the linear space L_m over F. $L(x)$ satisfies a minimal equation

$$P[x;L] \equiv L^n + P_1 L^{n-1} + \cdots + P_n = 0, \tag{5.2}$$

which holds for every general element $L(x) \in L_m$. If A is a simplicial algebra, then P_i's are symmetric homogeneous polynomials (SHP's) in x and are given by[1]

$$P_r = \sum_{[a_1 \cdots a_r]} a^r_{[a_1, a_2, \ldots, a_r]} \sum_{i_1 < i_2 < \cdots < i_r} x_{i_1}^{a_1} x_{i_2}^{a_2} \cdots x_{i_r}^{a_r} \tag{5.3}$$

for $r = 1, \ldots, n$, where $i_j \in [1, 2, \ldots, m]$ and $[a_1, a_2, \ldots, a_r]$ is a composition of r, i.e., integers $a_i > 0$ are such that $\sum a_i = r$. In particular, if A is a polynomial algebra, the degree of Eq. (5.2) is independent of the number of the basis elements $[\alpha^i \mid i = 1, \ldots, m]$. Substituting (5.1) in (5.2) and making use of (5.3) to find the coefficient of the general expression $x_1 x_2 \cdots x_n$ where $n \leq m$, we obtain

$$\begin{aligned}
&\sum \alpha_1 \cdots \alpha_n + a_1^1 \sum \alpha_1 \cdots \alpha_{n-1}\delta_n + a^2_{[1^2]} \sum \alpha_1 \cdots \alpha_{n-2}\,\delta_{n-1}\,\delta_n \\
&\quad + a^2_{[2]} \sum \alpha_1 \cdots \alpha_{n-2}\,\delta_{n-1,n} + \cdots + \sum_{[a_1 \cdots a_r]} a^r_{[a_1 \cdots a_r]} \\
&\quad \times \sum \alpha_1 \cdots \alpha_{n-r}\,\delta_{n-r+1, \cdots, n-r} + a_1\,\delta_{n-r+a+1, \ldots, n-r+a_1+a_2} \\
&\quad \times \delta_{n-ar+1, x-ar+2, \ldots, n} = 0,
\end{aligned} \tag{5.4}$$

where

$$\begin{aligned}
\delta_{i_1 i_2 \cdots i_r} &= 1 \quad \text{if } i_1 = i_2 = \cdots = i_r \\
&= 0 \quad \text{otherwise.}
\end{aligned} \tag{5.5}$$

Note that in (5.4) $\sum$ is over all the $n!$ permutations of $\{1, \ldots, n\}$ and δ_i is introduced to keep track of all the symbols permuted. Further note that the general term in (5.4) can also be written as

$$\sum = {}_nC_{[a_1, a_2, \ldots, a_r]} \sum{}', \tag{5.6}$$

where now $\sum'$ is over distinct terms only and ${}_nC_{[a_1 \cdots a_r]}$ is the generalized combination symbol defined by

$${}_nC_{[a_1, a_2, \ldots, a_r]} = n!/a_1!\,a_2! \cdots a_r!\,(n-r)!\,.$$

Now, multiplying (5.4) by b_n and making use of (4.10) which is true for a set of n symbols for which associative law multiplication holds to eliminate $b_n \sum_p \alpha_1 \cdots \alpha_n$, we obtain the general polynomial commutation relation given by

$$\begin{aligned}
&a_n C(\alpha_1 \alpha_2 \cdots \alpha_n) - \Delta_{n+1} + b_n\, {}_nC_{[a_1 \cdots a_r]} \sum_{r=1}^{n} \\
&\quad \times \sum_{[a_1 \cdots a_r]} a^r_{[a_1 \cdots a_r]} \sum_{\{p\}}{}' \alpha_1 \alpha_2 \cdots \alpha_{n-r}\ \Delta_{[a_1 \cdots a_r]} = 0,
\end{aligned} \tag{5.7}$$

where

$$a_1 \cdots a_r = \delta_{n-r+1, \ldots, n-r+a_1} \cdots \delta_{n-a_r+1, n-a_r+2, \ldots, n}. \tag{5.8}$$

In general it so happens that one knows $[\alpha_i \alpha_j \alpha_k]$ in terms of α_i's. Then substituting for Δ_{n+1} in the above expression, we get the required commutation relations.

Commutation relations of spin and parafield algebras

Now let us consider the special case of derived polynomial algebras for which the value of $[\alpha_i\, \alpha_j\, \alpha_k]$ in terms of α_i are known. To consider them, let $A[\alpha]$ be a simplicial algebra (polynomial algebra) and let $\sum_{\oplus}^{s} A[\alpha] \equiv A[\alpha] + \cdots + A[\alpha]$ be the sth derived algebras by the additive process. As noted earlier[1] these are also simplicial algebras for all values of $s \geq 1$. Further, the roots of the minimal polynomial equations of $\sum_{\oplus}^{s} A[\alpha]$ are sums of the roots of the minimal polynomial equations $\sum_{\oplus}^{s-1} A[\alpha]$ and $A[\alpha]$. The commutation relations of these algebras that are independent of s are postulated to be

$$[\alpha^k, I^{ij}] = \delta^{jk}\,\alpha^i - \delta^{ik}\,\alpha^j, \tag{5.9}$$

where $I^{ij} = \alpha^i\,\alpha^j - \alpha^j\,\alpha^i$ for the spin algebra and

$$\begin{aligned}
&[a^k, a^{i^+} a^j - a^j a^{i+}] = \delta^{ki} a^j, \\
&[a^k, a^i a^j - a^j a^i] = 0
\end{aligned} \tag{5.10}$$

for the parafield algebras associated with the ordinary Clifford algebras. Now the minimal polynomial equations satisfied by spin $\sum_{\oplus}^{s} A_c$ and parafield $\sum_{\oplus}^{s} A_{ac}$ algebras are easily obtained as

$$(L^2 - \tfrac{1}{4}s^2 \mathcal{L})\,(L^2 - \tfrac{1}{4}(s-1)^2 \mathcal{L}) \cdots (L - \tfrac{1}{4}\mathcal{L}) = 0 \tag{5.11}$$

if s is half-integral and

$$(L^2 - s^2 \mathcal{L})\,(L^2 - (s-1)^2) \cdots (L^2 - \mathcal{L})\,L = 0 \tag{5.12}$$

if s is integral where

$$L = x_1\alpha_1 + \cdots + x_n\alpha_n \quad \text{and} \quad \mathcal{L} = x_1^2 + \cdots + x_n^2 \tag{5.13}$$

for spin algebras; and

$$L = (Z_i a^i + \overline{Z}_i a^i +) \quad \text{and} \quad \mathcal{L} = (Z_1 \overline{Z}_1 + Z_z \overline{Z}_z + \cdots +) \tag{5.14}$$

for the parafield algebras respectively. By the general methods developed in I, these considerations can be extended to the associative algebras of the generalized Clifford algebras too. Now, in the half-integral spin case expanding (5.11), we obtain

$$\begin{aligned}
&L^{2s} - P_1 L^{2s-2}\,\mathcal{L} + P_2\, L^{2s-4} \mathcal{L}^2 + \cdots + (-1)^r L^{2s-2r} \mathcal{L}^r + \cdots + \\
&(-1) P_s\ \mathcal{L}^s = 0,
\end{aligned} \tag{5.15}$$

where P_r is the sum of the products of the rth roots of (5.11). Now, the polynomial commutation relation reduces to

$$\sum_{r=0}^{s} (-1)^r\, P_r \sum \alpha_1 \cdots \alpha_{n-2r}\ \delta_{n-2r+1, n-2r+2} \cdots \delta_{n-1,n} = 0, \tag{5.16}$$

where $n = 2s$. Now the sum $\sum$ over all the $n!$ permutations of the indices can be written as

$$\sum_{\{p\}} = \frac{n!}{2^p (n-2p)!} \sum{}'$$

where $\sum'$ is over distinct terms of the summation. Now, proceeding in the same way as is done in the case of (5.7), we obtain

$$a_n C(\alpha_1 \cdots \alpha_n) - \Delta_n + b_n \sum_{r=1}^{n} P_r \frac{n!}{2^p (n-2r)!}$$
$$\times \sum{}^1 \alpha_1 \cdots \alpha_{n-2r} \delta^r = 0, \quad (5.17)$$

where

$$\delta^r = \delta_{n-2r+1, n-2r+2} \cdots \delta_{n-1, n}, \quad (5.18)$$

Now, using (5.9) the mixed permutations Δ_n containing the triple commutators $[\alpha_i \alpha_j \alpha_k]$ can be simplified. Similar procedure can be applied in the integral spin case also.

However, in the case of parafield algebras an interesting complication arises as the index set over which the algebras are set up are given by $I \otimes I$. For example, when we consider parafield algebras of order $2s+1$, when s is half-integral, we have to take in Eq. (5.15) L and $\underline{L}$ given by Eq. (5.14). Now, enumerating the integers in $I \otimes I$ by unbarred and barred integers in each I and introducing $\bar{\delta}$ symbols which are given by

$$\bar{\delta}_{p,q} = 1 \text{ if } q = \bar{p}$$
$$= 0 \text{ otherwise}, \quad (5.19)$$

let us consider the coefficient of $\underline{Z}_1 \underline{Z}_2 \cdots \underline{Z}_n$, where $n = 2s$ with the auxiliary variables $\underline{Z}_i$ which are equal either to Z_i, $\bar{Z}_i$, in terms of the auxiliary operators $\underline{a}_i$ if $\underline{Z}_i = Z_i$ and a_i^+ if $\underline{Z}_i = \bar{Z}_i$ and obtain

$$a_n C(\underline{a}_1 \underline{a}_2 \cdots \underline{a}_n) - \Delta_n + b_n \sum_{r=1}^{n} P_r \sum \underline{a}_1 \underline{a}_2 \cdots \underline{a}_{n-2r} \delta^r = 0 \quad (5.20)$$

where

$$\delta^r = \bar{\delta}_{n-2r+1, \underline{Z}n-2r+2} \, \bar{\delta}_{n-2r+3, \underline{Z}n-2r+4} \cdots \bar{\delta}_{\underline{Z}n-1, \underline{Z}n}. \quad (5.21)$$

The δ symbols involving $\underline{Z}$ are simplified according to the rule that Z_i is replaced by i and $\bar{Z}_i$ is replaced by $\bar{i}$ to reduce to the $\bar{\delta}$ given by (5.19).

Making use of Eq. (5.20) and considering systematically commutation relations which contain 0, 1, 2, ..., $[(2s+1)/2]+1$ bared symbols we obtain $[(2s+1)/2]+1$ commutation relations for a parafield algebra of order $2s+1$. All the other commutation relations can be obtained from these either by simple complex conjugation or by using the general commutation relations given by (5.10) as this is equal to using the Eq. (4.22).

As an example, by choosing in Eq. (5.20) $\underline{a}_i = a_i$ for all i, and noting by Eq. (5.10) that $[a_i a_j a_k] = 0$, we obtain

$$C(a_1 a_2 \cdots a_n) = 0 \quad (5.22)$$

for the case of the nth order parafield algebra.

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Lie theory and separation of variables. 4. The groups $SO(2,1)$ and $SO(3)$

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Winternitz and coworkers have shown that the eigenfunction equation for the Laplacian on the hyperboloid $x_0^2-x_1^2-x_2^2=1$ separates in nine orthogonal coordinate systems, associated with nine symmetric quadratic operators L in the enveloping algebra of $SO(2,1)$. Corresponding to each of the operators L, we employ the standard one-variable model for the principal series of representations of $SO(2,1)$ and compute explicitly an L basis for the Hilbert space as well as the unitary transformations relating different bases. We also compute the associated results for realizations of these representations on the hyperboloid. Three of our bases are related to well-known subgroup reductions of $SO(2,1)$. Of the remaining six, one is related to Bessel functions, two to Legendre functions, and three to Lamé functions. We show that there is virtually a perfect correspondence between the known theory of the Lamé functions and the representation theory of $SO(2,1)$ and $SO(3)$.

1. INTRODUCTION

As is well known, the group $SO(2,1)$ acts on the hyperboloid $x_0^2-x_1^2-x_2^2=1$, $x_0>0$, with induced Lie derivatives K_1, K_2, M_3 given by

$$K_1=-x_0\partial_{x_2}-x_2\partial_{x_0},\quad K_2=-x_0\partial_{x_1}-x_1\partial_{x_0},$$
$$M_3=x_1\partial_{x_2}-x_2\partial_{x_1} \tag{1.1}$$

and commutation relations (2.3). Consider the eigenvalue equation

$$Qf(x_0,x_1,x_2)=l(l+1)f(x_0,x_1,x_2), \tag{1.2}$$

where $Q=K_1^2+K_2^2-M_3^2$ is the Casimir operator of the Lie algebra $so(2,1)$ expressed in terms of (1.1) and f is a function on the hyperboloid. Olevsky[1] has shown that Eq. (1.2) separates in nine orthogonal coordinate systems and Winternitz and coworkers[2,3] have shown that these coordinate systems correspond to nine quadratic symmetric operators L in the enveloping algebra U of $SO(2,1)$. Indeed, let S be the space of all symmetric second order elements in U, let C be the center of U and form the factor space $T=S/S\cap C$. (In this case $S\cap C=\{\alpha Q\}$, α any constant). Then $SO(2,1)$ acts on T via the adjoint representation and splits it into nine types of orbits. Choosing an operator L from each orbit, we find that for each such L the pair of equations

$$Qf=l(l+1)f,\quad Lf=\lambda f, \tag{1.3}$$

corresponds to one of the nine coordinate systems in which (1.2) separates. In fact, λ corresponds to a separation constant.

We choose our nine operators L as M_3^2, K_2^2, $(K_1+M_3)^2$, $L_E, L_H, L_{SH}, L_{EP}, L_{HP}, L_{CP}$, where the last six are given by (3.1). For the explicit derivation of these operators and the orthogonal coordinates to which they correspond see Ref. 2.

In the present paper, rather than study (1.2) directly, we employ the standard one-variable model (2.6) for the principal series representations of $SO(2,1)$ and explicitly compute an L basis for the Hilbert space corresponding to each of our nine L operators. We also compute unitary transformations relating different bases. Our results on the spectral resolutions of the L operators, though determined for the simple one-variable model, are obviously valid for any model of the principal series. The spectral resolutions for the "subgroup operators" M_3^2, K_2^2, and $(K_1+M_3)^2$ are well known, e.g., Refs. 4–6 and partial results for L_E and L_H can be found in Ref. 3. However, the remaining four cases are treated here for the first time. The operators L_E, L_H, L_{SH} lead to expansions in Lamé functions, L_{CP} to Bessel functions and the Hankel transform, and L_{EP}, L_{HP} to expansions in Legendre functions.

In Sec. 4 of this paper we construct models of the principal series in terms of solutions of (1.2), thus making explicit the relationship between the above results and separation of variables. This is accomplished via the Gel'fand–Graev transform which maps functions on the unit circle to functions on the hyperboloid and is an intertwining operator for the group action. We obtain a number of new results relating solutions of (1.2) in various bases.

Recently Patera and Winternitz[7] have introduced a new basis for the representations of the rotation group $SO(3)$. Their basis consists of the eigenfunctions of the symmetric operator $E=-4(L_1^2+rL_2^2)$, where $0<r<1$ and $[L_i,L_j]=\epsilon_{ijk}L_k$. In the two-variable model of the irreducible representations of $SO(3)$, functions on a sphere, the eigenfunctions are products of Lamé polynomials. However, the only one-variable model computed in Ref. 7 was one in which the basis functions appeared as complicated Heun polynomials. In Sec. 5 we show that, in fact, by a suitable change of variable and phase, one can construct a one-variable model in which the basis functions are exactly the Lamé polynomials. We show that there is a one-to-one relationship between the results of Ref. 7 and the standard theory of Lamé polynomials as presented in Ref. 8 or Ref. 9. This permits the use of tabulated properties of Lamé polynomials to implement the theory of Ref. 7. In general our results show an intimate relationship between the representation theory of $SO(2,1)$ and $SO(3)$ on the one hand and the theory of Lamé functions on the other.

We have not attempted to compute the matrix elements for the principal series representations of $SO(2,1)$ in any of the nonsubgroup bases. The practical computation of such results awaits the introduction of appropriate coordinates on the group manifold such that variables separate in the differential equations for the matrix elements. Work is in progress on this problem.

This paper is one of a series analyzing the relationship between Lie theory and separation of variables in the partial differential equations of mathematical physics.[10–12]

2. SUBGROUP BASES

In this section we establish notation and review those properties of $SO(2,1)$ that we will need in the sequel.

The group $SO(2,1)$ consists of those proper linear transformations acting on a three-dimensional vector $\mathbf{x}=(x_0, x_1, x_2)$ which preserve the infinitesimal distance

$$ds^2 = dx_0^2 - dx_1^2 - dx_2^2. \tag{2.1}$$

(These are the Lorentz transformations in the plane.) The group $SO(2,1)$ is 2—1 homomorphic to the group $SU(1,1)$ of quasiunitary unimodular matrices

$$g=\begin{pmatrix}\alpha & \beta\\ \bar{\beta} & \bar{\alpha}\end{pmatrix}, \quad |\alpha|^2-|\beta|^2=1. \tag{2.2}$$

The generators of the Lie algebra of $SO(2,1)$ are denoted by K_1, K_2, and M_3. Here K_1, K_2 are the generators of the pure Lorentz transformations along the 1 and 2 axes, respectively, and M_3 is the generator of rotations in the 1, 2 plane. The defining commutation relations of this algebra are

$$[K_1,K_2]=-M_3, \quad [K_2,M_3]=K_1, \quad [M_3,K_1]=K_2. \tag{2.3}$$

All unitary faithful irreducible representations are labeled by the eigenvalue of the Casimir operator Q, where

$$Q=K_1^2+K_2^2-M_3^2=l(l+1). \tag{2.4}$$

All such irreducible representations are infinite dimensional. We now give the spectrum of l corresponding to the unitary irreducible representations and the eigenvalues m of the operator iM_3 in each such representation.

(i) Principal series: $l=-\frac{1}{2}+i\rho$, $0<\rho<\infty$, $m=0, \pm1, \pm2, \cdots$ or $\pm\frac{1}{2}, \pm\frac{3}{2}, \cdots$.

(ii) Complementary series: $\mathrm{Im}\, l=0$, $-1<l<0$, $m=0, \pm1, \pm2, \cdots$.

(iii) Positive discrete series: $2l=$ integer, $m=l+1, l+2, \cdots$.

(iv) Negative discrete series: $2l=$ integer, $m=-l-1, -l-2, \cdots$.

For the purposes of this paper we only consider the single valued representations of the principal series. For a more detailed treatment of $SO(2,1)$ we refer to the standard references, 4, 13. The principal series of $SU(1,1)$ can be realized on the Hilbert space $\mathcal{H}$ of square integrable functions f on the unit circle with the scalar product

$$\langle f,h\rangle=\int_0^{2\pi}\overline{f(e^{i\theta})}\; h(e^{i\theta})d\theta. \tag{2.5}$$

The action of a group element g on a function f is specified by

$$T(g)f(e^{i\theta})=|\beta e^{i\theta}+\bar{\alpha}|^{2l} f\left(\frac{\alpha e^{i\theta}+\bar{\beta}}{\beta e^{i\theta}+\bar{\alpha}}\right), \tag{2.6}$$

and the generators of the Lie algebra have the form

$$K_1=l\cos\theta-\sin\theta\frac{d}{d\theta},$$
$$K_2=-l\sin\theta-\cos\theta\frac{d}{d\theta}, \tag{2.7}$$
$$M_3=\frac{d}{d\theta}.$$

Of the nine possible bases for $SO(2,1)$ as given by Winternitz *et al.*[2], three are of the subgroup type and have been treated in some detail in the literature.[4–6] We now give the explicit form of each of these subgroup bases for the principal series. In the section on the two variable model we also give the expansions in the subgroup bases. These results are not new,[6] but we present them here in summarized form in the interest of completeness.

1. *Spherical system*: The explicit form of the principal series in this basis has already been presented in our definition of the principal series. The basis functions of the spherical system are just the eigenfunctions $\exp(im\theta)/\sqrt{2\pi}$ of the operator M_3. This is the canonical or standard basis to which we will relate all subsequent bases.

2. *Equidistant system*: The basis defining operator for this system is K_2.

The representation space of the principal series splits into two spaces. The basis vectors in each space are

$$f^l_{\tau\epsilon}=(\cosh q)^l\exp(i\tau q)\,C_\epsilon, \quad -\infty<\tau<\infty, \tag{2.8}$$

where $\epsilon=\pm1$ is a reflection label which distinguishes the two spaces and $C_{+1}=\binom{1}{0}$, $C_{-1}=\binom{0}{1}$. The variable q is related to θ by

$$e^q=\tan\tfrac{1}{2}\theta, \qquad 0\le\theta\le\pi,$$
$$e^{-q}=\tan\tfrac{1}{2}(\theta-\pi), \qquad \pi\le\theta\le2\pi. \tag{2.9}$$

On each of the spaces K_2 is essentially the momentum operator with a unitary continuous spectrum, the real line. For further details concerning this basis see Refs. 5, 6.

3. *Horocyclic system*: The basis defining operator for this system is K_1+M_3. The representation space of the principal series is then spanned by a single set of basis vectors given by

$$f^l_s=[\tfrac{1}{2}(1+z^2)]^l\exp(isz), \quad -\infty<s<\infty, \tag{2.10}$$

where the variable z is related to θ by

$$z=\tan\tfrac{1}{2}\theta. \tag{2.11}$$

This basis has been considered to a limited extent in Ref. 13. The choice of basis operator is more convenient but still equivalent to that used in Ref. 13. (Similar remarks apply to the equidistant system.)

3. NONSUBGROUP BASES

Now we enumerate the six types of orbits in T which do not correspond to subgroup bases. Choosing a standard element on each of the orbits, we obtain the following list of six operators.

(1) Elliptic system: $L_E = M_3^2 + k^2 K_2^2, \quad k \in R$,

(2) Hyperbolic system: $L_H = K_2^2 - r^2 M_3^2, \quad 0 < r < 1$,

(3) Semihyperbolic system: $L_{SH} = M_3 K_1 + K_1 M_3 + r K_2^2, \quad 0 < r < \infty$, (3.1)

(4) Elliptic-parabolic system: $L_{EP} = \gamma K_2^2 + K_1^2 + M_3^2 + K_1 M_3 + M_3 K_1, \quad \gamma > 0$,

(5) Hyperbolic-parabolic system: $L_{HP} = -\gamma K_2^2 + K_1^2 + M_3^2 + K_1 M_3 + M_3 K_1, \quad \gamma > 0$,

(6) Semicircular-parabolic system: $L_{CP} = K_1 K_2 + K_2 K_1 + K_2 M_3 + M_3 K_2$.

We will show that each of these operators corresponds naturally to a symmetric operator on the Hilbert space $\mathcal{H} = L_2[0, 2\pi]$ corresponding to the principal series representations of $SO(2,1)$. Furthermore, we will show that each such symmetric operator has equal deficiency indices and can be extended to one or more self-adjoint operators on $\mathcal{H}$. Finally we will compute the spectral resolutions of these self-adjoint extensions and relate them to the spectral resolution of $L_S = M_3^2$.

Recall that for the principal series the Lie algebra generators are given by (1.7) and $l = -\frac{1}{2} + i\rho, \ \rho > 0$.

A. Elliptic parabolic system

For our first example we consider the operator L_{EP} normalized so that $\gamma = 1$:

$$L_{EP} = 2(1 - \sin\theta)\frac{d^2}{d\theta^2} + (2l - 1)\cos\theta\frac{d}{d\theta} + [l(l+1) - l\sin\theta]. \tag{3.2}$$

This operator can be defined on the domain of all C^∞ functions on the circle which vanish near $\theta = \pi/2$. It is straightforward to show that L_{EP} is essentially self-adjoint on this domain and that the self-adjoint extension, which we also call L_{EP}, has continuous spectrum only, covering the negative real axis. The normalized generalized eigenfunctions are

$$F_\xi^{EP}(\theta) = \alpha_\xi (\sin\tfrac{1}{2}\phi)^{-1/2+i\rho} P^{i\xi}_{-1/2+i\rho}(\cos\tfrac{1}{2}\phi),$$
$$\alpha_\xi = \left(\frac{4\pi\xi \sinh \pi\xi}{\cosh\pi\xi + \cosh\pi\rho}\right)^{1/2}, \quad \theta = \tfrac{1}{2}\pi + \phi, \ 0 \le \phi < 2\pi, \tag{3.3}$$

and the orthogonality relations are

$$\int_0^{2\pi} \overline{F_{\xi'}^{EP}(\theta)} F_\xi^{EP}(\theta)\, d\theta = \delta(\xi' - \xi). \tag{3.4}$$

Here, $L_{EP} F_\xi^{EP}(\theta) = -\xi^2 F_\xi^{EP}(\theta), \ 0 < \xi < \infty$, and $P_l^\mu(z)$ is a Legendre function.[8] A tedious computation for the overlap functions between the S and EP bases yields

$$\begin{aligned} U_{n,\xi}^{S,EP} &= \int_0^{2\pi} \overline{F_n^S(\theta)} F_\xi^{EP}(\theta)\, d\theta \\ &= \frac{\alpha_\xi}{\sqrt{2\pi}}(-i)^n \int_0^{2\pi} \exp(-in\phi)(\sin\tfrac{1}{2}\phi)^l P_l^{i\xi}(\cos\tfrac{1}{2}\phi)\, d\phi \\ &= \alpha_\xi(\tfrac{1}{2}\pi)^{1/2}(-i)^n\, 2^{i\xi}\, \frac{(-1)^n 2^{2(n+1)}\Gamma(n+\frac{1}{2})\Gamma((l+i\xi+1)/2)\Gamma((-2n+l-i\xi+1)/2)}{\Gamma(-n+l+1)\Gamma((l-i\xi+2)/2)\Gamma((-2n-i\xi-l+1)/2)} \\ &\quad \times {}_4F_3\left(\left.\begin{matrix} n-l,\ n+\frac{1}{2},\ n,\ n+\frac{1}{2} \\ (1+2n+i\xi-l)/2,\ (1+2n-i\xi-l)/2,\ 1+2n \end{matrix}\right| 1\right) \pm \frac{i\pi\, 2^{2n}\,\Gamma((i\xi-l+1)/2)\Gamma((l-2n+i\xi+1)/2)}{\Gamma((2l-2n+3)/2)\Gamma((-l-i\xi)/2)\Gamma((1+2n-l+i\xi)/2)} \\ &\quad \times \frac{1}{(|n|)!}\, {}_4F_3\left(\left.\begin{matrix} n-l-\frac{1}{2},\ n+\frac{1}{2},\ n+1,\ n \\ (1+2n-l+i\xi)/2,\ (1+2n-l-i\xi)/2,\ 2n \end{matrix}\right| 1\right) \end{aligned} \tag{3.5}$$

where the plus sign applies to the case $n \le 0$ and the minus sign to $n > 0$. The ${}_4F_3$ is a generalized hypergeometric function.[8]

B. Elliptic system

Corresponding to the elliptic system we have

$$L_E = (1 + k^2\cos^2\theta)\frac{d^2}{d\theta^2} + k^2(2l-1)\sin\theta\cos\theta\frac{d}{d\theta} + k^2(l^2\sin^2\theta + l\cos^2\theta). \tag{3.6}$$

Initially we define this operator on the domain of C^∞ functions on the circle. However, it is easy to see that L_E has a unique self-adjoint extension. Indeed, it corresponds to a regular Sturm–Liouville operator on the interval $[0, 2\pi]$ with periodic boundary conditions. Thus the spectrum is discrete. To solve the eigenvalue equation $L_E f_\lambda^E = \lambda f_\lambda^E$, we set

$$f_\lambda(\theta) = (1 + k^2\cos^2\theta)^{l/2} g_\lambda(w),$$

$\theta = \phi - \pi/2$ and $\sin\phi = \mathrm{sn}(w, ik)$, where $\mathrm{sn}(z,k)$ is a Jacobi elliptic function (Ref. 8, Chap. 13). Then the eigenvalue equation becomes

$$\left(\frac{d^2}{dz^2} - r^2 l(l+1)\,\mathrm{sn}^2(z,r) + l(l+1)r^2 - \frac{\lambda}{1+k^2}\right) g_\lambda(z) = 0, \tag{3.7}$$

$$z = (1+k^2)^{1/2} w, \quad r^2 = \frac{k^2}{1+k^2}, \quad -K(\gamma) \le z \le 3K(\gamma),$$

with periodic boundary conditions $g_\lambda(z)|_{-K}^{3K}=0$, $g'_\lambda(z)|_{-K}^{3K}=0$. This is the Lamé equation and the required eigenfunctions are the periodic Lamé functions with period $4K$. We can divide the eigenfunctions into symmetry classes by noting that L_E commutes with the unitary commuting idempotent operators R_1, R_2, where

$$(R_1 f)(\phi)=f(-\phi), \quad (R_2 f)(\phi)=f(\pi-\phi)$$

with ϕ as in (3.3) and $f(\phi)$ a function on the unit circle.

Since the eigenvalues of R_1 and R_2 are ± 1 the eigenfunctions of L_E fall into four classes labeled by these eigenvalues. In terms of the notation given in Ref. 8, Sec. 15.5.1, the results are

$\lambda(1+k^2)^{-1}$	$g_\lambda(z)$	period	R_1	R_2
$a_l^{2m}(r^2)$	$Ec_l^{2m}(z, r^2)$	$2K$	1	1
$a_l^{2m+1}(r^2)$	$Ec_l^{2m+1}(z, r^2)$	$4K$	-1	1
$b_l^{2m+2}(r^2)$	$Es_l^{2m+2}(z, r^2)$	$2K$	1	-1
$b_l^{2m+1}(r^2)$	$Es_l^{2m+1}(z, r^2)$	$4K$	-1	-1

(3.8)

for $m=0,1,2,\cdots$. Here the multiplicity of each eigenvalue is one, and the superscripts m are related to the number of zeros of the corresponding eigenfunctions in a period. We normalize each eigenfunction f_λ^E to have unit length in $\mathcal{H}$, leaving a phase factor undetermined.

Note that the action of R_1 and R_2 on the spherical basis functions $f_m^S(\theta)=\exp(im\theta)/\sqrt{2\pi}=(-i)^m\exp(im\phi)/\sqrt{2\pi}$ is

$$R_1 f_m^S=(-1)^m f_{-m}^S, \quad R_2 f_m^S=f_{-m}^S. \tag{3.9}$$

The overlap functions relating the f_m^S basis to the f_λ^E basis are the coefficients $U_{\lambda,m}^{E,S}$ in the expansion

$$f_\lambda^E=\sum_{m=-\infty}^{\infty} U_{\lambda,m}^{E,S} f_m^S. \tag{3.10}$$

We can obtain recurrence relations for these coefficients by substituting (3.10) into the eigenvalue equation $L_E f_\lambda^E=\lambda f_\lambda^E$ and equating coefficients of f_m^S on both sides of the resulting identity. For example, the basis function $h_m(\phi)=(1+k^2\sin^2\phi)^{1/2}Ec_l^{2m}(z, r^2)$ satisfies $R_1 h_m=R_2 h_m=h_m$ so that the expansion (3.10) takes the form

$$h_m(\phi)=\tfrac{1}{2}C_0+\sum_{n=1}^{\infty} C_{2n}\cos(2n\phi).$$

Substituting this expression into the eigenvalue equation, we find

$$\begin{aligned}&[k^2 l(l+1)-2\lambda]C_0-k^2(l^2-5l-2)C_2=0,\\ &k^2[\tfrac{1}{2}(n-1)(3-2l)+\tfrac{1}{4}l(1-l)]C_{2n-2}\\ &\quad+\{\tfrac{1}{2}k^2[l(l+1)-4n]-(\lambda+4n^2)\}C_{2n}\\ &\quad+k^2[\tfrac{1}{2}(n+1)(1+2l)+\tfrac{1}{4}l(1-l)]C_{2n+2}=0.\end{aligned} \tag{3.11}$$

These expressions are closely related (but not identical) to recurrence formulas derived in Section 15.5.1 of Ref. 8. There are similar formulas for the other three types of periodic Lamé functions.

C. Semicircular parabolic system

The basis defining operator L_{CP} has the form

$$\begin{aligned}L_{CP}&=2\cos\theta(1-\sin\theta)\frac{d^2}{d\theta^2}+(2l-1)(1-\sin\theta)\\ &\quad\times(1+2\sin\theta)\frac{d}{d\theta}+l\cos\theta[1+2(l-1)\sin\theta].\end{aligned} \tag{3.12}$$

Before discussing the self-adjoint extension of L_{CP} it is convenient to use instead of the functions f defined on the unit circle, the functions $g^\epsilon(v)$,

$$f(\theta)=[2v/(1+v^4)]^l g^\epsilon(v), \tag{3.13}$$

where $\epsilon=+1$, $v=\sqrt{\cot\frac{1}{2}\phi}$ $(0<\phi<\pi)$, and $\epsilon=-1$, $v=\sqrt{-\cot\frac{1}{2}\phi}$ $(\pi<\phi<2\pi)$. The space of functions $f(\theta)$ is then replaced by the pair of functions (g^+, g^-), and so we need to consider L_{CP} acting on the direct sum of two Hilbert spaces which we call $\mathcal{H}^+$ and $\mathcal{H}^-$ $(H=\mathcal{H}^+\oplus\mathcal{H}^-)$. On each of these spaces L_{CP} has the form

$$L_{CP}=\frac{1}{4}\left(\frac{d^2}{dv^2}-\frac{l(l+1)}{v^2}\right).$$

This operator has deficiency indices (1,1) on each of the two Hilbert spaces $\mathcal{H}^+$ and $\mathcal{H}^-$. There is thus a two-parameter family of possible self-adjoint extensions of L_{CP} acting on the space of functions defined on H. We choose one of these which immediately suggests itself and relate it to the standard S basis. The normalized generalized eigenfunctions we choose are

$$f_{\lambda\epsilon}^{CP}(\theta)=[2v/(1+v^4)]^l\sqrt{\lambda v}\,J_{l+1/2}(\sqrt{2}\lambda v)\,C_\epsilon, \tag{3.14}$$

with C_ϵ as in (2.8). This choice of basis corresponds to the choice of eigenvalue $\epsilon\lambda^2$ $(0<\lambda<\infty)$ for the basis vector $f_{\lambda\epsilon}^{CP}(\theta)$, i.e.,

$$L_{CP}f_{\lambda\epsilon}^{CP}=\epsilon\lambda^2 f_{\lambda\epsilon}^{CP}.$$

The orthogonality relations are

$$\int_0^{2\pi} f_{\lambda'\epsilon'}^{CP\dagger}(\theta)f_{\lambda\epsilon}^{CP}(\theta)\,d\theta=\delta(\lambda'-\lambda)\,\delta_{\epsilon'\epsilon}. \tag{3.15}$$

The relation of this basis to the spherical basis can be readily computed:

$$\begin{aligned}U_{-n,\lambda+}^{S,CP}&=2^{l+1}\sqrt{\lambda}\int_0^\infty v^{l+3/2}J_{l+1/2}(\sqrt{2}\lambda v)\\ &\quad\times(v^2+i)^{2n}(1+v^4)^{-n-l-1}\,dv\\ &=\Bigg[2\sqrt{\pi}\left(\frac{\lambda}{2}\right)^{-l-1}\sum_{r=0}^{2n} i^{2n-r}C\binom{2n}{r}\\ &\quad\times\frac{\Gamma(-l-n)}{\Gamma(-l-r)\,\Gamma(r+l+1)}\left(\frac{1}{\lambda}\frac{\partial}{\partial\lambda}\right)^r\left(\frac{1}{16z^3}\frac{\partial}{\partial z}\right)^{n-r}\\ &\quad\times\left(\frac{8z^2}{\lambda^2}\right)^{l+1/2-r}J_{-l-1/2+r}(\lambda z)K_{-l-1/2+r}(\lambda z)\Bigg]_{z=1},\end{aligned} \tag{3.16}$$

where $n>0$ and $K_l(z)$ is a MacDonald function.[8]

For $n<0$ it is only necessary to make the substitution $l\to -l-1$. The only modification of these results for the overlap function $U_{-n,\lambda-1}^{S,CP}$ is the replacement of the i^{2n-r} term in the above expression by $(-i)^{2n-r}$.

D. Hyperbolic system

The basis defining operator L_H has the form

$$\begin{aligned}L_H&=(r^2-\cos^2\theta)\frac{d^2}{d\theta^2}+(1-2l)\sin\theta\cos\theta\frac{d}{d\theta}\\ &\quad-l^2\sin^2\theta-l\cos^2\theta.\end{aligned} \tag{3.17}$$

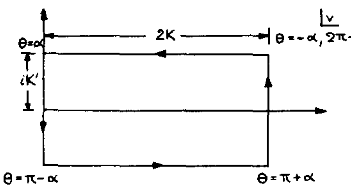

FIG. 1. The θ coordinate in the v plane for the hyperbolic system.

This operator is defined in the domain of all C^∞ functions which vanish near those four points for which $|\cos\theta| = r$ $(r>0)$. It is convenient at this point to split the space H into a direct sum of four spaces which we label by a discrete index i $(i=1,2,3$ or $4)$. The splitting is achieved according to the prescriptions $\mathcal{H}^1 \leftrightarrow (-\alpha<\theta<\alpha)$, $\mathcal{H}^2 \leftrightarrow (\alpha<\theta<\pi-\alpha)$, $\mathcal{H}^3 \leftrightarrow (\pi-\alpha<\theta<\pi+\alpha)$, $\mathcal{H}^4 \leftrightarrow (\pi+\alpha<\theta<2\pi-\alpha)$ so that

$$H=\sum_{i=1}^{4}\oplus\mathcal{H}^i. \tag{3.18}$$

(note: we assume $r=\cos\alpha$, $0<\alpha<\pi/2$). The functions $f(\theta)$ are then replaced by functions $h_i(v)$, given by

$$f_i(\theta)=[ir'/\mathrm{cn}(v,r)]^l\, h_i(v), \tag{3.19}$$

where $r'=(1-r^2)^{1/2}$ and $\cos\theta=\mathrm{dn}(v,r)/\mathrm{cn}(v,r)$.

The ranges of the parameters are shown in Fig. 1, and it can be seen that as θ runs from $-\alpha\to 2\pi-\alpha$, the parameter v describes a closed path as indicated in Fig. 1.

On each of the Hilbert spaces $\mathcal{H}^i$ the operator $L_{\rm H}$ has the form

$$L_{\rm H}=\frac{d^2}{dv^2}-r^2\,l\,(l+1)\,\mathrm{sn}^2(v,r). \tag{3.20}$$

We are then concerned with four eigenvalue problems each of which is such that the operator $L_{\rm H}$ is singular at each of the two corresponding end points. Let us first consider the choice of basis for $\mathcal{H}^1$. For this space $v\in(iK', iK'+2K)$. Following Erdelyi,[8] Chap. 15, we choose the boundary conditions for a basis as

$$\text{(i)}\ [\mathrm{sn}(v,r)]^{1/2}\,\Lambda(v)\ \text{bounded at}\ v=iK',\qquad \Lambda'(K+iK')=0. \tag{3.21}$$

The corresponding solution is denoted by $\Lambda=F_l^{2m}(v,r)$ and has $2m$ zeros in the interval $(iK',\ iK'+2K)$

$$\text{(ii)}\ [\mathrm{sn}(v,r)]^{1/2}\,\Lambda(v)\ \text{bounded at}\ v=iK',\qquad \Lambda(K+iK')=0. \tag{3.22}$$

The corresponding solutions are denoted by $F_l^{2m+1}(v,r)$. In the above $\Lambda(v)$ is the corresponding solution of the equation $L_{\rm H}\Lambda=\lambda_m\Lambda$. Here m is the number of zeros of the eigenfunction Λ in the interval $(iK',\ iK'+2K)$. These are the finite Lamé or Lamé Wangerin functions. The solution of the corresponding boundary value problem gives these functions as expansion functions with the discrete spectrum of $L_{\rm H}$ labeled by the upper index. [This index is also the number of zeros of the solution in the interval $(iK', iK'+2K)$.] The problem for the basis of $\mathcal{H}^3$ is exactly similar so that we then have the basis

$$f^{\rm H}_{m,i}(v)=F_l^m(v,r)\,\lambda_i,\quad i=1,3. \tag{3.23}$$

The λ_i are 4×1 column vectors having 1 in the ith row and zero elements elsewhere. For the choice of basis in the spaces $\mathcal{H}^2$ and $\mathcal{H}^4$ the corresponding eigenfunction expansion problem is similar to that considered already but the variable v is now in the range $(iK',\ -iK')$ or $(2K+iK', 2K-iK')$. The corresponding boundary value problem of interest is now given by the requirement that $(\mathrm{sn}v)^{1/2}\,\Lambda(v)$ be bounded at the end points $v=\pm iK'$ and that $\Lambda'(0)=0$ or $\Lambda(0)=0$ according as Λ is even or odd about $v=0$. The complete set of eigenfunctions are the Lamé Wangerin functions $F_l^m(v,r)$. The corresponding basis functions are then given as in (3.23) with $i=2,4$. In particular we have for each eigenfunction $f^{\rm H}_{m,i}$ $(i=1,2,3,4)$ as θ varies from $-\alpha$ to $2\pi-\alpha$, that v varies continuously around the rectangle drawn in Fig. 1. The corresponding eigenfunction $[ir'/\mathrm{cn}(v,r)]^l f^{\rm H}_{m,i}$ corresponds to a continuous differentiable function of θ and is therefore an element of the original representation space. This requirement picks out this solution and does not require us to consider the deficiency indices in each subspace. (We have essentially periodic boundary conditions). The latter procedure in general leads to sectionally continuous eigenfunctions on H. The orthogonality of the basis functions is written

$$(f^{\rm H}_{m,i},\, f^{\rm H}_{m',j})=\delta_{ij}\,\delta_{mm'}\,N^i_m \tag{3.24}$$

with N^i_m a normalization factor. The eigenfunctions $f^{\rm H}_{m,i}$ defined as above are nonzero only in the corresponding Hibert space $\mathcal{H}^i$.

We now proceed to calculate a recurrence relation for the overlap functions between hyperbolic and spherical bases.

We consider in detail overlaps associated with the spaces $\mathcal{H}^1$ and $\mathcal{H}^3$. As with the elliptic system it is convenient to consider a number of discrete transformations. The first of these is reflection R about the line $\mathrm{Re}\,v=K$. This corresponds to the transformation $\theta\to-\theta$. We have accordingly

$$Rf^{\rm H}_{m,i}(v)=(-1)^m f^{\rm H}_{m,i}(v),\quad i=1,3. \tag{3.25}$$

In addition, if we consider the reflection $\bar{R}:\theta\to\pi-\theta$, then we have

$$\bar{R}f^{\rm H}_{m,i}(v)=(-1)^m f^{\rm H}_{m,j}(v),\quad i\neq j,\ i,j=1,3. \tag{3.26}$$

From these equations we can form the linear combinations $F^{\rm H\pm}_m=f^{\rm H}_{m,i}(v)\pm f^{\rm H}_{m,j}(v)$ [with i,j as in (3.23)] having eigenvalues $(-1)^m$, $\pm(-1)^m$ respectively, of the operators R and $\bar{R}$.

It is these functions for which we can form the overlap functions, i.e., instead of relating the normal basis $f^{\rm H}_{m,i}(v)$ to the spherical basis $f^{\rm S}_n$ via $f^{\rm H}_{m,i}=\sum_{n=-\infty}^{\infty}U^{\rm H,S}_{m,n}f^{\rm S}_n$ we write each $F^{\rm H\pm}_m$ as a Fourier series in θ and find recurrence relations for the coefficients. This involves extending the domain of the functions $F^{\rm H\pm}_m$ to be defined on the unit circle, $0<\theta\leq 2\pi$.

The symmetrized basis function $G^{\rm H\pm}_{2p}=(r^2-\cos^2\theta)^{l/2}\times F^{\rm H\pm}_{2p}$ has eigenvalues $+1$ for the both the reflections R and $\bar{R}$ and so can be represented by the series

$$G^{\rm H+}_{2p}(\theta)=\tfrac{1}{2}C_0+\sum_{n=1}^{\infty}C_{2n}\cos(2n\theta) \tag{3.27}$$

for $\alpha < \theta < \pi/2 - \alpha$. Applying the operator L_H to both sides, we obtain the recurrence relations

$$-[l(l+1)+2\lambda_m]C_0+[2+l(3l-1)]C_2=0,$$
$$[\tfrac{1}{2}(p-1)(2l-2p-1)+\tfrac{1}{4}(l-1)]C_{2p-2}$$
$$+[2p^2(1-2r^2)-\tfrac{1}{2}l(l+1)-\lambda_m]C_{2p}$$
$$+[\tfrac{1}{2}(p+1)(2l+2p+1)+\tfrac{1}{4}l(l-1)]C_{2p+2}=0 \qquad (3.28)$$

for $p \geq 1$.

Similar recurrence relations can be derived for the other symmetrized basis functions. Identical arguments can be applied to overlap functions associated with the Hilbert spaces $\mathcal{H}^2$ and $\mathcal{H}^4$. In this case it is convenient to introduce the same discrete transformations as previously but with θ replaced by $\phi(\theta=\pi/2+\phi)$. With this change the analysis goes through as before.

E. Semihyperbolic system

The basis defining operator L_{SH} has the form

$$L_{SH}=(r\cos^2\theta-2\sin\theta)\frac{d^2}{d\theta^2}+(2l-1)\cos\theta(1+r\sin\theta)\frac{d}{d\theta}$$
$$+r(l^2\sin^2\theta+l\cos^2\theta)-l\sin\theta. \qquad (3.29)$$

This operator is defined on the domain of all C^∞ functions which vanish near the two points at which $\sin\theta = 1/r[(1+r^2)^{1/2}-1]$. It is convenient to split the space H into the direct sum of two spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ defined according to the prescription $\mathcal{H}_1 \leftrightarrow (\alpha<\theta<\pi-\alpha)$, $\mathcal{H}_2 \leftrightarrow (\pi-\alpha<\theta<2\pi+\alpha)$ so that

$$H=\mathcal{H}_1\oplus\mathcal{H}_2.$$

The functions $f(\theta)$ are then replaced by the pair of functions h_i $(i=1,2)$, where

$$f(\theta)=\left(\frac{N\,\mathrm{sn}(v,s)\,dn(v,s)}{[-(1+r^2)^{1/2}+r+1]\,\mathrm{sn}^2(v,s)-2r}\right)^l h_1(v),$$
$$\alpha<\theta<\pi-\alpha,$$
$$=\left(\frac{N\,\mathrm{sn}(u,q)\,dn(u,q)}{[(1+r^2)^{1/2}+r-1]\,\mathrm{sn}^2(u,q)-2r}\right)^l h_2(u),$$
$$\pi-\alpha<\theta<2\pi+\alpha, \qquad (3.30)$$

where

$$N^2=\frac{8(1+r^2)^{1/2}}{r^2}[(1+r^2)^{1/2}-1],$$
$$s^2=\frac{(1+r^2)^{1/2}-r}{2(1+r^2)^{1/2}},\quad q^2=\frac{(1+r^2)^{1/2}+r}{2(1+r^2)^{1/2}}$$

and

$$\sin\theta=\frac{2[1-(1+r^2)^{1/2}]+[(1+r^2)^{1/2}-1-r]\,\mathrm{sn}^2(v,s)}{[1+r-(1+r^2)^{1/2}]\,\mathrm{sn}^2(v,s)-2r},$$
$$\alpha<\theta<\pi-\alpha,$$
$$=\frac{[(1+r^4)^{1/2}-1+r^2]\,\mathrm{sn}^2(u,q)-2[(1+r^4)^{1/2}-1]}{[(1+r^4)^{1/2}-1+r^2]\,\mathrm{sn}^2(u,q)-2r^2},$$
$$\pi-\alpha<\theta<2\pi+\alpha. \qquad (3.31)$$

The corresponding ranges of the variables are $0<v<2K(s)$, $0<u<2K(q)$. In terms of the new variables the operator L_{SH} assumes the forms

$$(1+r^2)^{-1/2}L_{SH}=-\left(\frac{d^2}{dv^2}+l(l+1)\frac{\mathrm{cn}^2(v,s)}{\mathrm{sn}^2(v,s)\,\mathrm{dn}^2(v,s)}+\frac{r\,l(l+1)}{(1+r^2)^{1/2}}\right)$$
$$=\frac{d^2}{du^2}-l(l+1)\frac{\mathrm{cn}^2(u,q)}{\mathrm{sn}^2(u,q)\,\mathrm{dn}^2(u,q)}-\frac{r\,l(l+1)}{(1+r^2)^{1/2}}. \qquad (3.32)$$

It is possible to make further transformations and write L_{SH} in the form of the standard Lamé operator as for instance in (3.20). The resulting elliptic functions then have a complex molulus $k=\exp(i\psi)$ (ψ real) and the range of variation of the new variables is not parallel to either of the directions of periodicity. It is more convenient to consider the operator L_{SH} in one of the forms (3.30). The problem of the self-adjoint extension of L_{SH} on each of the spaces $\mathcal{H}_i$ is exactly analogous to that considered in each of the spaces $\mathcal{H}_i$ of the hyperbolic system. In particular we choose the boundary conditions which require that $[\mathrm{sn}(v,s)]^{-1/2}\Lambda(v,s)$ be bounded in the interval $(0,2K(s))$. Here $\Lambda(v,s)$ is a solution of $L_{SH}\Lambda=\bar{\lambda}_m\Lambda$. More precisely the boundary conditions are:

(i) $[\mathrm{sn}(v,s)]^{-1/2}\Lambda(v,s)$ bounded at $v=0$, $2K(s)$ and $\Lambda'(K,s)=0$. The corresponding solution is denoted by $K_l^{2m}(v,s)$ and has $2m$ zeros in the interval $(0,2K(s))$.

(ii) $[\mathrm{sn}(v,s)]^{-1/2}\Lambda(v,s)$ bounded at $v=0$, $2K(s)$ and $\Lambda(K,s)=0$. The corresponding solution is denoted by $K_l^{2m+1}(v,s)$ and has $2m+1$ zeros in the interval $[0,2K(s)]$. Similar remarks apply to the related problem on $\mathcal{H}_2$. The corresponding solutions are denoted by $M_l^m(u,q)$. The spectrum in each case is discrete. A complete set of eigenfunctions for the Hilbert space H is then

$$f^{SH}_{m,1}(v)=K_l^m(v,s)C_+,$$
$$f^{SH}_{n,2}(v)=M_l^m(v,q)C_-. \qquad (3.33)$$

Satisfying the normalization conditions, we have

$$(f^{SH}_{m,\eta},f^{SH}_{m',\eta'})=\delta_{mm'}\delta_{\eta\eta'},\quad \eta,\eta'=1,2.$$

The functions $K_l^m(v,s)$ and $M_l^m(u,q)$ that we have introduced are closely related to the Lamé Wangerin functions which appear in the hyperbolic basis. In fact if we take the operator L_{SH} in the standard Lamé form we have in the space $\mathcal{H}_1$

$$[r+(r^2+1)^{1/2}]^{1/2}L_{SH}$$
$$=\frac{d^2}{dw^2}-k^2l(l+1)\,\mathrm{sn}^2(w,k)+\frac{r\,l(l+1)}{[r+(r^2+1)^{1/2}]^{1/2}} \qquad (3.34)$$

where $k=[q-i(1-q^2)^{1/2}]/[q+i(1-q^2)^{1/2}]$ and $w=[q+i(1-q^2)^{1/2}]v-iK'(k)$.

The corresponding eigenfunctions of this operator are then Lamé Wangerin functions. These solutions can be represented in a series as Erdeyli has done for the case of complex k, e.g.,

$$F_l^{2m}(w,k)=\sum_{r=0}^{\infty}A_r\exp[-i(l+1+2r)\xi], \quad (3.35)$$

where $\cos\xi=\mathrm{sn}(w,k)$ and the coefficients A_r satisfy the recurrence relations

$$[H-(l+1)^2(2-k^2)]A_0+(2l+3)k^2A_1=0,$$
$$(2r-1)(l+r)k^2A_{r-1}+[H-(l+1+2r)^2(2-k^2)]A_r$$
$$+(r+1)(2l+2r+3)k^2A_{r+1}=0,$$
$$r\geq 1 \quad\text{and}\quad H=2\bar{\lambda}_{2m}-l(l+1)k^2. \quad (3.36)$$

In this way we can write a series expansion for each of our basis functions K_l^m and M_l^m. It is again straightforward to calculate recurrence relations for the overlap functions between the semihyperbolic system and the spherical or canonical basis. This again depends on the fact that a given basis function consisting of two components represents a continuous function of θ for $\theta\in[0,2\pi]$. We merely note here that this can be done and omit the calculation which leads to rather lengthy recurrence relations.

F. The hyperbolic parabolic system

The operator L_{HP} has the form

$$L_{\mathrm{HP}}=2\sin\theta(\sin\theta-1)\frac{d^2}{d\theta^2}+(2l-1)\cos\theta(1-2\sin\theta)\frac{d}{d\theta}$$
$$-2l^2\sin^2\theta-2l\cos^2\theta-l\sin\theta, \quad \gamma=1. \quad (3.37)$$

We consider this operator to be defined initially on the C^∞ functions of θ which vanish near the points $\theta=\pi/2$, π, $3\pi/2$, where L_{HP} is singular. It is convenient to consider the space H divided into four subspaces $\mathcal{H}^i$ as with the hyperbolic system, i.e., $H=\sum_{i=1}^4\oplus\mathcal{H}^i$. Each of these subspaces corresponding to functions of θ defined over an interval of length $\pi/2$, e.g., $\mathcal{H}^1\longrightarrow(0<\theta<\pi/2)$ etc. It is then convenient to consider the operator L_{HP} acting on new functions h_i in each of these spaces where

$$f_i(\theta)=[\sqrt{2}\sinh b/(1+\cosh^2 b)]^l h_i(b), \quad i=1,2,$$
$$=[\sqrt{2}\sin\psi/(1+\cos^2\psi)]^l h_i(\psi), \quad i=3,4. \quad (3.38)$$

The variables b and ψ are given by

$$[(1+\sin\theta)/2\sin\theta]^{1/2}=\coth b \quad\text{if}\quad 0<\theta<\pi$$
$$=i\cot\psi \quad\text{if}\quad \pi<\theta<2\pi. \quad (3.39)$$

For $i=1,2$, L_{HP} acting on the functions $h_i(b)$ has the form

$$L_{\mathrm{HP}}=\frac{d^2}{db^2}-\frac{l(l+1)}{\sinh^2 b}$$

and for $i=3,4$ it is just required to make the substitution $b\rightarrow i\psi$. For $i=1,2$ the solutions of the eigenvalue equation $L_{\mathrm{HP}}\,h=\mu^2h$ are the functions $(\sinh b)^{1/2}$ $P_{-1/2-\mu}^{-l-1/2}(\cosh b)$. From this observation it is immediately seen that a complete set of basis functions does exist if we take $\mu=-i\rho$ (ρ real and positive). The corresponding completeness properties follow from the properties of the generalized Mehler transform. A complete set of orthonormal basis functions is then

$$f_{\rho,i}^{\mathrm{HP}}(b)=[(\rho\sinh\pi\rho/\pi)\,\Gamma(1+l+i\rho)\,\Gamma(1+l-i\rho)]^{1/2}$$
$$\times(\sinh b)^{1/2}P_{-1/2+i\rho}^{-l-1/2}(\cosh b), \quad (3.40)$$

$i=1,2$, satisfying the orthogonality relations

$$\langle f_{\rho,i}^{\mathrm{HP}},f_{\rho',i}^{\mathrm{HP}}\rangle=\delta(\rho-\rho').$$

The spaces $\mathcal{H}_3$ and $\mathcal{H}_4$ can be combined by defining the variable ψ as in (3.37) with $0<\psi<\pi$ but now taking into account the sign of the square root. The corresponding eigenvalue problem is singular at both ends of the interval $\psi\in(0,\pi)$. There is a two-parameter family of self-adjoint extensions of L_{HP} since the deficiency indices are (2, 2).

Each linearly independant solution is square integrable so that the spectrum is discrete for each self-adjoint extension. The computation of an orthonormal basis of eigenfunctions is straightforward but complicated and unenlightening and so we omit it. Also, the integrals relating these bases to the standard spherical basis appear intractable.

4. THE TWO VARIABLE MODEL

The group $SO(2,1)$ acts on 3-space according to $\mathbf{x}\rightarrow L(g)\mathbf{x}$, where $\mathbf{x}=(x_0,x_1,x_2)$ is a column 3-vector and $L(g)$ is the 3×3 matrix representation of $SU(1,1)$ defined as in Ref. 13, p. 289. This action induces a representation of $SU(1,1)$ on the space $\mathcal{F}$ of C^∞ functions in 3-space, defined by operators $\mathbf{T}(g)$:

$$[\mathbf{T}(g)F](\mathbf{x})=F(L(g^{-1})\mathbf{x}), \quad F\in\mathcal{F}. \quad (4.1)$$

To be precise, we choose the action so that the corresponding Lie derivatives are as in (1.1). Clearly the quadratic form $x_0^2-x_1^2-x_2^2$ is preserved by this action. In this section we will construct models of the principal series representations of $SO(2,1)$ in which the Hilbert space consists of functions $F(\mathbf{x})$ defined on the hyperboloid $x_0^2-x_1^2-x_2^2=1$, $x_0>0$, and the group acts via (4.1). In particular we will explicitly construct in this space the various basis functions listed above. Furthermore, we will use the Gel'fand—Graev transform to expand an arbitrary function, square integrable on the hyperboloid, in terms of each type of basis. We note that the basis functions are exactly those which appear when one uses separation of variable methods to find solutions of the wave equation

$$\left(\frac{\partial^2}{\partial y_0^2}-\frac{\partial^2}{\partial y_1^2}-\frac{\partial^2}{\partial y_2^2}\right)\phi(\mathbf{y})=0, \quad (4.2)$$

which are homogeneous in y_0, y_1, y_2.

We use the Gel'fand—Graev transform[14] to map functions on the unit circle corresponding to a principal series representation of $SO(2,1)$ to functions on the hyperboloid. Thus, corresponding to $f\in\mathcal{H}$ and the representation $l=-\frac{1}{2}+i\rho$, we define a function $F(\mathbf{x})$ on the hyperboloid by the integral

$$F(\mathbf{x})=\int_0^{2\pi}(x_0+x_1\sin\theta-x_2\cos\theta)^{-l-1}f(\theta)d\theta=I[f]. \quad (4.3)$$

It is easy to check that the operator $\mathbf{T}(g)$, (2.6), acting on f induces the operator $T(g)$, (4.1), acting on F:

$$T(g)F=I[\mathbf{T}(g)f].$$

It follows that the Lie derivatives (2.7) acting on f induce the Lie derivatives (1.1) acting on F.

If $\{f_n^G\}$ is a basis for $\mathcal{H}$ corresponding to the operator L_G, then

$$(K_1^2+K_2^2-M_3^2)f_n^G=l(l+1)f_n^G,$$
$$L_Gf_n^G=\lambda_nf_n^G. \tag{4.4}$$

It follows that the functions $F_n^G=I(f_n^G)$ satisfy the equations

$$(K_1^2+K_2^2-M_3^2)F_n^G=l(l+1)F_n^G,$$
$$L_GF_n^G=\lambda_nF_n^G, \tag{4.5}$$

where now the operators K_1, K_2, M_3 are given by (1.1) and L_G is expressed in terms of these operators by one of the Eqs. (3.1). We shall see that each choice of L_G in (3.1) corresponds to a separation of variables in the first equation (4.5).

We can now employ any one of our bases $\{F_n^G\}$ to expand functions on the hyperboloid. Thus, if $H(\mathbf{x})$ is square integrable on the hyperboloid $x_0^2-x_1^2-x_2^2=1$, $x_0>0$, with respect to the measure dx_1dx_2/x_0, then the Gel'fand–Graev integral transform yields the expansion

$$H(\mathbf{x})=\frac{1}{8\pi^2i}\int_{-1/2-i\infty}^{-1/2+i\infty} I[f_l]\,l\cot\pi l\,dl, \tag{4.6}$$

where $f_l(\theta)$ is a function on the circle defined by

$$f_l(\theta)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}H(\mathbf{x})\,(x_0+x_1\sin\theta-x_2\cos\theta)^l\,\frac{dx_1dx_2}{x_0}. \tag{4.7}$$

Since $f_l(\theta)$ can be expanded in a $\{f_n^G\}$ basis, we obtain

$$f_l(\theta)=\sum_n A_l^{G,n}f_n^G,\quad A_l^{G,n}=\langle f_n^G,f_l\rangle,$$

or

$$H(\mathbf{x})=\frac{1}{8\pi^2i}\int_{-1/2-i\infty}^{-1/2+i\infty} l\cot\pi l\,dl\sum_n A_l^{G,n}F_n^G(\mathbf{x}),$$
$$A_l^{G,n}=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}H(\mathbf{x})\,\overline{F_n^G(\mathbf{x})}\,\frac{dx_1dx_2}{x_0}. \tag{4.8}$$

Formulas (4.8) apply directly in the case L_G has discrete spectrum. When L_G has continuous spectrum, it is necessary to replace the sum over n by an integral.

Note: In the usual treatments of the Gel'fand–Graev integral transforms, our $I[f_l]$ is replaced by an integral over an arbitrary contour Γ on the cone $x_0^2-x_1^2-x_2^2=0$, which intersects every generator once. In this paper that contour is always chosen to be the circle $(x_0,x_1,x_2)=(1,-\sin\theta,\cos\theta)$.

We can view the transform (4.4) in another way: namely as the inner product of the functions $h_\mathbf{x}(\theta)$, $f(\theta)\in\mathcal{H}$,

$$F(\mathbf{x})=\langle h_\mathbf{x},f\rangle, \tag{4.9}$$
$$h_\mathbf{x}(\theta)=(x_0+x_1\sin\theta-x_2\cos\theta)^l\in\mathcal{H}.$$

Then the formula $F_n^G=\langle h_\mathbf{x},f_n^G\rangle$ yields immediately the expansion

$$h_\mathbf{x}(\theta)=\sum_n \overline{F}_n^G(\mathbf{x})f_n^G(\theta) \tag{4.10}$$

for the kernel function $h_\mathbf{x}(\theta)$. Furthermore, a direct computation yields the result

$$\langle h_\mathbf{x},h_\mathbf{y}\rangle=2\pi P_l(x_0y_0-x_1y_1-x_2y_2), \tag{4.11}$$

where $P_l(z)$ is a Legendre function. Substituting (4.10) into (4.11), we find

$$2\pi P_l(x_0y_0-x_1y_1-x_2y_2)=\sum_n \overline{F}_n^G(\mathbf{x})F_n^G(\mathbf{y}). \tag{4.12}$$

Finally, if two $\mathcal{H}$ bases $\{f_n^G\}$, $\{f_m^K\}$ are related by overlap functions $U_{n,m}^{G,K}$,

$$f_n^G=\sum_m U_{n,m}^{G,K}f_m^K,$$

it follows immediately that

$$F_n^G=\sum_m U_{n,m}^{G,K}F_m^K. \tag{4.13}$$

We now list the functions F_n^G for each choice of G. In several cases the integral $I[f_n^G]$ appears not to be known, and we have to make explicit use of the fact that, in each of the appropriate coordinates tabulated in Ref. 2, $I[f_n^G]$ satisfies a simple second order ordinary differential equation. Thus F_n^G can be expressed as products of solutions of such equations with coefficients determined by evaluating the integral for special values of the parameters $\mathbf{x}$. We now give explicit expressions for seven of the nine bases discussed.

A. Spherical system

$$F_m^S(a,\psi)=\int_0^{2\pi}[\cosh a-\sinh a\sin\theta\sin\psi-\sinh a\cos\theta\cos\psi]^{-l-1}\times\exp(im\theta)\,d\theta \tag{4.14}$$
$$=\frac{-1}{2\sqrt{2\pi}}\,\frac{\Gamma(l+1-m)}{\Gamma(l+1)}\,P_l^m(\cosh a)\exp(im\phi)$$

with $(x_0,x_1,x_2)=(\cosh a,\ -\sinh a\sin\psi,\ \sinh a\cos\psi)$, $0\le a<\infty$, $0\le\psi\le2\pi$.

B. Equidistant system

$$F_{\tau\epsilon}^{\mathrm{Eq}}(a,b)=\int_{-\infty}^{\infty}[\cosh a\cosh b\cosh q-\cosh a\sinh b\sinh q-\epsilon\sinh a]^{-l-1}\exp(i\tau q)\,dq$$
$$=\frac{4}{(\cosh a)^{1/2}}\exp[-i\pi(l+1/2)/4]\,\frac{\Gamma(l+1+i\tau)\Gamma(l+1-i\tau)}{\Gamma(l+1)}$$
$$\times P_{-1/2+i\tau}^{-(l+1/2)}(-\epsilon\tanh a)\exp(i\tau b) \tag{4.15}$$

with $(x_0,x_1,x_2)=(\cosh a\cosh b,\ -\sinh a,\ \cosh a\sinh b)$, $-\infty<a<\infty$, $-\infty<b<\infty$.

C. Horicyclic system

$$F_s^O(a,r)=\int_0^{2\pi}[\tfrac12(\exp(-a)+(r^2+1)\exp(a))-re^a\cos\theta-\tfrac12(\exp(-a)+(r^2-1)\exp(a))\sin\theta]^{-l-1}\times(2\cos^2\tfrac12\theta)^l\times\exp(is\tan\tfrac12\theta)\,d\theta$$
$$=\frac{2\sqrt{\pi}}{\Gamma(l+1)}\left|\frac{s}{2}\right|^{l+1/2}\exp(-a/2)K_{l+1/2}(e^{-a}|s|)\exp(isr) \tag{4.16}$$

with

$$(x_0,x_1,x_2)=(\tfrac12[\exp(-a)+(r^2+1)e^a],\ -\tfrac12[\exp(-a)+(r^2-1)e^a],\ re^a),\quad 0<r<\infty,\ -\infty<a<\infty.$$

D. Elliptic-parabolic system

$$F_\xi^{\mathrm{EP}}(a,\theta)=\alpha_\xi[2\cosh a\cos\theta]^{l+1}\times\int_0^{2\pi}[\cosh^2a+\cos^2\theta-\cos\phi(\cosh^2a+\cos^2\theta-2)-2\sin\phi\sinh a\sin\theta]^{-l-1}(\sin\tfrac12\phi)^l\times P_l^{i\xi}(\cos\tfrac12\phi)\,d\phi. \qquad (4.17)$$

Here,

$$x_0=\frac12\left(\frac{\cosh^2a+\cos^2\theta}{\cosh a\cos\theta}\right),$$

$$x_1=\frac12\left(\frac{\sin^2\theta-\sinh^2a}{\cosh a\cos\theta}\right),$$

$$x_2=-\frac{\sinh a\sin\theta}{\cosh a\cos\theta}.$$

Using Ref. 2 and symmetry in a and $i\theta$, we have

$$F_\xi^{\mathrm{EP}}(a,\theta)=A\,P_l^{i\xi}(\tanh a)P_l^{i\xi}(i\tan\theta)+B\,(P_l^{i\xi}(\tanh a)Q_l^{i\xi}(i\tan\theta)+Q_l^{i\xi}(\tanh a)\times P_l^{i\xi}(i\tan\theta))+C\,Q_l^{i\xi}(\tanh a)Q_l^{i\xi}(i\tan\theta). \qquad (4.18)$$

Setting $P_0=P_l(0)$, $P_0'=[dP_l(x)/dx]_{x=0}$, etc., (these values are listed explicitly in 8, Vol. 1), and computing $F_\xi^{\mathrm{EP}}(0,0)$, $\partial_aF_\xi^{\mathrm{EP}}(0,0)$, and $\partial_a\partial_\theta F_\xi^{\mathrm{EP}}(0,0)$ directly from (4.17) and from (4.18), we obtain the equations

$$\begin{pmatrix}P_0P_0 & P_0Q_0+Q_0P_0 & Q_0Q_0\\ P_0'P_0 & P_0'Q_0+Q_0'P_0 & Q_0'Q_0\\ P_0'P_0' & P_0'Q_0'+Q_0'P_0' & Q_0'Q_0'\end{pmatrix}\begin{pmatrix}A\\B\\C\end{pmatrix}=\begin{pmatrix}E_1\\0\\E_3\end{pmatrix}, \qquad (4.19)$$

where

$$E_1=\frac{\alpha_\xi 2^{2i\xi+1}\pi\,\Gamma((l+1+2i\xi)/2)\,\Gamma((l+1-2i\xi)/2)}{\Gamma(l+1)\,\Gamma(\frac12)\,\Gamma(l-2i\xi+2)/2)\,\Gamma((-l-2i\xi+1)/2)},$$

$$E_2=\frac{-\alpha_\xi 2^{l+3+2i\xi}\pi\,\Gamma((l+2-2i\xi)/2)\,\Gamma((l+2+2i\xi)/2)}{\Gamma(l+1)\,\Gamma(\frac12)\,\Gamma((l-2i\xi+1)/2)\,\Gamma((-l-2i\xi)/2)}.$$

Equations (4.19) can be solved via Cramer's rule to give explicit values for the constants A, B, C.

E. Elliptic system

$$F_{P,m}^{\mathrm{E}}(\alpha,\beta)=\int_0^{2\pi}[\mathrm{dn}\alpha\,\mathrm{dn}\beta-\mathrm{cn}\alpha\,\mathrm{cn}\beta\sin\theta+(i/\sqrt2)\,\mathrm{sn}\alpha\,\mathrm{sn}\beta\cos\theta]^{-l-1}\times(1+\cos^2\theta)^{1/2}\,Ep_l^m(z)\,d\theta. \qquad (4.20)$$

Here for simplicity the moduli of all elliptic and Lamé functions are chosen to be r, where $r=r'=1/\sqrt2$, and we have introduced coordinates α, β on the hyperboloid via the expressions

$$x_0=\sqrt2\,\mathrm{dn}\alpha\,\mathrm{dn}\beta,\quad x_1=-\mathrm{cn}\alpha\,\mathrm{cn}\beta,\quad x_2=-(i/\sqrt2)\,\mathrm{sn}\alpha\,\mathrm{sn}\beta,$$

$$0\le\alpha\le4K,\quad 0\le\beta<iK'$$

(see Ref. 3). The letter p in $Ep_l^m(z)$ stands for either c or s from expressions (3.8). Finally,

$$\mathrm{sn}(z,r)=\frac{-(1+k^2)^{1/2}\cos\theta}{(1+k^2\cos^2\theta)^{1/2}},\quad r=\frac{1}{\sqrt2},\quad k=1.$$

Making use of the facts that $F_{P,m}^{\mathrm{E}}(\alpha,\beta)$ is symmetric in α and β, that it satisfies the Lamé equation in α, and that $F_{P,m}^{\mathrm{E}}(\alpha,\beta)=F_{P,m}^{\mathrm{E}}(\alpha+4K,\beta)$, we easily obtain

$$F_{P,m}^{\mathrm{E}}(\alpha,\beta)=C_{P,m}Ep_l^m(\alpha)Ep_l^m(\beta), \qquad (4.21)$$

where the constant $C_{P,m}$ can be determined by evaluating the integral for a fixed choice of α and β.

Substituting this result into (4.12) and using the orthogonality relations for the elliptic basis, we obtain the integral

$$A_{P,m}Ep_l^m(\alpha')\overline{Ep_l^m(\beta)}Ep_l^m(\beta')=2\pi\int_0^{4K}P_l(2\,\mathrm{dn}\alpha\,\mathrm{dn}\alpha'\,\mathrm{dn}\beta\,\mathrm{dn}\beta'-\mathrm{cn}\alpha\,\mathrm{cn}\alpha'\,\mathrm{cn}\beta\,\mathrm{cn}\beta'-\tfrac12\,\mathrm{sn}\alpha\,\mathrm{sn}\alpha'\,\mathrm{sn}\beta\,\mathrm{sn}\beta')\times Ep_l^m(\alpha)\,d\alpha, \qquad (4.22)$$

where $A_{P,m}$ is a constant.

F. Semicircular parabolic system

$$F_{\lambda+}^{\mathrm{CP}}(\xi,\eta)=2\sqrt{\lambda}\,(2\xi\eta)^{l+1}\int_0^\infty\frac{J_{l+1/2}(\sqrt2\,\lambda v)\,v^{l+3/2}\,dv}{\{[v^2+(\xi-i\eta)^2][v^2+(\xi+i\eta)^2]\}^{l+1}}=\frac{2^{-2l}\lambda^{l+1}(2\pi\xi\eta)^{1/2}}{\Gamma(l+1)}J_{l+1/2}(\lambda\xi)K_{l+1/2}(\lambda\eta). \qquad (4.23)$$

The remaining integral is given by interchanging ξ and η, i.e.,

$$F_{\lambda-}^{\mathrm{CP}}(\xi,\eta)=F_{\lambda+}^{\mathrm{CP}}(\eta,\xi);$$

the coordinates on the hyperboloid are

$$x_0=\frac{(\xi^2+\eta^2)^2+4}{8\xi\eta},\quad x_1=\frac12\left(\frac{\eta}{\xi}-\frac{\xi}{\eta}\right),\quad x_2=\frac{(\xi^2+\eta^2)^2-4}{8\xi\eta}$$

with $\xi,\eta>0$.

G. Hyperbolic system

$$F_{m,i}^{\mathrm{H}}(\alpha,\beta)=(ir')^{l+1}\int_A^B F_l^m(v,r)\left(\frac{ir}{r'}\,\mathrm{cn}\alpha\,\mathrm{cn}\beta\,\mathrm{cn}v+rr'\,\mathrm{sn}\alpha\,\mathrm{sn}\beta\,\mathrm{sn}v+\frac{i}{r'}\,\mathrm{dn}\alpha\,\mathrm{dn}\beta\,\mathrm{dn}v\right)^{-l-1}dv=\lambda_m^iF_l^m(\alpha,r)F_l^m(\beta,r), \qquad (4.24)$$

where the integration region is over the appropriate side of the rectangle in Fig. 1 corresponding to the Hilbert space $\mathcal{H}^i$, e.g., if $i=1$, $(A,B)=(iK'+2K,\ iK')$.

The coordinates on the hyperboloid are

$$x_0=(ir/r')\,\mathrm{cn}(\alpha,r)\,\mathrm{cn}(\beta,r),$$

$$x_1=-ir\,\mathrm{sn}(\alpha,r)\,\mathrm{sn}(\beta,r),$$

$$x_2=(i/r')\,\mathrm{dn}(\alpha,r)\,\mathrm{dn}(\beta,r),$$

where $\alpha\in(iK',iK'+2K)$, $\beta\in(iK',-iK')$. The constants appearing in (4.24) are numbers which can in principle be determined by calculation in special cases of the integrand.

5. THE ROTATION GROUP IN AN ELLIPTIC BASIS

There has recently been an investigation by Patera and Winternitz[7] of the rotation group in a basis alternate to the usual one in which the component of angular momentum in a fixed direction is diagonalized. If the components of angular momentum are denoted by L_i $(i=1,2,3)$, satisfying the usual commutation relations $[L_i, L_j]=\epsilon_{ijk}L_k$, the operator which is diagonalized is $E=-4(L_1^2+r^2L_2^2)$, where $0<r^2<1$. In their work Patera and Winternitz examined the two variable realization on the sphere of $SO(3)$ and showed that in this basis the corresponding basis functions are ellipsoidal harmonics or products of Lamé polynomials as opposed to the conventional spherical harmonics in the canonical basis. The two-variable realization was discussed in detail in that paper together with the properties of the matrix relating the two bases. In that paper the authors were not, however, able to produce a realization of the single-variable model in which the basis functions were single Lamé polynomials. It is the purpose of this section to show that this can be done in a quite straightforward way. We also show how to relate the overlap coefficients to the coefficients of the Lamé polynomials.

The one-parameter model of the representations of the rotation group is realized on the space of polynomials $f(z)$ of order less than or equal to $2J$ (J = angular momentum) in the complex variable z. The invariant scalar product is so defined that

$$(z^{J-M}, z^{J-N})=(J-M)!\,(J+M)!\,\delta_{MN}. \tag{5.1}$$

A canonical basis in this realization (i.e., one in which L_3 is diagonal) is

$$f_M^J=\frac{z^{J-M}}{[(J-M)!\,(J+M)!]^{1/2}}, \quad -J\le M\le J. \tag{5.2}$$

The generators of $SO(3)$ are

$$L_1=\tfrac{1}{2}i(1-z^2)\frac{d}{dz}+iJz, \quad L_2=\tfrac{1}{2}(1+z^2)\frac{d}{dz}-Jz,$$

$$L_3=iz\frac{d}{dz}-iJ. \tag{5.3}$$

The operator E can then be written

$$E=[(1-r)z^2-(1+r)][(1+r)z^2-(1-r)]\frac{d^2}{dz^2}$$
$$+(2J-1)2z[1+r^2-z^2(1-r^2)]\frac{d}{dz}$$
$$+2J[1+r^2+(1-r^2)(2J-1)z^2]. \tag{5.4}$$

If we now write the eigenfunctions f of E in terms of new functions h, where

$$f(z)=(r')^J[(b-z^2)(1-bz^2)]^{J/2}h(z), \quad b=\frac{1+r}{1-r}, \tag{5.5}$$

and make the change of variable

$$\operatorname{sn}(w,r)=\frac{-i(1+b)z}{[(b-z^2)(1-bz^2)]^{1/2}}, \tag{5.6}$$

the operator E acting on the h functions has the form

$$\tfrac{1}{4}E=\frac{d^2}{dw^2}-r^2J(J+1)\operatorname{sn}^2(w,r). \tag{5.7}$$

The eigenvalue equation for E acting on the h functions is then the Lamé equation. The corresponding solutions are the Lamé polynomials. There are two cases to consider, viz., when J is even or odd.

Arscott[9] has shown that there are eight species of Lamé polynomials, four corresponding to even J and four to odd J. We shall consistently use his notation for the Lamé polynomials as it is very suggestive of the corresponding expansion of the Lamé polynomials in terms of Jacobi elliptic functions. In each case (J even or odd) the four corresponding polynomials form a complete basis for representation space. We now make these statements explicit.

Case 1, $J=2N$ $(N=1,2,\cdots)$

The complete basis set is

$$\Lambda_{Jm}^{++}=F^{2N}uE_{2N+2}^m(w), \quad \Lambda_{Jm}^{-+}=F^{2N}scE_{2N+2}^m(w),$$
$$\Lambda_{Jm}^{--}=F^{2N}sdE_{2N+2}^m(w), \quad \Lambda_{Jm}^{+-}=F^{2N}cdE_{2N+2}^m(w), \tag{5.8}$$

where $F=r'[(b-z^2)(1-bz^2)]^{1/2}$.

F can also be expressed in terms of w via Eq. (5.6), but we not do this here. The pair of discrete indices labeling the Λ functions are the eigenvalues of two discrete operators. The first of these is the reflection operator R which acts on functions f according to

$$Rf(z)=f(-z)$$

so that $R\Lambda_{Jm}^{pq}=p\Lambda_{Jm}^{pq}$. The second discrete label is related to the inversion operation I which acts on functions f according to

$$If(z)=z^{2J}f(1/z)$$

so that $I\Lambda_{Jm}^{pq}=q\Lambda_{Jm}^{pq}$. This method of labeling basis functions has been employed by Patera and Winternitz. The index m in each case labels the number of zeros of each Lamé polynomial appearing in the basis and hence also labels the basis vectors of a given type. For the basis function Λ_{Jm}^{++}, m lies in the range $0\le m\le N+1$; for all other basis functions we have the range $0\le m\le N$.

Case 2, $J=2N+1$ $(N=1,2,\cdots)$

The complete basis set is

$$\Lambda_{Jm}^{++}=F^{2N+1}cE_{2N+3}^m(w), \quad \Lambda_{Jm}^{+-}=F^{2N+1}dE_{2N+3}^m(w),$$
$$\Lambda_{Jm}^{--}=F^{2N+1}scdE_{2N+3}(w), \quad \Lambda_{Jm}^{-+}=F^{2N+1}sE_{2N+3}^m(w). \tag{5.9}$$

Here m varies between $0\le m\le N$ for Λ_{Jm}^{--} but varies between $0\le m\le N+1$ otherwise.

The calculation of the nonzero elements of the overlap matrix relating the E or Lamé basis to the canonical basis can be achieved by writing down the equation

$$\Lambda_{Jm}^{pq}=\sum_{M>0}(X_J^p)_{m,M}\frac{1}{[(J-M)!\,(J+M)!]^{1/2}}(z^{J-M}+pz^{J+M}), \tag{5.10}$$

where the summation extends over those M for which $(-1)^{J+M}=q$. All that is required is then the writing out of the left-hand side as a polynomial in z and equating coefficients. We shall illustrate this calculation in the particular case of the coefficient $(X_{2N}^{+})_{m,2q}$ corresponding to the basis function Λ_{2Nm}^{++} on the left-hand side of (5.10).

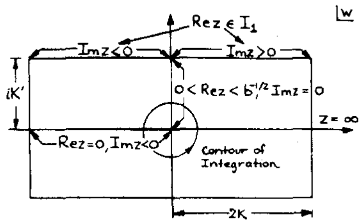

FIG. 2. The mapping $\operatorname{sn}w=-i(1+b)z/[(1-bz^2)(b-z^2)]^{1/2}$ in the w plane. In order to make this a single valued map, the z plane has two cuts along the intervals $I_1=[b^{-1/2}, b^{1/2}]$ and $I_2=[-b^{-1/2}, -b^{1/2}]$. The lines $w=2K+iv$ and $w=-2K+iv$ with $-K'<\operatorname{Im}v<K'$ are identified.

Written in terms of the variable z the basis function Λ^{++}_{2Nm} can be expressed in the form

$$\Lambda^{++}_{2N,m}=r'^{2N}\sum_{p=0}^{N}(-1)^p(1+b)^{2p}a^m_{2p}\times[(b-z^2)(1-bz^2)]^{N-p}z^{2p}, \tag{5.11}$$

where $uE^m_{2N+2}(w)=\sum_{p=0}^N a^m_{2p}\, sn^{2p}w$ and the coefficients satisfy the recurrence relations

$$\lambda^{++}_m a^m_0+2a^m_2=0,$$

$$(2N-2p+2)(2N+2p-1)r^2a^m_{2p-2}+[4(1+r^2)p^2-\lambda^{++}_m]a^m_{2p}-(2p+1)(2p+2)a^m_{2p+2}=0, \tag{5.12}$$

where $4\lambda^{++}_m$ is the eigenvalue of the operator E. Equating coefficients on both sides of (5.10), we obtain

$$(X^+_{2N})_{m,2q}=[(2N-2q)!(2N+2q)!]^{1/2}\sum_{p=0}^{N}2^{2p}a^m_{2p}\times\sum_{u,v}(-1)^{p+u+v}C\binom{N-p}{u}\binom{N-p}{v}(1+r)^{2N-p-u+v}(1-r)^{u-p-v}. \tag{5.13}$$

For $0\le p<N-q$ the u, v summation is over integers u, v such that $0\le u+v\le N-q-p$. For $N-q\le p\le N$, $u=v=0$. This expression then relates the overlap matrix to the coefficients a^m_{2p} of the expansion of Lamé polynomials in terms of Jacobi elliptic functions as given by Arscott. Similar calculations can be made for the other nonzero elements of the matrix $(X^p_J)_{m,M}$.

It is also possible to map the one-variable model we have examined thus far, into the two variable model of the rotation group realized as square integrable functions on the three-dimensional sphere. This is achieved by the following means. With each function $f(z)$ we associate a function on the sphere given by

$$F_J(\mathbf{x})=\frac{J!}{2\pi i}\int_C\left(\frac{\mathbf{x}\cdot\mathbf{v}}{z^2}\right)^J f(z)\frac{dz}{z}. \tag{5.14}$$

Here $\mathbf{x}$ is a point on the two-dimensional unit sphere, i.e., $\mathbf{x}=(x_1,x_2,x_3)$, $x_1^2+x_2^2+x_3^2=1$ and $\mathbf{v}=[\frac12 i(z^2-1), \frac12 i(z^2+1), z]$. The contour of integration is any closed path around the origin.

1. *Canonical basis*: Substituting the basis vector f^J_M in this expression, we get

$$F_{JM}(\theta,\phi)=\frac{(J!)^2}{(J-M)!(J+M)!}i^M P^J_{M0}(\cos\theta)\exp(-iM\phi), \tag{5.15}$$

where $P^J_{MN}(\cos\theta)$ is the matrix element of a rotation about the x axis in the canonical basis. The point $\mathbf{x}$ on the sphere is parametrized as

$$\mathbf{x}=(\sin\theta\cos\phi,\ \sin\theta\sin\phi,\ \cos\theta).$$

2. *The elliptic basis*: In this case it is convenient to make the change of variable indicated in Eq. (5.6). The resulting integral is then

$$F^{pq}_{Jm}(\alpha,\beta)=\frac{J!}{2\pi i}\int_C(1-r)^J[iK\operatorname{sn}\alpha\operatorname{sn}\beta\operatorname{sn}w-\operatorname{dn}\alpha\operatorname{dn}\beta\operatorname{dn}w-r\operatorname{cn}\alpha\operatorname{cn}\beta\operatorname{cn}w]^J(\operatorname{sn}w)^{-2J}E^{pq}_{Jm}(w)\frac{dw}{\operatorname{sn}w}, \tag{5.16}$$

where $E^{pq}_{Jm}(w)$ is one of the Lamé polynomials which form the particular basis for given J, e.g., $E^{++}_{2Nm}(w)=uE^m_{2N+2}(w)$. The integration is over a contour which encloses the origin in the w plane and lies strictly inside the square in the complex w plane with vertices $(2K, \pm iK')$ and $(2K, \pm iK')$. The situation is illustrated in Fig. 2, where the details of the mapping are shown together with a possible contour. The coordinates on the sphere are given by the relations

$$\mathbf{x}=((1/r')\operatorname{dn}(\alpha,r)\operatorname{dn}(\beta,r),\ -(ir/r')\operatorname{cn}(\alpha,r)\operatorname{cn}(\beta,r),\ -r\operatorname{sn}(\alpha,r)\operatorname{sn}(\beta,r))$$

with $\alpha\in(-2K, 2K)$, $\beta\in(-K, -K+2iK')$.

In each case the integral (5.16) and hence $F^{pq}_{Jm}(\alpha,\beta)$ is expressible in terms of a product of Lamé polynomials of the type appearing in the integral, e.g.,

$$F^{++}_{2Nm}(\alpha,\beta)=\lambda^m_N uE^m_{p2N+2}(\alpha,\beta)=\lambda\, uE^m_{2N+2}(\alpha)uE^m_{2N+2}(\beta),$$

where we have used the notation of Arscott for the product of two Lamé polynomials. In each case λ is a constant of proportionality which can in principle be calculated. This result can readily be obtained by considering the properties of the integral under the discrete operators R and I as well as using the fact that the integral satisfies the Laplace equation and is symmetric in α and β.

In order to make this a single valued map, the z plane has two cuts along the intervals $I_1=[b^{-1/2}, b^{1/2}]$ and $I_2=[-b^{-1/2}, -b^{1/2}]$. Because of the periodicity of the elliptic functions the lines $2K+iv$ and $-2K+iv$, where $-K'<v<K'$ are identified.

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Composition of coherent spin states

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Clebsch–Gordan coefficients for the $SU(2)$ group are computed in the coherent spin state basis introduced by Radcliffe.

Coherent spin states have previously been defined by Radcliffe.[1] This note is devoted to the calculation of Clebsch–Gordan coefficients in this new basis.

As is well known, coherent states for boson systems are defined according to

$$|\alpha\rangle = k\exp(\alpha a^{+})|0\rangle, \tag{1}$$

where k is a normalization factor, α a complex number, and a^{+} the boson creation operator. In very much the same way Radcliffe has defined coherent spin states $|s,\mu\rangle$ with total spin s according to

$$|s,\mu\rangle = \exp\mu S^{-}|0\rangle, \tag{2}$$

where μ runs over the entire complex plane. S^{-} creates spin deviation and $|0\rangle$ is the ground state $|s, m=s\rangle$. It is convenient[2,3] to introduce the Fock space built in the two-dimensional complex space $\mathbf{C}^2$ which is isomorphic to a space $\mathcal{J}$ of square integrable entire analytic functions[3] of two complex variables z and z':

$$f\in\mathcal{J} \Longleftrightarrow \begin{cases} f(z,z') = \sum\limits_{\substack{p\in\mathbf{N}\\ p'\in\mathbf{N}}} C_{pp'}(z^{p}/\sqrt{p!})(z'^{p'}/\sqrt{p'!}) \\ \|f\|^2 = \sum\limits_{\substack{p\in\mathbf{N}\\ p'\in\mathbf{N}}} C_{pp'}{}^2 < +\infty. \end{cases}$$

TABLE I. Particular values of $\langle s_1s_2, s, \lambda | s_1s_2, \mu_1\mu_2\rangle$.

	$s=0$	$s=1$		
$\frac12\otimes\frac12$	$(1/\sqrt{2})(\mu_2-\mu_1)$	$(1+\lambda^*\mu_1)(1+\lambda^*\mu_2)$		
	$s=\frac12$	$s=\frac32$		
$1\otimes\frac12$	$(\frac23)^{1/2}(\mu_2-\mu_1)(1+\lambda^*\mu_1)$	$(1+\lambda^*\mu_1)^2(1+\lambda^*\mu_2)$		
	$s=1$	$s=2$		
$\frac32\otimes\frac12$	$(\frac34)^{1/2}(\mu_2-\mu_1)(1+\lambda^*\mu_1)^2$	$(1+\lambda^*\mu_1)^3(1+\lambda^*\mu_2)$		
	$s=s_1-\frac12$	$s=s_1+\frac12$		
$s_1\otimes\frac12$	$[2s_1/(2s_1+1)]^{1/2}(\mu_2-\mu_1)(1+\lambda^*\mu_1)^{2s_1-1}$	$(1+\lambda^*\mu_1)^{2s_1}(1+\lambda^*\mu_2)$		
	$s=0$	$s=1$	$s=2$	
$1\otimes1$	$(1/\sqrt{3})(\mu_2-\mu_1)^2$	$(\mu_2-\mu_1)(1+\lambda^*\mu_1)(1+\lambda^*\mu_2)$	$(1+\lambda^*\mu_1)^2(1+\lambda^*\mu_2)^2$	
	$s=\frac12$	$s=\frac32$	$s=\frac52$	
$\frac32\otimes1$	$(1/\sqrt{2})(\mu_2-\mu_1)^2(1+\lambda^*\mu_1)$	$(6/5)^{1/2}(\mu_2-\mu_1)(1+\lambda^*\mu_1)^2(1+\lambda^*\mu_2)$	$(1+\lambda^*\mu_1)^3(1+\lambda^*\mu_2)^2$	
	$s=1$	$s=2$	$s=3$	
$2\otimes1$	$(3/5)^{1/2}(\mu_2-\mu_1)^2(1+\lambda^*\mu_1)^2$	$(4/3)^{1/2}(\mu_2-\mu_1)(1+\lambda^*\mu_1)^3(1+\lambda^*\mu_2)$	$(1+\lambda^*\mu_1)^4(1+\lambda^*\mu_2)^2$	
	$s=0$	$s=1$	$s=2$	$s=3$
$\frac32\otimes\frac32$	$\frac12(\mu_2-\mu_1)^3$	$(\frac{9}{10})^{1/2}(\mu_2-\mu_1)^2(1+\lambda^*\mu_1)$ $\times(1+\lambda^*\mu_2)$	$(\frac32)^{1/2}(\mu_2-\mu_1)^2(1+\lambda^*\mu_1)^2(1+\lambda^*\mu_2)^2$	$(1+\lambda^*\mu_1)^3(1+\lambda^*\mu_2)^3$
	$s=\frac12$	$s=\frac32$	$s=\frac52$	$s=\frac72$
$2\otimes\frac32$	$(2/5)^{1/2}(\mu_2-\mu_1)^3(1+\lambda^*\mu_1)$	$(6/5)^{1/2}(\mu_2-\mu_1)^2(1+\lambda^*\mu_1)^2$ $\times(1+\lambda^*\mu_2)$	$(12/7)^{1/2}(\mu_2-\mu_1)(1+\lambda^*\mu_1)^3(1+\lambda^*\mu_2)^2$	$(1+\lambda^*\mu_1)^4(1+\lambda^*\mu_2)^3$
	$s=1$	$s=2$	$s=3$	$s=4$
$\frac52\otimes\frac32$	$(1/\sqrt{2})(\mu_2-\mu_1)^3(1+\lambda^*\mu_1)^2$	$(10/7)^{1/2}(\mu_2-\mu_1)^2(1+\lambda^*\mu_1)^3$ $\times(1+\lambda^*\mu_2)$	$(15/8)^{1/2}(\mu_2-\mu_1)(1+\lambda^*\mu_1)^4(1+\lambda^*\mu_2)^2$	$(1+\lambda^*\mu_1)^5(1+\lambda^*\mu_2)^3$
	$s=\frac32$	$s=\frac52$	$s=\frac72$	$s=\frac92$
$3\otimes\frac32$	$(4/7)^{1/2}(\mu_2-\mu_1)^3(1+\lambda^*\mu_1)^3$	$(45/28)^{1/2}(\mu_2-\mu_1)^2(1+\lambda^*\mu_1)^4$ $\times(1+\lambda^*\mu_2)$	$\sqrt{2}(\mu_2-\mu_1)(1+\lambda^*\mu_1)^5(1+\lambda^*\mu_2)^2$	$(1+\lambda^*\mu_1)^6(1+\lambda^*\mu_2)^3$

In $\mathcal{J}$ the generators of $SU(2)$ are

$$S_1 = -\tfrac{1}{2}\left(z\frac{\partial}{\partial z'} + z'\frac{\partial}{\partial z}\right),$$
$$S_2 = -\frac{i}{2}\left(z\frac{\partial}{\partial z'} - z'\frac{\partial}{\partial z}\right), \tag{3}$$
$$S_3 = -\tfrac{1}{2}\left(z\frac{\partial}{\partial z} - z'\frac{\partial}{\partial z'}\right),$$

with $N = z(\partial/\partial z) + z'(\partial/\partial z')$ and $S^2 = \frac{1}{2}N(\frac{1}{2}N+1)$, where N is the operator "number of particles."

With this notation the states $|s, m=s\rangle$ such that

$$S^2|s,s\rangle = s(s+1)|s,s\rangle, \tag{4}$$
$$S^+|s,s\rangle = 0 \quad (S^+ = S_1 + iS_2), \tag{5}$$
$$\langle s,s|s,s\rangle = 1, \tag{6}$$

can be chosen as the homogeneous polynomials $V_{ss} = z'^{2s}/\sqrt{2s!}$. A coherent spin state is then defined according to

$$|s,\mu\rangle = \exp(\mu S^-)|s,s\rangle = (z' - \mu z)^{2s}/\sqrt{2s!}\ , \tag{7}$$

where $S^- = S_1 - iS_2 = -z(\partial/\partial z')$. Two such states $|S,\mu\rangle$ and $|s,\lambda\rangle$ are not orthogonal to one another. Their scalar product is

$$\langle s,\lambda|s,\mu\rangle = (1+\lambda^*\mu)^{2s}. \tag{8}$$

The essential property of such a set of states is its completeness

$$\int_{\mathbf{C}^2}|s,\mu\rangle\langle s,\mu|\,dM(\mu) = \sum_{m=-s}^{+s}|s,m\rangle\langle s,m| = \mathbb{1}_s, \tag{9}$$

where the weight is given by

$$dM(\mu) = [(2s+1)/\pi][d^2\mu/(1+|\mu|^2)^{2s+2}]. \tag{10}$$

The integration is carried out over the whole complex plane.

We now consider the addition of two spins $\mathbf{S}_1$ and $\mathbf{S}_2$. In the tensor product of two Bargmann's spaces $\mathcal{J}_1(z_1, z'_1)$ and $\mathcal{J}_2(z_2, z'_2)$ the infinitesimal generator of $SU(2)$ is

$$S = S_1 + S_2. \tag{11}$$

Looking for the vectors $|s_1s_2, s, s\rangle$ satisfying the relations (4), (5), and (6) among the eigenvectors of $\mathbf{S}_1^2$ [with the eigenvalue $s_1(s_1+1)$] and $\mathbf{S}_2^2$ [with the eigenvalue $s_2(s_2+1)$] one finds

$$|s_1s_2, s, s\rangle \propto z_1'^{\,s_1-s_2+s} z_2'^{\,s_2-s_1+s}(z_1z'_2 - z_2z'_1)^{s_1+s_2-s}. \tag{12}$$

The corresponding coherent spin states are calculated from the relation

$$\exp(\lambda s^-)|s_1s_2, s, s\rangle = |s_1s_2, s, \lambda\rangle. \tag{13}$$

With the notation $|s_1,\mu_1\rangle \otimes |s_2,\mu_2\rangle = |s_1s_2, \mu_1\mu_2\rangle$, one finds

$$\langle s_1s_2, s, \lambda|s_1s_2, \mu_1\mu_2\rangle = k(\mu_2-\mu_1)^{s_1+s_2-s}(1+\lambda^*\mu_1)^{s_1-s_2+s} \times (1+\lambda^*\mu_2)^{s_2-s_1+s}, \tag{14}$$

with

$$k = \left(\frac{(2s+1)!(2s_1)!(2s_2)!}{(s_1+s_2-s)!(s_1-s_2+s)!(s_2-s_1+s)!(s_1+s_2+s+1)!}\right)^{1/2}.$$

These polynomials are the coefficients of the expansion

$$|s_1s_2, \mu_1\mu_2\rangle = \sum_{s=|s_1-s_2|}^{s_1+s_2}\int dM(\lambda)|s_1s_2, s, \lambda\rangle\langle s_1s_2, s\lambda|s_1s_2, \mu_1\mu_2\rangle. \tag{15}$$

They are the "coherent" analogs of the well-known Clebsch–Gordan coefficients $\langle s_1s_2, s, m|s_1s_2, m_1m_2\rangle$. The connection between these two kinds of coefficients is given by the relation

$$\langle s_1s_2, s, \lambda|s_1s_2, \mu_1\mu_2\rangle = \sum_{m=-s}^{+s}\sum_{\substack{m_i=-s_i\\ i=1,2}}^{+s_i}\binom{2s}{s-m}^{1/2}\binom{2s_1}{s_1-m_1}^{1/2}\binom{2s_2}{s_2-m_2}^{1/2} \times \lambda^{*s-m}\mu_1^{\,s_1-m_1}\mu_2^{\,s_2-m_2}\langle s_1s_2, s, m|s_1s_2, m_1m_2\rangle. \tag{16}$$

Particular cases of formulas are listed in Table I.

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Null electromagnetic fields in spaces of high symmetry

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The paper investigates the solutions of Maxwell–Einstein equations for null electromagnetic fields with or without matter in case of spaces of high symmetry. For the spherically symmetric space no such solution exists, while for cylindrically symmetric spaces, there arises a wide variety of situations. In reality, for the solutions that emerge, the spaces should more appropriately be termed plane symmetric. Some solutions are exhibited.

I. THE SPHERICALLY SYMMETRIC SPACE

It is well known that if one assumes the space to be spherically symmetric, then one cannot have a solution of the Einstein—Maxwell equations corresponding to a radially expanding field of pure electromagnetic radiation. Thus with the line element

$$dz^2 = -e^{\lambda}dr^2 - r^2 d\Omega^2 + e^{\nu}dt^2, \tag{1}$$

where λ and ν are functions of r and t, the equations

$$R_{\mu\nu} - \tfrac{1}{2}Rg_{\mu\nu} = -8\pi[(1/4\pi)F_{\mu\alpha}F^{\alpha}{}_{\nu}], \tag{2}$$

$$*F^{\mu\alpha}{}_{;\alpha} = F^{\mu\alpha}{}_{;\alpha} = 0, \quad *F^{\mu\alpha}F_{\mu\alpha} = F^{\mu\alpha}F_{\mu\alpha} = 0 \tag{3}$$

do not have any nontrivial solution. Vaidya[1] by relaxing the Maxwell conditions for a charge free space did obtain a solution in which the current vector is null. Such a current may be interpreted as a charge moving with the velocity of light.[2]

A charge moving with the velocity of light and having no rest mass: This may not conflict with the equations of Maxwell and Einstein; nevertheless, the idea is unconventional and foreign to physics as we know it right now. It seems therefore interesting to investigate whether other solutions exist where the Einstein-Maxwell equations are rigorously satisfied but the energy tensor may be modified in a more conventional manner by the presence of ponderable matter.

For the discussion of null fields it is more convenient to take the line element in the form

$$dz^2 = B du^2 + 2A du dr - r^2 d\Omega^2, \tag{4}$$

where r is now a null coordinate and A, B are functions of u and r. It is easy to verify by direct calculation that the null vector $K^{\mu} = \delta^{\mu}_1$ is geodetic and shear free. Hence from Robinson's theorem[3] we may construct a null electromagnetic field tensor of the form

$$F_{\mu\nu} = \alpha[K_{\mu}(a_{\nu}\cos\beta + b_{\nu}\sin\beta) - K_{\nu}(a_{\mu}\cos\beta + b_{\mu}\sin\beta)] \tag{5}$$

which will satisfy the Maxwell equations. α and β in the above expression are the "amplitude" and "polarization" factors and the unit spacelike vectors a^{ν} and b^{ν} are given by

$$a^{\nu} = r^{-1}\delta^{\nu}_2, \quad b^{\nu} = (r\sin\theta)^{-1}\delta^{\nu}_3,$$

where we have numbered the coordinates u, r, θ, ϕ as $0, 1, 2, 3$, respectively. The Maxwell equations now give after some algebraic simplifications

$$\sin\theta\beta_{,2} + (\alpha_3/\alpha) = 0, \tag{6}$$

$$(\alpha_{,2}/\alpha)\sin\theta + \cos\theta + \beta_{,3} = 0. \tag{7}$$

The above two equations do not possess any solution with α independent of the angle coordinates. Thus the only nonvanishing energy tensor component of the field T_{00} $(=2\alpha^2K_0^2)$ would be angle-dependent. Thus if the Einstein gravitational equations are to be satisfied there must be an angle-dependent matter distribution compensating for the above dependence. However, the actual situation is even more complicated. The general solution of Eqs. (6) and (7) is given by

$$\alpha\sin\theta = \exp[f(u-\phi) + g(u+\phi)],$$

where

$$\beta = f'(u-\varphi) - g'(u+\phi)$$

$$u = \log\tan\theta/2,$$

and f and g indicate arbitrary functions of their arguments. The radiation energy tensor will thus have singularities in particular directions.

II. THE CYLINDRICALLY SYMMETRIC SPACES

(A) The simplest case of cylindrical symmetry corresponds to the Marder metric

$$dz^2 = \exp[2(\gamma-\psi)](dt^2 - dr^2) - \exp(-2\psi)r^2 d\varphi^2 - \exp[2(\psi+\mu)]dZ^2. \tag{8}$$

The above line element may also be written

$$dz^2 = 2\exp[2(\gamma-\psi)]d\eta d\xi - \exp(-2\psi)(\eta-\xi)^2 d\varphi^2 - \exp[2(\psi+\mu)]dZ^2, \tag{9}$$

where η, ξ are both null coordinates. We shall number the coordinates ξ, η, ϕ, Z as $0, 1, 2, 3$ and consider the null vector $K^{\mu} = \delta^{\mu}_1$. The vector is geodetic and the condition of vanishing shear gives

$$2\psi_1 + \mu_1 - (\eta-\xi)^{-1} = 0, \tag{10}$$

where the subscripts indicate differentiation with respect to the coordinate concerned. Equation (10) integrates to

$$\exp(2\psi+\mu)/(\mu-\xi) = f_1(\xi), \tag{11}$$

where $f_1(\xi)$ is an arbitrary function of ξ. The nonvanishing $R_{\mu\nu}$'s are

$$R_{11} = [\psi_1 - (\eta-\xi)^{-1}]^2 + (\psi_1+\mu_1)^2 - 2(\gamma_1-\psi_1)[\mu_1 + (\eta-\xi)^{-1}] + [\mu_1 + (\eta-\xi)^{-1}]_{,1}, \tag{12}$$

$$R_{00} = [\psi_0 + (\eta-\xi)^{-1}]^2 + (\psi_0+\mu_0)^2 - 2(\gamma_0-\psi_0)[\mu_0 - (\eta-\xi)^{-1}] + [\mu_0 - (\eta-\xi)^{-1}]_{,0}, \tag{13}$$

$$R_{01}=[\psi_0+(\eta-\xi)^{-1}][\psi_1-(\eta-\xi)^{-1}]+(\psi_0+\mu_0)(\psi_1+\mu_1)+[2\gamma_0-2\psi_0+\mu_0-(\eta-\xi)^{-1}]_{,1}, \quad (14)$$

$$R_{22}[\exp(2\gamma)/(\eta-\xi)^2]=2\psi_{10}+\mu_0[\psi_1-(\eta-\xi)^{-1}]+\psi_0[\mu_1+(\eta-\xi)^{-1}]+(\eta-\xi)^{-1}\times(\mu_1-\psi_1), \quad (15)$$

$$R_{33}\exp[-2(2\psi+\mu-\gamma)]=-2(\psi_{01}+\mu_{01})-\psi_0[\mu_1+(\eta-\xi)^{-1}]-\mu_0[\psi_1+(\eta-\xi)^{-1}]-2\mu_0\mu_1+(\eta-\xi)^{-1}(\psi_1+\mu_1). \quad (16)$$

III. THE ENERGY STRESS TENSOR AND THE FIELD EQUATIONS

We have

$$T_{\mu\nu}=(T_{\mu\nu})_{\text{rad}}+(T_{\mu\nu})_{\text{mat}}, \quad (17)$$

$$(T_{\mu\nu})_{\text{rad}}=+2\alpha^2\kappa_0^2\delta_{\mu0}\delta_{\nu0},$$
$$(T_{\mu\nu})_{\text{mat}}=(p+\rho)v_\mu v_\nu-pg_{\mu\nu}, \quad (18)$$

where we have assumed the matter to be a perfect fluid. If now the only nonvanishing v^μ's are v^0 and v^1, we get

$$v^1v_1=v^0v_0=\tfrac{1}{2}, \quad (19)$$

$$(T_{11})_{\text{mat}}=(p+\rho)v_1^2, \quad (20)$$

$$(T_2^2)_{\text{mat}}=(T_3^3)_{\text{mat}}=-p,$$
$$(T_1^1)_{\text{mat}}=(T_0^0)_{\text{mat}}=\tfrac{1}{2}(\rho-\phi), \quad (21)$$

so that finally

$$R_2^2=R_3^3=(8\pi/2)(\rho-\phi), \quad (22)$$

$$g^{01}R_{01}=R_1^1=R_0^0=-8\pi p, \quad (23)$$

$$R_{00}=-2\alpha^2K_0^2-8\pi(p+\rho)v_0^2, \quad (24)$$

$$R_{11}=-8\pi T_{11}=-8\pi(p+\rho)v_1^2. \quad (25)$$

The null electromagnetic field is given by

$$F_{\mu\nu}=\alpha[K_\mu(a_\nu\cos\beta+b_\nu\sin\beta)-K_\nu(a_\mu\cos\beta+b_\mu\sin\beta)],$$

where

$$a_\alpha=\exp(-\psi)(\eta-\xi)\delta_{2\alpha},$$
$$b_\alpha=\exp(\psi+\mu)\delta_{3\alpha}.$$

The Maxwell equations give

(i) β is an arbitrary functions of ξ alone

(ii) $\alpha=G(\xi)\exp(\psi)/(\eta-\xi)\exp(2\gamma-2\psi)$,

where $G(\xi)$ is an arbitrary function of ξ.

The electromagnetic energy-stress tensor $T_{\mu\nu}$ has only one nonvanishing component:

$$T_{00}=H(\xi)\exp(2\psi)/(\eta-\xi)^2,$$

where $H(\xi)$ is a positive function of ξ.

The condition $R_2^2=R_3^3$ gives, using (15), (16), and (10),

$$[\psi_1-(\eta-\xi)^{-1}][\mu_0+2\psi_0+(\eta-\xi)^{-1}]=0, \quad (26)$$

so that either

$$\psi_1-(\eta-\xi)^{-1}=0 \quad (27a)$$

or

$$\mu_0+2\psi_0+(\eta-\xi)^{-1}=0. \quad (27b)$$

With (27a) satisfied, R_2^2, R_3^3, as well as R_{11} vanish so that this is consistent only with a pure radiation field as is evident from equation (22), and (25). The complete solution in this case can be easily obtained. From equations (27a), (10), and (11),

$$e^\psi=f_2(\xi)(\eta-\xi), \quad (28)$$

$$e^\mu=f_3(\xi)(\eta-\xi), \quad f_3(\xi)=f_1/f_2^2. \quad (29)$$

From Eq. (23) R_{01} would vanish for the pure radiation field and this gives

$$e^\nu=(\eta-\xi)f_4(\xi)g_1(\eta). \quad (30)$$

Substitution into (24) and (13) gives α^2 in terms of the functions of ξ.

In case (27b) is satisfied, Eq. (11) becomes

$$\exp(2\psi+\mu)/(\eta-\xi)=\text{const.} \quad (31)$$

The field may now be either a pure radiation field or be associated with matter. For the pure radiation field $R_2^2=R_3^3=0$ and $R_2^2+R_3^3=0$ gives

$$\mu_{01}+[\mu_0/(\eta-\xi)]+\mu_0\mu_1-[\mu_1/(\eta-\xi)]=0, \quad (32)$$

which integrates to

$$e^\mu(\eta-\xi)=f_5(\xi)+g_2(\eta), \quad (33)$$

so that from (31)

$$e^\psi=(\eta-\xi)/(f_5+g_2)^{1/2}. \quad (34)$$

The vanishing of R_{11} and R_{01} gives, using Eqs. (10) and (27b)

$$\lambda_1+2(\gamma_1-\psi_1)-(\lambda_{11}/\lambda_1)=0, \quad (35)$$

$$\lambda_0\lambda_1+[\gamma_1-2\psi_1+(\eta-\xi)^{-1}]_{,0}=0, \quad (36)$$

where

$$\lambda=\psi-\log(\eta-\xi). \quad (37)$$

Eliminating γ_1 from Eqs. (35) and (36), one gets

$$\lambda_0\lambda_1+[-\tfrac{3}{2}\lambda_1+\tfrac{1}{2}(\lambda_{11}/\lambda_1)]_{,0}=0. \quad (38)$$

In view of (34) and (37), Eq. (38) is identically satisfied and Eq. (35) gives

$$e^\gamma=[(g_2')^{1/2}f_6/(f_5+g_2)^{3/4}](\eta-\xi).$$

We then get from (24) and (13) α^2 in terms of f_6, f_5 and their derivatives.

In case there is a fluid along with radiation, the field equations may be written as

$$-8\pi H(\xi)\exp(2\lambda)-8\pi(p+\rho)v_0^2=R_{00}=2\lambda_0^2=4(\nu_0-\lambda_0)\lambda_0-2\lambda_{00}, \quad (39)$$

$$-8\pi(p+\rho)v_1^2=R_{11}=2\lambda_1^2+4(\nu_1-\lambda_1)\lambda_1-2\lambda_{11}, \quad (40)$$

$$4\pi(\rho-p)=R_2^2=-2\exp[2(\lambda-\nu)](\lambda_{10}-2\lambda_0\lambda_1), \quad (41)$$

$$2g^{01}(\lambda_0\lambda_1+\nu_{10}-2\lambda_{10})=-8\pi p, \quad (42)$$

where

$$\nu=\gamma-\log(\eta-\xi).$$

Physically the integration of the set would require a knowledge of the equation of state—in any case the integration looks difficult. We have been able to find a mathematical solution which however gives a value of p/ρ greater than $\frac{1}{3}$. The solution is as follows:

$$e^{\lambda}=(\xi+\eta)^{-1}, \quad e^{\nu}=(\xi+\eta)^{\alpha},$$

$$8\pi p=2(\xi+\eta)^{-2(2+\alpha)}(1+\alpha),$$

$$8\pi p=2(\xi+\eta)^{-2(2+\alpha)}(3+\alpha),$$

$$v_1^2=[(\alpha+1)/(2+\alpha)](\xi+\eta)^{2(1+\alpha)},$$

$$v_0^2=\tfrac{1}{4}[(2+\alpha)/(\alpha+1)](\xi+\eta)^{2(1+\alpha)},$$

$$8\pi H(\xi)=\alpha(3\alpha+4)/(\alpha+1)$$

so that for H to be positive α must be greater than 0.

(B) Dutta and Raychaudhuri[4] considered stationary null fields for which they took the line element in the form

$$dz^2=f\,dt^2-\exp(2\psi)(dx^2+dy^2)-l\,dZ^2+2m\,dZ\,dt, \tag{43}$$

where f, ψ, l, m are considered functions of x alone. We shall number the coordinates t, x, y, z as 0, 1, 2, 3, respectively. The null vector is taken to have components K^0 and K^3 only. The condition that the vector is null gives

$$-l\alpha^2+2m\alpha+f=0, \tag{44}$$

where

$$\alpha=K^3/K^0. \tag{45}$$

Thus

$$\alpha=[m\mp(m^2+fl)^{1/2}]/l. \tag{46}$$

Again the condition that the vector is geodetic gives

$$-l_1\alpha^2+2m_1\alpha+f_1=0. \tag{47}$$

As the quadratics (44) and (45) must have a common root, this root may be written as

$$\alpha=-\tfrac{1}{2}(v_1/u_1), \tag{48}$$

where we have written

$$v=f/l, \quad u=m/l. \tag{49}$$

Differentiating (46) and eliminating v_1 with the help of (48), we get $\alpha_1=0$ so that Eq. (48) integrates to

$$f/l=-2\alpha(m/l)+b. \tag{50}$$

Substituting from (50) in (46), we get

$$f/l=-2\alpha(m/l)+\alpha^2. \tag{51}$$

If now the energy-stress tensor be due to this null field alone, $R_1^1=R_2^2=0$ and we get

$$e^{\psi}=Ax^b \tag{52}$$

and

$$f_1l_1+m_1^2=-4b. \tag{53}$$

Substituting from (51) in (53), we get

$$(f_1+\alpha m_1)^2=-4b\alpha^2$$

so that b must be negative, say $-c^2$. Integrating we get

$$f+\alpha m=2c\alpha x+d. \tag{54}$$

Combining (51) with (54)

$$m=\alpha l-2cx-(d/\alpha), \tag{55}$$

$$f=4c\alpha x+2d-\alpha^2 l, \tag{56}$$

so that

$$fl+m^2=[2cx+(d/\alpha)]^2.$$

Making a suitable transformation, we may now write

$$fl+m^2=x^2, \tag{57}$$

$$m=\alpha l\pm x, \tag{58}$$

$$f=-\alpha^2 l\mp 2\alpha x, \tag{59}$$

$$e^{\psi}=x^{-1/4}. \tag{60}$$

IV. THE ELECTROMAGNETIC FIELD AND THE FIELD EQUATIONS

The vector K^μ is already shear free and the null electromagnetic field is of the form

$$F_{\mu\nu}=K_\mu(a_\nu\cos\beta+b_\nu\sin\beta)-K_\nu(a_\mu\cos\beta+b_\mu\sin\beta), \tag{61}$$

with

$$a_\alpha=e^{\psi}\delta_{\alpha 1}, \quad b_\alpha=e^{\psi}\delta_{\alpha 2}. \tag{62}$$

The Maxwell equations give

$$\beta=By+C \tag{63}$$

and

$$K^3=A\exp(Bx)/x^{3/4}, \tag{64}$$

where A and B are constants and C is an arbitrary function of the argument $(z-\alpha t)$. The Einstein equations now give

$$x\psi_{11}-\psi_1-(2x)^{-1}(f_1l_1+m_1^2)=0, \tag{65}$$

$$x\psi_{11}+\psi_1=0, \tag{66}$$

$$[2(-g)^{1/2}]^{-1}[(fl_1+mm_1)/x]_{,1}=2K^3K_3, \tag{67}$$

$$[2(-g)^{1/2}]^{-1}[(lf_1+mm_1)/x]_{,1}=2K^0K_0, \tag{68}$$

$$[2(-g)^{1/2}]^{-1}[(mf_1-fm_1)/x]_{,1}=2K^3K_0, \tag{69}$$

$$[2(-g)^{1/2}]^{-1}[(lm_1-ml)/x]_{,1}=2K^0K_3. \tag{70}$$

Equations (65) and (66) have already been dealt with. Equation (67) gives, using Eqs. (58), (59), and (64),

$$l/x=-(4A^2/\alpha^3)f(x)+b\log x+c, \tag{71}$$

with

$$f(x)=\int[\exp(2Bx)/2Bx]\,dx \quad \text{if } B\neq 0$$

and

$$f(x)=x \quad \text{if } B=0.$$

The solution (71) was given by Dutta and Raychaudhuri for the case $B=0$.

The solutions as given above break down for $l=0$. In that case one gets

$$K^3=A/x^{3/4},$$

$$K_0=Ax^{1/4},$$

and the field equations give

$$f/x = 4A^2x + B\log x + c,$$

$$m = x.$$

V. CONCLUDING REMARKS

While in the usual cosmologies, one either considers a pure matter universe or one which has besides a distribution of blackbody radiation; it seems plausible that in the earlier epochs nonequilibrium processes led to a directed flux of radiation in a background distribution of matter. The present investigation was motivated by a desire to throw some light on such situations. However, so far we have been able to present only pure radiation solutions and they too exhibit unwelcome singularities. It seems that the solutions that we envisage would require space—times of lesser symmetry.

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Superpropagators as boundary values of analytic distributions

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In this paper we give a rigorous analysis for defining a class of superpropagators as boundary values of analytic distributions and discuss the ambiguities connected with this definition.

I. INTRODUCTION

Ambiguities[1] are inherent in the construction of superpropagators of nonpolynomial Lagrangian field theories,[1,2] and in the many approaches that have been proposed for evaluating the superpropagators the sources of the ambiguity appear to be different. For example, in the Mellin transform approach[1,3] there is nonuniqueness in interpolating the Taylor coefficients of the superpropagators by an analytic function or in the continuation of the coupling constant which is employed when the Mellin transform does not converge. In general, to fix the arbitrariness it is necessary to impose physical requirements, one of them being unitarity which fixes the imaginary part. For the exponential interactions[4] the arbitrariness in the real part is eliminated by demanding "minimally singular" behavior of the solution.

In this paper we should like to examine the problem of the definition of a class of superpropagators as boundary values of analytic distributions and discuss the ambiguities linked with this procedure. We analyze the superpropagators rigorously in the correct distribution theory framework, thereby avoiding difficulties connected with the Euclidicity postulate[3] and methods like the Mellin transform approach. We show that the ambiguities arise because of the existence of a brach point in the analytic distribution whose boundary value is the superpropagator.

II. SUPERPROPAGATORS AS DISTRIBUTIONS

The superpropagator of a massless theory with Lagrangian of interaction $L_{\text{int}}(\phi)$ is given by

$$\Phi[\kappa^2 D(x_1-x_2)] = \langle 0 |\, T\{L_{\text{int}}[\phi(x_1)]L_{\text{int}}[\phi(x_2)]\}\,| 0\rangle \qquad (2.1)$$

$$= \sum_{n=2}^{\infty} C_n[\kappa^2 D(x_1-x_2)]^n,$$

where $D(x)=1/(-x^2+iO)$ is the causal propagator (the numerical factor $1/4\pi^2$ has been absorbed in the coupling constant κ^2).

As a distribution $\Phi[\kappa^2/(-x^2+iO)]$ is by definition the boundary value (as $Y\to 0^+$) of $\Phi[\kappa^2/(-x^2+iY)]$ on the real axis of the plane $P=-x^2+iY$, where Y is a positive definite real form. The distribution $\Phi[\kappa^2/(-x^2+iY)]$ can be obtained in the upper half-plane of P by the analytic continuation of its values on a half-line of some argument θ, where $\theta=\theta_0+2\pi m$ and $0<\theta_0<\pi$ (m integer). Thus the problem reduces to defining $\Phi[\kappa^2/(e^{i\theta}\tau)]$ as a distribution, where $\tau=a_{\mu\nu}x_\mu x_\nu$ is a positive definite real form. This can be done under the following two conditions:

(a) $\Phi(z)$ is an entire function of z, of order of growth $\rho>0$ and type σ.

(b) There is a θ, as specified before, such that $\tau^{2-\epsilon}\Phi[\kappa^2/(e^{i\theta}\tau)]$ is continuous in x_μ ($\epsilon>0$).

The exponential-type interactions satisfy these conditions whereas the rational interactions violate the first condition.

The procedure for evaluating the superpropagators is thus split into three steps, shown schematically as follows:

Step 1: $\left(\Phi\ \dfrac{\kappa^2}{e^{i\theta}\tau}\right)$ Define and evaluate

Step 2: $\longrightarrow \Phi\left(\dfrac{\kappa^2}{-x^2+iY}\right)$ Analytically continue

Step 3: $\longrightarrow \Phi\left(\dfrac{\kappa^2}{-x^2+i0}\right)$. Boundary value as $Y\to 0^+$

Step 1: Since $\Phi[\kappa^2/(e^{i\theta}\tau)]$ satisfies condition (b), it is locally summable and therefore defines a regular distribution by

$$I=\langle\Phi(\kappa^2/e^{i\theta}\tau),\ \varphi\rangle = \int dx\,\Phi(\kappa^2/e^{i\theta}\tau)\varphi(x), \qquad (2.2)$$

where φ belongs to some test function space (e.g., the S-type spaces).[5]

Let $x_\mu=b_{\mu\nu}x'_\nu$ such that

$$b_{\mu\nu}a_{\mu\rho}b_{\rho\sigma}=\kappa^2\delta_{\nu\sigma}; \qquad (2.3)$$

then

$$I=(\det b)\int dx\Phi(e^{-i\theta}/r^2)f(x), \qquad (2.4)$$

where $r^2=x_0^2+x_1^2+x_2^2+x_3^2$ and $f(x)=\varphi(bx)$.

For convenience, in the following we write $\Delta=e^{-i\theta}/r^2$ and consider

$$E\equiv\int dx\,\Phi(\Delta)f(x)$$
$$=\int dx[\Phi(\Delta)-C_2\Delta^2][f(x)-f(0)\Theta(1-r)]$$
$$+f(0)\int dx\,\Phi(\Delta)\Theta(1-r)$$
$$+C_2\int dx\Delta^2[f(x)-f(0)\Theta(1-r)]$$

$$= \int dx[\Phi(\Delta) - C_2\Delta^2 - C_3\Delta^3][f(x) - f(0)\Theta(1-r) - (1/2!)x_\mu x_\nu f_{\mu\nu}(0)\Theta(1-r)] + f(0)\int dx\,\Phi(\Delta)\Theta(1-r) + (1/2!)f_{\mu\nu}(0) \times \int dx\, x_\mu x_\nu[\Phi(\Delta) - C_2\Delta^2]\Theta(1-r) + C_2\int dx\Delta^2[f(x) - f(0)\Theta(1-r)] + C_3\int dx\Delta^3[f(x) - f(0)\Theta(1-r) - (1/2!)x_\mu x_\nu f_{\mu\nu}(0)\Theta(1-r)], \quad (2.5)$$

where $f_{\mu\nu\cdots\lambda}(0) = \partial_\mu\partial_\nu\cdots\partial_\lambda f(0)$.

Continuing in this way we obtain

$$E = \int dx\left(\Phi(\Delta) - \sum_{n=2}^{\infty} C_n\Delta^n\right)\left(f(x) - \sum_{n=2}^{\infty}\frac{1}{(2n-4)!} \times x_{\mu_1}\cdots x_{\mu_{2n-4}} f_{\mu_1\cdots\mu_{2n-4}}(0)\Theta(1-r)\right) + \sum_{n=2}^{\infty} C_n\int dx\Delta^n\left(f(x) - \sum_{l=2}^{n}\frac{1}{(2l-4)!} \times x_{\mu_1}\cdots x_{\mu_{2l-4}} f_{\mu_1\cdots\mu_{2l-4}}(0)\Theta(1-r)\right) + \sum_{n=2}^{\infty}\frac{1}{(2n-4)!}f_{\mu_1\cdots\mu_{2n-4}}(0)\int_{r\le 1} dx\, x_{\mu_1}\cdots x_{\mu_{2n-4}} \times\left(\Phi(\Delta) - \sum_{l=2}^{n-1}C_l\Delta^l\right). \quad (2.6)$$

The first term in the above equation is defined as

$$\lim_{N\to\infty}\int dx\left(\Phi(\Delta) - \sum_{n=2}^{N}C_n\Delta^n\right)\left(f(x) - \sum_{n=2}^{N}\frac{1}{(2n-4)!} \times x_{\mu_1}\cdots x_{\mu_{2n-4}}f_{\mu_1\cdots\mu_{2n-4}}(0)\Theta(1-r)\right)$$

$$= \lim_{N\to\infty}\int_{r\ge 1} dx\left(\Phi(\Delta) - \sum_{n=2}^{N}C_n\Delta^n\right)f(x) + \lim_{N\to\infty}\int_{r\le 1}dx\left(\Phi(\Delta) - \sum_{n=2}^{N}C_n\Delta^n\right)\frac{1}{(2n-2)!} \times x_{\mu_1}\cdots x_{\mu_{2N-2}}f_{\mu_1\cdots\mu_{2N-2}}(\lambda x),$$

where $0 \le \lambda \le 1$. (2.7)

Condition (a) ensures the vanishing of the first term in Eq. (2.7) as $N\to\infty$. For the second term we consider

$$\Psi = \int_{r\le 1}dx\left(\Phi(\Delta) - \sum_{n=2}^{N}C_n\Delta^n\right)\frac{1}{(2N-2)!} \times x_{\mu_1}\cdots x_{\mu_{2N-2}}f_{\mu_1\cdots\mu_{2N-2}}(\lambda x)$$

$$= \int_{r=0}^{1}dr\, r^{2N+1}\left(\Phi\left(\frac{e^{-i\theta}}{r^2}\right) - \sum_{n=2}^{N}C_n e^{-in\theta}r^{-2n}\right)F_N(r^2), \quad (2.8)$$

where $F_N(r^2) = \int[d\Omega/(2N-2)!]\eta_{\mu_1}\cdots\eta_{\mu_{2N-2}}f_{\mu_1\cdots\mu_{2N-2}}(\lambda x)$ is the integral over the angular variables and η_μ are the direction cosines.

If $\varphi \in S^\beta$,[5] then

$$|f^{(2N-2)}(x)| \le AB^{2N-2}(2N-2)^{\beta(2N-2)}, \quad (2.9)$$

where $f^{(\kappa)}(x)$ is a κth derivative of $f(x)$. Thus

$$|F_N(r^2)| \le CB^{(2N-2)}(2N-2)^{\beta(2N-2)}/(2N-3)!. \quad (2.10)$$

By condition (b), splitting the range of integration in Eq. (2.8) into $(0, N^{-1/\rho})$ and $(N^{-1/\rho}, 1)$ and applying the first law of mean for integrals, we obtain

$$|\Psi| \le \tfrac{1}{2}N^{-1/\rho}|F_N(\mu)|\left[\mu^N\left|\Phi\left(\frac{e^{-i\theta}}{\mu}\right)\right| + \sum_{n=2}^{N}|C_n|\mu^{N-n}\right] + \tfrac{1}{2}(1-N^{-1/\rho})|F_N(\xi)|\sum_{n=N+1}^{\infty}|C_n|\xi^{N-n}, \quad (2.11)$$

where μ and ξ are obviously N-dependent and satisfy $0 \le \mu \le N^{-1/\rho} \le \xi \le 1$.

By Eq. (2.10)

$$|\Psi| \le \frac{C'B^{2N-2}(2N-2)^{\beta(2N-2)}}{(2N-3)!}\left[\mu^N\left|\Phi\left(\frac{e^{-i\theta}}{\mu}\right)\right|N^{-1/\rho} + N^{-1/\rho}\sum_{n=2}^{N}|C_n|\mu^{N-n} + \sum_{n=N+1}|C_n|\xi^{N-n}\right]. \quad (2.12)$$

Condition (b) implies that

$$\mu^N\left|\Phi\left(\frac{e^{-i\theta}}{\mu}\right)\right|N^{-1/\rho} \le MN^{-(1/\rho)(N-1+\epsilon)} \le MN^{-(1/\rho)(N-1)}e^{\sigma N},$$

and

$$N^{-1/\rho}\sum_{n=2}^{N}|C_n|\mu^{N-n} \le N^{-1/\rho}\sum_{n=2}^{N}|C_n|N^{-(1/\rho)(N-n)} \le FN^{-(1/\rho)(N+1)}e^{\sigma N} \le FN^{-(1/\rho)(N-1)}e^{\sigma N},$$

and

$$\sum_{n=N+1}^{\infty}|C_n|\xi^{N-n} \le N^{-(1/\rho)N}\sum_{n=N+1}^{\infty}|C_n|N^{n/\rho} \le FN^{-(1/\rho)N}e^{\sigma N} \le FN^{-(1/\rho)(N-1)}e^{\sigma N},$$

where M and F are constants.

$$\therefore |\Psi| \le DN(2N-2)^{(2N-2)[\beta-1-(1/2\rho)]}\exp N[2+\sigma+\ln(B^2 2^{1/\rho})], \quad (2.13)$$

where D is another constant.

We therefore see that for

$$\beta < \beta_0 = 1 + (2\rho)^{-1} \quad (2.14)$$

the second term in Eq. (2.7) vanishes as $N\to\infty$. Even when $\beta = \beta_0$ this can be made to hold by choosing an appropriate B which is equivalent to restricting φ to a countably normed subspace of S^{β_0}. By a similar analysis it can be seen that the last two series in Eq. (2.6) converge under the same conditions for β.

Thus for every $\varphi \in S^\beta$, $\beta < \beta_0$ or $\varphi \in S^{\beta_0, B}$ with B appropriately chosen, E is well-defined and equals (see Appendix)

$$E = \sum_{n=2}^{\infty}C_n e^{in\theta}\left\langle\left(\frac{1}{r^2}\right)^n_{\text{assoc}(n)}, f\right\rangle + \sum_{n=2}^{\infty}\frac{2\pi^2}{4^{n-2}\Gamma(n)\Gamma(n-1)}\Lambda(n)\left\langle \Box^{n-2}\delta(x), f\right\rangle, \quad (2.15)$$

where

$$\Lambda(n)=\int_{\tau=1}^{\infty} d\tau\,\tau^{2n-1}\sum_{l=n+1}^{\infty} C_l\Delta^l+\int_{\tau=0}^{1} d\tau\,\tau^{2n-1}\left(\Phi(\Delta)-\sum_{l=2}^{n-1} C_l\Delta^l\right).$$

From Eqs. (2.2) and (2.4) we get

$$I=\langle\Phi(\kappa^2e^{-i\theta}/\tau),\varphi\rangle=(\det b)E. \qquad (2.16)$$

From Eqs. (2.15), (2.16) and the Appendix it can be easily seen that the Fourier transform of the distribution $\Phi(\kappa^2e^{-i\theta}/\tau)$ is equal to

$$\mathcal{F}\left[\Phi\left(\frac{\kappa^2e^{-i\theta}}{\tau}\right)\right]=\sum_{n=2}^{\infty}\frac{(\det b)\pi^2}{\Gamma(n)\Gamma(n-1)}\left(-\frac{(bp)^2}{4}\right)^{n-2}C_ne^{-in\theta}$$
$$\times\{\psi(n)+\psi(n-1)-\ln[(bp)^2/4]+[2\Lambda(n)/C_n]e^{in\theta}\}. \qquad (2.17)$$

The Fourier transform clearly[5] converges to a distribution in $S_\beta'(\beta<\beta_0)$. It should be noted that this convergence is uniform with respect to $b_{\mu\nu}$ and therefore allows us to continue the parameters $b_{\mu\nu}$ under the summation in Eq. (2.17).

Step 2 *and Step* 3: So far we have defined $\Phi[\kappa^2/(g_{\mu\nu}x_\mu x_\nu)]$ for $g_{\mu\nu}=e^{i\theta}a_{\mu\nu}$. We now continue this result to $g_{\mu\nu}=-\eta_{\mu\nu}+i\epsilon_{\mu\nu}$, where $\eta_{\mu\nu}$ is the usual Minkowskian metric and $\epsilon_{\mu\nu}=\epsilon\mathbb{1}$, $\epsilon>0$ and $0<\arg(-\eta_{\mu\nu}+i\epsilon_{\mu\nu})<\pi$.

From Eq. (2.3), as $\epsilon\to0^+$, we obtain

$$(bp)^2\to\kappa^2e^{i\theta}(-p^2-i0),$$
$$\det b\to -i\kappa^4e^{i2\theta},$$

and

$$\log[(bp)^2/4]\to\log[(\kappa^2e^{i\theta}/4)(-p^2-i0)],$$
$$=\ln[(\kappa^2/4)|p^2|]+i(\theta-\pi),\quad \text{for } p^2>0,$$
$$=\ln[(\kappa^2/4)|p^2|]+i\theta,\quad \text{for } p^2<0. \qquad (2.18)$$

$$\therefore i\mathcal{F}\left[\Phi\left(\frac{\kappa^2}{-x^2+i0}\right)\right]=\sum_{n=2}^{\infty}\frac{(\kappa^2)^2C_n\pi^2}{\Gamma(n)\Gamma(n-1)}\left(\frac{\kappa^2(p^2+i0)}{4}\right)^{n-2}$$
$$\times\{\psi(n)+\psi(n-1)-\ln[(\kappa^2/4)|p^2|]+i\Theta(p^2)\pi-i\theta+[2\Lambda(n)/C_n]e^{in\theta}\}. \qquad (2.19)$$

From the equation for $\Lambda(n)$ [Eq. (2.15)] it is easily seen that the last term of Eq. (2.19) depends on θ_0, and not on $m(\theta=\theta_0+2m\pi)$. From the uniqueness of the analytic continuation $\mathcal{F}\{\Phi[\kappa^2/(-x^2+i0)]\}$ cannot depend on θ_0; however, it does depend on the arbitrary integer m. For example, for the exponential superpropagator for which $\pi/2\le\theta_0<\pi$,

$$\Lambda(n)=\int_{\tau=1}^{\infty} d\tau\,\tau^{2n}\sum_{l=n+1}\frac{e^{-i\theta_0 l}}{l!\,(\tau^2)^l}-\int_{\tau=0}^{1} d\tau\,\tau^{2n-1}\sum_{l=0}^{n-1}\frac{e^{-i\theta_0 l}}{l!\,(\tau^2)^l}$$
$$+\int_{\tau=0}^{1} d\tau\,\tau^{2n-1}\exp\left(\frac{e^{-i\theta_0}}{\tau^2}\right),$$
$$=\frac12\sum_{\substack{l=0\\ l\ne n}}^{\infty}\frac{e^{-i\theta_0 l}}{l!\,(l-n)}+\tfrac12E_{n+1}(-e^{-i\theta_0}),$$

where E_n is the exponential integral function.[6]

$$\therefore\Lambda(n)=\tfrac12(e^{-i\theta_0 n}/n!)[-i(\pi-\theta_0)+\psi(n+1)]. \qquad (2.20)$$

Hence

$$i\mathcal{F}\left[\exp\left(\frac{\kappa^2}{-x^2+i0}\right)-1-\frac{\kappa^2}{(-x^2+i0)}\right]$$
$$=\sum_{n=2}^{\infty}\frac{(\kappa^2)^2\pi^2}{\Gamma(n-1)\Gamma(n)\Gamma(n+1)}\left(\frac{\kappa^2p^2}{4}\right)^{n-2}\left[\psi(n)+\psi(n-1)\right.$$
$$\left.+\psi(n+1)-\ln\frac{\kappa^2|p^2|}{4}+i\pi(\Theta(p^2)-1-2m)\right]. \qquad (2.21)$$

By suitable averaging over some values of m, it is possible to obtain a unitary result. A claim has been made in Ref. 7 that a unitary and unambiguous result can be obtained by a method analogous to ours. This is contrary to our result. The averaging procedure, however, introduces an ambiguity in the real part of the superpropagator and this is eliminated by demanding a "minimally singular" solution.[4]

III. CONCLUSIONS

We have shown that under two conditions—

(a) $\Phi(z)$ is an entire function of z of order of growth $\rho>0$ and type σ;

(b) there exists a θ_0, $0<\theta_0<\pi$, such that $\tau^{2-\epsilon}\Phi[(\kappa^2e^{-i\theta})/\tau]$ is continuous in $\tau(\epsilon>0)$—

the superpropagator $\Phi[\kappa^2/(-x^2+i0)]$ can be defined as a boundary value of an analytic distribution in the space $(S^\beta)'$, where $\beta<\beta_0=1+1/2\rho$ or in the space $(S^{\beta_0,B})'$ for a suitably chosen B depending on ρ and σ. We obtain a series representation for the superpropagator and this representation converges as a distribution in the space above. The ambiguity in the result is due to the existence of a branch point in the analytic distribution which is a reflection of the fact that the function $\Phi(z)$ has an essential singularity at infinity.

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APPENDIX[8]

We briefly consider the distribution $(1/r^2)^z$ and the associate function $(1/r^2)^n_{\mathrm{assoc}(n)}$. Here $r^2=x_0^2+x_1^2+x_2^2+x_3^2$.

The function $(1/r^2)^z$ is locally summable for Re $z<2$ and therefore defines in this region a regular distribution which is also analytic in z. By analytically continuing $(1/r^2)^z$ beyond this range, one obtains for

$n-1<\mathrm{Re}\,z<n+1, \quad n=2,3,\cdots,$

$$\left\langle\left(\frac{1}{r^2}\right)^z, \varphi\right\rangle=\int dx\left(\frac{1}{r^2}\right)^z\left(\phi(x)-\phi(0)-\frac{1}{2!}\phi_{\mu\nu}(0)\right.$$
$$\left.x^\mu x^\nu-\cdots-\frac{1}{(2n-4)!}\phi_{\mu_1\cdots\mu_{2n-4}}(0)\,x^{\mu_1}\cdots x^{\mu_{2n-4}}\Theta(1-r)\right)$$
$$+\frac{\pi^2}{\Gamma(n)\Gamma(n-1)}\left(\frac{\Box}{4}\right)^{n-2}\phi(0)\frac{1}{n-z}$$
$$\equiv\left\langle\left(\frac{1}{r^2}\right)^z_{\mathrm{assoc}(n)},\varphi\right\rangle+\frac{\pi^2}{\Gamma(n)\Gamma(n-1)}\left\langle\left(\frac{\Box}{4}\right)^{n-2}\delta(x),\varphi\right\rangle\frac{1}{n-z},\qquad\text{(A1)}$$

where φ is a test function in an S-type space[5] (S^8 in our case).

The distribution $(1/r^2)^z$ is therefore meromorphic in z with simple poles at $z=n$, $n=2,3,\cdots$. Equation (A1) also defines the associated function $(1/r^2)^z_{\mathrm{assoc}(n)}$ in the range $n-1<\mathrm{Re}\,z<n+1$.

The Fourier transform of $(1/r^2)^z$ is given by

$$\mathcal{F}\left[\left(\frac{1}{r^2}\right)^z\right]=\pi^2\left(\frac{p^2}{4}\right)^{z-2}\frac{\Gamma(2-z)}{\Gamma(z)},\qquad\text{(A2)}$$

which has the same analytic structure as $(1/r^2)^z$.

In the neighborhood of the pole at $z=n$, $n=2,3,\cdots$ the Laurent expansion of $\mathcal{F}[(1/r^2)^z]$ is

$$\mathcal{F}\left[\left(\frac{1}{r^2}\right)^z\right]=\frac{\pi^2}{\Gamma(n)\Gamma(n-1)}\left(-\frac{p^2}{4}\right)^{n-2}$$
$$\times\left(\frac{1}{n-z}+\psi(n)+\psi(n-1)-\ln\frac{p^2}{4}+\cdots\right).\qquad\text{(A3)}$$

Thus the Fourier transform of the associated function at $z=n$ is

$$\mathcal{F}\left[\left(\frac{1}{r^2}\right)^n_{\mathrm{assoc}(n)}\right]=\frac{\pi^2}{\Gamma(n)\Gamma(n-1)}\left(-\frac{p^2}{4}\right)^{n-2}\left(\psi(n)+\psi(n-1)\right.$$
$$\left.-\ln\frac{p^2}{4}\right).\qquad\text{(A4)}$$

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On a boundary value problem for integro-differential equations*

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A boundary value problem of a linear differential-integral equation is converted to a Cauchy system by means of parameter imbedding. Numerical results are shown for an equation from nuclear physics.

1. INTRODUCTION

In the mathematical description of physical processes, boundary value problems for integro-differential equations frequently arise. Example of such processes are the distribution of a drug in the body[1] and elastic scattering of nucleons, such as α particles and protons, from medium sized nucleii.[2] The conversion of such problems to Cauchy systems has previously been discussed,[3,4] and numerical experiments have demonstrated that such Cauchy systems can feasibly be solved.[5,6] In this paper we show another method of reducing integro-differential equations to Cauchy systems by means of parameter imbedding, and we show numerical results for a degenerate kernel.

2. DERIVATION OF CAUCHY SYSTEM

Let $u(r)$ be a solution of the linear differential integral equation

$$u''(r) + \lambda q(r)u(r) = \int_0^L K(r,r')u(r')dr', \quad 0 \le r \le L, \; 0 \le \lambda \le \Lambda, \tag{1}$$

with boundary conditions

$$u(0) = 0, \tag{2}$$

$$u'(L) = c. \tag{3}$$

We shall consider a degenerate kernel of the form

$$K(r,r') = \sum_{i=1}^{N} f_i(r) g_i(r'). \tag{4}$$

We regard u as a function of both r and the parameter λ, so we write, where necessary,

$$u = u(r,\lambda). \tag{5}$$

Introduce the auxiliary function $z(r,\lambda)$ that is a solution of the linear differential equation

$$z''(r,\lambda) + \lambda q(r)z(r,\lambda) = 0, \quad 0 \le r \le L, \; 0 \le \lambda \le \Lambda, \tag{6}$$

with the boundary conditions

$$z(0,\lambda) = 0, \tag{7}$$

$$z'(L,\lambda) = 1. \tag{8}$$

Next, consider the differential equation

$$w''(r,\lambda) + \lambda q(r)w(r,\lambda) = \varphi(r), \quad 0 \le r \le L, \; 0 \le \lambda \le \Lambda, \tag{9}$$

$$w(0,\lambda) = 0, \tag{10}$$

$$w'(L,\lambda) = 0. \tag{11}$$

Introduce the Green's function, $G(r,r',\lambda)$, in terms of which the solutions of Eqs. (9)–(11) can be written

$$w(r,\lambda) = \int_0^L G(r,r',\lambda)\varphi(r')dr'. \tag{12}$$

In terms of the auxiliary functions z and G, the solution of Eqs. (1)–(3) can be written

$$u(r,\lambda) = cz(r,\lambda) + \sum_{i=1}^{N} m_i(\lambda) \int_0^L G(r,r',\lambda)f_i(r')dr', \tag{13}$$

where

$$m_i(\lambda) = \int_0^L g_i(r')u(r',\lambda)dr', \quad i = 1,2,\ldots,N. \tag{14}$$

Using the two auxiliary functions z and G, we have converted the differential integral equation of Eqs. (1)–(3) into a linear integral equation. We next shall obtain a Cauchy system for these auxiliary functions, and then we shall obtain a Cauchy system for the integral equation.

Differentiate Eqs. (6)–(8) with respect to λ to obtain

$$z''_\lambda(r,\lambda) + \lambda q(t)z_\lambda(r,\lambda) + q(t)z(r,\lambda) = 0, \tag{15}$$

$$z_\lambda(0,\lambda) = 0, \tag{16}$$

$$z'_\lambda(L,\lambda) = 0. \tag{17}$$

Here we regard z_λ as a new function of r and λ. In terms of the Green's function, the solution of Eqs. (15)–(17) is

$$z_\lambda(r,\lambda) = -\int_0^L G(r,r',\lambda)q(r')z(r',\lambda)dr'. \tag{18}$$

This is a differential equation for the function $z(r,\lambda)$. The initial condition at $\lambda = 0$ is

$$z(r,0) = r, \quad 0 \le r \le L. \tag{19}$$

Next, differentiate Eqs. (9)–(11) with respect to λ to obtain

$$w''_\lambda(r,\lambda) + \lambda q(r)w_\lambda(r,\lambda) + q(r)w(r,\lambda) = 0, \tag{20}$$

$$w_\lambda(0,\lambda) = 0, \tag{21}$$

$$w'_\lambda(L,\lambda) = 0. \tag{22}$$

In terms of the Green's function, we can write

$$w_\lambda(r,\lambda) = -\int_0^L G(r,r',\lambda)q(r')w(r',\lambda)dr'. \tag{23}$$

Next, differentiate Eq. (12) with respect to λ to obtain

$$w_\lambda(r,\lambda) = \int_0^L G_\lambda(r,r',\lambda)\varphi(r')dr'. \tag{24}$$

Using Eq. (12), we can write Eq. (23) as

$$w_\lambda(r,\lambda) = -\int_0^L G(r,r',\lambda)q(r') \int_0^L G(r',r'',\lambda)\varphi(r'')dr''dr'. \tag{25}$$

Since Eqs. (25) and (25) must hold for all arbitrary functions $\varphi(r)$, it must follow that

$$G_\lambda(r,r',\lambda) = \int_0^L G(r,r'',\lambda)q(r'')G(r'',r',\lambda)dr'', \quad 0 \le \lambda \le \Lambda. \tag{26}$$

This is a differential equation for $G(r,r',\lambda)$. The initial condition on G is

$$G(r,r',0) = \begin{cases} -r', & 0 \le r' \le r, \\ -r, & r \le r' \le L. \end{cases} \tag{27}$$

Equations (18), (19), (26), and (27) comprise the Cauchy system for the auxiliary functions z and G. We now consider the integral equation Eq. (13). To evaluate $u(r,\lambda)$, we need the values of $m_i(\lambda)$. Substitute for $u(r,\lambda)$ from Eq. (13) in Eq. (14) to obtain

$$m_i(\lambda) = \int_0^L g_i(r')\Big[cz(r',\lambda) + \sum_{j=1}^N m_j(\lambda) \times \int_0^L G(r',r'',\lambda)f_j(r'')dr''\Big]dr', \quad i = 1,2,\ldots,N. \tag{28}$$

This we recognize as a set of linear algebraic equations for $m_1(\lambda), m_2(\lambda), \ldots, m_N(\lambda)$.

It is expedient to adopt matrix notation. Let a be the $N \times 1$ vector whose elements are

$$a_i(\lambda) = \int_0^L g_i(r')z(r',\lambda)dr', \quad i = 1,2,\ldots,N. \tag{29}$$

Next, let B be the $N \times N$ matrix whose elements are

$$b_{ij}(\lambda) = \int_0^L g_i(r') \int_0^L G(r',r'',\lambda)f_j(r'')dr''dr', \quad i,j = 1,2,\ldots,N. \tag{30}$$

If m is the $N \times 1$ vector whose elements are $m_i(\lambda)$, we can write Eq. (28) as

$$m(\lambda) = ca(\lambda) + B(\lambda)m(\lambda). \tag{31}$$

Introduce the resolvent matrix $R(\lambda)$, in terms of which the solution of Eq. (31) is

$$m(\lambda) = ca(\lambda) + cR(\lambda)\,a(\lambda). \tag{32}$$

The matrices B and R are related by

$$R(\lambda) = B(\lambda) + B(\lambda)R(\lambda). \tag{33}$$

We now obtain a Cauchy system for R. Differentiate Eq. (33) to obtain

$$R_\lambda(\lambda) = B_\lambda(\lambda) + B_\lambda(\lambda)R(\lambda) + B(\lambda)R_\lambda(\lambda), \tag{34}$$

which can be written

$$R_\lambda(\lambda) = [B_\lambda(\lambda) + B_\lambda(\lambda)R(\lambda)] + R(\lambda)[B_\lambda(\lambda) + B_\lambda(\lambda)R(\lambda)] \tag{35}$$

or

$$R_\lambda(\lambda) = [I + R(\lambda)]B_\lambda(\lambda)[I + R(\lambda)], \tag{36}$$

where I is the identity matrix. Equation (36) is the desired Riccati equation for the matrix R. The initial condition on R is found from Eq. (33),

$$R(0) = [I - B(0)]^{-1}B(0). \tag{37}$$

Expressions for the elements of the matrix $B_\lambda(\lambda)$ are obtained by differentiating Eq. (30),

$$(b_{ij})_\lambda = \int_0^L g_i(r') \int_0^L G_\lambda(r',r'',\lambda)f_j(r'')dr''dr', \quad i,j = 1,2,\ldots,N. \tag{38}$$

The functions $g_1(r), g_2(r), \ldots, g_N(r)$ and $f_1(r), f_2(r), \ldots, f_N(r)$ are known functions, and $G_\lambda(r,r',\lambda)$ is given by Eq. (26).

3. SUMMARY OF CAUCHY SYSTEM

The functions z, G, and R are defined to be solutions of the differential equations

$$z_\lambda(r,\lambda) = -\int_0^L G(r,r',\lambda)g(r')z(r',\lambda)dr', \tag{39}$$

$$G_\lambda(r,r',\lambda) = -\int_0^L G(r,r'',\lambda)\,q(r'')\,G(r'',r',\lambda)dr'', \tag{40}$$

$$R_\lambda(\lambda) = [I + R(\lambda)]B_\lambda(\lambda)[I + R(\lambda)], \quad 0 \le r \le L,\; 0 \le \lambda \le \Lambda \tag{41}$$

with initial conditions

$$z(r,0) = r, \tag{42}$$

$$G(r,r',0) = \begin{cases} -r', & 0 \le r' \le r, \\ -r, & r \le r' \le L, \end{cases} \tag{43}$$

$$R(0) = [I - B(0)]^{-1}B(0). \tag{44}$$

The elements of the matrix $B_\lambda(\lambda)$ are defined by

$$(b_{ij})_\lambda = \int_0^L g_i(r') \int_0^L G_\lambda(r',r'',\lambda)f_j(r'')dr''dr', \quad i,j = 1,2,\ldots,N. \tag{45}$$

At the points λ^* where the values of $u(r,\lambda^*)$ are desired, we evaluate the vector $m(\lambda)$ by

$$m(\lambda^*) = c[I + R(\lambda^*)]a(\lambda^*), \tag{46}$$

where the elements of the vector a are given by

$$a_i(\lambda^*) = \int_0^L g_i(r')\,z(r',\lambda^*)\,dr', \quad i = 1,2,\ldots,N. \tag{47}$$

To evaluate $u(r,\lambda^*)$, we use Eq. (13),

$$u(r,\lambda^*) = cz(r,\lambda^*) + \sum_{i=1}^N m_i(\lambda) \int_0^L G(r,r',\lambda^*)f_i(r')dr', \quad 0 \le r \le L. \tag{48}$$

4. COMPUTATIONAL TECHNIQUES

One numerical technique that has been shown to be feasible[5-7] is that of semidiscretization, or the method of lines.[8] In this method, the Cauchy system of Eqs. (39)–(44) is integrated numerically from $\lambda = 0$ to $\lambda = \Lambda$ along lines of constant values of r. At each step in the numerical integration, the right-hand sides of these equations are evaluated by an appropriate quadrature formula using the values of the functions z, G, and R at each of the lines of constant r. It is clear that the type and order of the quadrature formula dictate the locations of the lines of constant r.

In the numerical example to follow, Simpson's rule with twenty intervals is used to evaluate the definite integrals, and a fourth order Adams–Moulton procedure is used to integrate the differential equations. Computations were performed using an IBM 360/65 digital computer.

5. A NUMERICAL EXAMPLE

To describe elastic scattering of nucleons, such as α particles, protons, etc., from medium size nucleii, such as Fe^{54}, Pb^{208}, etc., optical model potentials can be used.[2,9] In this model, the complex many-body effects introduce a nonlocal potential in the Schrödinger equation governing the motion of the particle.[10,11] The reduced S-wave Schrödinger equation is a one-dimensional differential-integral equation where the kernel of the integral term represents the nonlocal interactions. The equation is[11]

$$u''(r,\lambda) + [\lambda + V(r)]u(r,\lambda) = \int_0^L K(r,r')u(r',\lambda)\,dr', \quad 0 \le r \le L,\ 0 \le \lambda \le \Lambda, \tag{49}$$

with boundary conditions

$$u(0,\lambda) = 0, \tag{50}$$

$$u'(L,\lambda) = A\sqrt{\lambda}\ \cos(\sqrt{\lambda}\ L + \delta). \tag{51}$$

We here consider the special case of a degenerate kernel of the form

$$K(r,r') = rr'[\exp(-\tfrac{1}{2}r^2 - \tfrac{1}{4}r'^2) + \exp(-\tfrac{1}{4}r^2 - \tfrac{1}{2}r'^2)]. \tag{52}$$

The local potential, $V(r)$, is given by

$$V(r) = -\exp(-\tfrac{1}{4}r^2). \tag{53}$$

The coefficient A is a known constant.

In the second boundary condition, Eq. (51), the phase angle δ is unknown. An additional relationship exists at the boundary, namely,

$$u(L,\lambda) = A\sin(\sqrt{\lambda}L + \delta). \tag{54}$$

We now show how the value of δ is determined. The values of the function $u(r,\lambda)$ are given by [Eq. (48)]

$$u(r,\lambda) = cz(r,\lambda) + \sum_{i=1}^{N} m_i(\lambda) \int_0^L G(r,r',\lambda)f_i(r')\,dr', \tag{55}$$

and the values of m are given by [Eq. (46)]

$$m(\lambda) = c[I + R(\lambda)]a(\lambda). \tag{56}$$

In Eqs. (55) and (56), c represents the value of $u'(L,\lambda)$, or

$$c = A\sqrt{\lambda}\ \cos(\sqrt{\lambda}\ L + \delta). \tag{57}$$

In view of Eqs. (55) and (56), we can write

$$u(L,\lambda) = c\varphi(\lambda), \tag{58}$$

where $\varphi(\lambda)$ is a function of $z(L,\lambda), G(L,r',\lambda), R(\lambda)$, and $a(\lambda)$, all of which are being computed in the Cauchy system. Next, using a trigonometric identity, we write

$$u^2(L,\lambda) + u'^2(L,\lambda)/\lambda = A^2, \tag{59}$$

which can also be written, using Eqs. (57) and (58),

$$c^2\varphi^2 + c^2/\lambda = A^2 \tag{60}$$

or

$$c = \pm\,[A^2\lambda/(\lambda\varphi^2 + 1)]^{1/2}. \tag{61}$$

The phase angle δ is given by

$$\delta = \tan^{-1}(\sqrt{\lambda}\,\varphi) - \sqrt{\lambda}\,L. \tag{62}$$

A Cauchy system was developed for Eqs. (49)–(53), and a computer program was written in the FORTRAN language. Several sample cases were run, and we present here some results. Table I shows the phase angle δ for various values of λ. Table II shows values of $u(r,\lambda)$ for $\lambda = 0.10$ and $\lambda = 0.25$. In all cases, the parameters A and L were both arbitrarily set equal to 1.0. Numerical quadrature was accomplished via 20-interval Simpson's rule, and integration of the differential equations was performed using an Adams–Moulton method with a step size of 0.01.

TABLE I. Phase angle (δ) for various values of $\lambda (L = 1, A = 1)$.

λ	δ (degrees)
0.0	180.000
0.05	176.393
0.10	174.919
0.15	173.802
0.20	172.872
0.25	172.063

TABLE II. Values of $u(r,\lambda)$ for $\lambda = 0.1$ and 0.25 $(L = 1, A = 1)$

	$u(r,\lambda)$	
r	$\lambda = 0.1$	$\lambda = 0.25$
0.00	0.0	0.0
0.10	0.018 25	0.029 29
0.20	0.036 78	0.058 98
0.30	0.055 85	0.089 44
0.40	0.075 73	0.121 07
0.50	0.096 69	0.154 22
0.60	0.118 96	0.189 23
0.70	0.142 78	0.226 41
0.80	0.168 36	0.266 05
0.90	0.195 90	0.308 40
1.00	0.225 59	0.353 65

Other methods, such as effective mass approximations and iterative techniques,[11,12] have been used to solve equations involving nonlocal potentials. These values compare favorably with the values found using the imbedding approach, as indicated in this paper. The imbedding approach has the advantage of giving the wave solution inside the potential region. This is useful in understanding such phenomena as the Perey effect.[12]

6. DISCUSSION

The imbedding approach, as used in this paper, yields numerical results consistent with those found by other methods. In subsequent papers, we shall extend these results to problems with general (nondegenerate) kernels and problems with nonlinear boundary conditions.

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Generalized covariance principles and neutrino physics

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The zero-mass Dirac equation admits a simple generalized covariance group which is an inhomogeneous Lorentz group G different from the Poincaré group. Its mathematical structure and unitary irreducible representations have been studied by Flato and Hillion [Phys. Rev. D 1, 1667 (1970)]. Physical consequences concerning neutrino physics were then obtained by introduction of the Stokes parameters. The present article is divided into three parts: (1) Introduction, in which we present briefly the idea of generalized convariance, summarize the main results obtained by Flato and Hillion, and introduce the 14-dimensional unification group proper for the generalized convariance of the free neutrino equation. (2) In the second part, we study by the well-known method of induced representations all the strongly continuous unitary irreducible representations of the 10-dimensional Dirac group G as well as of the 14-dimensional unification group G'. (3) Physical applications: in this chapter, we concentrate on particular zero-mass representations of G' which are of interest at least for the study of the neutrino free-field theory. These classes of unitary irreducible representations of G' permit us to have two possible physical alternatives which are discussed.

I. INTRODUCTION

To begin with, we summarize the essential ideas in Ref. 1: In classical theory, the field belongs to a certain linear space of functions on Minkowski space with values in $\mathbb{C}^n$. This tensor or spinor field satisfies a classical field equation of the type $A(\partial)\ \psi(x)=0$ where $A(\partial)$ is a differential operator. $\mathbb{C}^n$ is also a representation space of a *finite-dimensional* non-unitary representation of $SL(2,\mathbb{C})$, the universal covering of the connected component of the homogeneous Lorentz group. The equation $A(\partial)\ \psi(x)=0$ is said to be relativistic covariant if when we make the transformation $x\to x'=\tilde{\Lambda}x+a$ in Minkowski space (where $\pm\Lambda\to\tilde{\Lambda}$ in the covering map) and, at the same time, cotransform the field $\psi(x)\to\psi'(x')=S(\Lambda)\psi(x)$, our original equation $A(\partial)\psi(x)=0$ goes into $A(\partial')\psi'(x')=0$.

One can ask what are the most general transformations of the field $\psi(x)$ compatible with the Poincaré transformation $x\to x'=\tilde{\Lambda}x+a$, which lead to the equation $A(\partial')\psi'(x')=0$. A general cotransformed field which meets our purpose is, e.g., of the form $\psi'(x')=S(\Lambda)\psi(x)+\varphi'(x')$, where $\varphi'(x')$ is a solution of the field equation $A(\partial')\varphi'(x')=0$. Thus, we have to introduce a generalized covariance group which is, e.g., a semidirect product of $SL(2,\mathbb{C})$ by the space of solutions of the field equation. The multiplication law is directly obtained by

$$(\Lambda_1,\varphi_1(x))(\Lambda,\varphi(x))=(\Lambda_1\Lambda,\varphi(x)+S(\Lambda^{-1})\varphi_1(x)).$$

The space of the solutions of the field equation is in general infinite-dimensional and the mathematical study of this kind of groups sets some yet unsolved problems. In particular, the exhaustive classification of its unitary irreducible representations (UIR) in unknown. However, the special case of zero-mass Dirac operator $A(\partial)=\gamma^\mu\partial_\mu$ can be partially studied by considering only the subspace of constant solutions. We obtain a generalized covariance group which is the Dirac group $G=SL(2,C)\circledS\mathbb{R}^4$, with the multiplication law $(\Lambda_1,a_1)(\Lambda_2,a_2)=(\Lambda_1\Lambda_2,a_2+S(\Lambda_2^{-1})a_1)$ which is equivalent to $(\Lambda_1,a_1)(\Lambda_2,a_2)=(\Lambda_1\Lambda_2,a_1+S(\Lambda_1)a_2)$ and where S is a real-irreducible representation equivalent to

$$D(\tfrac{1}{2},0)\oplus D(0,\tfrac{1}{2}):$$

$$\Lambda\in SL(2,\mathbb{C}),\ \Lambda\to S(\Lambda)=\begin{pmatrix}\mathrm{Re}\Lambda & \mathrm{Im}\Lambda\\ -\mathrm{Im}\Lambda & \mathrm{Re}\Lambda\end{pmatrix}.$$

The faithful UIR (which belong to the principal series) can be obtained by direct methods[1]:

$$U_g f(Z)=\alpha(Z,g)f(Zg),\quad \text{where } Z=(Z_1,Z_2)\in\mathbb{C}^2, f(Z)\in L^2(\mathbb{C}^2),$$

$$g=(\Lambda,a),\quad \Lambda=\begin{pmatrix}\alpha&\beta\\ \gamma&\delta\end{pmatrix}\in SL(2,\mathbb{C}),\quad a=(h_1,h_2,h_3,h_4)\in\mathbb{R}^4,$$

$$Zg=(\alpha Z_1+\gamma Z_2,\ \delta Z_2+\beta Z_1),$$

$$\alpha(Z,g)=\exp[i(t\beta Z_2^{-1}(\delta Z_2+\beta Z_1)^{-1}+CC)]\times\exp[i((h_1+ih_3)Z_1+(h_2+ih_4)Z_2+CC)].$$

Next, we introduce the Stokes parameters as a kind of internal variables like in Ref. 1. Either in terms of two perpendicular plane polarizations or in terms of two circular polarizations, the state of polarization of a beam of photons is described by a linear superposition of two states $\chi=C_1\chi_1+C_2\chi_2$ and we have $|C_1|^2+|C_2|^2=1$. The Stokes parameters P_μ are then defined by the relations:

$$P_0=|C_1|^2+|C_2|^2,\quad P_1=|C_1|^2-|C_2|^2,$$

$$P_2=C_1\bar{C}_2+C_2\bar{C}_1,\qquad P_3=i(C_2\bar{C}_1-C_1\bar{C}_2).$$

It is quite interesting to notice that they define a mapping of the unit ball in $\mathbb{C}^2\simeq SL(2,\mathbb{C})\cdot\mathbb{C}^2/SL(2,\mathbb{C})$ on the "Stokes cone" $P_\mu P^\mu=0$, a thing related to the fact that we deal here with zero-mass particles. This formalism works with the electromagnetic field as following: Let $F_{\mu\nu}$ be the electromagnetic field and $\zeta_i (i=1,2,3)$ a complex vector defined by $\zeta_i=F_{i4}+\sqrt{-1}\,F_{jk}$ where (i,j,k) is a cyclic permutation of (1, 2, 3). For plane waves, this vector is isotropic: $\zeta_1^2+\zeta_2^2+\zeta_3^2=0$, and there exist

$$\varphi=\begin{pmatrix}\varphi_1\\ \varphi_2\end{pmatrix}\in\mathbb{C}^2$$

such that $\zeta_1=\varphi_1\varphi_2$, $\zeta_2=\frac{1}{2}(\varphi_2^2-\varphi_1^2)$, $\zeta_3=\frac{1}{2}i(\varphi_1^2+\varphi_2^2)$. Then, one can verify that a sufficient condition for having energy conservation with time is $\sigma^\mu\partial_\mu\varphi=0$ where σ^0 is the 2×2 identity matrix and σ^i $(i=1,2,3)$ the Pauli matrices. Conversely, for fully polarized plane waves of a time-independant electromagnetic field, in virtue of Maxwell equations, the Stokes spinor φ is shown to satisfy the equation $\sigma^\mu \partial_\mu \varphi = 0$.

We know that the two-component free neutrino Weyl equation $\sigma^\mu \partial_\mu \psi = 0$ can be derived from the zero-mass Dirac equation by adding subsidiary conditions and analogously, we may consider the two-component spinor field as a Stokes spinor. The differences, from our point of view, between neutrinos and photons, which are a natural consequence of the formalism developed in Ref. 1, are

(1) For neutrinos, the Dirac group is the covariance group of the field equation while for photons, it is only the covariance group of the polarization equation.

(2) In terms of Stokes parameters, neutrinos are always fully polarized while this is not the case for photons.

In the internal space of the neutrino Stokes parameters, one then distinguishes like in Ref. 1 among four principal types of operations extendible to four types of automorphisms of the Dirac group (the identity automorphism plus three different ones) which are identified with the four types of neutrinos existing in Nature.

Thus, in the example of neutrino physics, we use two groups: the Poincaré group acting on the "external space" (which is the Minkowski space T^4) and the Dirac group acting on the "internal space" of the Stokes parameters $\mathbb{R}^4$. The natural idea is then to look for a formalism which could describe these two aspects. The *simplest* mathematical unification (in the sense of Ref. 2) of the Dirac group and the Poincaré group which acts as it should act separately on $\mathbb{R}^4$ and on T^4 is the semidirect product $SL(2,\mathbb{C})(\mathbb{R}^4 \times T^4)$ denoted by G'. For what additional reasons are we led to the unification group G'?

The first reason is that space-time translations should commute with the field translations since these two types of translations act on two different and disconnected spaces $\mathbb{R}^4$ and T^4.

The second reason is that in Ref. 1 a generalized covariance principle for the second-quantized neutrino equation was obtained.

This principle was compatible with the usual Wightman covariance principle (which is also postulated by us) only if the reduction of the representation of the Dirac group on $SL(2,\mathbb{C})$ coincides with the reduction of the representation of the Poincaré group on $SL(2,\mathbb{C})$. This fact is ensured if we take a unification group of the Poincaré and the Dirac groups with $SL(2,\mathbb{C})$ as intersection. The preceding two reasons determine uniquely the unification group G'.

Therefore, our first aim in the second chapter will be the study of the UIR of the 10 dimensional Dirac group and its 14-dimensional unification with the Poincaré group. These groups are semidirect products of a semisimple group by an abelian normal subgroup and the complete classification of their unitary, strongly continuous, irreducible representations is obtained by the Mackey theory of induced representations. Among the UIR of G', we are certainly *a priori* interested only by those representations for which the Poincaré Casimir $P^\mu P_\mu = 0$ since the one-particle neutrino states are massless. Among these, of particular interest for us are two classes of UIR of G': the first class consists of such UIR that, when restricted to the Dirac subgroup, remain irreducible and when restricted to the Poincaré subgroup are reducible into two continuous-spin irreducible Poincaré representations. The second class is composed of such UIR (obtained as a limiting case of the first class) which are irreducible with respect to the Dirac subgroup but reducible with respect to the Poincaré subgroup giving rise, after decomposition, to all possible discrete spin representations with multiplicity one. Finally in chapter three we utilize these classes of representations to sketch briefly two possible physical alternatives for the construction of a neutrino Fock space and a free field theory *incorporating both* external and internal symmetry groups.

II. UNITARY STRONGLY CONTINUOUS IRREDUCIBLE REPRESENTATIONS OF G AND G'

Let $G = SL(2,\mathbb{C})\mathbb{R}^4$ be the Dirac group and (Λ, h) its elements. Let $\hat{\mathbb{R}}^4$ be the dual space of $\mathbb{R}^4$. The dual action of G on $\hat{\mathbb{R}}^4$ is: $\hat{h} \to {}^T S(\Lambda^{-1})\hat{h}$ where $\hat{h}$ is a "four spinor", $\Lambda \in SL(2,\mathbb{C})$, S the representation of $SL(2,\mathbb{C})$ defined above and ${}^T\Lambda$ denotes the transposed of Λ. This action determines two orbits in $\hat{\mathbb{R}}^4$: the trivial one $\{0\}$, and $\hat{\mathbb{R}}^4 - \{0\}$. The stabilizer of the first one is $SL(2,\mathbb{C})$ and the corresponding induced representations, with kernel $\mathbb{R}^4$, are the unitary continuous irreducible representations of $SL(2,\mathbb{C})$. On the second orbit, we choose the stabilized point $(1,0,0,0)$, the stabilizer of which is the nilpotent group of the 2×2 complex lower triangular matrices N. The irreducible unitary representations of this group form the one complex parameter class $L(t)$ of the unitary characters of the complex plane. Almost everywhere, we can choose the matrix

$$\Lambda(\hat{h}) = \begin{pmatrix} 0 & \beta \\ -\beta^{-1} & \delta \end{pmatrix}_{\substack{\beta = \hat{h}_2 + i\hat{h}_4 \\ \delta = \hat{h}_1 + i\hat{h}_3}} \quad \text{so that} \begin{pmatrix} \hat{h}_1 \\ \hat{h}_2 \\ \hat{h}_3 \\ \hat{h}_4 \end{pmatrix} = {}^T S(\Lambda^{-1}(\hat{h})) \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

The Hilbert space of the induced representation ${}_G U^{L(t)}$ is $L^2(\hat{\mathbb{R}}^4 - \{0\})$ (the space of square integrable functions defined on the orbit $\hat{\mathbb{R}}^4 - \{0\}$ with values in the space $\mathbb{C}$ of the representations $L(t)$ of the little group).

Let

$$\Lambda_0 = \begin{pmatrix} \alpha_0 & \beta_0 \\ \gamma_0 & \delta_0 \end{pmatrix} \in SL(2,\mathbb{C});$$

by a straightforward calculation, one gets

$$\Lambda^{-1}(\hat{h})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{h}) = \begin{pmatrix} 1 & 0 \\ -\beta_0(\delta_0\beta - \beta_0\delta)^{-1} & 1 \end{pmatrix}$$

and the standard form of Wigner of the induced representation is then

$$[{}_G U^{L(t)}(\Lambda_0, h)F](\hat{h}) = \langle \hat{h}, h\rangle L(t)(\Lambda^{-1}(\hat{h})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{h}))F(\Lambda_0^{-1}\hat{h})$$

TABLE I. Nontrivial orbits for G'.

Orbit (X,Ω)	Stabilized point $(\hat{h}_x, \hat{x}_\Omega)$	Stabilizer group
(E_k, Ω_+^m)	$(k,0,0,0)(m,0,0,0)$	$\{I\}$
(E_k, Ω_-^m)	$(k,0,0,0)(-m,0,0,0)$	$\{I\}$
(O_ρ, Ω^{im})	$(\rho,0,0,1)(0,m,0,0)$	$\{I\}$
$(O_{0\lambda}, \Omega^{im})$	$(1,0,\lambda,0)(0,m,0,0)$	N_r
$(O_{0\infty}, \Omega^{im})$	$(0,0,1,0)(0,m,0,0)$	N_r
(C_k, Ω_+^0)	$(0,k,0,0)(1,0,0,1)$	$\{I\}$
(C_{0l}, Ω_+^0)	$(l,0,0,0)(1,0,0,1)$	N
(C_k, Ω_-^0)	$(0,k,0,0)(-1,0,0,1)$	$\{I\}$
(C_{0l}, Ω_-^0)	$(l,0,0,0)(-1,0,0,1)$	N

$$= \exp[i(\hat{h}_1 h_1 + \hat{h}_2 h_2 + \hat{h}_3 h_3 + \hat{h}_4 h_4)] \exp[i(-t\beta_0\beta^{-1}(\delta_0\beta - \beta_0\delta)^{-1} + CC)]F(\Lambda_0^{-1}\hat{h})$$

with $F \in L^2(\hat{\mathbb{R}}^4 - \{0\})$.

By a straightforward calculation, these representations are shown to be equivalent to those found in Ref. 1.

Next, we are interested in the UIR of the unification group $G' = SL(2,\mathbb{C})\ (\mathbb{R}^4 \times T^4)$. The dual space is $(\hat{\mathbb{R}}^4 \times \hat{T}^4)$ and the dual action of G' is given by: $(\hat{h}, \hat{x}) \to ({}^T S(\Lambda^{-1})\hat{h}, {}^T\tilde{\Lambda}^{-1}\hat{x})$ where $\pm\Lambda \to \tilde{\Lambda} \in L_+^\uparrow$. Except for the orbit $\{0\}\times\{0\}$ which leads to the representations of $SL(2, C)$, we find three kinds of orbits:

(1) The first ones are the Cartesian products of the trivial orbit $\{0\}$ in $\hat{\mathbb{R}}^4$ by the well-known orbits of the Poincaré group. It is clear that the corresponding induced representations of G' are unfaithful, with kernel $\mathbb{R}^4$, and coincide with the usual UIR of the Poincaré group.

(2) The second type consists of the unique orbit $\{\hat{\mathbb{R}}^4 - \{0\}\}\times\{0\}$ and the corresponding UIR are those of the Dirac group discussed above.

(3) We are interested in the third type of orbits which will give us the faithful UIR of G'. These are subsets of the products $\{\hat{\mathbb{R}}^4 - \{0\}\}\times\Omega$ where Ω is a nontrivial orbit of the Poincaré group P, which are not expressible as Cartesian subproducts. Let $(\hat{h}_0, \hat{x}_0)$ be a point in $\{\hat{\mathbb{R}}^4 - \{0\}\}\times\Omega$, where Ω is a fixed orbit of P. All points belonging to the orbit generated by the point $(\hat{h}_0, \hat{x}_0)$, that can be written as $(\hat{h}, \hat{x}_0)$, verify $(\hat{h}) = {}^T S(\Lambda^{-1})(\hat{h}_0)$ where Λ belongs to the stabilizer of $\hat{x}_0$.

Therefore, it is clear that there exist in $\{\hat{\mathbb{R}}^4 - \{0\}\}\times\Omega$ as many orbits as in $\hat{\mathbb{R}}^4 - \{0\}$ under the action of the stabilizer of $\hat{x}_0$. Thus, we have to choose one fixed point $\hat{x}_\Omega$ on each orbit Ω of P and next to determine the orbits in $\hat{\mathbb{R}}^4 - \{0\}$ under the action of its stabilizer. Notice that we could have chosen first a point in $\hat{\mathbb{R}}^4 - \{0\}$ and then look for the orbits in Ω. This way is clearly equivalent but leads to a different parametrization of the orbits. Our choice is made so as to put an accent on the space-time parametrization of the orbits. Of course, for the study of the reduction of the UIR of G' on P and G, it will be quite important to be able to pass from one point of view to the other.

Let $\Omega_\pm^m$ (positive mass), Ω^{im} (imaginary mass), $\Omega_\pm^0$ (mass zero) be the orbits in $\hat{T}^4$ and $(\pm m, 0, 0, 0)$, $(0, m, 0, 0)$, $(\pm 1, 0, 0, 1)$ respectively, be the corresponding stabilized points on each one. The corresponding stabilizers are $SU(2)$, $SL(2,\mathbb{R})$, $\tilde{E}_2$ ($\tilde{E}_2$ being the twofold covering of the Euclidean group E_2 in two dimensions). By an easy calculation, the orbits in $\hat{\mathbb{R}}^4 - \{0\}$ are found to be:

under the action of $SU(2)$,

$$E_k = \{\hat{h}; \hat{h}_1^2 + \hat{h}_2^2 + \hat{h}_3^2 + \hat{h}_4^2 = k^2\}, \quad k \in]0+\infty[,$$

under the action of $SL(2, \mathbb{R})$,

$$0_\rho = \{\hat{h}; \hat{h}_1\hat{h}_4 - \hat{h}_2\hat{h}_3 = \rho\}, \quad \rho \in \mathbb{R} - \{0\},$$

$$0_{0\lambda} = \{\hat{h}; \hat{h}_3 = \lambda\hat{h}_1, \hat{h}_4 = \lambda\hat{h}_2\}, \quad \lambda \in \mathbb{R},$$

$$0_{0\infty} = \{\hat{h}; \hat{h}_1 = \hat{h}_2 = 0\},$$

under the action of $\tilde{E}_2$,

$$C_k = \{\hat{h}; \hat{h}_2^2 + \hat{h}_4^2 = k^2\}, \quad k \in]0+\infty[,$$

$$C_{0l} = \{\hat{h}; \hat{h}_2 = \hat{h}_4 = 0, \hat{h}_1^2 + \hat{h}_3^2 = l^2\}, \quad l \in]0+\infty[.$$

We shall denote by (X, Ω) the orbit generated by the point $(\hat{h}, \hat{x}_\Omega)$ where $\hat{x}_\Omega$ is the point chosen on Ω and X is one of the orbits in $\hat{\mathbb{R}}^4 - \{0\}$, $(\hat{h} \in X)$.

At this point, a Borel set having only one intersection point with each orbit can be easily built up and we know that this is the only condition needed for the UIR of G' to be obtained by the Mackey method.

On each orbit with a nontrivial projection on $\hat{\mathbb{R}}^4$ and $\hat{T}^4$, we need to choose a particular point and to determine its stabilizer. This is what we do in Table I, where N_r denotes the real lower triangular matrices: Let L be a representation of the stabilizer of the orbit (X, Ω) in the Hilbert space $\mathcal{H}$. The induced representation can be written formally

$$[{}_{G'}U^L(\Lambda_0, h_0, x_0)F](\hat{h}, \hat{x}) = \langle\hat{x}, x_0\rangle\langle\hat{h}, h_0\rangle L(\Lambda^{-1}(\hat{h}, \hat{x})\Lambda_0 \times \Lambda(\Lambda_0^{-1}(\hat{h}, \hat{x})))F(\Lambda_0^{-1}\hat{h}, \Lambda_0^{-1}\hat{x})$$

where $F(\hat{h}, \hat{x}) \in L^2[(X, \Omega), \mathcal{H}]$ (the space of square integrable functions defined on the orbit (X, Ω) with values in $\mathcal{H}$) and $\Lambda(\hat{h}, \hat{x})$ is a fixed matrix satisfying $(\hat{h}, \hat{x}) = \Lambda(\hat{h}, \hat{x}) \cdot (\hat{h}_x, \hat{x}_\Omega)$. We also know that $\Lambda^{-1}(\hat{h}, \hat{x})\Lambda_0 \times \Lambda(\Lambda_0^{-1}(\hat{h}, \hat{x}))$ is always an element of the stabilizer of the orbit. When the stabilizer is $\{I\}$, for any choice of the matrix $\Lambda(\hat{h}, \hat{x})$, we have $\Lambda^{-1}(\hat{h}, \hat{x})\Lambda_0\Lambda(\Lambda_0^{-1}(\hat{h}, \hat{x})) = I$. Therefore, in such cases, we find only one representation which is

$$f(\hat{h}, \hat{x}) \xrightarrow{(\Lambda_0, h_0, x_0)} \langle\hat{x}, x_0\rangle\langle\hat{h}, h_0\rangle f(\Lambda_0^{-1}\hat{h}, \Lambda_0^{-1}\hat{x}), f(\hat{h}, \hat{x}) \in L^2((X, \Omega)).$$

The stabilizer N_r is isomorphic to the additive group of the real numbers. Its unitary representations are the unitary characters $L(t)$ $(t \in R)$.

On the orbit $(0_{0\lambda}, \Omega^{im})$, we choose the matrix:

$$\Lambda(\hat{h}, \hat{x}) = \begin{pmatrix} K(1-\lambda i)^{-1}(\hat{h}_1 - i\hat{h}_3) & -(1+\lambda i)^{-1}(\hat{h}_2 + i\hat{h}_4) \\ K(1-\lambda i)^{-1}(\hat{h}_2 - i\hat{h}_4) & (1+\lambda i)^{-1}(\hat{h}_1 + i\hat{h}_3) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ iu & 1 \end{pmatrix}$$

$K=(1+\lambda^2)(\hat{h}_1^2+\hat{h}_2^2+\hat{h}_3^2+\hat{h}_4^2)^{-1}$ with $u\in R$

The point $\binom{1+i\lambda}{0}$ is stabilized by the matrix $\begin{pmatrix}1&0\\iu&1\end{pmatrix}$ so that we have

$$\begin{pmatrix}\hat{h}_1+i\hat{h}_3\\ \hat{h}_2+i\hat{h}_4\end{pmatrix}={}^T(\Lambda^{-1}(\hat{h},\hat{x}))\begin{pmatrix}1+i\lambda\\ 0\end{pmatrix}$$

and therefore the matrix

$$\begin{pmatrix}K(1-\lambda i)^{-1}(\hat{h}_1-i\hat{h}_3) & -(1+\lambda i)^{-1}(\hat{h}_2+i\hat{h}_4)\\ K(1-\lambda i)^{-1}(\hat{h}_2-i\hat{h}_4) & (1+\lambda i)^{-1}(\hat{h}_1+i\hat{h}_3)\end{pmatrix}$$

belongs to the coset space $SL(2,\mathbb{C})/N$ and $\Lambda(\hat{h},\hat{x})$ span the coset space $SL(2,\mathbb{C})/N_r$. Notice that we have thus parametrized the orbit by five real numbers: $\hat{h}_1,\hat{h}_2,\hat{h}_3,\hat{h}_4,u$.

To simplify writing, we put

$$\delta=(1+\lambda i)^{-1}(\hat{h}_1+i\hat{h}_3),\quad \beta=-(1+\lambda i)^{-1}(\hat{h}_2+i\hat{h}_4)$$

so that

$$K=(\beta\bar{\beta}+\delta\bar{\delta})^{-1}.$$

We have

$$\Lambda_0^{-1}\Lambda(\hat{h},\hat{x})=\begin{pmatrix}\cdot & \delta_0\beta-\beta_0\delta\\ \cdot & -\gamma_0\beta+\alpha_0\delta\end{pmatrix}$$

and we obtain the form of the matrix $\Lambda(\Lambda_0^{-1}(\hat{h},\hat{x}))$:

$$\Lambda(\Lambda_0^{-1}(\hat{h},\hat{x}))=\begin{pmatrix}K'(\overline{-\gamma_0\beta+\alpha_0\delta})+iu'(\delta_0\beta-\beta_0\delta) & \delta_0\beta-\beta_0\delta\\ -K'(\overline{\delta_0\beta-\beta_0\delta})+iu'(-\gamma_0\beta+\alpha_0\delta) & -\gamma_0\beta+\alpha_0\delta\end{pmatrix},$$

where $u'\in\mathbb{R}$ and $K'=[(\delta_0\beta-\beta_0\delta)(\overline{\delta_0\beta-\beta_0\delta})+(-\gamma_0\beta+\alpha_0\delta)(\overline{-\gamma_0\beta+\alpha_0\delta})]^{-1}$. Next, a straightforward calculation leads to

$$\Lambda^{-1}(\hat{h},\hat{x})\Lambda_0\Lambda(\Lambda_0^{-1}(\hat{h},\hat{x}))=\begin{pmatrix}1 & 0\\ KK'[(\alpha_0\bar{\beta}+\gamma_0\bar{\delta})(\overline{-\gamma_0\beta+\alpha_0\delta})-(\beta_0\bar{\beta}+\delta_0\bar{\delta})(\overline{\delta_0\beta-\beta_0\delta})+i(u'-u) & 1\end{pmatrix}$$

But this matrix belongs a priori to N_r. From this, we deduce

$$u'-u=-\operatorname{Im}[KK'[(\alpha_0\bar{\beta}+\gamma_0\bar{\delta})(\overline{-\gamma_0\beta+\alpha_0\delta})-(\beta_0\bar{\beta}+\delta_0\bar{\delta})(\overline{\delta_0\beta-\beta_0\delta})]].$$

We now define

$$b=\operatorname{Re}[KK'[(\alpha_0\bar{\beta}+\gamma_0\bar{\delta})(\overline{-\gamma_0\beta+\alpha_0\delta})-(\beta_0\bar{\beta}+\delta_0\bar{\delta})(\overline{\delta_0\beta-\beta_0\delta})]]$$

and the representation induced from $L(t)$ $(t\in\mathbb{R})$ is

$$F(\hat{h},u)\xrightarrow{(\Lambda_0,h_0,x_0)}[{}_G\mathcal{U}^{L(t)}(\Lambda_0,h_0,x_0)F](\hat{h},u)=\langle\hat{x},x_0\rangle\langle\hat{h},h_0\rangle e^{itb}\times F(\Lambda_0^{-1}\hat{h},u').$$

The orbit $(0_{\rho\infty},\Omega^{im})$ is treated in a similar way. Setting $\delta=-i(\hat{h}_1+i\hat{h}_3)$, $\beta=i(\hat{h}_2+i\hat{h}_4)$, we find the same expression for the matrix $\Lambda(\hat{h},\hat{x})$. We are therefore led in this case to the same calculations and to a similar result.

Next, we consider the orbit (C_{0l},Ω_+^0). Its stabilizer is N, the representations of which are the unitary characters $L(t)$ $(t\in\mathbb{C})$.

Therefore, the representation space will be the space of square integrable complex valued functions defined on the orbit. We choose the matrices

$$\Lambda(\hat{h})=\begin{pmatrix}Kl^{-1}(\hat{h}_1-i\hat{h}_3) & -l^{-1}(\hat{h}_2+i\hat{h}_4)\\ Kl^{-1}(\hat{h}_2-i\hat{h}_4) & l^{-1}(\hat{h}_1+i\hat{h}_3)\end{pmatrix}$$

which span the coset space $SL(2,\mathbb{C})/N$, and which verify

$$\begin{pmatrix}\hat{h}_1+i\hat{h}_3\\ \hat{h}_2+i\hat{h}_4\end{pmatrix}={}^T(\Lambda^{-1}(\hat{h}))\begin{pmatrix}l\\ 0\end{pmatrix}\quad\text{with } K=l^2(\hat{h}_1^2+\hat{h}_2^2+\hat{h}_3^2+\hat{h}_4^2)^{-1}.$$

Therefore, in this case, a complete parametrization of the orbit is given by the four real numbers $\hat{h}_1,\hat{h}_2,\hat{h}_3,\hat{h}_4$. We now set $\delta=l^{-1}(\hat{h}_1+i\hat{h}_3)$, $\beta=-l^{-1}(\hat{h}_2+i\hat{h}_4)$ and find

$$\Lambda^{-1}(\hat{h})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{h})=\begin{pmatrix}1 & 0\\ KK'[(\alpha_0\bar{\beta}+\gamma_0\bar{\delta})(\overline{-\gamma_0\beta+\alpha_0\delta})-(\beta_0\bar{\beta}+\delta_0\bar{\delta})(\overline{\delta_0\beta-\beta_0\delta}) & 1\end{pmatrix}$$

with $K=(\beta\bar{\beta}+\delta\bar{\delta})^{-1}$, $K'=(\delta\alpha_0-\beta\gamma_0)(\overline{\alpha_0\delta-\beta\gamma_0})+(\beta\delta_0-\beta_0\delta)(\overline{\beta\delta_0-\beta_0\delta})$, which is an element of N. The corresponding induced representations are

$$F(\hat{h})\xrightarrow{(\Lambda_0,h_0,x_0)}[{}_G\mathcal{U}^{L(t)}(\Lambda_0,h_0,x_0)F](\hat{h})=\langle\hat{x},x_0\rangle\langle\hat{h},h_0\rangle\times\exp[i(tB+\bar{t}\bar{B})]F(\Lambda_0^{-1}\hat{h})$$

with $B=KK'[(\alpha_0\bar{\beta}+\gamma_0\bar{\delta})(\overline{-\gamma_0\beta+\alpha_0\delta})-(\beta_0\bar{\beta}+\delta_0\bar{\delta})(\overline{\delta_0\beta-\beta_0\delta})]$.

Finally, the last class of representations, corresponding to the orbit (C_{0l},Ω_-^0) and stabilizer N, has the same form as the preceding one. Since the physical interest of G' is related to the study of massless particles, we shall now pay a particular attention to the zero-mass representations of G'. The orbit (C_{0l},Ω_+^0) is homeomorphic to $\hat{\mathbb{R}}^4-\{0\}$ and the associated representations are labeled by the complex parameter t. These representations restricted to the Dirac group G are exactly the UIR induced by $L(t)$ for the particular choice of $\Lambda(\hat{h})$. (This choice of representative is different from the one we made at the beginning.)

Next, we restrict our ${}_G\mathcal{U}^{L(t)}$ to the Poincaré subgroup:

Let

$$\Lambda(\hat{x})=\begin{pmatrix}p^{-1/2}\cos\theta/2 & -p^{1/2}e^{-i\varphi}\sin\theta/2\\ p^{-1/2}e^{i\varphi}\sin\theta/2 & p^{1/2}\cos\theta/2\end{pmatrix}$$

be the matrix which transforms the point $(1,0,0,1)$ into $\hat{x}=(p,p\sin\theta\sin\varphi,\ p\sin\theta\cos\varphi,\ -p\cos\theta)$ on the orbit Ω_+^0 in the helicity formalism. The ranges of the parameters are

$$-\infty<p<+\infty,\quad 0\leqslant\theta\leqslant\pi,\quad -\pi\leqslant\varphi<\pi.$$

The family of these matrices spans the coset space $SL(2, \mathbb{C})/\tilde{E}_2$, so that an element of the coset space $SL(2, \mathbb{C})/N$ (which is homemorphic to the orbit $\hat{\mathbb{R}}^4 - \{0\}$) can be written in a unique way as $\Lambda(\hat{h}) = \Lambda(\hat{x})\Lambda(\psi)$ where

$$\Lambda(\psi) = \begin{pmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{pmatrix} \in \tilde{E}_2/N \quad \text{with } 0 \leqslant \psi < 2\pi$$

and we can explicitly realize the homeomorphism $SL(2, \mathbb{C})/N \longleftrightarrow (C_{0l}, \Omega_+^0)$ by

$$\left[\begin{pmatrix} l \\ 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}\right] \xrightarrow{\Lambda(\hat{x})\ \Lambda(\psi)} \left[\begin{pmatrix} lp^{1/2}\cos\theta/2\cos\psi \\ lp^{1/2}\sin\theta/2\cos(\psi-\varphi) \\ lp^{1/2}\cos\theta/2\sin\psi \\ lp^{1/2}\sin\theta/2\sin(\psi-\varphi) \end{pmatrix}, \begin{pmatrix} p \\ p\sin\theta\sin\varphi \\ p\sin\theta\cos\varphi \\ -p\cos\theta \end{pmatrix}\right].$$

One can verify that $\Lambda(\hat{x})\ \Lambda(\psi)$ is exactly the matrix $\Lambda(\hat{h})$ that we have considered before. We now can parametrize our representation with the parameters $\hat{x}, \psi$. One has

$$\Lambda(\Lambda_0^{-1}\hat{h}) = \Lambda(\Lambda_0^{-1}\hat{x})\Lambda(\psi') \text{ and } \Lambda^{-1}(\hat{h})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{h})$$
$$= \Lambda^{-1}(\psi)\Lambda^{-1}(\hat{x})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{x})\Lambda(\psi')$$

where ψ' has to be determined. But we know that $\Lambda^{-1}(\hat{x})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{x})$ belongs to $\tilde{E}_2$ and by putting

$$\Lambda^{-1}(\hat{x})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{x}) = \begin{pmatrix} e^{-i\phi} & 0 \\ Z & e^{i\phi} \end{pmatrix}, \quad (Z \in \mathbf{C})$$

we have $\Lambda^{-1}(\hat{h})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{h}) = \begin{pmatrix} e^{-(\phi+\psi'-\psi)} & 0 \\ Ze^{-i(\psi+\psi')} & e^{i(\phi+\psi'-\psi)} \end{pmatrix}$.

The last matrix belonging to N, we finally get

$$\phi + \psi' - \psi = 0 \pmod{2k\pi}$$
$$B = Ze^{-i(\psi+\psi')} = Z^{-i(2\psi-\phi)}$$

The restriction of our representation on the Poincaré subgroup can be written as

$$[{}_{G'}U^{L(t)}|_P(\Lambda_0, x_0)F](\hat{x}, \psi) = \langle\hat{x}, x_0\rangle \exp[i(tB + \overline{tB})]F(\Lambda_0^{-1}\hat{x}, \psi - \phi),$$

where $F(\hat{x}, \psi)$ is a complex-valued square integrable function defined on $\Omega_+^0 \times \Gamma$ (Γ the unit circle).

Next, (by utilizing the Fubini theorem) we pass from the space $L^2(\Omega_+^0 \times \Gamma)$ to the space $L^2(\Omega_+^0, L^2(\Gamma))$ of $L^2(\Gamma)$-valued square integrable functions defined on Ω_+^0 by the isomorphism:

$$f(\hat{x}, \psi) \longrightarrow F'(\hat{x}) = f(\hat{x},\ ).$$

The representation becomes

$$[{}_{G'}U^{L(t)}|_P(\Lambda_0, x_0)F'](\hat{x}) = \langle\hat{x}, x_0\rangle L(\Lambda^{-1}(\hat{x})\Lambda_0\Lambda(\Lambda_0^{-1}\hat{x}))F'(\Lambda_0^{-1}\hat{x}),$$

where L is a representation of $\tilde{E}_2$ defined by

$$\left[L\begin{pmatrix} e^{-i\phi} & 0 \\ Z & e^{i\phi} \end{pmatrix}\right] f(\psi) = \exp[i(tB + \overline{tB})f(\psi - \phi)$$

with $B = Z\exp[-i(2\psi - \phi)]$ and $f \in L^2(\Gamma)$.

Thus, the representation ${}_{G'}U^{L(t)}$ restricted to the Poincaré subgroup is induced by the representation L of the stabilizer $\tilde{E}_2$. We know that $\tilde{E}_2$ has two series of UIR: the discrete one L^j (j integer or half-integer) and the continuous one $L^{[\epsilon, r]}$ ($\epsilon = \pm 1$, $r > 0$). The representation L is then easily shown to be reducible into the sum of the two representations $L^{[+1, |t|]}$ and $L^{[-1, |t|]}$ for $t \neq 0$.

From this, we obtain (for $t \neq 0$) the reducibility of the restricted representation ${}_{G'}U^{L(t)}|_P$ into the sum of the two corresponding continuous-spin UIR of the Poincaré group (containing, respectively, all integer and half-integer helicities).

For $t = 0$, the representation becomes:

$$[{}_{G'}U^{L(0)}(\Lambda_0, x_0)F'](\hat{x}) = \langle\hat{x}, x_0\rangle F'(\Lambda_0^{-1}\hat{x})$$

and it is induced by the representation $f(\psi) \to f(\psi - \phi)$. This last *unfaithful* representation of $\tilde{E}_2$ is actually the regular representation of the twofold covering of the group of plane rotations. One then deduces that, for $t = 0$, the representation ${}_{G'}U^{L(0)}|_P$ is reducible into a direct sum of all the discrete spin zero-mass UIR of the Poincaré group with multiplicity one.

III. POSSIBLE PHYSICAL APPLICATIONS

What was our line of thought until now? We have begun with a generalized covariance principle, and applied it to the classical free neutrino equation.

When we wanted to implement this generalized covariance principle to the *second-quantized* neutrino equation, two things occured: (1) We had to parametrize the Hilbert space of the one-particle neutrino states as square integrable functions defined on a new type of internal variables: the neutrino Stokes parameters. In this way, we account for a type of internal structure of the neutrino, and also parametrize some of the phenomena of its weak interactions (cf., Ref. 1). (2) The parametrization of the Hilbert space of the one-particle neutrino states explained in point (1) enabled us to extract finally the abstract form of a generalized Wightman covariance principle for our problem, which stressed the important role that the unitary representations of the Dirac group play in our formalism. If we insist upon having also the usual Wightman covariance principle for our quantized field, we are led to a compatibility condition which (in addition to a simplicity argument) gives rise to the unification group G' as explained in the introduction. In other terms, from the action of the unification group G' on $\hat{\mathbb{R}}^4 \times \hat{T}^4$, plus the neutrino second-quantized free-field theory (and of course assuming the conservation of transition amplitudes), one can axiomatize a unification-covariance principle in which the unitary representations of the 14-*dimensional unification group* G' play the predominant role.

This unification-covariance principle incorporates two aspects: if the *field translations* are equal to zero we get the usual Wightman covariance axiom, and if the space-time translations are equal to zero we get our generalized covariance principle.

G' is therefore a kind of unification group between external and "internal" symmetries, which plays also in our approach a field theoretical role.

As was noticed by us in section two, there are two types of UIR of G' of interest for us: those which are irreducible when restricted to the Dirac subgroup and reducible into two continuous-spin UIR of the Poincaré group P when restricted to the latter, and those which are irreducible when restricted to the Dirac subgroup and reducible into an infinite sum of all discrete spin zero-mass UIR of P with multiplicity one, when restricted to the Poincaré subgroup. This fact gives us two interesting mathematical possibilities, which we shall have now to confront with the physical aspects of our problem. It was guessed by some people in the last decade that the so-called continuous-spin representations (often refered to as infinite-spin representations) might have to do with zero-mass particles occuring in Nature and in particular with neutrinos. This point of view was studied in detail in Ref. 3: in this work, it was suggested that the continuous-spin UIR of the Poincaré group with a small $\rho > 0$ ($-\rho^2 = W^\mu W_\mu$ where W^μ is the Pauli–Lubanski vector) might be utilized as a representation acting on a one-particle *physical neutrino space*. Infinite component fields were constructed which correspond to these representations (suffering from the usual diseases of this kind of theories), and a generalized $V-A$ theory was constructed for the interacting case.

In the limit when $\rho \to 0$, the infinite component field theory in question goes to a usual field theory of a fixed-helicity zero-mass particle and the generalized interaction goes in the limit to the *usual* $V-A$ interaction. It is now evident how to construct the free-field neutrino theory which incorporates also the "internal structure" of neutrinos. Actually we shall mention two possibilities. However, since there exists an unusual feature common for the two possibilities to be mentioned, we discuss this feature before.

We focused our attention on two particular classes of UIR of G'. Both remain irreducible when restricted to the Dirac subgroup. However, both are *reducible* when restricted to the Poincaré subgroup. In one case, we obtain after reduction on Poincaré two continuous-spin UIR of the Poincaré group: one containing all integer helicities, the other containing all half-integer helicities. In the second case, we obtain after reduction on P *all* discrete-spin UIR of the Poincaré group (integer as well as half-integer helicities) with multiplicity one.

Evidently, the second case is a limiting case of the first one. A question arises whether we shall choose the first or the second of the physical alternatives to be mentioned later, how comes and what can be done about the fact that in both cases we have already on the level of one-particle states both integer *as well as* half-integer helicity states occuring together?

The first half of the question can be simply answered: group theoretically the result is not astonishing since G' contains an eight-dimensional abelian normal subgroup "half" of which having a vector character and "half" of which having a spinor character.

From the physical point of view we have to remember that the Dirac group was also the covariance group (in our generalized sense) of the polarization equation of a fully polarized plane wave (for time-independent electromagnetic field).

Thus it is not astonishing that we find in the end at least a trace of a fully polarized photon state.

As to the second half of the question, we shall rather adopt the point of view that as far as we are interested in the neutrino free field or in the neutrino leptonic weak interactions, we shall systematically (when looking at the usual space-time behavior of our system) retain only the half-integer helicity part of the reduction and ignore the integer helicity part. It should be mentioned however, that the integer helicity part might play an important role in systems involving e.g., neutrinos and photons.

What are now the two physical alternatives that we got by means of our study?

(1) To take the idea of continuous-spin representations seriously. In such a case, we shall utilize this class of UIR of G' which are irreducible when restricted to the Dirac group and reducible into two *continuous-spin* UIR of P when restricted to the Poincaré subgroup (we shall utilize this subclass of representations which corresponds to a small value of ρ after reduction on P).

The construction of the Fock space is straightforward: the one-particle representation space will be the Hilbert space $\mathcal{H}$ of the UIR of G' which we utilize here, and the n-particle states space $\mathcal{H}_n$ will be constructed as usual as a completed skew-symmetric tensor product of n factors of $\mathcal{H}$:

$$\mathcal{H}_n = \underbrace{\mathcal{H}\,\hat{\otimes}_A \cdots \hat{\otimes}_A\,\mathcal{H}}_{n}.$$

If we denote by $\{\Omega\}$ the one-dimensional vacuum space, our Fock space will finally be

$$F = \{\Omega\} + \bigoplus_{n=0}^{\infty} \mathcal{H}_n.$$

The remaining of the free field construction in this formalism is straightforward. (Evidently as was said before, when concentrating on the Poincaré behavior of such a system, we shall only retain the half-integer continuous-spin UIR part for the one-particle states.)

(2) To utilize those UIR of G' which are reducible on the Poincaré subgroup, *giving rise to all discrete spin zero-mass* representations of P, and of course are irreducible when restricted to the Dirac subgroup. In such a case, we are led to the usual space-time description of the neutrino—by the ordinary *finite component* field theory—but with an unusual feature, that already the *one-particle states* will contain all possible helicites. Physically, this means the following: either we are dealing with neutrinos that can exist in all helicity (half-integer) excitation states, or that once we passed from the neutrino equation to the groups G and G' (by the generalized covariance principle) and then came back to, e.g., the corresponding free-field theory, we built a theory not only of the neutrino but also, in addition, of all other possible zero-mass discrete spin particles (which are yet to be discovered!).

Of course, in this case, the construction of the corresponding free-field theory is as before. The advantages and disadvantages of the two alternatives which were discussed are rather clear from the context. However, it should be noticed that both alternatives [mentioned in

(1) and (2)] have interesting space-time features (these features are of course seen in the limit when the field translations are set equal to zero and the theory then shows only its usual space-time aspects) and certainly both alternatives have also nice features concerning the "internal structure" of zero-mass particles since in both cases the corresponding UIR of G' is *irreducible* when restricted to the Dirac subgroup G.

It is this last condition which is necessary in order to utilize and develop the results concerning the Dirac-group aspect of our problem, mentioned in Ref. 1, such as parity violation, number of the different types of neutrinos occuring in Nature, conservation of lepton-number, leptonic-weak interactions and so on.

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Canonical transforms. I. Complex linear transforms

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Recent work by Moshinsky *et al.* on the role and applications of canonical transformations in quantum mechanics has focused attention on some complex extensions of linear transformations mapping the position and momentum operators $\hat{x}$ and $\hat{p}$ to a pair $\hat{\eta}$ and $\hat{\xi}$ of canonically conjugate, but not necessarily Hermitian, operators. In this paper we show that for a continuum of complex linear canonical transformations, a related Hilbert space of entire analytic functions exists with a scalar product over the complex plane such that the pair $\hat{\eta}, \hat{\xi}$ can be realized in the Schrödinger representation η and $-id/d\eta$. We provide a unitary mapping onto the ordinary Hilbert space of square-integrable functions over the real line through an integral transform. The transform kernels provide a representation of a subsemigroup of $SL(2,\mathbb{C})$. The well-known Bargmann transform is the special case when $\hat{\eta}$ and $i\hat{\xi}$ are the harmonic oscillator raising and lowering operators. The Moshinsky–Quesne transform is regained in the limit when the canonical transformation becomes real, a case which contains the ordinary Fourier transform. We present a realization of these transforms through hyperdifferential operators.

I. INTRODUCTION

The purpose of this work is to explore some of the consequences of the use of general canonical transformations in quantum mechanics. We shall concentrate here in studying complex linear transformations between the quantum mechanical operators of position and momentum $\hat{x}$ and $\hat{p}$, and a new pair of quantities given by

$$\hat{\eta} = a\hat{x} + b\hat{p},$$

$$\hat{\xi} = c\hat{x} + d\hat{p}, \quad a, b, c, d \in \mathbb{C} \text{ complex field}, \tag{1.1a}$$

with the unimodularity condition

$$ad - bc = 1 \tag{1.1b}$$

which ensures that, if $\hat{x}$ and $\hat{p}$ are canonically conjugate operators, then $\hat{\eta}$ and $\hat{\xi}$ will also be canonically conjugate, namely

$$[\hat{x}, \hat{p}] = i\,\mathbb{1} \Leftrightarrow [\hat{\eta}, \hat{\xi}] = i\,\mathbb{1} \tag{1.2}$$

in units where $\hbar \equiv 1$. In the usual Hilbert space $\mathcal{H}$ of quantum mechanical states,[1] we have the space of square integrable functions over the real line $\mathbb{R}$ with the scalar product

$$(f, g)_0 = \int_{\mathbb{R}} dx\, f(x)^* g(x) \tag{1.3}$$

for $f, g \in \mathcal{H}$. (The star denotes complex conjugation.) The Stone–von Neumann theorem states, moreover, that we can always (through a unitary transformation if necessary) use the Schrödinger realization of the realization of the Heisenberg algebra (1.2), i.e., represent $\hat{x}$ and $\hat{p}$ by x and $-id/dx$ over a set dense in $\mathcal{H}$.

When the transformation (1.1) is real, a scalar product where $\hat{\eta}$ and $\hat{\xi}$ are Hermitian and realized by the Schrödinger representation as η and $-i\,d/d\eta$ on functions of η in $\mathcal{H}' \approx \mathcal{H}$, with a scalar product analogous to (1.3) leads to the Moshinsky–Quesne transform[2] between $\mathcal{H}$ and $\mathcal{H}'$. The ordinary Fourier transform is a special case of this for $a = 0 = d$, $b = 1 = -c$.

The use of a complex linear transformation (1.1) with

$$a = 2^{-1/2} = d, \quad b = -i2^{-1/2} = c \tag{1.4}$$

has proven to be of great importance, as developed by Bargmann[3,4] and applied to the coherent-state formulation of quantum optics.[5] Equation (1.1) with (1.4) gives to $\hat{\eta}$ and $i\hat{\xi}$ (notice that Bargmann's $\hat{\xi}$ is here $i\hat{\xi}$) the meaning of creation and annihilation operators with respect to the harmonic oscillator states. Hermitian conjugation in $\mathcal{H}$ induces the properties $\hat{\eta}^+ = i\hat{\xi}$ and $(i\hat{\xi})^+ = \hat{\eta}$. In order to find a Hermitian form where the Schrödinger realization for $\hat{\eta}$ and $\hat{\xi}$ can be implemented, Bargmann introduced a space $\mathcal{J}$ of entire analytic functions $\bar{f}$ in $\eta \in \mathbb{C}$—the complex field—restricted by the condition $|\bar{f}(\eta)| \le \gamma \exp(\frac{1}{2}\alpha\eta^*\eta)$ for finite $\gamma > 0$ and $0 < \alpha < 1$, with a scalar product given by

$$(\bar{f}, \bar{g}) = \int_{\mathbb{C}} d\mu(\eta) \bar{f}(\eta)^* \bar{g}(\eta), \tag{1.5a}$$

$$d\mu(\eta) = \nu(\eta, \eta^*)\, d\mathrm{Re}\,\eta\, d\mathrm{Im}\,\eta \tag{1.5b}$$

for $\bar{f}, \bar{g} \in \mathcal{J}$, where the integration is extended over the complex η-plane (with a definite limiting procedure, see Ref. 3) and, in Bargmann's case, the weight $\nu(\eta, \eta^*) = \pi^{-1}\exp(-\eta^*\eta)$. It was also shown in Ref. 3 that $\mathcal{J}$ completed with respect to the norm induced by (1.5) is a Hilbert space and, moreover, a unitary mapping $\mathcal{A}: \mathcal{H} = \mathcal{J}$ can be implemented through the transform pair

$$\bar{f}(\eta) = \int_{\mathbb{R}} dx A(\eta, x) f(x), \tag{1.6a}$$

$$f(x) = \int_{\mathbb{C}} d\mu(\eta) A(\eta, x)^* \bar{f}(\eta), \tag{1.6b}$$

with the kernel $A(\eta, x) = \pi^{-1/4}\exp[-\frac{1}{2}(x^2 + \eta^2) + 2^{1/2}x\eta]$.

In a recent work, Kramer, Moshinsky, and Seligman[6] have considered a class of complex linear transformations of the type (1.1) and applied them to the study of clustering in nuclei, thereby achieving significant conceptual and calculational simplifications. We have taken their motivation to study the general case of complex linear transformations and set up a continuum of spaces $\mathcal{J}$ of entire analytic functions with different growth restrictions in the complex η-variable and a scalar product of the general type (1.5) with appropriate measures $\nu(\eta, \eta^*)$, where the Schrödinger representation is realized. As in Bargmann's case, completion with respect to the norm induced by (1.5) shows that the $\mathcal{J}$'s are Hilbert spaces and that unitary maps $\mathcal{A}: \mathcal{H} = \mathcal{J}$ can be implemented through transforms of the type (1.6). We shall call these *canonical* transforms.

In Sec. II we construct and characterize the spaces $\mathcal{J}$ and find the transform kernels in Sec. III. In Sec. IV we determine the behavior of the transforms in the limit where the parameters a, b, c, d become real. The scalar product (1.5) is shown to collapse to an integral over $\mathbb{R}$, so that the Moshinsky—Quesne transform is regained. As the composition of two canonical transformations is of the same type, the composition of the corresponding transforms is developed in Sec. V. In Sec. VI, the transform kernels are shown to provide, when bounded, representations of a semigroup $HSL(2, \mathbb{C})$ of the group $SL(2, \mathbb{C})$ of canonical transformations (1.1). In Appendix A we give a realization of canonical transforms through hyperdifferential operators, while in Appendix B results for general n-dimensional spaces are presented.

In a future series of articles we intend to explore the consequences of more general complex canonical transformations in quantum mechanics. In Ref. 6 it was shown that a transformation in the radial coordinate[7] of a higher-dimensional space undergoing a linear transformation is related with the Barut—Girardello transform.[8] Among the classes of canonical transformations where classical and quantum mechanics follow each other[9] are point transformations followed by linear ones. This has been used to relate[10] the representation of the algebra $so(2,1)$ given by the dynamical algebra of a harmonic oscillator (with the addition of an inverse-square potential) and its exponentiation to the discrete series representations of the group $SO(2,1)$, with Bargmann's realization[11] of the same series. Finally, many-sheeted canonical mappings of phase space into itself such as those considered in Ref. 12 can be implemented with the help of the representations of the group of automorphisms and an associated transform.[6]

II. THE SPACE $\mathcal{J}$

Consider the complex unimodular linear transformation (1.1) written in matrix form as

$$\mathbf{Z} \equiv \begin{pmatrix} \hat{\eta} \\ \hat{\xi} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{p} \end{pmatrix} \equiv M\mathbf{Z}_0, \quad \det M = 1 \tag{2.1}$$

(i.e., $M \in SL(2,\mathbb{C})$). The corresponding adjoint operators, relative to the scalar product in $\mathcal{H}$, where $\hat{x}$ and $\hat{p}$ are Hermitian, can be then written in terms of the original ones as

$$\mathbf{Z}^+ \equiv \begin{pmatrix} \hat{\eta}^+ \\ \hat{\xi}^+ \end{pmatrix} = M^*\mathbf{Z}_0 = M^*M^{-1}\mathbf{Z} \equiv C\mathbf{Z} \tag{2.2a}$$

where the *conjugation* matrix

$$C = \begin{pmatrix} u & iv \\ iw & u^* \end{pmatrix} \tag{2.2b}$$

is such that $\det C = 1$, $CC^* = 1$ and its elements are given and restricted by

$$u = a^*d - b^*c \in \mathbb{C}, \tag{2.3a}$$

$$v = 2\,\mathrm{Im}\, b^*a, \quad w = 2\,\mathrm{Im}\, c^*d \in \mathbb{R}, \tag{2.3b}$$

$$|u|^2 + vw = 1. \tag{2.3c}$$

For every $M \in SL(2,\mathbb{C})$ we have thus a conjugation matrix $C(M)$. In particular, if $R \in SL(2,\mathbb{R})$, then $C(R) = \mathbb{1}$ and $\hat{\eta}$ and $\hat{\xi}$ are Hermitian, and $C(MR) = C(M)$. Bargmann's case (1.4) corresponds to the imaginary antidiagonal matrix with $u=0$, $v=1=w$. Since from (1.2), $\hat{\eta}$ and $\hat{\xi}$ are canonically conjugate, we want to implement the Schrödinger representation

$$\hat{\eta}\bar{f}(\eta) = \eta\bar{f}(\eta), \tag{2.4a}$$

$$\hat{\xi}\bar{f}(\eta) = -i\frac{d}{d\eta}\bar{f}(\eta) \tag{2.4b}$$

on any suitable function $\bar{f}$ of the complex variable η. In order that the total derivative in (2.4b) be well defined, the function $\bar{f}$ must be analytic in η. The conditions we are asking for a scalar product to satisfy can then be formulated, through (2.2), as

$$(\hat{\eta}\bar{f}, \bar{g}) = (\bar{f}, [u\hat{\eta} + iv\hat{\xi}]\bar{g}), \tag{2.5a}$$

$$(\hat{\xi}\bar{f}, \bar{g}) = (\bar{f}, [iw\hat{\eta} + u^*\hat{\xi}]\bar{g}). \tag{2.5b}$$

We can see that an ordinary scalar product of the type (1.3) cannot fulfill this requirement. One must look for a more general kind of scalar product. Proposing the form (1.5) we can turn Eqs. (2.5) into differential equations for the weight function $\nu(\eta, \eta^*)$. Using (1.5), (2.4) and performing an integration by parts [provided that the boundary value of $\bar{f}(\eta)^*\nu(\eta,\eta^*)\bar{g}(\eta)$ at infinity be zero], the conditions (2.5) can be given as

$$\eta^*\nu(\eta,\eta^*) = (u\eta - v\frac{\partial}{\partial\eta})\nu(\eta,\eta^*), \tag{2.6a}$$

$$\frac{\partial}{\partial\eta^*}\nu(\eta,\eta^*) = -\left(w\eta + u^*\frac{\partial}{\partial\eta}\right)\nu(\eta,\eta^*). \tag{2.6b}$$

The solution of (2.6) with a specific choice of normalization is

$$\nu(\eta,\eta^*) = 2(2\pi v)^{-1/2}\exp\left\{\frac{1}{2v}[u\eta^2 - 2\eta\eta^* + u^*\eta^{*2}]\right\}$$
$$= \nu(\eta^*,\eta)^*. \tag{2.7a}$$

A convenient representation is obtained when we write in polar form $\eta = \rho e^{i\theta}$, $u = \omega e^{i\phi}$, whereupon (2.7a) becomes

$$\nu(\eta,\eta^*) \equiv \nu[\rho,\theta] = 2(2\pi v)^{-1/2}\exp\left\{-\frac{\rho^2}{v}[1 - \omega\cos(\varphi + 2\theta)]\right\}. \tag{2.7b}$$

The boundary condition on $\bar{f}(\eta)^*\nu(\eta,\eta^*)\bar{g}(\eta)$ can now be made explicit: we write $\bar{f}(\eta) = f_b(\eta v^{-1/2})\exp[(-u/2v)\eta^2]$, imposing the condition $v > 0$, then the scalar product (1.5)—(2.7) becomes the Bargmann scalar product[3] between $f_b(\eta')$ and $g_b(\eta')$ for $\eta' = \eta v^{-1/2}$. The growth conditions imposed on these functions imply then that $\bar{f}$ and $\bar{g}$ must satisfy

$$|\bar{f}(\rho e^{i\theta})| \le \gamma\exp\left\{\frac{\rho^2}{v}[\alpha - \omega\cos(\varphi + 2\theta)]\right\}, \tag{2.8}$$

for finite $\gamma > 0$ and $0 < \alpha < 1$, which is dependent on the direction θ in the complex η-plane. This is sufficient to characterize the space $\mathcal{J}$ of entire analytic functions for which the scalar product (1.5) is finite. Bargmann's analysis[3] can now be translated to state that for $v > 0$, the space $\mathcal{J}$ with the scalar product (1.5) is a Hilbert space, unitarily equivalent to $\mathcal{H}$ through a transform of the kind (1.6). It should be noticed that Bargmann's transform is indeed regained in the particular case (1.4), allowing for the choice in the measure normalization: here it is chosen as $2(2\pi v)^{-1/2}$ so that it go over smoothly to the Moshinsky—Quesne transform (Sec. IV), while in the original work[3] it is set as π^{-1}. For every matrix $M \in SL(2,\mathbb{C})$ such that $C(M)$ satisfies $v>0$ we have thus a Hilbert space $\mathcal{F}$.

A dense orthonormal basis for $\mathcal{F}$ can now be constructed as

$$\bar{u}_n(\eta) = [(2\pi v)^{1/2} n!]^{-1/2} \exp\left(-\frac{u}{2v}\eta^2\right)(\eta v^{-1/2})^n, \qquad n = 0,1,2,\ldots. \tag{2.9}$$

These functions satisfy the following recursion relations:

$$[v^{-1/2}\eta]\bar{U}_n(\eta) = (n+1)^{1/2}\bar{U}_{n+1}(\eta), \tag{2.10a}$$

$$\left[uv^{-1/2}\eta + v^{1/2}\frac{d}{d\eta}\right]\bar{U}_n(\eta) = n^{1/2}\bar{U}_{n-1}(\eta), \tag{2.10b}$$

and, in particular,

$$\left[u\eta + v\frac{d}{d\eta}\right]\bar{U}_0(\eta) = 0. \tag{2.10c}$$

They are, thus, eigenfunctions of a number operator

$$\hat{N}_u\bar{U}_n(\eta) \equiv \left[uv^{-1}\eta^2 + \eta\frac{d}{d\eta}\right]\bar{U}_n(\eta) = \frac{1}{v}\hat{\eta}\hat{\eta}^\dagger\bar{U}_n(\eta) = n\bar{U}_n(\eta). \tag{2.11}$$

From the orthonormal basis (2.9) we can build the generating function

$$K(\eta,\eta') \equiv \sum_{n=0}^{\infty}\bar{U}_n(\eta)\bar{U}_n(\eta')^* = (2\pi v)^{-1/2} \times \exp\left\{-\frac{1}{2v}[u\eta^2 - 2\eta\eta'^* + u^*\eta'^{*2}]\right\} = K(\eta',\eta)^*, \tag{2.12a}$$

which acts as the reproducing kernel under the scalar product (1.5):

$$(K(\cdot,\eta'),\bar{f}) = \int_{\mathbb{C}} d\mu(\eta)K(\eta,\eta')^*\bar{f}(\eta) = \bar{f}(\eta'). \tag{2.12b}$$

III. THE TRANSFORMATION KERNEL AND PAIRS OF TRANSFORM BASES

We want to establish a mapping between the elements f of the Hilbert space $\mathcal{H}$ and the elements $\bar{f}$ in $\mathcal{F}$, as given by (1.6) in such a way that if $f(x)$ is mapped into $\bar{f}(n)$, then $\hat{\eta}f(x)$ maps into $\eta\bar{f}(\eta)$ and $\hat{\xi}f(x)$ into $-i(d/d\eta)\bar{f}(\eta)$. Through (2.1), this means

$$\eta\bar{f}(\eta) = \int_{\mathbb{R}} dx A(\eta,x)\hat{\eta}f(x) = \int_{\mathbb{R}} dx\left(\left[ax + ib\frac{\partial}{\partial x}\right]A(\eta,x)\right)f(x), \tag{3.1a}$$

$$-i\frac{d}{d\eta}\bar{f}(\eta) = \int_{\mathbb{R}} dx A(\eta,x)\hat{\xi}f(x) = \int_{\mathbb{R}} dx\left(\left[cx + id\frac{\partial}{\partial x}\right]A(\eta,x)\right)f(x), \tag{3.1b}$$

and hence the transformation kernel $A(\eta,x)$ must satisfy the differential equations

$$\eta A(\eta,x) = \left[ax + ib\frac{\partial}{\partial x}\right]A(\eta,x), \tag{3.2a}$$

$$-i\frac{\partial}{\partial\eta}A(\eta,x) = \left[cx + id\frac{\partial}{\partial x}\right]A(\eta,x). \tag{3.2b}$$

The solution, with proper normalization, is

$$A(\eta,x) = \varphi_A(2\pi|b|)^{-1/2}\exp\left\{\frac{i}{2b}[ax^2 - 2x\eta + d\eta^2]\right\}, \tag{3.3a}$$

where we choose the phase factor to be

$$\varphi_A = \exp\left(-\frac{i}{2}\left[\frac{\pi}{2} + \Phi(b)\right]\right), \tag{3.3b}$$

where $\Phi(b) \equiv$ phase of $b \in [-\pi, \pi)$. This choice of phase has been made so that the representation properties of the $A(\eta,x)$ be simple (Sec. VI) and for $M \in SL(2,\mathbf{R})$ they agree with Ref. 2. The integrability condition in (1.6a) requires that $\mathrm{Im}(a/b) \geq 0$ (i.e., $v \geq 0$) and that if $a=0$, then b should be real. The integrability of Eq. (1.6b) can then be seen to hold through the identity $ub = -ivd + b^*$ since this implies that $|id/2b| \leq |1-\omega|/2v$. The normalization makes the transforms (1.6) be inverse to each other, as

$$\int_{\mathbb{R}} dx A(\eta,x)A(\eta',x)^* = K(\eta,\eta'), \tag{3.4a}$$

$$\int_{\mathbb{C}} d\mu(\eta)A(\eta,x)^*A(\eta,x') = \delta(x-x'). \tag{3.4b}$$

Equation (3.4a) can be verified directly, while Eq. (3.4b) will be shown to hold when we will write the transform kernel $A(\eta,x)$ as the generating function linking two orthonormal bases, one in $\mathcal{H}$ and one in $\mathcal{F}$.

We have constructed an orthonormal basis of functions $\{\bar{U}_n(\eta)\}$ for $\mathcal{F}$ in (2.9). In searching for a corresponding basis $\{U_n(x)\}$ for $\mathcal{H}$ we can go directly through the transform definition (1.6b) or, preferably, use the independent method of using the raising operators (2.10) for $\{\bar{U}_n(\eta)\}$ translated to operators in x and d/dx through (2.1). The extremum $U_0(x)$ of the ladder is found from (2.10c) as

$$U_0(x) = \varphi_A^{-1}\left(\pi/\mathrm{Im}\,\frac{a}{b}\right)^{-1/4}\exp\left(-i\frac{a^*}{2b^*}x^2\right) \tag{3.5a}$$

normalized with respect to the scalar product in $\mathcal{H}$, with φ_A given by (3.3b). From $U_0(x)$ and the raising operator (2.10a) we find

$$U_n(x) = [v^n n!]^{-1/2}\left[ax - ib\frac{d}{dx}\right]^n U_0(x) = \varphi_A^{-1}\varphi_n\left[2^n n!\left(\pi/\mathrm{Im}\,\frac{a}{b}\right)^{1/2}\right]^{-1/2} \times \exp\left(-i\frac{a^*}{2b^*}x^2\right)H_n\left(\left[\mathrm{Im}\,\frac{a}{b}\right]^{1/2}x\right). \tag{3.5b}$$

with

$$\varphi_n = \exp\left[in\left(\frac{\pi}{2} + \Phi(b)\right)\right]. \tag{3.5c}$$

The basis $\{U_n(x)\}$ can be checked to be indeed orthonormal under the scalar product in $\mathcal{H}$ and we can verify directly that the transformation kernel is indeed the generating function between the bases:

$$A(\eta, x)=\sum_{n=0}^{\infty} \bar{U}_n(\eta)U_n(x)^*. \tag{3.6}$$

In particular, notice that for Bargmann's case (1.4), $\{\bar{U}_n(\eta)\}$ is the basis of monomials in η while $\{U_n(x)\}$ are the harmonic oscillator wavefunctions $\psi_n(x)$.

There are reasons for not being satisfied with the basis $\{\bar{U}_n(\eta)\}$ alone. There is the problem of not having a manifest limit as $v\to 0$ (when the transformation matrix M becomes real) and that of being eigenfunctions of the number operator (2.11) which in $\mathcal{H}$ reads $v^{-1}(ax-ib\,d/dx)\times(a^*x-ib^*\,d/dx)$. Thus, we introduce the well-known harmonic oscillator wavefunction basis (with the usual phase convention)

$$\psi_n(x)=[2^n n!\,\pi^{1/2}]^{-1/2}\exp(-\tfrac{1}{2}x^2)H_n(x), \quad n=0,1,2,\ldots. \tag{3.7}$$

The raising, lowering, and number operators are simple and can be translated to operators in η and $d/d\eta$ through (2.1) in order to find the transform basis. The differential equation for the ground function yields

$$\bar{\psi}_0(\eta)=[\pi^{1/2}(a+ib)]^{-1/2}\exp\left(-\frac{d-ic}{a+ib}\,\frac{\eta^2}{2}\right), \tag{3.8a}$$

where we must take the sheet given by $(a+b)^{-1/2}=|a+ib|^{-1/2}\exp-\tfrac{1}{2}i\,\Phi(a+ib)$, and the rest of the basis can be generated through the application of the raising operator, i.e.,

$$\bar{\psi}_n(\eta)=[2^n n!]^{-1/2}\left[(d+ic)\eta+(-a+ib)\frac{d}{d\eta}\right]^n\bar{\psi}_0(\eta)$$

$$=\left[\left(2\frac{a+ib}{a-ib}\right)^n n!\,\pi^{1/2}(a+ib)\right]^{-1/2}$$

$$\times\exp\left[-\frac{d-ic}{a+ib}\,\frac{\eta^2}{2}\right]H_n\left([a^2+b^2]^{-1/2}\eta\right), \tag{3.8b}$$

which reduces to (3.7) when M becomes $\mathbb{1}$. It is also interesting to notice that Bargmann's case (1.4) gives back the basis $\{\bar{U}_n(\eta)\}$ with the proper normalization. (Notice that only the leading term of the Hermite polynomial survives). As a final check of the calculation we can verify that the transformation kernel $A(\eta,x)$ in (3.3) is the generating function between the bases $\{\psi_n(x)\}$ and $\{\bar{\psi}_n(\eta)\}$, i.e.,

$$A(\eta, x)=\sum_{n=0}^{\infty}\bar{\psi}_n(\eta)\psi_n(x)^* \tag{3.9}$$

implemented through the use of an integral representation for one of the Hermite functions.[13]

IV. THE LIMIT OF REAL TRANSFORMATIONS

We now want to examine the behavior of our construction when the parameters $a,b,c,d\in\mathbb{C}$ in (2.1) become real. Notice that the basis functions $\{\bar{\psi}_n(\eta)\}$ present no peculiar behavior and indeed go smoothly into $\{\psi_n(x)\}$ when $M\to\mathbb{1}$. The transformation kernel $A(\eta,x)$ in (3.3) is uneventful when a,b,c,d become real and only when b approaches zero does the expression become indeterminate at first sight. The analysis in Ref. 2 leads us to expect that the kernel will become a Dirac δ in $\eta-x$. This has to be examined further. Indeed, we intend to show that the scalar product (1.5) collapses to a line integral as $v\to 0$.

Consider the measure (1.5b) parametrized in its polar decomposition (2.7b) as $d\mu(\eta)=\nu[\rho,\theta]\rho d\rho d\theta$. When $v\to 0$, $\omega=|1-vw|^{1/2}\approx 1-\tfrac{1}{2}vw\to 1$. Recalling that for real, positive $\epsilon\to 0$, $\mathrm{l.i.m.}\,\epsilon^{-1/2}\exp(-q^2/\epsilon)=\pi^{1/2}\delta(q)$, we can write

$$\begin{aligned}\underset{\nu\to 0}{\mathrm{l.i.m.}}\ \nu[\rho,\theta]&=\underset{\nu\to 0}{\mathrm{l.i.m.}}\ 2(2\pi v)^{-1/2}\exp\left\{-\frac{\rho^2}{v}[1-(1-\tfrac{1}{2}vw)\times\cos(\varphi+2\theta)]\right\}\\&=2^{1/2}\delta(\rho[1-\cos(\varphi+2\theta)]^{1/2})\\&\quad\times\exp[-\tfrac{1}{2}\rho^2 w\cos(\varphi+2\theta)]\\&=\rho^{-1}\delta(\sin(\tfrac{1}{2}\varphi+\theta))\exp[-\tfrac{1}{2}\rho^2 w\cos(\varphi+2\theta)]\\&=\rho^{-1}[\delta(\theta+\tfrac{1}{2}\varphi)+\delta(\theta+\tfrac{1}{2}\varphi-\pi)]\exp[-\tfrac{1}{2}\rho^2 w].\end{aligned} \tag{4.1}$$

All of these steps should be done remembering that the functions are under the double integral $\int_0^\infty \rho\,d\rho\int_0^{2\pi}d\theta$, in particular, the third step takes into account the fact that the point $\rho=0$ is immaterial for the δ as it is cancelled by the measure in ρ, and the last step makes use of the consequence that the δ will act only in picking out values in the integration over θ. The growth condition (2.8) on the function space is such that the scalar product is finite and for the line $\theta_0\equiv-\tfrac{1}{2}\varphi$, $\pi-\tfrac{1}{2}\varphi$ is

$$|\bar{f}(\rho e^{i\theta_0})|\leqslant\gamma\exp\left(\frac{\rho^2}{2v}[\alpha-\omega]\right)<\gamma\exp(\tfrac{1}{4}w\rho^2) \tag{4.2}$$

when we write $\omega\approx 1-\tfrac{1}{2}vw$, $\alpha=1-A(v)$ and let $A(v)$ be any function of v which decreases faster than v as $v\to 0$. Similarly for $\bar{g}$. If we now define for $\bar{f}(\eta)=\bar{f}[\rho,\theta]$, $\bar{f}(x)\equiv\bar{f}[x,-\tfrac{1}{2}\varphi]$ and $\bar{f}(-x)\equiv\bar{f}[x,\pi-\tfrac{1}{2}\varphi]$ for $x\geqslant 0$, the limit indicated follows, i.e.,

$$\lim_{v\to 0}\int_{\mathbb{C}}d\mu(\eta)\bar{f}(\eta)^*\bar{g}(\eta)=\int_{\mathbf{R}e^{-i\varphi/2}}dx\,e^{-w|x|^2/2}\bar{f}(x)^*\bar{g}(x) \tag{4.3}$$

with the condition, in effect, that $\bar{f}$ be such that $\bar{f}(x)\times\exp(-\tfrac{1}{4}wx^2)$ is square integrable over $\mathbf{R}$, and similarly for $\bar{g}$.

As can be seen, as $v\to 0$ the integral over $\eta\in\mathbb{C}$ becomes an integral over a straight line passing through the origin and with a phase $-\tfrac{1}{2}\varphi=-\tfrac{1}{2}\Phi(u)=\Phi(a)$. When the transformation matrix M is real, $u=1$ and the integration path becomes the real axis. By a similar argument, the reproducing kernel $K(\eta,\eta')$ in (2.12) becomes the Dirac $\delta(x-x')$. The behavior of the transformation kernel $A(\eta,x)$ at the limit $b\to 0$ can be analized when this takes place from any direction in the complex plane. Using (1.1b),

$$\begin{aligned}A(x',x)&=(2\pi)^{-1/2}\varphi_A|b|^{-1/2}\exp\{-|b|^{-1}[\varphi_A(2/a)^{-1/2}x\\&\quad-\varphi_A(2a)^{-1/2}x']^2\}\exp\left(\frac{ic}{2a}x'^2\right)\\&\underset{|b|\to 0}{\to}a^{-1/2}\delta(x-a^{-1}x')\exp\left(\frac{ic}{2a}x'^2\right)\end{aligned} \tag{4.4}$$

and the phase of the direction in which the inverse transform takes place, $\Phi(a)=-\frac{1}{2}\Phi(u)$, is the appropriate one which will make use of the Dirac δ.

We can make explicit the condition that a transformation M in (2.1) lead to a transform involving only a line integral. Notice first that $C(M)=\mathbb{1}$ if and only if $M \in SL(2,\mathbb{R})$, the measure in the transform space being simply dx. Next, we can examine the cases when $C(M)$ is a lower triangular matrix ($v=0$). We consider the case $u=1$ so that the integral be along the real axis. Analysis of the conditions (2.3) leads us to the restrictions: a, b real. An important subclass is that considered in Ref. 6, namely $b=0$, $a=d^{-1}$ real, where (4.4) simulates the matrix elements of a Gaussian potential for $c=iq$, $q>0$.

Transforms involving line integrals along a path tilted by a phase α can be obtained multiplying the transformation matrix M on the left by a diagonal matrix with elements $\exp(i\alpha)$, $\exp(-i\alpha)$ as then $u=\exp(-2i\alpha)$. In particular, for $b=i=-c^{-1}$, $d=0$ ($\alpha=\pi/2$) we obtain a Laplace transform with kernel (3.3) given by $-i(2\pi)^{-1/2}\times\exp(-xx')$, which is off by a factor and a phase from the usual Laplace transform. The condition "b real when $a=0$" for the kernel (3.3) is now violated, so it is not surprising that the integral in (1.6a) can diverge for $f\in\mathcal{H}$. A restriction on $\mathcal{H}$ [for instance $f(x)=0$ for $x<0$] may make the transform meaningful. The inverse transform is an integral over a Bromwich contour up along the imaginary axis.

V. COMPOSITION OF TRANSFORMS

For every matrix $M\in SL(2,\mathbb{C})$ in (2.1) satisfying $\mathrm{Im}(a/b)\geq 0$ we have associated a canonical transform (1.6) from the Hilbert space $\mathcal{H}$ to a Hilbert space $\mathcal{F}$ characterized by (1.5), (2.7), and (2.8). Take now two such spaces $\mathcal{F}_1$ and $\mathcal{F}_2$ associated to the transformations $\mathbf{z}_1=M_1\mathbf{z}_0$ and $\mathbf{z}_2=M_2\mathbf{z}_0$, with transformation kernels $A_1(\eta,x)$ and $A_2(\eta,x)$. Then, since $\mathbf{z}_2=M_2M_1^{-1}\mathbf{z}_1\equiv M_{21}\mathbf{z}_1$, we want to find the unitary mapping between $\mathcal{F}_1$ and $\mathcal{F}_2$. Labelling $\bar{f}^{(k)}(\eta)\in\mathcal{F}_k$ and the corresponding measures $d\mu_k(\eta)$, we obtain from (1.6),

$$\bar{f}^{(2)}(\eta)=\int_{\mathbb{C}}d\mu_1(\eta')A_{21}(\eta,\eta')\bar{f}^{(1)}(\eta'), \tag{5.1a}$$

$$\bar{f}^{(1)}(\eta')=\int_{\mathbb{C}}d\mu_2(\eta)A_{21}(\eta,\eta')^*\bar{f}^{(2)}(\eta), \tag{5.1b}$$

where the transform kernel $A_{21}(\eta,\eta')$ from $\mathcal{F}_1$ to $\mathcal{F}_2$ is

$$A_{21}(\eta,\eta')=\int_{\mathbb{R}}dx\,A_2(\eta,x)A_2(\eta',x)^*=A_{12}(\eta',\eta)^*. \tag{5.1c}$$

Explicitly, it is

$$A_{21}(\eta,\eta')=\Phi(b_2,-b_1^*;b)\exp[-\tfrac{1}{2}i(\pi/2+\Phi(b))](2\pi|b|^{-1/2}\times\exp\{(i/2b)[a\eta'^{*2}-2\eta'^*\eta+d\eta^2]\}, \tag{5.2a}$$

where

$$\begin{pmatrix}a & b\\ c & d\end{pmatrix}=\begin{pmatrix}a_2 & b_2\\ c_2 & d_2\end{pmatrix}\begin{pmatrix}a_1 & b_1\\ c_1 & d_1\end{pmatrix}^{*-1}, \tag{5.2b}$$

and

$$\Phi(b',b'';b)\equiv\exp\{-\tfrac{1}{2}i[\Phi(b')+\Phi(b'')-\Phi(b)-\Phi(b'b''/b)]\}=\pm 1 \tag{5.2c}$$

[compare with Eqs. (3.3)], and can be written as a generating function

$$A_{21}(\eta,\eta')=\sum_{n=0}^{\infty}\bar{\psi}_n^{(2)}(\eta)\bar{\psi}_n^{(1)}(\eta')^*. \tag{5.3}$$

In particular, this allows us to define $A_k(\eta,x)\equiv A_{k0}(\eta,x)$, $A_{0k}(x,\eta)\equiv A_k(\eta,x)^*$ and the reproducing kernel in each space as $K_k(\eta,\eta')=A_{kk}(\eta,\eta')$. The composition of transforms can then be effected through any (allowed) space $\mathcal{F}_3$ as

$$A_{21}(\eta,\eta'')=\int_{\mathbb{C}}d\mu_3(\eta')A_{23}(\eta,\eta')A_{31}(\eta',\eta''), \tag{5.4}$$

which generalizes (5.1c) when we understand that $\int_{\mathbb{C}}d\mu_0(\eta)\cdots=\int_{\mathbb{R}}dx\cdots$ and $\mathcal{H}\equiv\mathcal{F}_0$, it corresponds to $M_{21}=M_{23}M_{31}$ for $M_{31}=M_3M_1^{-1}$, etc. with the explicit forms as obtained from (5.2). Notice that when M_1 and M_2 belong to the class $v=0$, the transform (5.1) involves only line integrals although $M_2M_1^{-1}$ may not belong to this class. Similarly, the condition $\mathrm{Im}(a/b)\geq 0$ which must hold for M_1 and M_2 may not hold for their composition $M_2M_1^{-1}$. The existence of the transform (5.1) is assured, however, as $A_{21}(\eta,\eta')$ belongs to $\mathcal{F}_1$ as a function of its second argument and to $\mathcal{F}_2$ as a function of the first. Square integrability is only demanded in $\mathcal{H}$ or its isomorphic spaces.

VI. LINEAR OPERATORS AND REPRESENTATIONS OF HSL (2,C)

Let $\mathcal{P}$ be a bounded operator mapping $\mathcal{H}$ onto itself, represented by an integral kernel $P(x,x')$ through

$$f'(x)=\int_{\mathbb{R}}dx'P(x,x')f(x'). \tag{6.1}$$

It then follows from (1.6) that $\mathcal{P}$ will also map $\mathcal{F}$ onto $\mathcal{F}$ through

$$\bar{f}'(\eta)=\int_{\mathbb{C}}d\mu(\eta')\bar{P}(\eta,\eta')\bar{f}(\eta'), \tag{6.2}$$

represented by the integral kernel

$$\bar{P}(\eta,\eta')=\int\int_{\mathbb{R}}dx\,dx'A(\eta,x)P(x,x')A(\eta',x')^*. \tag{6.3}$$

To a product $\mathcal{R}=\mathcal{P}\mathcal{Q}$ of such bounded operator then corresponds

$$R(x,x'')=\int_{\mathbb{R}}dxP(x,x')Q(x',x'') \tag{6.4}$$

which is also bounded and

$$\bar{R}(\eta,\eta'')=\int_{\mathbb{C}}d\mu(\eta')\bar{P}(\eta,\eta')\bar{Q}(\eta',\eta''). \tag{6.5}$$

In particular, to the unit operator, whose representative in $\mathcal{H}$ is $\delta(x-x')$, will correspond through (3.4a) the reproducing kernel $K(\eta,\eta')$ in $\mathcal{F}$.

Now, for every $M\in SL(2,\mathbb{C})$, consider the operator $\mathcal{A}(M)$ with the integral kernel given by (3.3), when we restrict η to the real line. These are now operators mapping $\mathcal{H}$ onto $\mathcal{H}$, and can be seen as *passive* $SL(2,\mathbb{C})$ transformations, as opposed to the active transformations seen in the last section, which mapped $\mathcal{H}$ onto $\mathcal{F}$. We shall denote this integral kernel by

$$D_{xx'}^{(0)}(M)=A_M(x,x')=\exp[-\tfrac{1}{2}i(\pi/2+\Phi(b))](2\pi|b|)^{-1/2}\times\exp\{(i/2b)[ax'^2-2x'x+dx^2]\}. \tag{6.6}$$

When integration is possible, these kernels satisfy

$$\int_{\mathbb{R}}dx'D_{xx'}^{(0)}(M_1)D_{x'x''}^{(0)}(M_2)=\Phi(b_1,b_2;b_{12})D_{xx''}^{(0)}(M_1M_2) \tag{6.7}$$

and hence form a ray representation of a subset of

$SL(2,\mathbb{C})$: the subset for which the operators $\mathcal{A}(M)$ are bounded. As the product of two bounded operators is bounded, such a set must be a semigroup contained in $SL(2,\mathbb{C})$.

Notice first that the kernels representing $\mathcal{A}(M)$ with $M\in SL(2,\mathbb{R})$ are bounded. This is obvious when we examine the transform normalized basis (3.8), as here $\mathcal{J}\equiv\mathcal{H}$, $(\mathcal{A}(M)\psi_n, \mathcal{A}(M)\psi_n)_0=(\bar{\psi}_n,\bar{\psi}_n)_0=1$ and $\{\psi_n(x)\}$ is dense in $\mathcal{H}$ and $\mathcal{J}$. For $M\in SL(2,\mathbb{C})$ the operators $\mathcal{A}(M)$ will be Hilbert–Schmidt operators when the kernels (6.6) satisfy $\iint dx\,dx'\,|D^{(0)}_{xx'}(M)|^2<\infty$. In performing the integrals, we see that we obtain the conditions

$$\mathrm{Im}\, b^*a>0:v>0, \tag{6.8a}$$

$$\mathrm{Im}\, b^*a\,\mathrm{Im}\, b^*d>\mathrm{Im}^2 b. \tag{6.8b}$$

Now, the product of a Hilbert–Schmidt and a bounded one is a Hilbert–Schmidt operator, hence the set of matrices

$$\begin{pmatrix}\alpha & \beta\\ \gamma & \delta\end{pmatrix}\begin{pmatrix}\cosh\zeta & -i\sinh\zeta\\ i\sinh\zeta & \cosh\zeta\end{pmatrix}\begin{pmatrix}\alpha' & \beta'\\ \gamma' & \delta'\end{pmatrix} \tag{6.9}$$

($\alpha,\alpha',\beta,\ldots,\delta'$ real) will be represented by Hilbert–Schmidt operators for $\zeta>0$, as can be verified directly from (6.8). This is a semigroup which does not contain the identity. If we add to (6.9) the point $\zeta=0$, thereby making (6.9) contain $SL(2,\mathbb{R})$, we will have a set of bounded operators representing the semigroup denoted by $HSL(2,\mathbb{C})$ in Ref. 6. Notice that the matrix (1.4) corresponding to the Bargmann transform does not belong to this set.

An important subset of $HSL(2,\mathbb{C})$ is the set of matrices which we write and decompose as

$$\begin{pmatrix}\alpha'' & -i\beta''\\ i\gamma'' & \delta''\end{pmatrix}=\begin{pmatrix}1 & 0\\ iq & 1\end{pmatrix}\begin{pmatrix}D & 0\\ 0 & D^{-1}\end{pmatrix}\begin{pmatrix}1 & -iq'\\ 0 & 1\end{pmatrix} \tag{6.10}$$

with $\alpha'',\ldots,\delta''$, $q,q'\geq 0$, $D>0$, which are bounded, but not Hilbert–Schmidt operators [as conditions (6.8) may be violated]. The set (6.10) manifestly forms a semigroup denoted by $HSL(2,\mathbb{R})$ in Ref. 6, since it is related through a similarity transformation [by a diagonal matrix with elements $\exp(-i\pi/4)$, $\exp(i\pi/4)$] with the set of $SL(2,\mathbb{R})$ matrices with nonnegative elements. The parametrization (6.10) furthermore allows us to reach the special cases $\beta''=0$ [Eq. (4.4) which simulates the Gaussian potential] for which the decomposition (6.9) fails.

From the representation (6.6) we can build through (6.3) a continuum of representations of $HSL(2,\mathbb{C})$ through (5.1c) as

$$D^{(k)}_{\eta\eta'}(M)=D^{(0)}_{\eta\eta'}(M_k M M_k^{*-1}) \tag{6.11}$$

where $M_k\in SL(2,\mathbb{C})$ satisfying the conditions for the existence of a transform. Notice that the variable η' in (6.11) appears as η'^* in the explicit form (6.6). These D's will exhibit the composition

$$\int_{\mathbb{C}} d\mu_k(\eta')D^{(k)}_{\eta\eta'}(M_1)D^{(k)}_{\eta'\eta''}(M_2)=\varphi D^{(k)}_{\eta\eta''}(M_1M_2) \tag{6.12}$$

and the property

$$D^{(k)}_{\eta\eta'}(M)=D^{(k)}_{\eta'\eta}(M^{*-1})^* \tag{6.13}$$

so that the representation is unitary for $M\in SL(2,\mathbb{R})$.

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APPENDIX A: REALIZATION THROUGH HYPERDIFFERENTIAL OPERATORS

In this Appendix we want to introduce a Lie algebra structure for the set of canonical transforms as

$$\bar{f}(x)=[U_\tau f](x)=\exp(i\tau H)f(x)=\int_{\mathbb{R}}dx'A_\tau(x,x')f(x') \tag{A1}$$

where τ labels the elements of a one-parameter subgroup (or subsemigroup) of $SL(2,\mathbb{C})$. For our purposes it is sufficient to ask that the integral in (A1) to exist, so that we can disregard the Hilbert space structure of the functions involved, and the operator U_τ need not be bounded.[14,15]

We want to find a differential operator H which generates the transform (A1), i.e.,

$$H\left(x,\frac{d}{dx}\right)f(x)=-i\int_{\mathbb{R}}dx'\left[\frac{\partial}{\partial\tau}A_\tau(x,x')\Big|_{\tau=0}f(x')\right] \tag{A2a}$$

with the boundary condition

$$A_\tau(x,x')\big|_{\tau=0}=\delta(x-x'). \tag{A2b}$$

If we knew H and solved for $A_\tau(x,x')$, this would be a Green's function problem,[16] where $A_\tau(x,x')$ is the Green's function of $\exp(+i\tau H)$. Here we know $A_\tau(x,x')$ as given by (6.6) and [and (4.4)], so that we can build the operator $H(x,d/dx)$ by inspection of (A2a), for various one-parameter subgroups of $SL(2,\mathbb{C})$, viz.:

$$\exp[ic(\tfrac{1}{2}\hat{x}^2)]:\begin{pmatrix}1 & 0\\ c & 1\end{pmatrix}, \tag{A3a}$$

$$\exp[ib(\tfrac{1}{2}\hat{p}^2)]:\begin{pmatrix}1 & -b\\ 0 & 1\end{pmatrix}, \tag{A3b}$$

$$\exp[i\alpha\tfrac{1}{4}(\hat{p}^2-\hat{x}^2)]:\begin{pmatrix}\cosh\frac{1}{2}\alpha & -\sinh\frac{1}{2}\alpha\\ -\sinh\frac{1}{2}\alpha & \cosh\frac{1}{2}\alpha\end{pmatrix}, \tag{A3c}$$

$$\exp[i\beta\tfrac{1}{4}(\hat{x}\hat{p}+\hat{p}\hat{x})]:\begin{pmatrix}\exp(-\frac{1}{2}\beta) & 0\\ 0 & \exp(\frac{1}{2}\beta)\end{pmatrix}, \tag{A3d}$$

$$\exp[i\gamma\tfrac{1}{4}(\hat{p}^2+\hat{x}^2)]:\begin{pmatrix}\cos\frac{1}{2}\gamma & -\sin\frac{1}{2}\gamma\\ \sin\frac{1}{2}\gamma & \cos\frac{1}{2}\gamma\end{pmatrix}. \tag{A3e}$$

The last three generators can be seen to constitute the well-known $su(1,1)$ dynamical algebra of the harmonic oscillator,[2] (A3d) being a scale operator, i.e.,

$$\bar{f}(x)=\exp[i\beta\tfrac{1}{4}(\hat{x}\hat{p}+\hat{p}\hat{x})]f(x)=\exp(\tfrac{1}{4}\beta)f[\exp(\tfrac{1}{2}\beta)x] \tag{A4}$$

while Eq. (A3e), $\frac{1}{2}(\hat{x}^2+\hat{p}^2)$ being the oscillator Hamiltonian, gives the development in time $t=\frac{1}{2}\gamma$ of the system.

The association of hyperdifferential operators in (A3) with 2×2 matrices can yield a host of Baker–Campbell–Hausdorff relations between second order differential operators,[17] as

$$\begin{pmatrix}\cosh\theta & -\sinh\theta\\ \sinh\theta & \cosh\theta\end{pmatrix} = \begin{pmatrix}1 & -\tanh\theta\\ 0 & 1\end{pmatrix}\begin{pmatrix}1/\cosh\theta & 0\\ 0 & \cosh\theta\end{pmatrix}\begin{pmatrix}1 & 0\\ -\tanh\theta & 1\end{pmatrix} \quad \text{(A5a)}$$

which gives

$$\exp\left[-\tfrac{1}{2}i\theta\left(\frac{d^2}{dx^2}+x^2\right)\right] = \exp\left[-\tfrac{1}{2}i\tanh\theta\frac{d^2}{dx^2}\right]\exp\left[\tfrac{1}{2}\ln\cosh\theta\left(x\frac{d}{dx}+\frac{d}{dx}x\right)\right] \times\exp[-\tfrac{1}{2}i\tanh\theta x^2]. \quad \text{(A5b)}$$

Further, when allowed to act on specific functions f whose canonical transforms $\bar{f}$ are known, (A3) yield special function relations. For $\theta = i\pi/4$, (A5a) becomes the Bargmann transform matrix (1.4), thus

$$\bar{f}(x) = \exp\left[\tfrac{1}{8}\pi\left(\frac{d^2}{dx^2}+x^2\right)\right]f(x) = 2^{-1/4}\exp\left(\frac{1}{2}\frac{d^2}{dx^2}\right)\exp(\tfrac{1}{4}x^2)f(2^{-1/2}x). \quad \text{(A6)}$$

In particular, letting f be one of the harmonic oscillator wavefunctions $\psi_n(x)$ given by (3.7), $\bar{f}$ will be (2.9) for $u=0$, $v=1$. Eq. (A6) with a change of scale gives immediately

$$x^n = 2^{-n}\exp\left(\frac{1}{4}\frac{d^2}{dx^2}\right)H_n(x) \quad \text{(A7a)}$$

and its inverse

$$H_n(x) = \exp\left(-\frac{1}{4}\frac{d^2}{dx^2}\right)(2x)^n \quad \text{(A7b)}$$

which are formulas that do not commonly appear in special function tables.[14,18]

APPENDIX B; EXTENSION TO n DIMENSIONS

We shall sketch here some of the results for the case of n-dimensional spaces $\mathcal{F}^n$. The most general complex linear canonical transformation (2.1) now reads

$$\begin{pmatrix}\hat{\eta}\\ \hat{\xi}\end{pmatrix} = \begin{pmatrix}A & B\\ C & D\end{pmatrix}\begin{pmatrix}\hat{\mathbf{x}}\\ \hat{\mathbf{p}}\end{pmatrix} \quad \text{(B1)}$$

where $\hat{\mathbf{x}}$, $\hat{\mathbf{p}}$, $\hat{\eta}$, and $\hat{\xi}$ are n-component column vectors and $A,\ldots,D$ are $n\times n$ matrices satisfying[2] $A\tilde{B}=B\tilde{A}$, $C\tilde{D}=D\tilde{C}$, and $A\tilde{D}-B\tilde{C}=\mathbb{1}$ (the tilde means matrix transposition). Hermitian conjugation is achieved as

$$\begin{pmatrix}\hat{\eta}^+\\ \hat{\xi}^+\end{pmatrix} = \begin{pmatrix}A^* & B^*\\ C^* & D^*\end{pmatrix}\begin{pmatrix}\tilde{D} & -\tilde{B}\\ -\tilde{C} & \tilde{A}\end{pmatrix}\begin{pmatrix}\hat{\eta}\\ \hat{\xi}\end{pmatrix} = \begin{pmatrix}U & iV\\ iW & \tilde{U}^*\end{pmatrix}\begin{pmatrix}\hat{\eta}\\ \hat{\xi}\end{pmatrix}, \quad \text{(B2)}$$

where $U = A^*\tilde{D} - B^*\tilde{C}$, $V = 2\,\mathrm{Ah}(B^*\tilde{A})$, and $W = 2\,\mathrm{Ah}(C^*\tilde{D})$, the symbol $\mathrm{Ah}M = (2i)^{-1}(M - \tilde{M}^*)$ denotes the anti-Hermitian part of a matrix, so that V and W are Hermitian and their determinants are real. An analysis parallel to (2.4)–(2.7) yields a Hermitian form for the space $\mathcal{F}^n$ given by

$$(\bar{f},\bar{g}) = \int_{\mathbb{C}^n}\nu(\eta,\eta^*)d^n\mathrm{Re}\,\eta\, d^n\mathrm{Im}\,\eta f(\eta)^* g(\eta) \quad \text{(B3)}$$

with the weight

$$\nu(\eta,\eta^*) = ([\tfrac{1}{2}\pi]^n\det V)^{-1/2}\exp\{\tfrac{1}{2}\tilde{\eta}V^{-1}U\eta - \tilde{\eta}V^{-1}\eta^* + \tfrac{1}{2}\tilde{\eta}^*V^{*-1}U^*\eta^*\} \quad \text{(B4)}$$

the growth restrictions on $\bar{f}\in\mathcal{F}^n$ can be seen writing $\bar{f}(\eta) = f_b(V^{*-1/2}\eta)\exp\{-\tfrac{1}{2}\tilde{\eta}V^{-1}U\eta\}$ where $(V^{1/2})^2 = V$. As V is Hermitian, when we ask it to be positive definite, its positive definite square root is uniquely defined and f_b can be asked to be in the n-dimensional Bargmann space. The restrictions are then

$$|\bar{f}(\eta)| \le \gamma\exp\{\tfrac{1}{2}\alpha\tilde{\eta}V^{-1}\eta^* - \tfrac{1}{2}\mathrm{Re}[\tilde{\eta}V^{-1}U\eta]\},\quad \alpha<1. \quad \text{(B5)}$$

The transform kernel between $\mathcal{H}^n$ and $\mathcal{F}^n$ will be, in terms of the submatrices in (B1), up to a phase φ,

$$A(\eta,x) = \varphi([2\pi]^n|\det B|)^{-1/2}\exp i\{\tfrac{1}{2}\tilde{\mathbf{x}}B^{-1}A\mathbf{x} - \tilde{\mathbf{x}}B^{-1}\eta + \tfrac{1}{2}\tilde{\eta}DB^{-1}\eta\} \quad \text{(B6)}$$

out of an analysis parallel to (3.1)–(3.3).

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Causal boundaries for general relativistic space–times*

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Let M be a causally continuous space–time. Using indecomposable past and future sets in a symmetric way we construct a causal completion N for M. N is a causal space; the chronology of M in N is the chronology of M. The extended Alexandrov topology for N makes N Hausdorff and M a densely imbedded subspace. M is globally hyperbolic iff either the chronological future or the chronological past of each point in $N-M$ is empty, causally simple iff the causality of M in N is the causality of M. The standard examples of causal completions are special cases.

INTRODUCTION

Penrose's conformal completion method for certain general relativistic space–times[1] has proved useful in applications.[2,3] Various generalizations have been suggested.[4–7] In particular, Geroch, Kronheimer, and Penrose[5] have shown, under rather general assumptions, that certain open subsets of space–time can be used to assign a boundary to space–time. Some of the subsets simply represent points of the space–time itself. The others are interpreted as ideal points at a singularity, or at infinity, or at an event gratuitously amputated out of a larger space–time. Geroch, Kronheimer, and Penrose obtain a Hausdorff topological space, interpreted as the space–time with the ideal points attached as boundary points. The boundary might be regarded as the place where information, carried by particles or fields, enters that portion of physical space–time which can be described by nonquantum general relativity.

In general, the causality structure[8] of the space–time does not extend to the boundary. For example, it may not make sense to say a space–time even can signal to a boundary point at a speed less than that of light. Now causality structure is perhaps the deepest structure our physical models have. In general relativity, analyzing causality is central to the study of black holes,[2,3] to cosmology,[9,10] and to each of the major recent mathematical theorems.[2,11] Causality can be used to analyze in what sense properties of freely falling particles and photons determine a topology, differentiable structure, and Lorentzian structure for space–time.[12] In fact, causal structure determines these further structures up to a conformal factor.[13] In view of this basic character, one hates to lose the causality structure when attaching a boundary.

The main purpose of this paper is to show that if space–time is causally continuous,[14] the causality structure does extend to the ideal points. Roughly speaking, a causally continuous space–time is one with the following three properties: There are no closed timelike curves and this property persists even if sufficiently small but otherwise arbitrary perturbations of the metric are made; moreover, if there are "gaps" in the space–time, their "dimension" or "shape" is restricted; and finally, space–time is "not to concave" at infinity or other boundaries such as the big bang. In such a space–time the past and future of a local observer depend continuously on his location.[14] There is then apparently just one reasonable, conformally invariant way to attach a boundary. Causal continuity insures that for the boundary points causality and topology cooperate in a rather cunning way. Most known physically interesting examples, such as the maximally extended Reissner Nordstrom space–times, are causally continuous.

In Sec. 1 we shall review some known results and add a few preliminary propositions. Section 2 shows how to assign a causal structure to certain collections of space–time subsets. To avoid later redundancy, we work rather generally in these two sections, but we have in mind the ideal point boundary of a causally continuous space–time throughout. Section 3 reviews the technical definition of causal continuity and proves some results about causally continuous space–times. Section 4 discusses topology. Section 5 contains our main result. We there define the causal boundary of a causally continuous space–time and show how it is attached to the space–time.

The essential feature of our methods in Secs. 1–5 is indicated in Fig. 1. The standard conventions[2] for space–time diagrams are used. The figure shows a space–time conformal to an open submanifold of two-dimensional Minkowski space. The (closed) shaded regions are not part of the space–time. P and F, shown dotted, are sets of the kind which represent ideal points. The key question is the following. By what general method can one tell that P and F represent the same ideal point y rather than two different ideal points. Our answer here will be that P is the common past of F and F is the common future of P. Specifically, P is the largest open set each event in which can signal to each observer in F at a speed less than that of light; F is the largest open set each observer in which can receive such a signal from each event in P. We shall identify sets, and the points they represent, pairwise iff both these conditions, which do not imply each other, hold.

In Sec. 6 we show that once a boundary has been attached, one need not repeat the process: Completing

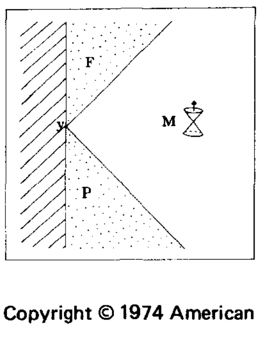

FIG. 1.

the completion gives nothing new. Section 7 discusses a byproduct of our investigations which has some independent interest. Any time-oriented space–time determines an algebraic structure, called a complete lattice. The geometric properties of the space–time are reflected in the algebraic properties[15] of the lattice. There is some hope that such lattices may be useful in analyzing global space–times properties and/or in quantizing. Finally, Sec. 8 mentions few unsolved problems.

1. PRELIMINARIES

This section reviews most of the standard definitions and results we shall need, sets the notation, and defines common pasts and futures. The latter are new, so we shall analyze some of their basic properties in subsections 1.4–1.8.

Let (M,g) be a time-oriented space–time.[2] Thus g is a smooth Lorentzian metric on the smooth manifold M. A smooth *future-directed* curve in (into[16]) M is a smooth curve whose tangent is never zero and always timelike or lightlike future-directed. Define binary relations $\leqslant$ and $\ll$ on M as follows: $x \leqslant y$, if there is a smooth, future directed curve from x to y; $x \ll y$ if there is a smooth, future-directed, timelike curve from x to y.

By abstraction, Kronheimer and Penrose[8] obtained an algebraic structure which has some, but in general not all, the properties of $(M,g,\leqslant,\ll)$. Suppose $\mathbf{Z}$ is a set, ρ is a binary relation on $\mathbf{Z}$, and $\mathbf{x},\mathbf{y},\mathbf{z}\in\mathbf{Z}$. Recall that ρ is *reflexive* if $\mathbf{x}\rho\mathbf{x}$ for all $\mathbf{x}$, *antireflexive* if $\mathbf{x}\rho\mathbf{x}$ for no $\mathbf{x}$, and *transitive* if $\mathbf{x}\rho\mathbf{y}$ and $\mathbf{y}\rho\mathbf{z}$ together imply $\mathbf{x}\rho\mathbf{z}$. A transitive ρ is a *partial ordering* if two distinct elements $\mathbf{x},\mathbf{y}$ cannot obey both $\mathbf{x}\rho\mathbf{y}$ and $\mathbf{y}\rho\mathbf{x}$. Let $\leqslant$, $\ll$, be binary relations on $\mathbf{Z}$. $\leqslant$, called the *causality relation*, will correspond intuitively to signals which travel no faster than light; $\ll$, called the *chronology relation*, will correspond to signals slower than light. As here we shall often use boldface to distinguish structures defined in general from corresponding structures defined on a space–time.

Definition 1.1[8]: $(\mathbf{Z},\leqslant,\ll)$ is a *causal space* if:

A. $\mathbf{x}\ll\mathbf{y}$ implies $\mathbf{x}\leqslant\mathbf{y}$;

B. $\leqslant$ is a reflexive partial ordering;

C. $\ll$ is antireflexive;

D. either $\mathbf{x}\leqslant\mathbf{y}\ll\mathbf{z}$ or $\mathbf{x}\ll\mathbf{y}\leqslant\mathbf{z}$ implies $\mathbf{x}\ll\mathbf{z}$.

Let $(\mathbf{Z},\leqslant,\ll)$ be a causal space. By Axioms 1.1.A and 1.1.D, $\ll$ is transitive. If $\mathbf{Y}\subseteq\mathbf{Z}$, $(\mathbf{Y},\leqslant,\ll)$ is a causal space.[8] Let X and Z be causal spaces and θ: $\mathbf{X}\to\mathbf{Z}$ be a function. θ is called *isocausal* if $\mathbf{x}\leqslant\mathbf{y}$ implies $\theta\mathbf{x}\leqslant\theta\mathbf{y}$ and $\mathbf{x}\ll\mathbf{y}$ implies $\theta\mathbf{x}\ll\theta\mathbf{y}$. θ is called a *causal isomorphism* if it is one-to-one, is onto, is isocausal, and has an isocausal inverse.

Let $\mathbf{Z}$ be a causal space, $\mathbf{S},\mathbf{P}\subseteq\mathbf{Z}$ be subsets. The *chronological past* $\mathbf{I}^-\mathbf{S}$ *of* $\mathbf{S}$ is $\mathbf{I}^-\mathbf{S}=\{\mathbf{x}\in\mathbf{Z}\colon \mathbf{x}\ll\mathbf{s}$ for some $\mathbf{s}\in\mathbf{S}\}$. Thus if $\mathbf{y}\in\mathbf{Z}$, $\mathbf{I}^-\{\mathbf{y}\}=\{\mathbf{x}\in\mathbf{Z}\colon\mathbf{x}\ll\mathbf{y}\}$, where $\{\mathbf{y}\}\subseteq\mathbf{Z}$ denotes the singleton subset. $\mathbf{P}$ is called a *past* set if $\mathbf{P}=\mathbf{I}^-\mathbf{S}$ for some $\mathbf{S}$. A past set $\mathbf{P}$ is called *indecomposable*[5] if it is not the empty subset and obeys the following restriction: Whenever $\mathbf{Q}$ and $\mathbf{R}$ are past sets such that $\mathbf{P}=\mathbf{Q}\cup\mathbf{R}$, then $\mathbf{Q}=\mathbf{P}$ or $\mathbf{R}=\mathbf{P}$. The *causal past* $\mathbf{J}^-\mathbf{S}$ *of* $\mathbf{S}$ is $\mathbf{J}^-\mathbf{S}=\{\mathbf{x}\in\mathbf{Z}\colon\mathbf{x}\leqslant\mathbf{s}$ for some $\mathbf{s}\in\mathbf{S}\}$. *Chronological* and *causal futures* $\mathbf{I}^+\mathbf{S}$ and $\mathbf{J}^+\mathbf{S}$, *future* sets, and *indecomposable* future sets are defined dually, i.e., with $\ll$ or $\leqslant$ replaced by the respective inverse relations $\gg$ or $\geqslant$. We shall often take dual results for granted.

The time-oriented space–time (M,g) is called *causal* if, for all $x,y\in M$, $x\leqslant y$ and $y\leqslant x$ together imply $x=y$. (M,g) is causal iff there are no self-intersecting future-directed curves which is true iff $(M,\leqslant,\ll)$ is a causal space.[2,11] For all $S\subseteq M$, $I^-S\subseteq M$ is open.[11]

Let (M,g) be a causal space–time, and $U\subseteq M$ an open subset. The *chronological common past* $\downarrow U$ *of* U is $\downarrow U = I^-\{x\in M\colon x\ll u$ for all $u\in U\}$. Since $\ll$ is transitive $I^-U\supseteq\downarrow U$ iff U is not the empty set $\emptyset\subseteq M$. The *chronological common future* $\uparrow U$ is defined dually.

1.2. *Notation and Conventions*: Throughout the rest of this paper: A. $M=(M,g)$ is a causal space–time with chronology $\ll$, causality $\leqslant$, topology $\mathcal{T}=\{U\subseteq M\colon U$ is open$\}$, and power set $\mathcal{S}=\{S\subseteq M\}$. The following two examples indicate the basic notations that will be used. (i) $\uparrow\mathcal{T}\equiv\{S\subseteq M\colon S=\uparrow U$ for some $U\in\mathcal{T}\}$, etc. (ii) Suppose $U\in\mathcal{T}$; then $\downarrow\uparrow U\equiv\downarrow(\uparrow U)\equiv\downarrow[\uparrow(U)]\equiv(\downarrow\circ\uparrow)U\equiv(\downarrow\circ\uparrow)(U)$, with the first form preferred, etc.

B. The *collection* $\mathcal{P}$ *of pasts* is $\mathcal{P}=I^-\mathcal{L}$; $\mathcal{F}=I^+\mathcal{L}$ is the *collection of futures*. The (past) *hull lattice* $\hat{\mathcal{L}}$ is $\hat{\mathcal{L}}=\downarrow\mathcal{T}$; dually, $\check{\mathcal{L}}=\uparrow\mathcal{T}$; the term "hull lattice" is suggested by the results of Sec. 7 following. $\hat{\mathcal{M}}$ is the collection of indecomposable past sets; dually, $\check{\mathcal{M}}$ is the collection of indecomposable future sets.

C. $(P,F)\in\mathcal{P}\times\mathcal{F}$ means $P\in\mathcal{P}$ and $F\in\mathcal{F}$, etc. (P,F) will be called a *hull pair* if $(P,F)\in\mathcal{P}\times\mathcal{F}$, $P=\downarrow F$ and $F=\uparrow P$. Define a relation $\sim$ on $\mathcal{P}\cup\mathcal{F}$ as follows. $A\sim A$ for all $A\in\mathcal{P}\cup\mathcal{F}$. If $A,B\in\mathcal{P}\cup\mathcal{F}$ then $A\sim B$ iff either (A,B) or (B,A) is a hull pair. We shall show below that $\sim$ is an equivalence relation and that each equivalence class contains at most two members.

D. $\hat{I}\colon M\to\mathcal{P}$ denotes the function with rule $\hat{I}x=I^-\{x\}$; dually $\check{I}x=I^+\{x\}$. For example, suppose $S\subseteq M$. Then I^-S is an open subset of M. But $\hat{I}S=\{\hat{I}s : s\in S\}\equiv\{I^-\{s\} : s\in S\}$ is a subset of $\mathcal{T}$; thus $\hat{I}S$ is a collection of open subsets of M.

The ideal points we eventually wish to discuss are the elements of $\hat{\mathcal{M}}\cup\check{\mathcal{M}}/\sim$. In the rest of this section we first analyze how the topology $\mathcal{T}$, the collection $\mathcal{P}$ of pasts, the hull lattice $\hat{\mathcal{L}}$, the collection $\hat{\mathcal{M}}$ of indecomposable past sets, etc., are interrelated. Then we examine common pasts and futures in some detail. We will base most of our proofs in the paper on the following standard proposition.

Proposition 1.3[2,11]: Suppose $U\in\mathcal{T}$, $S\subseteq M$, and $S\supseteq I^-S$; then:

A. Interior (Closure S) = Interior $S = I^-S$;

B. Closure (Interior S) = Closure $S = \{x\in M : S\supseteq\hat{I}x\}\supseteq J^-S$;

C. $I^-U\supseteq U$.

Lemma 1.4: Suppose $U, V \in \mathcal{T}$. Then:

A. $U \supseteq V$ implies $\uparrow U \subseteq \uparrow V$;

B. $\downarrow\uparrow U \supseteq U$;

C. $\uparrow U \supseteq V$ iff $U \subseteq \downarrow V$.

Proof: Part A follows directly from the definitions. For part B, first note than if $u \in U$ then $z \in \uparrow U$ implies $u \ll z$. Let $Q = \{x \in M : x \ll z$ for all $z \in \uparrow U\}$; thus $Q \supseteq U$. Therefore $\downarrow\uparrow U = I^- Q \supseteq I^- U \supseteq U$, where we have used Proposition 1.3.C. Finally, for part C, suppose $\uparrow U \supseteq V$. Then the dual of part A and part B itself together give $\downarrow V \supseteq \downarrow\uparrow U \supseteq U$. The dual argument gives the converse. ■

Proposition 1.5:

A. $\mathcal{T} \supseteq \mathcal{P} \supseteq \hat{\mathcal{L}} = \downarrow\mathcal{F}$;

B. $(\downarrow\circ\uparrow)_{\hat{\mathcal{L}}}$ is the identity; $\downarrow(\check{\mathcal{L}}) = \hat{\mathcal{L}}$;

C. $(I^-)_{\mathcal{P}}$ is the identity;

D. $\mathcal{P} \cap \mathcal{F} = \{\emptyset, M\} = \hat{\mathcal{L}} \cap \check{\mathcal{L}}$.

$$\mathcal{T} \supseteq \mathcal{P} \xrightarrow{\ \uparrow\ } \check{\mathcal{L}} \subseteq \mathcal{F}$$
$$\uparrow\downarrow$$
$$\mathcal{T} \supseteq \mathcal{F} \xrightarrow{\ \downarrow\ } \hat{\mathcal{L}} \subseteq \mathcal{P}$$

Proof: Part A. $\mathcal{T} \supseteq \mathcal{P}$ since $I^- S$ is open for all $S \subseteq M$. $\mathcal{P} = I^- \mathcal{S} \supseteq \hat{\mathcal{L}}$. Now $\mathcal{T} \supseteq \mathcal{F}$ by the dual of $\mathcal{T} \supseteq \mathcal{P}$ so $\downarrow\mathcal{F} \subseteq \downarrow\mathcal{T} = \hat{\mathcal{L}}$. Conversely, suppose $L = \downarrow U$, $U \in \mathcal{T}$. Then $\uparrow L \supseteq U$ by the dual of Lemma 1.4.B. Thus $\downarrow U \supseteq \downarrow\uparrow L$ by the dual of lemma 1.4.A. This gives $L \supseteq \downarrow\uparrow L$. Lemma 1.4.B. gives $\downarrow\uparrow L \supseteq L$. Thus $L = \downarrow\uparrow L \in \downarrow\mathcal{F}$; thus $\hat{\mathcal{L}} \subseteq \downarrow\mathcal{F}$. Thus $\hat{\mathcal{L}} = \downarrow\mathcal{F}$.

Part B. We have just shown that $(\downarrow\circ\uparrow)$ is the identity on $\hat{\mathcal{L}}$; dually, $(\uparrow\circ\downarrow)$ is the identity on $\check{\mathcal{L}}$. Thus $\downarrow(\check{\mathcal{L}}) = \hat{\mathcal{L}}$.

Part C. Suppose $P = I^- S$, $S \subseteq M$. $P \supseteq I^- P$ since $\ll$ is transitive. By Propositions 1.5.A. and 1.3.A, $P = \text{Interior } P = I^- P$. Thus I^- is the identity on $\mathcal{P}$.

Part D. Suppose $S \in \mathcal{P} \cap \mathcal{F}$. $I^+ I^- S \supseteq S$ since $\ll$ is a relation. By Proposition 1.5.C $S = I^- S$. Proposition 1.3.B and the transitivity of $\ll$ give I^- Closure $S = I^-\{x \in M : S \supseteq \hat{I}x\} \subseteq$ Closure S. By Proposition 1.3.A we now have $S = I^-$ Closure S. Thus Interior $S = S = I^+ I^-$ Closure $S \supseteq$ Closure S, so that S is open and closed. Since a space–time is connected, $S = \emptyset$ or $S = M$. Conversely $I^\pm \emptyset = \emptyset$ and, by Proposition 1.3.A, $M \supseteq I^\pm M = \text{Interior } M = M$. Thus $\mathcal{P} \cap \mathcal{F} = \{\emptyset, M\}$. Now by Proposition 1.5.A, $\hat{\mathcal{L}} \cap \check{\mathcal{L}} \subseteq \mathcal{P} \cap \mathcal{F}$. Conversely, $\downarrow\emptyset = M = \uparrow\emptyset$ and, since $\ll$ is antireflexive, $\downarrow M = \emptyset = \uparrow M$. Thus $\hat{\mathcal{L}} \cap \check{\mathcal{L}} = \{\emptyset, M\}$. ■

We shall henceforth regard the empty set $\emptyset \subseteq M$, the past copy $\emptyset \in \mathcal{P}$, and the future copy $\emptyset \in \mathcal{F}$ as in principle distinct. Unless explicitly indicated otherwise, $\emptyset$ in the following means $\emptyset \subseteq M$. The analogous comments apply to M; the distinction between $M \in \mathcal{P}$ and $M \in \mathcal{F}$ is sometimes essential.[1]

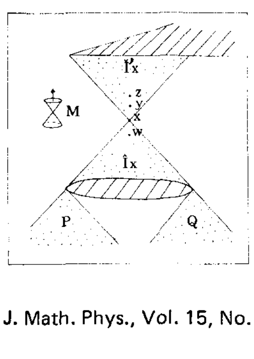

FIG. 2. Here $\downarrow\check{I}x = (\hat{I}x) \cup P \cup Q$, and $\downarrow\uparrow\hat{I}x = (\hat{I}x) \cup P$.

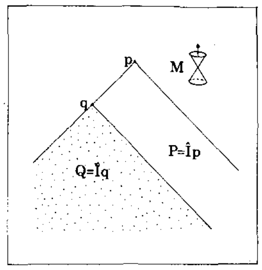

FIG. 3. $p \geq q$, $P \supseteq Q$.

The following miscellaneous results will be needed later.

Corollary 1.6: Suppose $U \in \mathcal{T}$ and $P, Q \in \mathcal{P}$. Then:

A. $P \not\supseteq Q$ implies Closure $P \not\supseteq Q$;

B. $P \cap U \neq \emptyset$ implies $P \supseteq \downarrow U$;

C. $\downarrow U = \text{Interior}\{x \in M : u \gg x$ for all $u \in U\}$.

Proof: By Propositions 1.5.C and 1.3.A, $P \not\supseteq Q$ implies Interior Closure $P = P \not\supseteq Q =$ Interior Q, so part A holds. For part B, we have $P = I^- P \supseteq I^-(P \cap U) \supseteq \downarrow(P \cap U) \supseteq \downarrow U$, where we have used Proposition 1.5.C, the definition of I^-, the definition of $\downarrow$, and the dual of Lemma 1.4.A. Finally, Propositions 1.3.A and 1.5.A imply part C. ■

Proposition 1.7: Suppose $P \in \mathcal{P}$ and $x \in M$. Then:

A. $P \cap (\check{I}x) \neq \emptyset$ iff $x \in P$;

B. $\downarrow\check{I}x \supseteq \downarrow\uparrow\hat{I}x \supseteq \hat{I}x$.

Proof: $x \in P$ iff $x \in I^- P$ iff there is a $y \in P$ such that $x \ll y$ iff $(\check{I}x) \cap P \neq \emptyset$. Thus part A holds. For part B first note that $\downarrow\uparrow Ix \supseteq \hat{I}x$ by Lemma 1.4.B. Now suppose $z \in \check{I}x$ (Fig. 2). Then $z \in I^+ \check{I}x$ by the duals of Propositions 1.5.A and 1.5.C. Thus there is a $y \in \check{I}x$ with $z \gg y$. $y \gg w$ for all $w \in \hat{I}x$ since $\gg$ is transitive. Thus $z \in \uparrow\hat{I}x$; thus $\uparrow\hat{I}x \supseteq \check{I}x$; by the dual of Lemma 1.4.A, $\downarrow\check{I}x \supseteq \downarrow\uparrow\hat{I}x$. ■

1.8: Figure 2, for an open submanifold of two-dimensional Minkowski space, shows that neither equality in Proposition 1.7.B need hold.

Proposition 1.9: The following three conditions are equivalent:

A. (P, F) is a hull pair;

B. $P \in \hat{\mathcal{L}}$ and $F = \uparrow P$;

C. $F \in \check{\mathcal{L}}$ and $P = \downarrow F$.

Proof: By Proposition 1.5.A, $P = \downarrow F$ implies $P \in \hat{\mathcal{L}}$; dually $F = \uparrow P$ implies $F \in \check{\mathcal{L}}$. Proposition 1.9 thus follows from Proposition 1.5.C and its dual. ■

By our conventions, $\mathcal{P}$ and $\mathcal{F}$ have no elements in common. Proposition 1.9 implies that the relation $\sim$ defined in 1.2.D is an equivalence relation which identifies a given $A \in \mathcal{P} \cup \mathcal{F}$ with at most one other element of $\mathcal{P} \cup \mathcal{F}$.

2. SET CAUSALITY

M, its topology $\mathcal{T}$, the collection $\mathcal{P} \subseteq \mathcal{T}$ of pasts, the

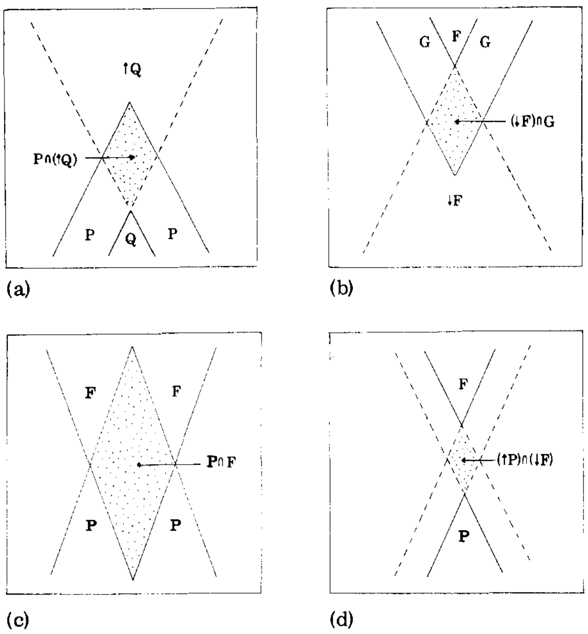

FIG. 4. Duality corresponds to turning the page upside down.

collection $\mathcal{F}$ of futures, the hull lattice $\hat{\mathcal{L}}$, its dual $\check{\mathcal{L}}$, $\hat{\mathcal{M}}$, $\check{\mathcal{M}}$, and the equivalence relation $\sim$ are as in subsection 1.2.

Ultimately we will consider space–times such that $(\hat{I}x, \check{I}x)$ is a hull pair for each event x, represent each event x by $\hat{I}x$ or equivalently $\check{I}x$, and use elements of $\hat{\mathcal{M}} \cup \check{\mathcal{M}}/\sim$ to represent ideal points. For awhile, we work more generally. The game is to make $\mathcal{P}$ and $\mathcal{F}$ into causal spaces, abstracting from simple situations such as those shown in Figs. 3 and 4. Then one must glue $\mathcal{P}$ and $\mathcal{F}$ together.

Various glueing constructions are possible algebraically, but most of these can be shot down by showing that they give unnaceptable answers in some of the standard examples[2] of black-hole, big bang, or other conformally completed space–times. The key idea of the method we shall use is to glue $\mathcal{P}$ and $\mathcal{F}$ together along the hull lattice and its dual.

2.1: Define relations $\geqslant$ and $\gg$ on $\mathcal{P} \cup \mathcal{F}$ by the table below, whose use is indicated by the following examples. Suppose $(P,Q) \in \mathcal{P} \times \mathcal{P}$, $(P,F) \in \mathcal{P} \times \mathcal{F}$ and $(F,P) \in \mathcal{F} \times \mathcal{P}$. The table specifies: $P \geqslant Q$ iff $P \supseteq Q$, as in Fig. 3; $P \gg Q$ iff $P \cap (\uparrow Q) \neq \phi$, as in Fig. 4A; $P \geqslant F$ iff there is a hull pair $(\hat{L}, \check{L})$ such that $P \geqslant \hat{L}$ and $\check{L} \geqslant F$ (i.e., $P \supseteq \hat{L}$ and $\check{L} \subseteq F$); etc.

2.2		$\cdot \geqslant \cdot$	$\cdot \gg \cdot$
A. $\mathcal{P} \times \mathcal{P}$		$\cdot \supseteq \cdot$	$\cdot \cap (\uparrow \cdot) \neq \phi$
B. $\mathcal{F} \times \mathcal{F}$		$\cdot \subseteq \cdot$	$(\downarrow \cdot) \cap \cdot \neq \phi$
C. $\mathcal{P} \times \mathcal{F}$	$\exists (\hat{L}, L)$:	$\cdot \supseteq \hat{L}$ and $L \subseteq \cdot$	$\cdot \cap \cdot \neq \phi$
D. $\mathcal{F} \times \mathcal{P}$	$\exists (L, L)$:	$\cdot \subseteq L$ and $\hat{L} \supseteq \cdot$	$(\downarrow \cdot) \cap (\uparrow \cdot) \neq \phi$

2.3: The dualities in the table are a little tricky: Line B is the dual of line A but both line C and line D are self-dual. Compare Fig. 4. Proposition 2.6.B and Example 2.7 following indicate on intrinsic difference between $\geqslant$ in line C and $\geqslant$ in line D. We now analyze the table, starting with line A.

Proposition 2.4: $(\mathcal{P}, \leqslant, \ll)$ is a causal space; $\hat{I}: M \to \mathcal{P}$ is isocausal.

Proof: $(\mathcal{P}, \subseteq)$ is a partially ordered set so that Axiom 1.1.B holds. Now suppose $P, Q, R \in \mathcal{P}$. To check Axiom 1.1.A, assume first $P \gg Q$. Then $P \cap (\uparrow Q) \neq \phi$. Corollary 1.6.B and Lemma 1.4.B give $P \supseteq \downarrow\uparrow Q \supseteq Q$, so that $P \geqslant Q$ as required. Now to check that $\gg$ is antireflexive, assume $P \gg Q$ and $Q \gg P$. Then $P = Q$ and $P \cap (\uparrow P) \neq \phi$ by the argument just given. But $x \in P (\uparrow P)$ implies $x \gg x$, the desired contradiction. Now suppose $P \geqslant Q \gg R$. Then $P \supseteq Q$ and $Q \cap (\uparrow R) \neq \phi$; thus $P \cap (\uparrow R) \neq \phi$ and $P \gg R$. Finally, assume $P \gg Q \geqslant R$. Then $P \cap (\uparrow Q) \neq \phi$ and $Q \supseteq R$. By Lemma 1.4.A $\uparrow R \supseteq \uparrow Q$. Thus $P \gg R$ also in this case. Thus Axiom 1.1.D holds; thus $(\mathcal{P}, \leqslant, \ll)$ is a causal space.

Now suppose $x, y \in M$. If $x \geqslant y$, $\hat{I}x \supseteq \hat{I}y$, since $x \geqslant y \gg z$ implies $x \gg z$ for any event z. Thus $\hat{I}x \geqslant \hat{I}y$. If $x \gg y$, then $y \in \check{I}x$ so $(\hat{I}x) \cap (\uparrow \hat{I}y) \supseteq (\hat{I}x) \cap (\check{I}y) \neq \phi$, where we have used Proposition 1.7. Thus $\hat{I}x \gg \hat{I}y$ in this case. Thus $\hat{I}$ is isocausal. ■

By the dual of Proposition 2.4, $(\mathcal{F}, \leqslant, \ll)$ is a causal space. To analyze how $\mathcal{P}$ and $\mathcal{F}$ are glued together, considerable casework will be required. Propositions 2.5 and 2.6 below give some of the interrelations. Example 2.7 shoots down various false conjectures. Proposition 2.8 shows that the relations defined in Table 2.2 cooperate with the equivalence relation $\sim$. Theorem 2.9 is the main result we shall need.

Proposition 2.5: $\uparrow: \mathcal{P} \to \mathcal{F}$ is isocausal; $\uparrow: \hat{\mathcal{L}} \to \check{\mathcal{L}}$ is a causal isomorphism.

Proof: Suppose $P, Q \in \mathcal{P}$. If $P \geqslant Q$, then by Lemma 1.4.A, $\uparrow P \geqslant \uparrow Q$. If $P \gg Q$, then, by Lemma 1.4.B applied to $P = U$, $\uparrow P \gg \uparrow Q$. Thus $\uparrow$ is isocausal. Dually, $\downarrow: \mathcal{F} \to \mathcal{P}$ is isocausal. Proposition 1.5.B now shows $\uparrow$: $\hat{\mathcal{L}} \to \check{\mathcal{L}}$ is a causal isomorphism. ■

Proposition 2.6: Suppose $P \in \mathcal{P}$, $F \in \mathcal{F}$, and r $\in \{\geqslant, \leqslant, \gg, \ll\}$. Then:

A. PrF iff, for some hull pair $(\hat{L}, \check{L})$, $Pr\hat{L}$ and $\check{L}rF$;

B. PrF implies $Pr(\downarrow F)$ and $(\uparrow P)rF$; $P \leqslant F$ iff $P \leqslant (\downarrow F)$ iff $(\uparrow P) \leqslant F$.

Proof: In part A, the cases $r = \leqslant$ and $r = \geqslant$ are trivial. Suppose $P \gg F$ or $F \gg P$. Then $P \cap F \neq \phi$ or $(\uparrow P) \cap (\downarrow F) \neq \phi$ respectively. So suppose $Q \in \mathcal{P}$, $G \in \mathcal{F}$, $x \in Q \cap G$. Let $\hat{L} = \downarrow \check{I}x$; then $\downarrow\uparrow \hat{L} = \hat{L}$. By Corollary 1.6.B, Proposition 1.7, and their duals $Q \cap (\uparrow \hat{L}) \neq \phi$ and $(\downarrow\uparrow \hat{L}) \cap G \neq \phi$. Substituting $P = Q$ and $F = G$ or $\uparrow P = G$ and $\downarrow F = Q$ finishes the proof of the direct assertion in A. To prove the converse, suppose first $P \gg \hat{L}$ and $\check{L} \gg F$. Then $P \cap \hat{L}$ and $\hat{L} \cap F$ are both nonempty. By Corollary 1.6.B and $\downarrow\uparrow \hat{L} = \hat{L}$ we get $P \gg F$. The remaining case, with $r = \ll$, is handled by the dual argument. Thus 2.6.A holds.

We start the proof of 2.6.B with the case $P \leqslant F$. Then $F \subseteq \uparrow\hat{L}$ and $\hat{L} \supseteq P$, $\hat{L} \in \hat{\mathcal{L}}$. $\uparrow P \supseteq \uparrow \hat{L}$ by Lemma 1.4.A, so that $\uparrow P \supseteq F$ and $F \geqslant \uparrow P$. Moreover, $\uparrow P \supseteq F$ iff $\downarrow F \supseteq P$ iff $\downarrow F \geqslant P$, where we have used Lemma 1.4.C. Now if $\downarrow F \supseteq P$, set $\hat{L} = \downarrow F$. Then $\hat{L} \in \hat{\mathcal{L}}$, $\hat{L} \supseteq P$, and $\uparrow \hat{L} \supseteq F$, so that $F \geqslant P$. Thus B is valid if $r = \leqslant$.

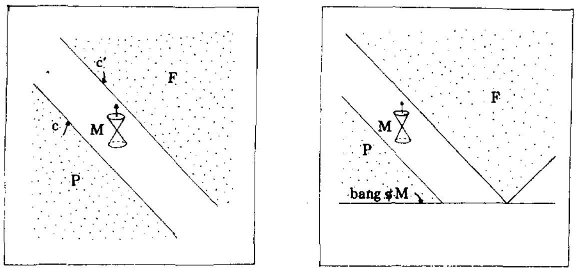

FIG. 5.

Now suppose $P \geqslant F$. Then $P \supseteq \hat{L}$, $\uparrow \hat{L} \subseteq F$, $\hat{L} \in \mathcal{L}$. Thus $P \supseteq \hat{L} = \downarrow\uparrow \hat{L} \supseteq \downarrow F$ and $P \geqslant \downarrow F$; dually $\uparrow P \geqslant F$. Suppose $P \gg F$. Then $P \cap F \neq \phi$. By Lemma 1.4.B and its dual, $\uparrow P \gg F$ and $P \gg \downarrow F$. Finally, $F \gg P$ implies $F \gg \uparrow P$ and $\downarrow F \gg P$ directly from the definitions. Thus 2.6.B is also valid. ■

Example 2.7: It is not true that $P \supseteq \downarrow F$ and $\uparrow P \subseteq F$ imply $P \geqslant F$. We give a counterexample. Let c be the image of an inextendible lightlike geodesic in Minkowski space, c' be another. Set $P = I^- c$, $F = I^+ c'$, as shown in Fig. 5A. Then $\uparrow P = \phi = \downarrow F$, so that $P \geqslant \downarrow F$ and $\uparrow P \geqslant F$; but $P \geqslant F$ need not hold, as the figure suggests. This example is important in applications. P represents a point at future lightlike infinity, F a point at past lightlike infinity.[2] Various geometric and physical arguments indicate that one must allow $P \not\geqslant F^2$. A similar situation arises in some of the cosmological models.[2] In Fig. 5B, F represents a point on the big bang. The definitions in Table 2.2 were designed to handle such cases.

Proposition 2.8: Suppose $(\hat{L}, \check{L})$ is a hull pair, $C \in \mathcal{P} \cup \mathcal{F}$, and r is as in Proposition 2.6. Then $\hat{L} r C$ iff $\check{L} r C$.

Proof: Suppose $P \in \mathcal{P}$ and $F \in \mathcal{F}$. By Proposition 2.6., $\check{L} r P$ implies $\hat{L} r P$ and $\hat{L} r F$ implies $\check{L} r F$. The remaining cases involving $r = \gg$ and $r = \ll$ follow directly from Table 2.2 and the definition of a hull pair. The remaining cases involving $r = \geqslant$ or $r = \leqslant$ can be proved by arguments of the following kind. Suppose $\check{L} \geqslant P$. Then $\hat{L} \supseteq P$ and $\hat{L} \supseteq \hat{L}$ so that $\check{L} \geqslant P$. ■

Suppose $\mathcal{C} \subseteq \mathcal{P} \cup \mathcal{F}$ is a subcollection. Proposition 2.8 shows that $\leqslant$ and $\ll$ are well defined on the quotient space $\mathcal{C}/\sim$. It is such quotient spaces which are of interest in what follows. However, since each equivalence class contains at most two members, it will be convenient to work with differences rather than quotients. Call $\mathcal{C} \subseteq \mathcal{P} \cup \mathcal{F}$ *causal* iff $\mathcal{C}$ does not contain both members $\hat{L}, \check{L}$ of any hull pair $(\hat{L}, \check{L})$. For example $\mathcal{C} = \mathcal{P} \cup \mathcal{F} - \mathcal{L}$ is a causal subcollection and has essentially the same structure as $\mathcal{P} \cup \mathcal{F}/\sim$.

Theorem 2.9: $(\mathcal{C}, \leqslant, \ll)$ is a causal space iff $\mathcal{C}$ is causal.

Proof: Assume $\mathcal{C}$ is not causal. Then there is a hull pair $(\hat{L}, \check{L})$ both of whose members are in $\mathcal{C}$. By Proposition 2.8, $\hat{L} \geqslant \check{L}$, $\check{L} \geqslant \hat{L}$; $\hat{L} \neq \check{L}$, so that $\mathcal{C}$ is not a causal space. Conversely, suppose $\mathcal{C}$ is causal. In checking Axioms 1.1 we need consider only cases where at least one element is in $\mathcal{P}$ and at least one element is in $\mathcal{F}$. Take $P, Q \in \mathcal{P}$ and $F \in \mathcal{F}$ throughout.

To check Axiom 1.1.A, suppose $P \gg F$. Then by Proposition 2.6.A there is a hull pair $(\hat{L}, \check{L})$ (neither of whose elements need be in $\mathcal{C}$) such that $P \gg \check{L}$ and $\check{L} \gg F$. Using Proposition 2.4 and its dual, together with Proposition 2.6.A again, we get $P \geqslant F$. The dual argument finishes the proof of Axiom 1.1.A.

Suppose now $P \geqslant F$ and $F \geqslant P$. By Proposition 2.6.B, $P \geqslant \downarrow F \geqslant P$ and $F \geqslant \uparrow P \geqslant F$. Thus $P = \downarrow F$ and $F = \uparrow P$. This is a contradiction since $\mathcal{C}$ cannot contain a hull pair. Thus, to show $\leqslant$ is a reflexive partial ordering, it remains to show that $\leqslant$ is transitive. Suppose first $P \geqslant Q \geqslant F$. Then, for some hull pair $(\hat{L}, \check{L})$, $P \geqslant Q \geqslant \hat{L}$ and $\check{L} \geqslant F$, so that $P \geqslant F$. Similarly trivial cases will be omitted in the rest of the proof. Now suppose $P \geqslant F \geqslant Q$. By Proposition 2.6.B, $P \geqslant \downarrow F \geqslant Q$, so that $P \geqslant Q$. The dual arguments finish the proof that Axiom 1.1.B holds.

If $P \gg F$ and $F \gg P$, then $P \geqslant F$ and $F \geqslant P$ by Axiom 1.1.A. By the above proof of Axiom 1.1.B this cannot occur. Thus $\ll$ is antireflexive and 1.1.C holds.

The proof of Axiom 1.1.D follow the above proof that $\geqslant$ is transitive almost *verbatim*. For example, if $P \gg F \geqslant Q$, then $P \gg \downarrow F \geqslant Q$, so that $P \gg Q$ by Proposition 2.4. ■

3. CAUSAL CONTINUITY

To proceed further, one needs a restriction on M. The appropriate condition can be motivated in various ways,[14] though it is not clear that all physically interesting space–times obey the condition. In the present context, the simplest motivation is the following. Since we eventually plan to represent each $x \in M$ by $\hat{I}x$ or $\check{I}x$, it seems reasonable to require that $\hat{I}$ and $\check{I}$ be one-to-one maps which leave chronology completely unaltered. This gives the following definition.

Definition 3.1: M is *causally continuous* iff for all $x, y \in M$:

A. $\hat{I}x \gg \hat{I}y$ iff $x \gg y$ iff $\check{I}x \gg \check{I}y$;

B. $\hat{I}x = \hat{I}y$ iff $x = y$ iff $\check{I}x = \check{I}y$.

Proposition 3.2: The following requirements are equivalent:

A. Requirement 3.1.A;

B. for all $x \in M$, $\uparrow \hat{I}x = \check{I}x$ and $\downarrow \check{I}x = \hat{I}x$;

C. for all $x, y \in M$, $x \in \text{Closure } J^+\{y\}$ iff $y \in \text{Closure } J^-\{x\}$.

Proof: In any case: (i) $x \gg y$ iff $y \in \hat{I}x$; and (ii) $\check{I}x \gg \check{I}y$ iff $(\downarrow \check{I}x) \cap (\check{I}y) \neq \phi$ iff $y \in \check{I}x$, where we have used the definitions in Table 2.2 and used Proposition 1.7.A. (i), (ii), and their duals show 3.2.A and 3.2.B are equivalent. The equivalence of 3.2.B and 3.2.C is proved elsewhere.[14] ■

Proposition 3.2 shows that if M is causally continuous, $(\hat{I}x, \check{I}x)$ is a hull pair for all $x \in M$. In our subsequent discussion we shall need two more definitions and two further results. The *Alexandrov topology* $\mathcal{T}'$ on M is the smallest topology $\mathcal{T}'$ on M such that $\hat{I}x$ and $\check{I}x$ are open for all $x \in M$ [8]; thus $\mathcal{T}' \subseteq \mathcal{T}$. A causal space $(Z, \leqslant, \ll)$ is *weakly distinguishing*[8] if, for all $w, z \in Z$,

$I^+\{w\}=I^+\{z\}$ and $I^-\{w\}=I^-\{z\}$ together imply $w=z$.

Proposition 3.3: If M is weakly distinguishing and obeys Condition 3.1.A then:

A. $\mathcal{T}'=\mathcal{T}$;

B. M is causally continuous.

Proof: Suppose the hypotheses of the proposition hold and $\mathcal{T}'\neq\mathcal{T}$; we will show a contradiction. There are distinct events $x,y\in M$ such that $x\geqslant y$ and $\downarrow\check{I}y\supseteq\hat{I}x$.[2,8,11] By Proposition 3.2.B, $\hat{I}y\supseteq\hat{I}x$; by Axiom 1.1.D, $\hat{I}x\supseteq\hat{I}y$. Thus $\hat{I}x=\hat{I}y$; the dual argument gives $\check{I}x=\check{I}y$. But $x\neq y$, the required contradiction. Now $\mathcal{T}'=\mathcal{T}$ implies that unless $x=y$, neither $\hat{I}x=\hat{I}y$ nor $\check{I}x=\check{I}y$ can hold.[2,8,11] Part B of the proposition follows. ∎

Corollary 3.4: If M is causally continuous, $\mathcal{T}'=\mathcal{T}$.

4. TOPOLOGY

Some of the examples given by Geroch, Kronheimer, and Penrose[5] indicate that in general one cannot hope to get a reasonable causal structure for ideal points which cooperates with any reasonable Hausdorff topology. When M is causally continuous, as we shall assume throughout this section, the situation is more cheerful.

4.1: Call $\mathcal{C}\subseteq\mathcal{P}\cup\mathcal{F}$ an *enlargement* of M iff $\mathcal{C}$ is causal and $\mathcal{C}$ contain either $\hat{I}x$ or $\check{I}x$ for all $x\in M$. The *extended Alexandrov topology* $\mathcal{T}$ on an enlargement $\mathcal{C}$ is defined as the smallest topology on $\mathcal{C}$ such that, for all $C\in\mathcal{C}$, each of the following four subcollections is open:

$$I^+\{C\},\quad I^-\{C\},\quad K^+\{C\}\equiv\mathcal{C}-J^-\{C\},\quad K^-\{C\}=\mathcal{C}-J^+\{C\}.$$

Suppose $\mathcal{C}$ is an enlargement of M. Because of Propositions 2.8 and 3.2.B we can, and shall, assume $\hat{I}x\in\mathcal{C}$ and $\check{I}x\notin\mathcal{C}$ for all $x\in M$ without essential loss of generality.

Theorem 4.2: $(\mathcal{C},\mathcal{T})$ is Hausdorff; $\hat{I}:M\to\mathcal{C}$ is an imbedding.

Proof: Throughout the proof P and Q are distinct elements of $\mathcal{C}\cap\mathcal{P}$ and F and G are distinct elements of $\mathcal{C}\cap\mathcal{F}$; "Closure" and "Interior" will refer to $\mathcal{T}$ on M, not to $\mathcal{T}$ on $\mathcal{C}$.

Since $\mathcal{C}$ is causal, either $Q\ngeqslant P$ or vice-versa; suppose $Q\ngeqslant P$. Then Closure $Q\nsupseteq P$ by Corollary 1.6.A. Choose $x\in P-\text{Closure } Q$. Then $P\in I^+\{\hat{I}x\}$ by causal continuity and Proposition 1.7.A. $Q\in K^-\{\hat{I}x\}$ by Proposition 1.3.B. For any $C\in\mathcal{P}\cup\mathcal{F}$, $I^+\{C\}$ and $K^-\{C\}$ are disjoint, since $B\gg C$ implies $B\geqslant C$. Thus we have found separating neighborhoods for P and Q.

Suppose $G\nleqslant F$. The dual of the argument just given shows there is an $x\in F-\text{Closure } G$ and that, within $(\mathcal{P}\cup\mathcal{F},\leqslant,\ll)$, $\check{I}x\gg F$, $\check{I}x\ngeqslant G$. Causal continuity and Proposition 2.8 now show that $F\in I^-\{\hat{I}x\}$ and $G\in K^+\{\hat{I}x\}$, which gives separating neighborhoods. Throughout the rest of the paper we will use "extended duality" to connote that duality, causal continuity, and Proposition 2.8 are being used simultaneously, as in the argument just given.

Either $F\geqslant P$ or $F\ngeqslant P$. Suppose first $F\ngeqslant P$. Then there is an x in $P-\text{Closure }(\downarrow F)$. $P\in I^+\{\hat{I}x\}$ as above. $F\in K^-\{\hat{I}x\}$ by Proposition 2.6.B with $r=\leqslant$, since $\downarrow F\nsupseteq\hat{I}x$ by Proposition 1.3.B. Thus we again have separating neighborhoods. Now suppose instead that $F\geqslant P$. Then $\downarrow F\supseteq P$ and $\uparrow P\supseteq F$. Since $\mathcal{C}$ is causal, either $\downarrow F\neq P$ or $\uparrow P\neq F$. If there is an $x\in\downarrow F-\text{Closure } P$, then $P\in K^-\{\hat{I}x\}$ and $\downarrow F\gg\hat{I}x$ as above. Since $\downarrow F\gg\hat{I}x$ iff $(\downarrow F)\cap(\uparrow\hat{I}x)\neq\emptyset$ iff $F\gg\hat{I}x$ iff $F\in I^+\{\hat{I}x\}$, there are separating neighborhoods in this case. An extended dual of the argument just given completes the proof that $(\mathcal{C},\mathcal{T})$ is Hausdorff.

$\hat{I}:M\to\mathcal{C}$ is one-to-one by Condition 3.1.B. Moreover, $\hat{I}:M\to\hat{I}M$ is open when $\hat{I}M$ is assigned the relative topology from $(\mathcal{C},\mathcal{T})$ since the Alexandrov topology of M is the manifold topology of M and Condition 3.1.A holds. To show $\hat{I}$ is continuous, we consider sets of the form $\hat{I}^{-1}\mathcal{B}$, where $\mathcal{B}$ is one of the subbasic open neighborhoods 4.1 and $\hat{I}^{-1}$ denotes the complete inverse image. Now $\hat{I}x\gg P$ iff $(\hat{I}x)\cap(\uparrow P)\neq\emptyset$ iff $x\in\uparrow P$, by the dual of Proposition 1.7.A. Thus $\hat{I}^{-1}I^+\{P\}=\uparrow P$ is open. Moreover, $P\gg\hat{I}x$ iff $P\cap(\uparrow\hat{I}x)\neq\emptyset$ iff $x\in P$, where we have used causal continuity. Thus $\hat{I}^{-1}I^-\{P\}=P$ is open. $\hat{I}x\ngeqslant P$ iff $x\in M-\text{Closure }(\uparrow P)$ by causal continuity, Proposition 2.8, and the dual of Proposition 1.7.A. Thus the complete inverse image of $K^-\{P\}$ is again open. Similarly, $P\ngeqslant\hat{I}x$ iff $x\in M-\text{Closure } P$. Extended duals of the above arguments show that each subbasic open neighborhood 4.1 has an open complete inverse image. Thus $\hat{I}$ is continuous. Thus it is an imbedding. ∎

5. IDEAL POINTS

We now apply our results to ideal points. The notation is that of 1.2.

Suppose $P\in\hat{\mathcal{M}}$. Then[5] $P=I^-c$, where $c\subseteq M$ is the image of some smooth, future-pointing, timelike curve. There are essentially just two different cases[5]: (i) c has a future end point $x\in M$; (ii) c is future inextendible. In case (i), $P=\hat{I}x$; in case (ii), P is interpreted as an ideal point. Compare Figs. 1 and 5.

Throughout the rest of this section, M is causally continuous. Define the *causal completion* $\mathbf{M}$ of M as $\mathbf{M}=\hat{\mathcal{M}}\cup\check{\mathcal{M}}-\downarrow(\check{\mathcal{M}}\cup\mathcal{L})$. Thus M has essentially the same structure as $\hat{\mathcal{M}}\cup\check{\mathcal{M}}/\sim$. Define the *casual boundary* $\partial\mathbf{M}\subseteq\mathbf{M}$ of M as $\partial\mathbf{M}=\mathbf{M}-\hat{I}M$. $\mathbf{M}$ is an enlargement of M. Assign $\mathbf{M}$ the causality $\leqslant$, chronology $\ll$, and extended Alexandrov topology $\mathcal{T}$). Thus $(M,\leqslant,\ll,\mathcal{T})$ is a causal space with Hausdorff topology. Suppose $x,y\in M$.

Theorem 5.1: $\hat{I}:M\to\mathbf{M}$ is a dense imbedding. $\hat{I}x\gg\hat{I}y$ iff $x\gg y$; $\hat{I}x\geqslant\hat{I}y$ iff $y\in\text{Closure }(\hat{I}x)$.

Proof: $\hat{I}$ is an imbedding by Theorem 4.2. To show that $\hat{I}M\subseteq\mathbf{M}$ is dense we will again analyze the subbasic open neighborhoods $\mathcal{B}$ given by 4.1. Suppose $P\in\mathcal{B}$. Define $P\cap(\hat{I}^{-1}\mathcal{B})=Z\subseteq M$ and define $Y=P-Z$. By casework we will show $Z\neq\emptyset$ and $I^-Y\subseteq Y$. Extended duality and indecomposability will then show $\hat{I}M$ is dense.

Suppose $\mathcal{B}=I^-\{B\}$, $B\in\mathbf{M}$. Then $x\in P$ implies $B\gg P\gg\hat{I}x$. Thus $Z=P$ in this case; Z is not empty since $P\in\hat{\mathcal{M}}$; Y is empty so $Y\supseteq I^-Y$. Now if $\mathcal{B}=K^-\{B\}$, we again have $Z=P$ and $Y=\emptyset$, since $P\gg\hat{I}x$, $P\ngeqslant B$, and $\hat{I}x\geqslant B$ cannot hold simultaneously. Next suppose $\mathcal{B}=I^+\{B\}$. Then, by the definitions in Table 2.2, $Z=P\cap F\neq\emptyset$, where $F=B$ or $F=\uparrow B$, according as $B\in\mathcal{F}$ or $B\in\mathcal{P}$ respectively. This gives $Y=P-F$. Since $I^-P=P$ and I^+F

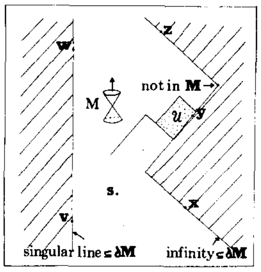

FIG. 6.

$=F$, $Y\supseteq I^-Y$. Finally, suppose $\mathcal{B}=K^+\{B\}$. Let $Q=B$ or $Q=\downarrow B$, according as $B\in\mathcal{P}$ or $B\in\mathcal{F}$ respectively. In both cases we have $Z=P-\text{Closure}_{\mathcal{T}}Q\neq\phi$, where we have used the definitions, Proposition 2.6, and Proposition 1.3.B. $Y=P\cap(\text{Closure}_{\mathcal{T}}Q)\supseteq I^-Y=P\cap Q$.

Now suppose $P\in\mathcal{B}_1\cap\mathcal{B}_2$, where $\mathcal{B}_1$ and $\mathcal{B}_2$ are subbasic open neighborhoods. Then $P=I^-P=[I^-(Z_1\cap Z_2)]\cup[I^-Y_1]\cup[I^-Y_2]$. We cannot have $Z_1\cap Z_2=\phi$. For if we did, indecomposability would give, say, $P=I^-Y_1$ which contradicts $I^-Y_1\not\supseteq Z_1$. By induction, each $\mathcal{B}\in\mathcal{T}$ which contains some $P\in\mathcal{P}$ contains the image of some $x\in M$. By extended duality each nonempty $\mathcal{B}\in\mathcal{T}$ contains the image of some $x\in M$. Thus $\hat{I}$ is a dense imbedding.

$\hat{I}x\geqslant\hat{I}y$ iff $\hat{I}x\supseteq\hat{I}y$ iff $y\in\text{Closure}(\hat{I}x)$ by the definitions and Proposition 1.3.B. $\hat{I}x\gg\hat{I}y$ iff $x\gg y$ by Condition 3.1.A.

A topologized causal space Z is *causally simple*[2] iff $J^+\{z\}$ and $J^-\{z\}$ are closed for all $z\in Z$. Trivially M is causally simple.

Corollary 5.2: $\hat{I}$: $M\to\hat{I}M$ is a causal isomorphism iff M is causally simple.

Example 5.3: Consider the submanifold of two dimensional Minkowski space shown, together with its completion M, in Fig. 6. This space—time and its completion mimic many of the properties of a maximally extended, causally completed Reissner—Nordstrom solution.[2] In addition, s represents a point amputated from the space—time and resurrected in M.

The reader may check the following points. As a point set, the boundary ∂M has the intuitively expected properties. For example $v\in\partial$M corresponds to a hull pair and is a single point of M. The topology is also the expected one. For example $\mathcal{U}$ is an open neighborhood of y. The causality is for the most part also obvious. Thus $w\gg v$, $z\gg v$, and $z\gg y\geqslant x$. $y\not\gg x$, which is acceptable, but not intuitively obvious.

6. PROPERTIES OF CAUSAL COMPLETIONS

Throughout this section M is a causally continuous space—time and **M** is its causal completion. Boldface denotes structures formed from $(\mathbf{M},\leqslant,\ll,\mathcal{T})$ by repeating exactly earlier definitions given for $(M,\leqslant,\ll,\mathcal{T})$. For example $\mathcal{P}=I^-\{S\subseteq\mathbf{M}\}$ is the generalization of the definition in 1.2.B. Similarly, suppose $U\in\mathcal{T}$ so that U is an open subset of M. Then $\downarrow U=I^-\{x\in M: x\ll u$ for all $u\in U\}$. We summarize some properties of M, with the rather tedious proofs omitted or drastically condensed.

It can be shown that M is causally continuous in the following sense (compare Sec. 3). M is weakly distinguishing; moreover, for all $x,y\in M$, $x\in\text{Closure }J^+\{y\}$ iff $y\in\text{Closure }J^-\{x\}$.

Theorem 6.1: M is causally isomorphic and homeomorphic to its own causal completion $\hat{\mathcal{M}}\cup\check{\mathcal{M}}/\sim$.

Proof: We outline the main steps. (A) Suppose $x,y\in M$ and $x\gg y$; then there exists a $z\in M$ such that $x\gg\hat{I}z\gg y$. (B) Suppose $P\in\mathcal{P}$; then $P=I^-P$. (C) $I^-\circ\hat{I}$: $\mathcal{P}\to\mathcal{P}$ is a one-to-one onto function with inverse $\hat{I}^{-1}$. (D) $P\subseteq\hat{\mathcal{M}}$ iff $\hat{I}^{-1}P\in\hat{\mathcal{M}}$. (E) Suppose $P\in\mathcal{P}$; then $\uparrow P=I^-\hat{I}\uparrow\hat{I}^{-1}P$. (F) Suppose $(P,F)\in\mathcal{P}\times\mathcal{F}$; then (P,F) is a hull pair iff $(\hat{I}^{-1}P,\hat{I}^{-1}F)$ is a hull pair. (A)—(F) and some of their extended duals imply that $\hat{\mathcal{M}}\cup\check{\mathcal{M}}/\sim$ is causally isomorphic to $\hat{\mathcal{M}}\cup\check{\mathcal{M}}/\sim$. Since the topologies are determined by the causal structure, M is also homeomorphic to its own completion. ∎

The following theorem has several applications which will be discussed elsewhere. It corresponds to a result proposed by Seifert[4] in a slightly different context.

Theorem 6.2: M is globally hyperbolic iff, for every $x\in\partial M$, either $I^-\{x\}$ or $I^+\{x\}$ is empty.

The result follows from the relation between boundary points and inextendible curves discussed in Sec. 5. We omit the proof.

7. LATTICE STRUCTURE

Let $\hat{\mathcal{L}}$ be the hull lattice of M, $\mathcal{N}\subseteq\hat{\mathcal{L}}$ be a subcollection.

Proposition 7.1: $(\hat{\mathcal{L}},\supseteq)$ is a complete lattice. The greatest lower bound $\sqcap\mathcal{N}$ and least upper bound $\sqcup\mathcal{N}$ of the elements of $\mathcal{N}$ are given by

$$\sqcap\mathcal{N}=\text{Interior}\bigcap_{N\in\mathcal{N}}N,\quad \sqcup\mathcal{N}=\downarrow\uparrow\bigcup_{N\in\mathcal{N}}N\ .$$

Proof: $(\mathcal{T},\supseteq)$ is a complete lattice, with Interior $\cap$ as meet and $\cup$ as join.[15] Lemmas 1.4.A and 1.4.B, together with their duals show that $\uparrow$ and $\downarrow$ are a Galois connection from $\mathcal{T}$ to itself. The result follows.[15]

Example 7.2: Let x and y be spacelike separated events in Minkowski space, c be the straight line between them. Then $\hat{I}x$ and $\hat{I}y$ are in $\hat{\mathcal{L}}$ since Minkowski space is causally continuous. The greatest lower bound of these two elements is $(\hat{I}x)\cap(\hat{I}y)\in\hat{\mathcal{L}}$. However, in four dimensions, $(\hat{I}x)\cup(\hat{I}y)$ is not in $\hat{\mathcal{L}}$. It turns out that the least upper bound of $\hat{I}x$ and $\hat{I}y$ is I^-c, the geodesic hull of $(\hat{I}x)\cup(\hat{I}y)$.

Example 7.3: Let $\hat{\mathcal{L}}$ be the hull lattice of the Einstein deSitter cosmological model. In $\mathbb{R}^3$, let $\mathcal{L}$ be the collection of all open, bounded, convex subsets together with the empty set and with $\mathbb{R}^3$ itself. $(\mathcal{L},\supseteq)$ is a complete lattice. The greatest lower bound of two elements in $\mathcal{L}$ is their set intersection; the least upper bound is their convex hull. It can be shown that $\mathcal{L}$ and $\hat{\mathcal{L}}$ are isomorphic as complete lattices.

By using the methods of Secs. 2—4, one can assign a causal structure and a Hausdorff topology to the hull lattice of a causally continuous space—time. Roughly speaking, the resulting structure is a big collection of fuzzy points.

8. CONCLUSION

For a causally continuous space—time the causal completion defined here seems quite satisfactory. But should one assume that all physically interesting space—times are causally continuous? If so, one would like a characterization of the above causal completion which does not involve the rather clumsy Table 2.2. If not, one might look for generalizations. We have tried many generalizations; each seems to have some incurable disease.

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Equilibrium statistical mechanics of relativistic particles with variable masses. I. Nonquantal theory

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The necessity for statistical mechanics of relativistic particles endowed with variable rest masses essentially arises from astrophysics (when dealing with clusters of stars or galaxies which do exhibit a mass spectrum) and from the statistical bootstrap model of Hagedorn and Frautschi for inclusive reactions of elementary particles. We begin this series with the simplest case of classical particles since this case demonstrates more clearly the main features of the theory. Moreover, this classical case is an excellent approximation for the statistical bootstrap near the "hadronic boiling point." We first derive the one-particle distribution function using the standard maximization procedure, in the implicit case of a uniform mass spectrum. It is shown that the actual mass spectrum possesses a part due to thermal agitation. An equation of states is derived. Other distributions are obtained (energy, 4-velocity). In the case of weak collisions, space–time correlations for the numerical and proper energy densities are derived and applied to the hadronic matter near the "hadronic boiling point." Finally, several extensions of these ideas are discussed.

1. INTRODUCTION

With the present article, we begin a series of papers devoted to the systematic study of the relativistic statistical mechanics of particles with variable masses. A few years ago such a subject could have been considered of mere academic interest. However, the situation has evolved mainly under the pressure of problems arising from astrophysics.

Accordingly, let us briefly mention some of these problems. A first one occurs when dealing with *statistical cosmology*, [1–4] where the universe is constituted of a gas whose particles are assumed to be of equal masses. These particles are generally considered as being galaxies and possibly clusters of galaxies. However, galaxies (and *a fortiori* clusters of galaxies) do not appear to possess identical masses. Therefore, a less crude approach to statistical cosmology should involve their *mass distribution*. A second problem where such an approach seems to be worth considering arises when treating in a statistical way clusters of galaxies themselves. Indeed a number of clusters (such as Coma or Virgo) contains large numbers of galaxies of unequal masses. At another scale star clusters could also be dealt with such an approach. Let us also mention a general statistical approach involving implicitly mass distributions, by Saslaw. [5–7] In this theory excitations of variable masses in a gravitational plasma are considered and discussed in connection with galaxy formation, etc. Other articles involving mass distributions have been published either in the context of stellar dynamics[8] or in cosmology.[9]

However, the necessity of such statistical mechanics appear more clearly when considering the very attractive *fireball model* of multiple production of particles in high energy reactions, i.e., the *statistical bootstrap* initiated by Hagedorn[10–12] (see also Frautschi's version[13]). In this theory a *mass spectrum* of the asymptotic form

$$\rho(m) \sim c\, m^a \exp(bm)$$

(where c, a, b are constants) is basic and leads to a good qualitative agreement with relevant experiments in high energy physics.

As a consequence, interesting applications of this theory have been considered[14,15] in the context of the big bang cosmology.

At this stage, and particularly when referring to star or galaxy clusters which do not exhibit a violent thermal agitation, the reader may wonder why should the theory be relativistic. The answer is both of theoretical and practical order. First it is clear that a relativistic treatment is needed for large masses or large velocities, and that such a relativistic treatment implies a Newtonian one. Second, in Newtonian physics, the mass is always decoupled from momentum or energy (i.e., there exists a superselection rule which guaranties the conservation of mass[16] while the situation is not so in relativity physics). This amounts to saying that an extension of Newtonian statistical mechanics to particles with a given mass spectrum does not present the same physical content as in relativity physics.

In this paper, we are mainly interested in treating the simplest case, i.e., equilibrium, which is of immediate importance in applications. A general relativistic theory does not present any particular difficulty, at least at a theoretical level.

In Sec. 2, the equilibrium distribution and the subsequent equation of states are obtained. Section 3 is devoted to the study and discussion of the thermal mass spectrum. In Sec. 4, connected distributions (for energy and 4-velocities) are derived. Section 5 is concerned with space–time correlations.

Conventions and notations

Throughout this paper, the signature of the metric tensor $g_{\mu\nu}$ is $+---$. Greek indices run from 0 to 3 while Latin indices run from 1 to 3.

2. THE EQUILIBRIUM DISTRIBUTION

Let us first derive the equilibrium distribution function of a relativistic gas of noninteracting[17] particles endowed with unprecisely defined masses (or, equivalently, with a mass spectrum), i.e., such that

$$p^\mu p_\mu \geq 0, \quad p^0 \geq 0. \tag{2.1}$$

The distribution function $N(x^\lambda, p^\lambda)$ we are looking for is normalized through

$$\int N(x^\lambda, p^\lambda)(p^\mu/m)\,d_4p = j^\mu(x^\lambda), \tag{2.2}$$

where the integral extends to the domain defined by Eq. (2.1). In Eq. (2.2), m must be considered as a mere notation standing for $(p^\lambda p_\lambda)^{1/2}$. It has, however, the physical meaning of a mass, and the normalization integral (2.2) will appear below to have the sense of the average over a mass spectrum of the current of particles of mass m. $j^\mu(x^\lambda)$ is the 4-current of the gas,

$$j^\mu(x^\lambda) = n(x^\lambda)\,\bar{u}^{\,\mu}(x^\lambda), \tag{2.3}$$

where $n(x^\lambda)$ is the invariant numerical world density of the gas, and $\bar{u}^{\,\mu}(x^\lambda)$ is its average local 4-velocity.

Since the mass m is no longer a disposable parameter but rather a function of the p^λ's, the normalization equation (2.2) has now to be justified. Let us start with the microscopic Feynman's current for n identical particles. Successively one gets

$$j^\mu_R(x^\lambda) = \sum_{i=1}^{i=n}\int_{-\infty}^{+\infty} d\tau\,\delta(x^\lambda - x_i^\lambda(\tau))\,u_i^\mu(\tau)$$

$$\equiv \sum_{i=1}^{i=n}\int_{-\infty}^{+\infty} d\tau\,\delta(x^\lambda - x_i^\lambda(\tau))\,\frac{p_i^\mu(\tau)}{m_i}$$

$$= \sum_{i=1}^{i=n}\int d\tau\,d_4p\,\delta(x^\lambda - x_i^\lambda(\tau))\delta(p^\lambda - p_i^\lambda(\tau))\,\frac{p^\mu}{m}. \tag{2.4}$$

The distribution function $N(x^\lambda, p^\lambda)$ is defined as the average value over the possible motions of the quantity[18,19]

$$N(x^\lambda, p^\lambda) = \langle R(x^\lambda, p^\lambda)\rangle \equiv \Big\langle \sum_{i=1}^{i=n}\int_{-\infty}^{+\infty} d\tau\,\delta(x^\lambda - x_i^\lambda(\tau))\delta(p^\lambda - p_i^\lambda(\tau))\Big\rangle,$$

from which [and from Eq. (2.4)] the normalization (2.2) follows. It should also be noticed that the variation of mass (and hence of the mass spectrum) is entirely due to dynamics through the terms $p_i^\lambda(\tau)$.

Let us now adopt another point of view. For like particles of fixed mass m, the normalization condition reads[20]

$$j^\mu(x^\lambda) = \int_{H_m} \frac{d_3p}{p_0}\,p^\mu\,N_m(x^\lambda, p^\lambda)$$

(with H_m defined by $p^\mu p_\mu = m^2$) or

$$j^\mu(x^\lambda) = \int_{H_m} m\,\frac{d_3p}{p_0}\,\frac{p^\mu}{m}\,N_m(x^\lambda, p^\lambda).$$

Suppose now that we are given a mixture of particles endowed with different masses m_j and that those particles of mass m_j have the weight $\omega(m_j)$; or, in other words, there exists a true mass spectrum. Then, instead of the preceding equation, we should have

$$j^\mu(x^\lambda) = \sum_j \omega(m_j)\int_{H_{m_j}} m_j\,\frac{d_3p}{p_0}\,\frac{p^\mu}{m_j}\,N_{m_j}(x^\lambda, p^\lambda),$$

and going to a continuous mass distribution

$$j^\mu(x^\lambda) = \int_0^\infty dm\,\omega(m)\int_{H_m} m\,\frac{d_3p}{p_0}\,\frac{p^\mu}{m}\,N_m(x^\lambda, p^\lambda),$$

which is easily seen to be rewritten as

$$j^\mu(x^\lambda) = \int_{p^\lambda p_\lambda \geq 0} d_4p\;\omega(m)\,N_m(x^\lambda, p^\lambda)\,\frac{p^\mu}{m}$$

$$\equiv \int_{p^\lambda p_\lambda \geq 0} d_4p\,N(x^\lambda, p^\lambda)\,\frac{p^\mu}{m} \qquad \text{QED} \tag{2.2$'$}$$

Once again—in a different physical context—the normalization equation (2.2) has been recovered.

With the normalization (2.4), the momentum—energy tensor reads

$$T^{\mu\nu}(x^\lambda) = \int N(x^\lambda, p^\lambda)\,\frac{p^\mu p^\nu}{m}\,d_4p. \tag{2.5}$$

Of course, j^μ and $T^{\mu\nu}$ must satisfy the conservation equations[21]

$$\partial_\mu j^\mu = 0, \quad \partial_\mu T^{\mu\nu} = 0 \tag{2.6}$$

The 4-entropy density[18,20] is given by

$$S^\mu(x^\lambda) = -\int \frac{p^\mu}{m}\,N(x^\lambda, p^\lambda)\ln[N(x^\lambda, p^\lambda)]\,d_4p \tag{2.7}$$

and should verify

$$\partial_\mu S^\mu = 0 \tag{2.8}$$

at equilibrium. In Eq. (2.7) we have dropped an unessential multiplicative constant. The simplest way to interpret Eq. (2.7) is to consider $S^\mu(x^\lambda)$ as the 4-entropy density in the sense of information[22,23] theory. However, if we go back to the Newtonian case, it is easily seen that a definition such as (2.7) amounts to adding to the usual Boltzmann entropy of kinetic theory a contribution due to the mass density. In the relativistic case the situation is not that simple so that it is preferable either to take (2.7) as a generalization of the usual entropy or to interpret it within the context of information theory.

Let us now derive the equilibrium distribution function. We follow the usual maximization procedure which in local form writes

$$\delta S^\mu(x^\lambda) = 0 \tag{2.9}$$

with account of the constraints (2.2) and (2.5). By introducing therefore five Lagrangian multipliers c and ξ^ν, the following variation equation,

$$\delta S^\mu(x^\lambda) + c\,\delta j^\mu(x^\lambda) + \xi_\nu T^{\mu\nu}(x^\lambda) = 0, \tag{2.10}$$

is obtained. Equivalently, it may be written as

$$\int_{\substack{p_\mu p^\mu \geq 0\\ p^0 \geq 0}} d_4p\,\frac{p^\mu}{m}\,\delta N(x^\lambda, p^\lambda)\{\ln[N(x^\lambda, p^\lambda)] + 1 + c + \xi_\nu p^\nu\} = 0, \tag{2.11}$$

from which we immediately get

$$N(x^\lambda, p^\lambda) = A\exp(-\xi_\nu p^\nu), \tag{2.12}$$

with $\ln A \equiv -1 - c$. This form for the equilibrium distribution function is quite similar to the Jüttner—Synge[20] one. This is by no means surprising since (i) the basic physical contents are alike and (ii) their derivation is formally analogous. The main difference comes from the domain where the integrals are evaluated: $\{p^\mu p_\mu \geq 0,\ p^0 \geq 0\}$ in our case and $\{p^\mu p_\mu = m^2,\ p^0 > 0\}$ in the Jüttner—Synge case.

Let us now calculate the Lagrange multiplier A. From dimensional arguments it is immediately seen that $A \propto n\xi^4$ (with $\xi^2 = \xi^\lambda \xi_\lambda$). Finally, using the fact that the only 4-vector at our disposal is ξ^μ and Eq. (2.3), we obtain

$$A = n(x^\lambda)\xi^4/4\pi\chi \tag{2.13}$$

with[24]

$$j^\mu(x^\lambda) = n(x^\lambda)\,\xi^\mu(x^\lambda)/\xi(x^\lambda), \tag{2.14}$$

where the x^λ dependance of ξ has been made explicit in the last equation. In Eq. (2.13), χ is the following constant:

$$\chi = \int_0^\infty x^2 K_2(x)\,dx = 3\pi/2, \tag{2.15}$$

where $K_2(x)$ is a modified Bessel function[25] of order 2.

As to the remaining Lagrange multiplier ξ, it can be identified with the reciprocal temperature

$$\xi = (kT)^{-1} \quad (k: \text{Boltzmann const}) \tag{2.16}$$

as in the Jüttner—Synge case. However, this last point has to be discussed a little bit further. It has indeed been shown that this identification is (in the Jüttner—Synge case) not the only possible one.[26] This is due to the fact that the relativistic perfect gas law may be written either as $p = nkT$ *or* as $p = \rho kT'$. Synge makes the first choice and, accordingly, the identification (2.16) follows. However, the second choice (ρ = mass density) leads to another expression.[26] Here, the identification (2.16) has been effected (i) for the sake of comparison with the Jüttner—Synge case and (ii) because, as we show below, we have *not* a perfect gas law in ρ as in n.

Equation of states

In order to find out the equation of states obeyed by this particular gas, let us calculate its momentum—energy tensor (2.5). This tensor has necessarily the form

$$T^{\mu\nu}(x^\lambda) = \rho(x^\lambda)\bar{u}^\mu\bar{u}^\nu - p(x^\lambda)\Delta^{\mu\nu}(\bar{u}^\lambda) \tag{2.17}$$

where $\rho(x^\lambda)$ is the invariant mass density of the gas and $p(x^\lambda)$ its pressure. $\Delta^{\mu\nu}(\bar{u}^\lambda)$ is the *local* projector on the spacelike 3-surface orthogonal to $\bar{u}^\mu$:

$$\Delta^{\mu\nu}(\bar{u}^\lambda) = g^{\mu\nu} - \bar{u}^\mu\bar{u}^\nu. \tag{2.18}$$

From Eq. (2.17) we get

$$\rho = T^{\mu\nu}\bar{u}_\mu\bar{u}_\nu, \quad p = \tfrac{1}{3}(\rho - T^\mu{}_\mu). \tag{2.19}$$

It follows that

$$\rho = A\int d_4\,p\,\frac{(p^\lambda\bar{u}_\lambda)^2}{m}\exp(-\xi\,\bar{u}_\mu p^\mu), \tag{2.20}$$

which is easily calculated in a comoving frame ($\bar{u}^0 = 1,\ \bar{u}^i = 0$):

$$\rho = 4n/\xi. \tag{2.21}$$

It remains to calculate the trace $T^\mu{}_\mu$ of the momentum—energy tensor. However, instead of using the second Eq. (2.19) to get the pressure, it is sufficient to notice that the usual momentum energy tensor (for particles endowed with a mass m) is[20]

$$T_m^{\mu\nu} = nm[K_3(m\xi)/K_2(m\xi)]\bar{u}^\mu\bar{u}^\nu - (n/\xi)g^{\mu\nu}, \tag{2.22}$$

and that $T^{\mu\nu}(x^\lambda)$ can be obtained from $T_m^{\mu\nu}$ with an average over masses; i.e., through

$$T^{\mu\nu}(x^\lambda) = \langle T_m^{\mu\nu}(x^\lambda)\rangle_{\text{mass}} \tag{2.23}$$

And since

$$\langle 1\rangle_{\text{mass}} = 1, \tag{2.24}$$

it follows that pressure is simply

$$p = n\,\xi^{-1}, \tag{2.25}$$

i.e., is the mass average of the coefficient of $g^{\mu\nu}$. Of course, we have anticipated a little bit on the next section; however, we see that the precise form of $\langle\ \rangle_{\text{mass}}$ has no importance at this stage. From Eqs. (2.21) and (2.24) we finally obtain

$$p = \tfrac{1}{4}\rho, \tag{2.26}$$

which may be considered as the equation of states of this gas. It should be emphasized, however, that the "good" one does depend on its future use. Both Eqs. (2.25) and (2.26) are equations of states, but they should not be employed without any precaution. For instance, if we had to introduce such an equation of states in cosmological equations, we should use Eq. (2.26) and *not* Eq. (2.25). In a sense, one could say that Eq. (2.25) reflects the fact that we deal with noninteracting particles, while Eq. (2.26) reflects the energy content of the model.

Remark

At first sight, it could be surprising not to find, as particular solutions of our variational problem (2.11), the usual Jüttner—Synge distribution for given masses; i.e., solutions of the form

$$N(x^\lambda, p^\lambda) = \sum_{i=1}^{\infty}\frac{n_i\xi}{4\pi m_i^2 K_2(m_i\xi)}\exp(-\xi m_i\bar{u}_\lambda p^\lambda) \times\delta(p^\lambda p_\lambda - m_i^2)\,2\theta(p^0)m_i. \tag{2.27}$$

In fact, solutions of this form are, of course, admissible, but they cannot be contained in the above derivation since our definition of the 4-entropy density implied the use of *continuous* distributions and not of the singular type (2.27). To obtain a general solution, we should use the following expression for the 4-entropy density;

$$S^\mu(x^\lambda) = -\int\frac{p^\mu}{m}N(x^\lambda, p^\lambda)\ln[N(x^\lambda, p^\lambda)]\,d_4p - \sum_{i=1}^{\infty}\frac{1}{m_i}\int_{\substack{p^\mu p_\mu = m_i^2\\ p^0>0}} N_i(x^\lambda, p^\lambda)\ln[N_i(x^\lambda, p^\lambda)]\,p^\mu\frac{d_3p}{p^0}, \tag{2.28}$$

and the usual constraints provided by the numerical 4-current and the momentum—energy tensor.

3. MASS DENSITY

Let us denote by $N_m(x^\lambda, p^\lambda)$ the usual Jüttner—Synge distribution[20]

$$N_m(x^\lambda, p^\lambda) = [n\xi/4\pi m^2 K_2(m\xi)]\exp(-\xi\,\bar{u}_\lambda\,p^\lambda) \tag{3.1}$$

This distribution being normalized on the mass shell

$\{p^\lambda p_\lambda = m^2,\ p^0 > 0\}$ appears in this context as being a *conditional* distribution. As a consequence, it is related to the equilibrium distribution (2.12) through

$$N(x^\lambda, p^\lambda) = \eta(m) N_m(x^\lambda, p^\lambda) \tag{3.2}$$

where $\eta(m)$ is the *mass density* we are looking for. Now from Eq. (2.12) and (3.1) we get

$$\eta(m) = (2\xi^3/3\pi) m^2 K_2(m\xi), \tag{3.3}$$

which is normalized as

$$\int_0^\infty \eta(m)\, dm = 1. \tag{3.4}$$

For $m \sim 0$, $\eta(m)$ reduces to

$$\eta(m) \sim \xi/3\pi \tag{3.5}$$

and for $m \sim \infty$ to

$$\eta(m) \sim (\xi/3)\sqrt{(2/\pi)}(m\xi)^{3/2} \exp(-m\xi). \tag{3.6}$$

The first two moments are given by

$$\langle m \rangle = (2/3\pi)\, \xi^{-1}, \quad \langle m^2 \rangle = 5\, \xi^{-2}, \tag{3.7}$$

from which follows that $\delta m \sim 5\, kT$, where δm is the mass dispersion.

More generally,

$$\langle m^l \rangle = \frac{2}{3\pi}\, \Gamma\left(\frac{l+5}{2}\right) \cdot \Gamma\left(\frac{l+1}{2}\right) 2^{l+1}\, \xi^{-l}. \tag{3.8}$$

Remarks and discussion

(1) The above mass density may be derived with several other methods. Among them, the following is useful and sheds some light on what is really done.

Let us calculate the local average value of an arbitrary function $\phi(m)$ submitted to the only constraints that (i) it does not grow faster than an exponential at infinity and (ii) it is locally integrable. We have[18,27]

$$\langle \phi(m) \rangle = \frac{1}{n} \bar{u}_\mu \int d_4p\, N(x^\lambda, p^\lambda) \frac{p^\mu}{m} \phi(m)$$
$$= \frac{A}{n} \int_0^\infty m^3 \phi(m)\, dm \int_{\substack{u^\mu u_\mu = 1 \\ u^0 \geq 1}} \exp(-m\xi u^0)\, d_3u, \tag{3.9}$$

$$= \frac{A}{n} \int_0^\infty m^3 \phi(m) \frac{4\pi K_2(m\xi)}{m\xi}\, dm \tag{3.10}$$

$$\equiv \int_0^\infty \phi(m)\eta(m) dm. \qquad \text{QED}$$

(2) The existence of such a mass spectrum might appear extremely surprising since we have not made any assumption involving mass, except, of course, the possibility of the existence of a mass spectrum.

In fact, we have made the *implicit* assumption that masses could take any values uniformly in the range $(0, \infty)$. Let us specify this point more precisely by saying that $\eta(m)$ depends only on the thermal state of the gas since it depends on the reciprocal temperature $\xi \cdot \eta(m)$ should therefore be considered, not as a true mass spectrum, but rather as a systematic contribution of thermal agitation to the mass. Consequently,

$$dF_\xi(m) \overset{\text{DEF}}{\equiv} \eta(m)\, dm \tag{3.11}$$

must be considered as a weight factor with respect to which we have to integrate quantities like $\phi(m)\ \sigma(m)$, where $\sigma(m)$ is the true spectrum. In the case considered above, $\sigma(m) \equiv 1$, i.e., any positive mass is uniformly allowed.

(3) The preceding argument can be supported by a more serious analysis of the derivation of the distribution function (2.12). We have indeed maximized the entropy of the distribution $N(x^\lambda, p^\lambda)$. However, what would have occured if we had maximized only the conditional entropy (m being fixed)? A simple calculation shows that we would have obtained the Jüttner–Synge distribution for N_m, leaving the mass density completely *undetermined* as expected. Let us pursue this brief analysis by looking at the entropy of the distribution written under the form (3.12). We get

$$S^\mu = -\int \eta(m) N_m(x^\lambda, p^\lambda) \ln[\eta(m) N_m(x^\lambda, p^\lambda)] \frac{p^\mu}{m}\, d_4p \tag{3.12}$$

for the entropy 4-density. This last equation can be rewritten as

$$S^\mu = \bar{u}^\mu S\{\eta(m)\} + \langle S_m^\mu \rangle \tag{3.13}$$

where the angle brackets denote an average over m and where $S\{\eta(m)\}$ stands for the entropy of the mass density $\eta(m)$. From Eq. (3.13) it is clear that the maximization of S^μ [with due account of the constraints (2.2) and (2.5)] yields the Jüttner–Synge distribution.

Let us now maximize the total entropy density (3.13) with respect to the variations of $\eta(m)$ only and let us also take the constraints (2.2) into account. We obtain the following equation:

$$\delta(\bar{u}_\mu S^\mu) + c\delta\langle 1 \rangle + \xi_\nu \delta \langle T_m^{\mu\nu} \bar{u}_\nu \rangle = 0 \tag{3.14}$$

where the brackets denote an average over mass and where the index m indicates a quantity in which the mass is fixed.[28] Equation (3.14) immediately provides

$$\eta(m) = \exp(-c - \bar{u}_\mu S_m^\mu - \xi T_m^{\mu\nu} \bar{u}_\mu \bar{u}_\nu). \tag{3.15}$$

In Eq. (3.15) the quantities S_m^μ and $T_m^{\mu\nu}$ are completely arbitrary. Therefore, $\eta(m)$ is itself completely arbitrary, which result is not surprising since no specific assumption has been effected for $\eta(m)$! However, this arbitrariness shows that the mass dependance of $\eta(m)$ depends entirely on what is assumed as to the thermal agitation of the gas through the terms S_m^μ and $T_m^{\mu\nu}$. If these last two quantities are specialized to the usual ideal[20] relativistic gas, then, with a simple calculation, expression (3.3) is recovered.

Accordingly, the mass density (3.3) must not be considered as a mass spectrum (either to be given or to be found from additional assumptions) but rather as a weight factor due to *thermal agitation*.

(4) Suppose we impose some conditions on $\eta(m)$, for instance, that

$$\langle m \rangle = m_0 \quad (m_0: \text{given constant}). \tag{3.16}$$

Then instead of Eq. (3.15) we should find

$$\eta(m) = \exp(-c - \alpha m - \bar{u}_\mu S_m^\mu - \xi T_m^{\mu\nu} \bar{u}_\mu \bar{u}_\nu) \tag{3.17}$$

and, instead of Eq. (3.3),

$$\eta(m)dm = D\exp(-\alpha m)\,dF_\xi(m), \qquad (3.18)$$

where D is a normalization factor and α, the Lagrange multiplier associated with condition (3.16). Note that, because of the asymptotic form (3.6), α can be positive or negative.

In this context, Hagdorn's mass spectrum (1.1) can be found anew by imposing a condition of the form

$$\langle m - a\ln m\rangle = \text{const}, \qquad (3.19)$$

whose physical meaning is not yet clear in this context.

Another case of interest, since it occurs frequently, is the case when m is bounded from above or/and has a minimum value. Then it is easily found that

$$\eta(m)\,dm = E\,\theta(m - m_{\min})\,\theta(m_{\max} - m)\,dF_\xi(m) \qquad (3.20)$$

(E : normalization constant)

where θ is the Heaviside step function.

(5) What about the nonrelativistic case? With similar methods, the distribution function is found to be infinite, because of the lack of convergence in m. More specifically

$$\eta(m) \sim m^{3/2}. \qquad (3.21)$$

This circumstance is due to the absence of link between mass and energy. It is therefore incorrect to say that Eq. (3.6) constitutes the nonrelativistic limit of the relativistic mass density, even though the Maxwell—Boltzmann distribution can be obtained from Jüttner and Synge's by using the low temperature limit.[29] Comparison of Eq. (3.21) with Eq. (3.6) shows that they differ by the exponential factor $\exp(-m\xi)$, which is a typically relativistic term.

(6) It should be emphasized that, in this model, the particles constituting the gas can actually modify their masses through interactions or any other processes. An example of such a situation is provided by Hagedorn's fireballs.

With this remark in mind, it is quite natural that our equilibrium distribution gives rise to an uniform true spectrum[30] in the simplest case where no extra assumption is made. Only with the introduction of basic dynamical processes, as to the mass loss (or gain), or with empirical or theoretical facts the "true" $\rho_{eq}(m)$ can be obtained.

When such an extra function is given [as, for instance, Eq. (1.1) in the statistical bootstrap], the equilibrium distribution function is simply written as

$$N(x^\lambda, p^\lambda) = \tilde{A}\rho_{eq}((g_{\mu\nu}p^\mu p^\nu)^{1/2})\exp(-\xi\,\bar{u}_\lambda p^\lambda) \qquad (3.22)$$

where $\tilde{A}$ is a new normalization constant and ρ_{eq} a given function.

(7) A remark similar to that effected at the end of the last section can be made—our procedure cannot contain singular distributions and, consequently, we have to impose them. Finally, the most general *thermal spectrum* has the form

$$\rho(m) = \frac{2\xi^3}{3\pi}m^2K_2(m\xi)\gamma + \sum_{i=1}^{\infty} q_i\ \delta(m - m_i)(1-\gamma) \qquad (3.23)$$

with

$$\sum_{i=1}^{\infty} q_i = 1, \quad q_i \geq 0, \ 0 \leq \gamma \leq 1.$$

4. CONNECTED DISTRIBUTIONS

In this section, we derive (1) the 4-velocity distribution and (2) the energy distribution.

4-velocity distribution

It is immediately obtained by taking the average over mass of the Jüttner—Synge distribution written in 4-velocity space,

$$\Phi(u^\lambda) = \left\langle \frac{nm\xi}{4\pi K_2(m\xi)}\exp(-m\xi\,u^\lambda\bar{u}_\lambda)\right\rangle \qquad (4.1)$$

$$= \frac{n(x^\lambda)}{\pi^2}\cdot\frac{1}{(\bar{u}^\lambda u_\lambda)^4}. \qquad (4.2)$$

Had we used a true spectrum uniform inside two values $m_{\min}$ and $m_{\max}$, we would have found (I am indebted to the referee for pointing out an error in the calculation)

$$\Phi(u^\lambda) = \frac{n(x^\lambda)}{(\bar{u}^\lambda u_\lambda)^4}\times(\text{normalization const})$$

$$\times[\exp(-m_{\min}\xi\,\bar{u}_\lambda u^\lambda)\cdot P(m_{\min}\xi\,\bar{u}^\lambda u_\lambda)$$
$$-\exp(-m_{\max}\xi\,\bar{u}_\lambda u^\lambda)\cdot P(m_{\max}\xi\,\bar{u}^\lambda u_\lambda)], \qquad (4.3)$$

where $P(x) = x^3/3! + x^2/2! + x + 1$. Such a minimum mass appears while dealing with galaxies ($m \sim 10^{44}g$) or in Hagedorn's fireballs, where it is considered to be the π meson mass.

In connection with these 4-velocity distributions it might be interesting to find out the mass spectrum which could give rise to the cosmic rays distribution,

$$\Phi_{\cos}(u^\lambda) = \text{const}(\bar{u}_\lambda u^\lambda)^{-\alpha}, \qquad (4.4)$$

where $\alpha \sim 2.5$, i.e., we look for a $\sigma(m)$ such that

$$\text{const}(\bar{u}_\lambda u^\lambda)^{-\gamma} = \int dm\,\sigma(m)\,\frac{\epsilon\xi^4 n}{\epsilon 6\pi^2}\,m^3\exp(-m\,\xi\,\bar{u}_\lambda u^\lambda). \qquad (4.5)$$

It is easily seen that $\sigma(m) \sim m^{\gamma-4}$ and that it should be limited from below ($m \geq m_{\min} > 0$). Naturally, this mass spectrum should not be taken too seriously and is, presently, a mere curiosity.

Energy distribution

Let us derive the distribution of the energy[27] $\epsilon = p^\mu\,\bar{u}_\mu$. We have

$$\psi(\epsilon) = \langle\delta(\epsilon - p^\mu\,\bar{u}_\mu)\rangle, \qquad (4.6)$$

where the brackets now denote an average over the p^μ's, x^λ being fixed. Thus,

$$\psi(\epsilon) = (A/n)\int_{\substack{p^\mu p_\mu > 0\\ p^0 \geq 0}} d_4p\,\delta(\epsilon - p^\mu\,\bar{u}_\mu)\exp(-\xi\,p^\mu\,\bar{u}_\mu)$$

$$\times\frac{p^\mu}{m}\,\bar{u}_\mu \qquad (4.7)$$

$$=(1/3!)\,\xi^4\epsilon^3\exp(-\xi\epsilon). \tag{4.8}$$

5. SPACE-TIME CORRELATIONS

Space—time correlations are of great interest in astrophysical applications, especially particle density correlations and mass density correlations. Naturally, applications require a more sophisticated true spectrum than the one used below. Here we derive what could be called "thermal correlations".

Particles density correlations

In Appendix A we derived the expression for such correlations (Eq. (A11)) in the case of particles with definite mass m. To obtain the particle density space—time correlations, we just have to take the average value of Eq. (A11) over the thermal mass spectrum. Therefore, we get

$$\langle \delta j^\mu(x^\lambda)\,\delta j^\nu(x'^\lambda)\rangle \equiv \langle \delta j^{\mu\nu}(X^\lambda)\rangle \tag{5.1}$$

(with $X^\lambda = x^\lambda - x'^\lambda$)

$$=\frac{X^\mu X^\nu}{T^5}\int_0^\infty dF_\xi(m)\,\frac{m\,\xi\,n}{4\pi K_2(m\xi)}\,\exp\frac{-m\,\xi\bar{u}_\lambda X^\lambda}{T} \tag{5.2}$$

$$=\frac{n}{\pi^2}\,\frac{X^\mu X^\nu}{T(\bar{u}_\lambda X^\lambda)^4}, \tag{5.3}$$

where $T^2 \equiv X_\lambda X^\lambda$. The space—time correlations for the invariant world density n are obtained by contracting the indices μ and ν, and hence

$$\langle \delta n(x^\lambda)\cdot\delta n(x'^\lambda)\rangle = \frac{4n}{\pi^2}\,\frac{((x^\lambda - x'^\lambda)(x_\lambda - x'_\lambda))^{1/2}}{(\bar{u}_\lambda x^\lambda)^4}. \tag{5.4}$$

They vanish on the light cone and decrease as $\sim t^{-4}$.

It should be noticed that, instead of Eq. (5.3), we would have obtained a temperature-dependant relation *if* we had used a spectrum with a nonvanishing minimum mass.

Mass density correlations

These correlations are easily obtained from the expression of

$$\langle T^{\mu\nu}(x^\lambda)T^{\mu'\nu'}(x'^\lambda)\rangle \tag{5.5}$$

by multiplication by $\bar{u}_\mu\bar{u}_\nu\bar{u}_{\mu'}\bar{u}_{\nu'}$. The evaluation of Eq. (5.5) does not present any particular difficulty and follows exactly the one given in Appendix A for $\delta j^{\mu\nu}$. The only changes required are the introduction of a factor $m\,u^{\mu'}u^{\nu'}$ in equations such as (A2). Finally, we get

$$\langle T^{\mu\nu}(x^\lambda)\,T^{\mu'\nu'}(x'^\lambda)\rangle_m = \frac{m^2\xi n}{4\pi K_2(m\xi)}\,\frac{X^\mu X^\nu X^{\mu'}X^{\nu'}}{T^7} \times\exp -\frac{m\,\xi\,\bar{u}_\lambda X^\lambda}{T}, \tag{5.6}$$

from which we have

$$\langle T^{\mu\nu}(x^\lambda)\,T^{\mu'\nu'}(x'^\lambda)\rangle = \frac{4n}{\xi\pi^2}\,\frac{1}{(\bar{u}_\lambda X^\lambda)^5}\,\frac{X^\mu X^\nu X^{\mu'}X^{\nu'}}{X^\lambda X_\lambda}. \tag{5.7}$$

Consequently, the mass density correlation is

$$\langle \delta\rho(x^\lambda)\,\delta\rho(x'^\lambda)\rangle = \frac{4n}{\xi\pi^2}\,\frac{1}{\bar{u}_\lambda X^\lambda}\,\frac{1}{(X^\lambda X_\lambda)} \tag{5.8}$$

It follows that (i) mass density correlations decrease more slowly in time than particle density correlations, (ii) unlike particle density correlations, mass density correlations do not vanish when x^λ and x'^λ are separated by a null 4-distance but rather tend to increase indefinitely. The latter circumstance is due to the absence of a minimum mass. If we had taken a uniform spectrum begining at $m_{\min}$, a multiplying factor of the form

$$\exp[-m_{\min}\,\xi\,\bar{u}_\lambda X^\lambda/(X_\lambda X^\lambda)^{1/2}] \tag{5.9}$$

would have prevented such infinite correlations, making them going to zero when $X^\lambda X_\lambda \to 0$.

Note also that Eq. (5.8) can be rewritten as

$$\langle \delta\rho(x^\lambda)\cdot\delta\rho(x'^\lambda)\rangle = \frac{\rho}{\pi^2}\,\frac{1}{\bar{u}_\lambda X^\lambda}\cdot\frac{1}{X^\lambda X_\lambda}, \tag{5.10}$$

where use has been made of Eq. (2.21).

Space-time correlations for the hadronic fireball[10-13]

The hadronic fireball is characterized by the mass spectrum (1.1) with $a=-3$ and $b\sim m_\pi^{-1}$, where m_π is the π meson mass. Moreover, this spectrum is limited from below by m_π:

$$\rho(m) = c\,m^{-3}\exp(bm). \tag{5.11}$$

Strictly speaking, Eq. (5.11) is only the asymptotic form of the actual spectrum. It is, however, used in most calculations since the low energy part is difficult to obtain.

In order to calculate the space—time correlations of the hadronic fireball, the 4-velocity distribution has to be derived. This distribution is given by Eq. (4.1) with another meaning for the average $\langle\ \rangle$, since we now have a "true" mass spectrum $\rho(m)$. This average is given by

$$\langle\cdots\rangle = H\int_{m_\pi}^\infty(\cdots)\,m^{-3}\exp(bm)\,dF_\xi(m), \tag{5.12}$$

where H is a normalization constant, i.e., such that $\langle 1\rangle = 1$. Note that, due to the asymptotic expression (3.6) for the thermal mass spectrum, ξ is always greater than b and hence b^{-1} is a limiting temperature[10] (i.e., the "hadronic boiling point"[10,31]).

The 4-velocity distribution is now easily computed and turns out to be

$$\phi_{\rm had}(u^\mu) = (Hn\xi^4/6\pi^2)\exp[-m_\pi(\xi\bar{u}_\lambda u^\lambda - b)]\,(\xi\bar{u}_\lambda u^\lambda - b)^{-1}. \tag{5.13}$$

Despite the denominator $(\xi\bar{u}_\lambda u^\lambda - b)$, this distribution is never singular provided $\xi > b$.

Using now Eq. (A10) with $N(u^\lambda)$ given by Eq. (5.13), we find that

$$\delta j^{\mu\nu}(X^\lambda) = \frac{Hn\xi^4}{6\pi^2}\times\frac{X^\mu X^\nu}{T^4}\,(\xi\bar{u}_\lambda X^\lambda - Tb)^{-1} \times\exp[-m_\pi T^{-1}(\xi\bar{u}_\lambda u^\lambda - bT)]. \tag{5.14}$$

This formula exhibits interesting properties. One can see that for $\mathbf{x}=0$, when $\xi \to b$, the density fluctuations (and correlations) tend to infinity. This is due to the fact that, at $\xi=b$, the hadronic fireball undergoes a *phase transition*. This property shows, as remarked by Carlitz[31] in another context, that a thermodynamical model is no longer valid for a description of hadronic matter. Note also that, on the light cone, $\delta j^{\mu\nu}=0$.

For the mass density space–time correlations, the same techniques yield

$$\begin{aligned}\langle T^{\mu\nu}(x^\lambda)\, T^{\mu'\nu'}(x'^\lambda)\rangle &\equiv \delta T^{\mu\nu\mu'\nu'}(X^\lambda)\\ &= \frac{Hn\xi^4}{6\pi^2}\cdot\frac{X^\mu X^\nu X^{\mu'} X^{\nu'}}{T^4}\\ &\times[(\xi\bar{u}_\lambda X^\lambda - bT)^{-3}\\ &\times\exp[-m_\pi T^{-1}(\xi\bar{u}_\lambda X^\lambda - bT)]\\ &\times[(\xi\bar{u}\, X^\lambda - bT)^2 m_\pi^2\\ &+2(\xi\bar{u}_\lambda X^\lambda - bT)m_\pi + 2].\end{aligned} \tag{5.15}$$

Contracting $\delta T^{\mu\nu\mu'\nu'}$ with $\bar{u}_\mu \bar{u}_\nu \bar{u}_{\mu'} \bar{u}_{\nu'}$, we get

$$\begin{aligned}\langle\delta\rho(x^\lambda)\delta\rho(x'^\lambda)\rangle &= \frac{Hn\xi^4}{6\pi^2}(\xi\bar{u}_\lambda X^\lambda - bT)^{-3}\,(X^\lambda\bar{u}_\lambda)^4\\ &\times\exp[-m_\pi(\bar{u}_\lambda X^\lambda - bT)T^{-1}]\\ \times[(\xi\bar{u}_\lambda X^\lambda - bT)^2 m_\pi^2 &\cdot 2(\xi\bar{u}_\lambda X^\lambda - bT)m_\pi + 2],\end{aligned} \tag{5.16}$$

which exhibits the same qualitative features (discussed above) as

$$\begin{aligned}\langle\delta n(x^\lambda)\cdot\delta n(x'^\lambda)\rangle &= \frac{Hn\xi^4}{6\pi^2}\times\frac{1}{T^2}\times\frac{1}{\xi\bar{u}_\lambda X^\lambda - bT}\\ &\times\exp[-m_\pi T^{-1}(\xi\bar{u}_\lambda X^\lambda - bT)]\\ \times[(\xi\bar{u}_\lambda X^\lambda - bT)^2 m_\pi^2 &+ 2(\xi\bar{u}_\lambda X^\lambda - bT)m_\pi + 2]\end{aligned} \tag{5.17}$$

obtained from Eq. (5.14) by contracting the indices μ and ν. The only qualitative difference between mass density and numerical density correlations (or fluctuations) is that the former begins much before the latter when $\xi\to b$.

Expression of this kind will be proved useful in big bang models or in hadron stars. However, we must bear in mind that Eqs. (5.14)–(5.17) are only approximate since (i) the number of particles has been implicitly considered as fixed and (ii) we have used Maxwell–Boltzmann statistics instead of the correct quantal ones.[32] We shall see[32] that the difference may be important.

6. DISCUSSION AND CONCLUSION

In this paper, we have given the most simple properties of relativistic gases at equilibrium (and possibly at local equilibrium) when their particles may exchange mass. This was essentially possible for, *at equilibrium*, we did not need any detailed dynamical mechanism for such exchanges. It is clear, however, that dynamics is (at least partially)[10] contained in the "true" mass spectrum has to be determined elsewhere: either experimentally or theoretically as in the statistical bootstrap models for hadronic matter.

It is also clear that the extremely simple properties derived here cannot be applied bluntly to physical situations. Some less trivial generalizations are required. Among them let us mention (1) microcanonical, canonical and grand canonical ensembles, (2) presence of an external force field, (3) gravitation, (4) quantum statistics, and (5) nonequilibrium phenomena.

Let us briefly review these various points.

(1) *The microcanonical ensemble* is easily written[18] in the absence of mass spectrum and next integrated over a given $\rho(m)$. From this microcanonical ensemble the canonical ensemble is derived, by using the method of structure functions. Although be it rather lengthy, this does not present any particular difficulty.[33,34] However, the most interesting generalization is the grand canonical ensemble since particles can also be exchanged. Here again things are simple (see Appendix B).

(2) The usual relativistic gas in an *external force field* has already been treated elsewhere[35] and the generalization is obvious. However, in the context of an eventual application to the primordial fireball (with $10^{-23}\,s \lesssim t \lesssim 1s$), the classical external mesic field deserves a particular consideration. First, this field contributes to the mass, adding a term in $\lambda\Phi$ (λ: coupling constant; Φ: mesic field). Second, such a classical field can be used to describe the interactions of a field containing a *large number* of π mesons. Third, in a model[15] based on the statistical bootstrap, very heavy fireballs (which ultimately will turn out to be protogalaxies) are produced (matter acquires a "grainy structure") in a sea of light particles, most of which are π mesons. Fourth, the relativistic scalar plasma (and at this stage of the evolution of universe, matter could be described as such, with suitable modifications) has been studied and presents particular instabilities[36,37] which could be interesting in this context.

(3) As to the extension of the previous results to include *gravitation*, most results of Secs. 2, 3, 4 are still valid, though some care is needed in handling indices, integration, etc. For instance, instead of Eq. (2.5), we would write

$$T^{\mu\nu}(x^\lambda) = \int_{\substack{g_{\sigma\rho}(x^\lambda)p^\sigma p^\rho \geq 0\\ p^0\geq 0}} (|g|)^{1/2}\, d_4p\, N(x^\lambda, p^\lambda)\frac{p^\mu p^\nu}{m} \tag{6.1}$$

It is also clear that the normalization constant A will not change since locally Minkowskian coordinates can always be used to evaluate this *invariant* quantity. In the same way, the thermal mass spectrum will not change since the general relativistic Jüttner–Synge distribution[38] preserves its special relativistic form.[39]

However, the main difference is that the distribution function has to satisfy a less trivial Liouville equation than the special relativistic one. Instead of

$$p^\mu\,\partial_\mu N = 0, \tag{6.2}$$

it should satisfy

$$L\,N \equiv p^\mu\,\partial_\mu N - \Gamma^\mu_{\alpha\beta}p^\alpha p^\beta\frac{\partial}{\partial p^\mu}\,N = 0, \tag{6.3}$$

where the $\Gamma^\mu_{\alpha\beta}$'s are the well-known Christoffel symbols of second kind. This equation demands the same constraints on ξ_μ as in the case considered by Chernikov[38]; i.e.,

$$\nabla_\mu \xi_\nu + \nabla_\nu \xi_\mu = 0 \tag{6.4}$$

and the only difference comes from the normalization constant which leads to $\partial_\mu A = 0$, or

$$n \xi^4 = \text{const.} \tag{6.5}$$

Had we also considered a "true" mass spectrum $\rho(m)$ in front of N [i.e., as in Eq. (3.23)], we would have obtained the same results essentially because of the fact that the quantity $m \equiv [g_{\mu\nu}(x^\lambda)p^\mu p^\nu]^{1/2}$ is a *constant of motion*. Accordingly, $\rho(m)$ is also a constant of motion and therefore is a solution of Eq. (6.3). Finally, since Eq. (6.3) is linear the function $\rho(m)\times N(x^\lambda, p^\lambda)$ is such that

$$\begin{aligned} L[\rho(m)\cdot N(x^\lambda, p^\lambda)] &= L\,\rho(m)\cdot N(x^\lambda, p^\lambda) + \rho(m)\, LN(x^\lambda, p^\lambda) \\ &= 0 \end{aligned}$$

provided $L\,N = 0$.

The only nontrivial generalization is that for the space–time correlations. This requires (i) the complete solution of the geodesic equations and (ii) extremely involved calculations. Fortunately, these calculations can be performed in the case of a big bang cosmology when correlation lengths are small compared with the radius of the universe. In such a case, the spatial curvature may be considered to be zero and the calculations (i) and (ii) can be performed.

Let us also note that the equilibrium distribution (2.12) is not a solution of Eq. (6.3) for an expanding homogeneous isotropic universe (except perhaps during an extremely short duration) since Eq. (6.4) is not satisfied. It can however be taken as an initial distribution whose evolution is governed by Eq. (6.3).[40]

Finally, it should be mentioned that the inclusion of gravitation in the theory is interesting not only in view of applications to astrophysics but also to elementary particle physics. Indeed, if Hagedorn–Frautschi statistical bootstrap has to be taken seriously, this theory will provides clues and suggestions as to possible tests for equality of gravitational and inertial masses etc.; of course, the latter assertion is true only if one thinks that general relativity is valid not only on a macroscopic scale but also at a microscopic level. These aspects are presently under current investigation.

(4) The *quantum case* is treated in a separate article[32] and does not present particular difficulties. Although we could start maximizing the expression for the entropy written as a functional of $\langle n_s\rangle$ (n_s: number of particles in the state s)[41] it is preferable to start directly from the density matrix. As an example, the thermal mass spectrum is found to be

$$\eta_{\substack{B\\F}}(m) = \frac{4\pi z}{n\pm} \sum_1^\infty (\mp z)^n \frac{m^2}{\xi} \frac{K_2(m\xi(n+1))}{(n+1)}, \tag{6.6}$$

where the upper sign stands for fermions and the lower one for bosons (z is linked to $n\pm$ and ξ through the normalization condition). In the case where the "true" mass spectrum is uniform, there exists a Bose–Einstein condensation on the state $p^\mu = 0$. When there exists a minimum mass, this condensation is on the state $p^\mu = (m_{\min}, 0)$, where $m_{\min}$ is the smallest mass *compatible* with the quantum numbers of the gas. This condensation might have interesting properties in big bang models.[32] It is also found that Fermi degeneracy presents peculiarities which might be used in the study of hadron stars.

APPENDIX A

In this appendix, we derive the expression of the correlation tensor $\langle \delta j_R^\mu(x^\lambda)\cdot \delta j_R^\nu(x'^\lambda)\rangle$ for a relativistic *perfect* gas. Let us write

$$\delta j^{\mu\nu} \overset{\text{DEF}}{\equiv} \langle \delta j_R^\mu(x^\lambda)\cdot \delta j_R^\nu(x'^\lambda)\rangle. \tag{A1}$$

$j_R^\mu(x^\lambda)$ is the *random* numerical 4-current[18] of the particles of the gas[42]:

$$j_R^\mu(x^\lambda) = \sum_{i=1}^{i=N} \int_{-\infty}^{+\infty} \delta(x^\lambda - x_i^\lambda - u_i^\lambda \tau_i) u_i^\mu \, d\tau_i \tag{A2}$$

(assuming weak collisions),

where τ_i is the proper time of the i-th particle while u_i^μ is its 4-velocity. Here $\tau_i^2 = x_i^\lambda x_{i\lambda}$, since the particles are not interacting. For the same reason particles move along straight lines between collisions.

Let us also recall that the average value of a given physical quantity $A^{\cdot\cdot}_{\cdot}$ is given by[18,20]

$$\langle A^{\cdot\cdot}_{\cdot}\rangle = \int_\Sigma \int_{\substack{u^\mu u_\mu = 1\\ u^0 > 0}} N(u^\lambda) A^{\cdot\cdot}_{\cdot}\; u^\mu \, d\Sigma_\mu \frac{d_3 u}{u_0} \tag{A3}$$

(Σ: spacelike surface)

and hence, as an example, we have[18]

$$\langle j_R^\mu(x^\lambda)\rangle = j^\mu(x^\lambda). \tag{A4}$$

In Eq. (A1), we defined

$$\delta j^\mu(x^\lambda) \equiv j_R^\mu(x^\lambda) - j^\mu(x^\lambda). \tag{A5}$$

Now, Eq. (A1) may be written as

$$\begin{aligned} \delta j^{\mu\nu}(x^\lambda, x'^\lambda) = \sum_i \int d\tau\, d\tau' \frac{d_3 u}{u_0} u^\alpha d\Sigma_\alpha(x_i) \\ \times u_i^\mu u_i^\nu N(x^\lambda, u_i^\lambda) \times \delta(x^\lambda - x_i^\lambda - u_i^\lambda \tau) \\ \times \delta(x'^\lambda - x_i^\lambda - u_i^\lambda \tau'), \end{aligned} \tag{A6}$$

where $d\Sigma_\alpha(x_i)$ is the 3-surface element relative to the ith variables. By using the properties of the Dirac distribution, Eq. (A6) reads

$$\begin{aligned} \delta j^{\mu\nu} = \sum_i \int d\tau\, d\tau' \frac{d_3 u}{u_0} u^\alpha d\Sigma_\alpha(x_i) u_i^\mu u_i^\nu\; N(u_i^\lambda) \\ \times \delta(x^\rho - x'_\rho - u_i^\rho(\tau - \tau')) \\ \times \delta(x'^\lambda - x_i^\lambda - u_i^\lambda \tau'). \end{aligned} \tag{A7}$$

The last δ term of this last expression is

$$\delta(t' - t_i - u_i^0 \tau')\cdot \delta(\mathbf{x}' - \mathbf{x}_i - \mathbf{u}_i \tau). \tag{A8}$$

The τ' integration yields

$$\delta(\mathbf{x}' - \mathbf{x}_i - \mathbf{u}_i (u^0)^{-1}(t_i - t'))u^{0-1}, \tag{A9}$$

which is next eliminated with the $\mathbf{x}_i$ integration [i.e., with $u^\alpha\, d\Sigma_\alpha(x_i)$]. Finally, it remains that

$$\delta j^{\mu\nu}(x^\lambda) = \int dT \int_{\substack{u^\mu u_\mu = 1\\ u^0>0}} N(u^\lambda)\, u^\mu u^\nu\, \delta(X^\lambda - u^\lambda T)\, \frac{d_3 u}{u_0}, \tag{A10}$$

where $X^\lambda \equiv x^\lambda - x'^\lambda$ and $T^2 \equiv X^\lambda X_\lambda$. The integrations occuring in Eq. (A10) are easily performed, and we find

$$\delta j^{\mu\nu}(X^\lambda) = \frac{m\,\xi\, n}{4\pi K_2(m\,\xi)}\, \frac{X^\mu X^\nu}{T^5}\, \exp\, \frac{-m\,\xi\, \bar{u}_\lambda X^\lambda}{T}. \tag{A11}$$

This expression agrees with the one already given by Sytenko[43] (in a noncovariant form) for the density correlation function.

APPENDIX B

In this appendix, starting from the microcanonical ensemble, we give a derivation of the distribution function (3.22)

$$N(x^\lambda, p^\lambda) = \tilde{A}\,\rho(m)\exp(-\xi\,\bar{u}_\lambda p^\lambda) \tag{B1}$$

The expression for the relativistic form of the microcanonical distribution for N free particles has been given elsewhere[18] and is easily generalized so as to take account of $\rho(m)$:

$$N^{(N)}_{\text{micr}}(P^\mu, \{p_i^\mu\}) = \text{const}\,\delta(P^\mu - \sum_{i=1}^{i=N} p_i^\mu) \times \prod_{i=1}^{i=N} 2m_i \rho(m_i)\theta(p_i^0)\delta(p_i^\lambda p_{\lambda i} - m_i^2), \tag{B2}$$

where θ is the Heaviside step function and where the normalization constant depends (i) on the number of particles N, (ii) on the *total* momentum energy P^μ of the gas, and (iii) on the spatial volume occupied. Note that $N^{(N)}_{\text{micr}}$ is normalized through[18]

$$\int N^{(N)}_{\text{micr}}(P^\mu, \{p_i^\mu\}) \prod_{i=1}^{i=N} d_4 p_i \frac{p_i^\mu}{m_i} \equiv J^{\mu_1\mu_2\cdots\mu_N} = \left(\frac{N}{V}\right)^{2N} \frac{P^{\mu_1}P^{\mu_2}\dots P^{\mu_N}}{M^N}, \tag{B3}$$

since P^μ is the only disposable 4-vector included in $N^{(N)}_{\text{micr}}$. In the preceding equation we have set $P^\lambda P_\lambda \equiv M^2$.

Instead of using $N^{(N)}_{\text{micr}}(P^\mu, \{p_i^\mu\})$ we shall rather use the conditional distribution[18] (x^λ being fixed)

$$N^{(N)}_{\text{micr}}(x^\lambda \,|\, P^\mu, \{p_i^\mu\}) = N^{(N)}_{\text{micr}}(P^\mu, \{p_i^\mu\}) \times \prod_{i=1}^{i=N} \frac{P^\mu p_{\mu i}}{M m_i}. \tag{B4}$$

The reason why we use this conditional distribution is the following. It is a true probability density in *momentum space*, while this is not the case for Eq. (B2) due to the normalization condition (B3).

It follows that the one-particle distribution function is given by

$$N(x^\lambda \,|\, p^\lambda) = \int \prod_i^N d_4 p_i \cdot \delta(p^\lambda - p_i^\lambda) N^{(N)}_{\text{micr}}(x^\lambda \,|\, P^\mu, \{p_i^\mu\}) \tag{B5}$$

where we have made clear in the notation for $N(x^\lambda | p^\lambda)$ the one-particle distribution that we calculate a *conditional* (x^λ being fixed; one could also say, a *local*$\cdots$) distribution. A simple calculation provides

$$N(x^\lambda \,|\, p^\lambda) = \rho(m)\, \frac{\Omega_{N-1}([(P^\lambda - p^\lambda)(P_\lambda - p_\lambda)]^{1/2})}{\Omega_N(M)}\, \frac{P^\mu p_\mu}{M_m}, \tag{B6}$$

where

$$\Omega_N(M) = \int \delta(P^\mu - \sum_{i=1}^{i=N} p_i^\mu) \times \prod_{i=1}^{i=N} \rho(m_i) 2m_i \theta(p_i^0)\delta(p_i^\lambda p_{\lambda i} - m_i^2)\, \frac{P^\mu p_{\mu i}}{M m_i}\, d_4 p_i \tag{B7}$$

An expression similar to $\Omega_N(M)$ has been evaluated by Lurçat and Mazur[33] using the central limit theorem.[44]

Their $\tilde{\Omega}_N(M)$ differs from ours by the absence of the term

$$\prod_{i=1}^{i=N} \rho(m_i) P^\mu p_{\mu i} M^{-1} m_i^{-1}.$$

In the limit $N \gg 1$, they found

$$\Omega_N(M) = \tilde{\phi}_N(\beta)\exp(\beta M) \times (2\pi)^{-2} \frac{\partial^2}{\partial\beta^2} \log \tilde{\phi}_N(\beta) \cdot \left(\frac{M^3}{\beta^3}\right)^{-1/2}, \tag{B8}$$

where $\tilde{\phi}_N(\beta)$ is the generating function[44] and where β may be identified[44] with $(kT)^{-1}$. In our case $\Omega_N(M)$ is given by a similar formula *except* that the generating function is different.

In our case, it turns out that the generating function is

$$\phi_N(\alpha) \overset{\text{DEF}}{\equiv} \int \Omega_N(M)\exp(-\alpha_\mu P^\mu)\, d_4 P \tag{B9}$$

$$= \left(\frac{1}{Mm}\right)^N \left(\frac{\partial^2}{\partial\alpha^2} + \frac{3}{\alpha}\frac{\partial}{\partial\alpha}\right)^N [X(\alpha)]^N, \tag{B10}$$

where

$$X(\alpha) = \frac{4\pi}{\alpha} \int_0^\infty dm\, \rho(m) m^2 K_1(m\alpha). \tag{B11}$$

(with $\alpha^2 \equiv \alpha^\mu \alpha_\mu$).

However, the important thing for the derivation of Eq. (B1) is the *form* of $\Omega_N(M)$ and, more particularly, the fact that

$$\Omega_N(M) \sim \exp(\beta M). \tag{B12}$$

Inserting Eq. (B12) in Eq. (B6), we find

$$N(x^\lambda \,|\, p^\lambda) = L(\beta, M)\exp[-\beta M + (M^2 + m^2 - 2P^\mu p_\mu)^{1/2}] \times \rho(m) \times P^\mu p_\mu (Mm)^{-1} \tag{B13}$$

$$\sim L(\beta, M)\rho(m)\, P^\mu p_\mu (Mm)^{-1} \exp(-\beta P^\mu M^{-1} p_\mu) \tag{B14}$$

since for $N \gg 1$, $M \gg m$.

This is almost Eq. (B1) except that the constant factor $L(\beta, M)$ has to be determined. In fact, for the sake of brevity, it can be determined by the normalization condition *although* it is actually furnished by the limit form of $\Omega_N(M)$.

Equation (B14) allows the identification of $\beta P^\mu M^{-1}$ with $\xi^\mu = \xi u^{-\mu}$. Next, after multiplying Eqs. (B13), (B14) by the invariant numerical density $n(x^\lambda)$ the final form (B1) is recovered.

In fact, the precise form (B1) could have been recovered rigorously from the generating function although the calculations are rather lengthy.

APPENDIX C: PROOF OF EQ. (2,15)

Since a number of calculations occuring in this paper are typically those leading to Eq. (2.15), this equation is proved here. First we start from the normalization equation (2.2) which we write as

$$\int_0^\infty m\,dm \int_{p^\lambda p_\lambda = m^2} \frac{d_3p}{p_0} \frac{p^\mu}{m} N(x^\lambda, p^\lambda) = J^\mu(x^\lambda). \qquad \text{(C1)}$$

Using the fact that $J^\mu(x^\lambda)$ is necessarily proportional to ξ^μ and a Lorentzian frame where ξ^μ reduces to $(1, 0, 0, 0)$ a straightforward calculation leads to

$$x = \int_0^\infty dm \int_{p^{0^2} - p^2 = m^2} \exp[-\xi p^0] p^0 \frac{\xi^4}{4\pi} \frac{d_3p}{P_0} \qquad \text{(C2)}$$

$$= \int_0^\infty dm \frac{\xi^4}{4\pi} \left(-\frac{\partial}{\partial \xi}\right) \int_{p^{0^2} - p^2 = m^2} \frac{d_3p}{p_0} \exp[-\xi p^0] \qquad \text{(C3)}$$

$$= \int_0^\infty dm \frac{\xi^4}{4\pi} \left(-\frac{\partial}{\partial \xi}\right) \left\{\frac{4\pi m K_1(m\xi)}{\xi}\right\}, \qquad \text{(C4)}$$

where the passage from Eq. (C3) to Eq. (C4) may be found in Ref. 18 (Eq. (108). Equivalently Eq. (C4) is rewritten as

$$x = \frac{\xi^4}{4\pi} \int_0^\infty dm \frac{4\pi m^2 K_2(m\xi)}{\xi} \qquad \text{(C5)}$$

$$\equiv \int_0^\infty dx\, x^2 K_2(x) \quad (\text{with } x = m\xi), \qquad \text{(C6)}$$

where use has been made of those recursion relations for the K_n's given in Ref. 18. Now using Cartesian coordinates, the normalization equation (2.2) leads immediately to

$$x = \xi^4 \int_0^\infty dp^0 \int_0^\infty dp \frac{p^2 p^0}{(p_0^2 - p^2)^{1/2}} \exp(-\xi p^0), \qquad \text{(C7)}$$

which reduces to

$$x = \xi^4 \int_0^\infty dp^0 (p^0)^3 \exp(-\xi p^0) \int_0^{\pi/2} \sin^2\theta\, d\theta \qquad \text{(C8)}$$

with the change of variable $p = p^0 \sin\theta$. Finally we obtain Eq. (2.15),

$$x = 3\pi/2. \qquad (2.15)$$

In conclusion, we have evaluated the same quantity in two different systems of coordinates in Minkowski space: Cartesian coordinates and relativistic polar coordinates.

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Clebsch–Gordan problem and coefficients for the three-dimensional Lorentz group in a continuous basis. I

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We have described a new approach to the Clebsch–Gordan problem for the unitary representations of the three-dimensional Lorentz group. We relate the various types of Clebsch–Gordan series to problems in the representation theory of four-dimensional orthogonal and pseudo-orthogonal groups, and thereby achieve a new and better understanding of the structures of the series. At the same time, the Clebsch–Gordan coefficients in a continuous basis are calculated. In this, the first of four papers, the case $D^+ \otimes D^+$ is worked out in detail.

INTRODUCTION

The problem of constructing the unitary irreducible representations (UIR's) of the three-dimensional Lorentz group $O(2, 1)$ was solved by Bargmann many years ago.[1] This work was partly motivated by the fact that knowledge of these UIR's was a necessary step in the construction of all the quantum mechanically acceptable unitary representations of the inhomogeneous Lorentz group.[2] For this reason both single- and double-valued representations of $O(2, 1)$, or in other words all the single-valued UIR's of the spinor group $SU(1, 1)$, were constructed by Bargmann. Following this work, many authors considered the Clebsch–Gordan (CG) problem for this group.[3] This problem naturally splits into two parts. The first is the determination of the Clebsch–Gordan series, namely the determination of which UIR's are present in the decomposition of the direct product of two given UIR's, and each how often. The second is the evaluation of the Clebsch–Gordan coefficients which effect the decomposition of a direct product into irreducibles.

The UIR's of the group $SU(1, 1)$ can be naturally divided into three classes: the discrete class, the continuous nonexceptional class, and the continuous exceptional class. We shall hereafter be concerned with the first two classes alone. The discrete class can be further subdivided into UIR's of the positive type, and those of the negative type. Let us generically denote these two types of UIR's as D^+ and D^-, respectively; for the UIR's of the continuous type we shall write C. (Further distinguishing labels will be appended in due course.) There is essentially just one nontrivial outer automorphism that can be defined for the group $SU(1, 1)$, and it has the effect of converting a UIR of type D^+ into one of the type D^- and vice versa, while it carries any UIR of type C into itself. Consequently, the only essentially distinct direct products to be considered are of the forms $D^+ \otimes D^+$, $D^+ \otimes D^-$, $D^+ \otimes C$, and $C \otimes C$; $D^- \otimes D^-$ and $D^- \otimes C$ are related to the first and third cases by the outer automorphism. The structure of the C–G series changes greatly as one goes from one of these four cases to another; but this structure has an intrinsic meaning in that it does not depend on the ways in which the various UIR's are realized. On the other hand, the C–G coefficients are always defined relative to a well-defined way of realizing the UIR's; that is to say they depend on the way in which basis vectors have been chosen in the spaces of the various UIR's.

In the three-dimensional Lie algebra of $SU(1, 1)$, one can distinguish three distinct types of elements, those of elliptic type, those of parabolic type, and those of hyperbolic type. The maximal compact subgroup of $SU(1, 1)$, [the $O(2)$ subgroup of $O(2, 1)$], is generated by an element of elliptic type. In Bargmann's paper, the UIR's of $SU(1, 1)$ were constructed in a basis in which the $O(2)$ generator is diagonal. In this basis, the breakup of a UIR of $SU(1, 1)$ into a discrete direct sum of one-dimensional representations of $O(2)$ is immediate. Further, the relationship of the representations of $SU(1, 1)$ to those of the compact group $SU(2)$, which is quite close, can be nicely displayed. In all the work done on the Clebsch–Gordan problem upto now, this same "$O(2)$-basis" has been used; so once again the expressions for the $SU(1, 1)$ C–G coefficients are intimately related to the $SU(2)$ case, and may be thought of as suitable analytic continuations of the latter.

An alternative basis in which to set up the UIR's of $SU(1, 1)$ is that in which the hyperbolic generator of an $O(1, 1)$ subgroup is diagonal.[4] We shall refer to such a basis as a continuous basis. This form for the representations has become quite important in recent analyses of generalized relativistic partial wave analysis.[5] The aim of the work to be described in the present series of papers was originally the determination of the C–G coefficients of $SU(1, 1)$ in a continuous basis, for all possible direct products of UIR's not belonging to the continuous exceptional class. We have described elsewhere a construction of the UIR's of $SU(1, 1)$, in which the generators are built up in a simple manner using oscillator operators, and in which a certain degree of uniformity is achieved in the treatment of the discrete class UIR's on the one hand, and the continuous class UIR's, on the other.[6] In this construction a particular $O(1, 1)$ generator has a specially simple structure not shared by the other two linearly independent generators. Using this construction as the basis for the calculation of the C–G coefficients in a continuous basis, it soon became apparent that there was a higher symmetry in the problem. The structure of the C–G series in each of the four cases $D^+ \otimes D^+$, $D^+ \otimes D^-$, $D^+ \otimes C$, $C \otimes C$ gets related to a problem in the representation theory of a four-dimensional real rotation group, the particular group depending on the type of direct product involved. By fully exploiting this connection, one now understands in a new light why the C–G series looks the way it does in each case; correspondingly, a certain amount of unification is achieved among results which might otherwise appear disjointed. The higher symmetry of course also helps us in computing the C–G coefficients in each case. But its greater value is in the explanation of the structures of the various C—G series; and these structures as we have already noted are intrinsic to the representation theory of $SU(1,1)$. It is interesting to note that this higher symmetry is not at all apparent in all the work done on the C—G problem for $SU(1,1)$, in the "$O(2)$-basis"; it results directly from the specific way in which we have set up the UIR's of the group, and this is geared to the use of the continuous basis.

It is worthwhile describing briefly at this point how the higher symmetry comes about. Recall that the discrete class UIR's of $SU(1,1)$ can be labeled by an index k with possible values $1/2$, 1, $3/2$, $\ldots$; for each value of k we have one UIR of positive type, D_k^+, and one of negative type, D_k^-. A UIR of continuous type is written $C_q^\epsilon : \epsilon = 0$ or $1/2$ accordingly as the UIR is of either integral or half-integral type, and q ranges from $1/4$ to ∞.[7] The value $q = 1/4$ is excluded if $\epsilon = 1/2$. The label q may be parametrized by $q = 1/4 + s^2$, with $0 \leqslant s < \infty$ if $\epsilon = 0$ and $0 < s < \infty$ if $\epsilon = 1/2$. In terms of oscillator operators, it is possible to set up three somewhat special unitary reducible representations of $SU(1,1)$, which we shall denote by $\mathcal{D}^+$, $\mathcal{D}^-$, and $\mathcal{C}$.[8] When expressed as a direct sum of UIR's, $\mathcal{D}^+$ contains the UIR $D_{1/2}^+$ once, and each D_k^+ for $k \geqslant 1$ twice. Similarly, $\mathcal{D}^-$ contains $D_{1/2}^-$ once, and each D_k^- for $k \geqslant 1$ twice. And $\mathcal{C}$ can be expressed as a direct integral of the UIR's C_q^ϵ, with each UIR for each pair ϵ, q occurring with multiplicity two. (All these properties will be explained in the subsequent sections.) Consider now the unitary representation $\mathcal{D}^+ \otimes \mathcal{D}^+$ of $SU(1,1)$: It is clear that every direct product of the form $D_k^+ \otimes D_{k'}^+$ is contained in this larger representation. It turns out that the generators of the product representation $\mathcal{D}^+ \otimes \mathcal{D}^+$ which are just sums of the generators of the individual factors, are invariant under a set of transformations that can be defined on the space of the representation $\mathcal{D}^+ \otimes \mathcal{D}^+$ and having the structure of the group $O(4)$, the group of real orthogonal rotations in four dimensions. And the Casimir invariant for the "total" $SU(1,1)$ representation is identical to one of the two $O(4)$ Casimir invariants. [The other $O(4)$ Casimir invariant vanishes.] In fact the representations of $O(4)$ appearing here are just those carried by "spherical harmonics" in four dimensions. By splitting up the space of the representation $\mathcal{D}^+ \otimes \mathcal{D}^+$ of $SU(1,1)$ into subspaces in which distinct $O(4)$ representations occur, and this is relatively easy, we obtain subspaces in which distinct UIR's of the "total" $SU(1,1)$ appear. By a further suitable choice of basis, we can then specialize to individual products of the form $D_k^+ \otimes D_{k'}^+$ contained in $\mathcal{D}^+ \otimes \mathcal{D}^+$, and easily read off the corresponding C—G series. The structure of the C—G series for this type of direct product is then seen to be essentially determined by the spectrum of $O(4)$ representations obtained by the action of this group on functions on the unit sphere in four dimensions.

In a similar way, the product representations $\mathcal{D}^+ \otimes \mathcal{D}^-$, $\mathcal{D}^+ \otimes \mathcal{C}$, and $\mathcal{C} \otimes \mathcal{C}$ are associated with the symmetry groups $O(2,2)$, $O(3,1)$, and $O'(2,2)$; and the structures of the C—G series for products of the form $D_k^+ \otimes D_{k'}^-$, $D_k^+ \otimes C_q^\epsilon$, and $C_q^\epsilon \otimes C_{q'}^{\epsilon'}$ are fully determined by the properties of "spherical harmonics" corresponding to $O(2,2)$, $O(3,1)$, and $O'(2,2)$, respectively. Here, the same group $O(2,2)$ describes the symmetry properties of both $\mathcal{D}^+ \otimes \mathcal{D}^-$ and $\mathcal{C} \otimes \mathcal{C}$; however, the "spherical harmonics" are needed in the two cases in different bases; in the former, the $O(2) \otimes O(2)$ subgroup of $O(2,2)$ is singled out, in the latter it is the subgroup $O(1,1) \otimes O(1,1)$. The construction of the "spherical harmonics" for the groups $O(2,2)$, $O'(2,2)$ can again be reduced to a simpler problem at the level of the group $SU(1,1)$: This happens because locally $O(2,2)$ has the same structure as $SU(1,1) \otimes SU(1,1)$. And the structure of the Plancherel formula for $SU(1,1)$, as derived by Bargmann, yields immediately the required spherical harmonics for $O(2,2)$; while the same formula written in a new basis is adequate for $O'(2,2)$.[9] In dealing with the intermediate case $\mathcal{D}^+ \otimes \mathcal{C}$, we were led to an interesting problem in the representation theory of the homogeneous Lorentz group $O(3,1)$, a partial solution to which is available in the literature.[10] The problem is to decompose the unitary representation of the $(3+1)$-homogeneous Lorentz group $O(3,1)$ acting on functions defined on the single sheeted spacelike hyperboloid in real four-dimensional space with metric $+++-$, into UIR's of $O(3,1)$. (The corresponding problem for the two sheeted timelike hyperboloid was solved long ago, and the results will be relevant in our work.) We have described elsewhere a complete solution to this problem, and the results will be used in the present work.[11]

We now outline the plan of the present and the succeeding papers of this series. Even though the spirit behind the solution is the same in all four types of direct products, the details differ. To avoid confusion, therefore, this paper mainly deals with the Clebsch—Gordan problem for the products of the form $D^+ \otimes D^+$, and the related case $D^- \otimes D^-$. In the second, third, and fourth parts of this work, we shall take up the cases $D^+ \otimes D^-$ (and $D^- \otimes D^+$), $D^+ \otimes C$ (and $D^- \otimes C$), and $C \otimes C$, respectively. In each case, all the relevant details of the corresponding symmetry group and its associated spherical harmonics will be developed. In Sec. I of this paper, we gather some information on the UIR's of the group $SU(1,1)$, and the particular construction of these UIR's that we will use later on. Section 2 contains a description of the three unitary representations $\mathcal{D}^+$, $\mathcal{D}^-$, and $\mathcal{C}$, as well as a concise statement of the structure of the C—G series in all four cases, and some comments on them. The material of Secs. 1 and 2 will be used in the succeeding papers as well. In Sec. 3, we describe the symmetry properties of the representation $\mathcal{D}^+ \otimes \mathcal{D}^+$ of $SU(1,1)$, and show how this leads to the well-known structure of the C—G series for two positive discrete UIR's. The results of Sec. 3 lead immediately to the C—G coefficients in a continuous basis; these are given in Sec. 4. Finally, in Sec. 5, the details for the case $D^- \otimes D^-$ are read off from the previous results using the outer automorphism of $SU(1,1)$.

1. STANDARD FORMS FOR THE UIR'S OF SU(1,1)

The group $SU(1,1)$ consists of all 2×2 complex matrices of the form

$$\begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}, \quad |\alpha|^2 - |\beta|^2 = 1. \tag{1.1}$$

In this defining representation, we identify the generators as $\frac{1}{2}\sigma_3$, $(i/2)\sigma_2$, and $-(i/2)\sigma_1$, where σ's are the 2×2 Pauli matrices. In a general representation, the corresponding generators will be written J_0, J_1, J_2 and they will obey the commutation rules

$$-i[J_0,J_1]=J_2, \quad -i[J_0,J_2]=-J_1, \quad -i[J_1,J_2]=-J_0. \tag{1.2}$$

In a unitary representation, the J_α are Hermitian. J_0 is elliptic, J_1 and J_2 hyperbolic. When we use a continuous basis, J_2 will be the preferred generator. The Casimir operator Q is defined by

$$Q=(J_1)^2+(J_2)^2-(J_0)^2. \tag{1.3}$$

It commutes with all the J_α. The outer automorphism τ may be defined to have the following actions on a general element of $SU(1,1)$ and on the generators:

$$\tau: \begin{pmatrix}\alpha & \beta\\ \beta^* & \alpha^*\end{pmatrix} \to \begin{pmatrix}\alpha^* & \beta^*\\ \beta & \alpha\end{pmatrix}, \tag{1.4a}$$

$$J_0\to -J_0, \quad J_1\to -J_1, \quad J_2\to J_2. \tag{1.4b}$$

Clearly, both the group composition law and the commutation relations (1, 2) are preserved by the mapping τ.

A UIR of $SU(1,1)$ is unambiguously specified by giving the value of the Casimir invariant Q, and in addition the eigenvalue spectrum of the generator J_0. In the discrete UIR's $D_k^\pm$, where k takes on one of the values 1/2, 1, 3/2, $\cdots$, the value of Q is $k(1-k)$; and the eigenvalues of J_0 are $m=k$, $k+1$, $k+2$, $\cdots$ in the positive discrete case, and $m=-k$, $-k-1$, $-k-2$, ... in the negative discrete case. Because the eigenvalues of J_0 are all of one sign, it is trivial to see that the automorphism τ cannot be unitarily implemented in these cases. On the other hand, τ preserves the value of Q; so it is equally obvious that it converts a UIR D_k^+ into D_k^- and conversely. In the continuous UIR's C_q^ϵ, the value of Q is $q=1/4+s^2$, where $s\geq 0$ or $s>0$ according as to whether $\epsilon=0$ or 1/2; and the eigenvalues of J_0 are $m=0$, ± 1, ± 2, $\cdots$ if $\epsilon=0$, and $m=\pm 1/2$, $\pm 3/2$, $\cdots$ if $\epsilon=1/2$. Since as we have said the value of Q and the spectrum of J_0 determine a UIR uniquely, τ must be unitarily implementable in a UIR C_q^ϵ; if we write $|s,\epsilon;m\rangle$ for the eigenvectors of J_0 and adopt a suitable phase convention for the matrix elements of J_1 and J_2 (the Bargmann choice),[12] then the unitary operator A that implements τ is given by

$$A|s,\epsilon;m\rangle=(-1)^{m-\epsilon}|s,\epsilon;-m\rangle. \tag{1.5}$$

Let us now summarize the nature of the eigenvalue spectrum of J_2, and then give the construction of the UIR's that will be used later. We will use letters p, p', $\cdots$ to denote eigenvalues of J_2. Then it turns out that in a UIR of discrete type, whether it be of positive type or of negative type and whatever be the value of k, the possible values of p are all real numbers from $-\infty$ to $+\infty$, and for each value of p, J_2 has precisely one eigenvector. In a UIR of continuous type, again the possible values of p are all real numbers from $-\infty$ to $+\infty$, independent of both s and ϵ, but now J_2 has two linearly independent eigenvectors for each value of p.[13] Therefore, within a discrete UIR, the elements of a continuous basis can be completely labeled by the eigenvalue p of J_2, but this is not so in a continuous type UIR. However, in the latter case we know that a unitary operator A can be found that will implement the automorphism τ, and A commutes with J_2. By specifying both the eigenvalue p of J_2, and $a=\pm 1$ of A, we can then unambiguously label the elements of the continuous basis in a UIR C_q^ϵ. Summarizing, in the UIR D_k^η, $\eta=\pm$, we have the continuous basis $|k,\eta;p\rangle$ obeying

$$J_2|k,\eta;p\rangle=p|k,\eta;p\rangle,$$
$$\langle k,\eta;p'|k,\eta;p\rangle=\delta(p'-p), \quad -\infty<p',p<\infty. \tag{1.6}$$

And in the UIR C_q^ϵ we have vectors $|s,\epsilon;p,a\rangle$ obeying

$$J_2|s,\epsilon;p,a\rangle=p|s,\epsilon;p,a\rangle, \quad A|s,\epsilon;p,a\rangle=a|s,\epsilon;p,a\rangle,$$
$$\langle s,\epsilon;p',b|s,\epsilon;p,a\rangle=\delta(p'-p)\delta_{ba}, \quad -\infty<p',p<\infty,$$
$$b=\pm 1, \quad a=\pm 1. \tag{1.7}$$

The question of a "phase convention" for such basis vectors is much more subtle than in the $O(2)$-basis, because the generators J_0 and J_1 cannot be described by means of "matrix elements" any more. All we shall insist on in a realization of a UIR is that choices of continuous basis vectors and of A be made consistent with the above equations.

For any chosen value of k, the UIR D_k^+ can be realized in the following fashion.[14] We define the Hilbert space $\mathcal{H}(k,+)$ to consist of functions on the positive real line, $f(r)$ for $0\leq r<\infty$, with the norm

$$\|f\|^2=\int_0^\infty r|f(r)|^2\,dr<\infty. \tag{1.8}$$

[Actually the space $\mathcal{H}(k,+)$ does not change with k, but we keep these labels to remind us of the UIR being constructed.] The generators of $SU(1,1)$ will be written $J_\alpha(k,+)$ and are

$$J_0(k,+)=\frac{1}{4}\left(r^2-\frac{d^2}{dr^2}-\frac{1}{r}\frac{d}{dr}+\frac{(2k-1)}{r^2}\right),$$
$$J_1(k,+)=\frac{-1}{4}\left(r^2+\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{(2k-1)}{r^2}\right),$$
$$J_2(k,+)=\frac{-i}{2}\left(r\frac{d}{dr}+1\right). \tag{1.9}$$

The dependence on k lies only in $J_0(k,+)$ and $J_1(k,+)$; it can be checked that Q has the value $k(1-k)$ and that $J_0(k,+)$ has the correct eigenvalues. The finite transformations generated by $J_2(k,+)$ are local but those generated by $J_0(k,+)$ and $J_1(k,+)$ are nonlocal. The first is easy to construct:

$$[\exp(i\zeta J_2(k,+))f](r)=\exp(\zeta/2)f[r\exp(\zeta/2)]. \tag{1.10}$$

For the others we can write the general forms

$$[\{\exp[i\mu J_0(k,+)] \text{ or } \exp[i\nu J_1(k,+)]\}f](r)=\int_0^\infty r'\,dr' \times\{L^{(k,+)}(r,r';\mu) \text{ or } M^{(k,+)}(r,r';\nu)\}f(r'). \tag{1.11}$$

The kernels L and M can be evaluated, and are given in Ref. 6, and will be omitted here. Finally, the vectors of the continuous basis, satisfying Eq. (1.6), may be chosen to be

$$|k,+;p\rangle\to(1/\sqrt{\pi})\,r^{2ip-1}. \tag{1.12}$$

For the UIR D_k^-, we define the Hilbert space $\mathcal{H}(k,-)$ in exactly the same way as $\mathcal{H}(k,+)$, but choose the generators $J_\alpha(k,-)$ thus:

$$J_0(k,-)=-J_0(k,+),\quad J_1(k,-)=-J_1(k,+),\quad J_2(k,-)=J_2(k,+). \tag{1.13}$$

The action of the finite transformation $\exp(i\zeta J_2(k,+))$ is unaltered, while the kernels $L^{(k,+)}$ and $M^{(k,+)}$ are replaced by new ones, $L^{(k,-)}$ and $M^{(k,-)}$, which are actually easily obtained from the former. Finally, there is no change in the continuous basis vectors:

$$|k,-;p\rangle \to (1/\sqrt{\pi})r^{2ip-1}. \tag{1.14}$$

Some subtleties are involved in setting up the UIR's C_q^ϵ. Just as the spaces $\mathcal{H}(k,\pm)$ did not change with k, we now have a Hilbert space $\mathcal{H}(s,\epsilon)$ which actually does not change with s or ϵ. It consists of pairs of functions on the positive real line,

$$f=\begin{pmatrix} f_1(r)\\ f_2(r)\end{pmatrix},\quad 0\le r<\infty, \tag{1.15}$$

with the norm

$$\|f\|^2=\int_0^\infty r(|f_1(r)|^2+|f_2(r)|^2)\,dr<\infty. \tag{1.16}$$

The generators $J_\alpha(s,\epsilon)$ will be simultaneously differential operators in r and 2×2 matrices; *formally* there seems to be no dependence on ϵ and we have

$$J_0(s,\epsilon)=\frac{1}{4}\left(-r^2+\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}+\frac{4s^2}{r^2}\right)\otimes\sigma_3,$$

$$J_1(s,\epsilon)=\frac{1}{4}\left(r^2+\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}+\frac{4s^2}{r^2}\right)\otimes\sigma_3,$$

$$J_2(s,\epsilon)=\frac{-i}{2}\left(r\frac{d}{dr}+1\right)\otimes 1. \tag{1.17}$$

But the dependence on ϵ comes in through the delicate dependence of the domains of $J_{0,1}(s,\epsilon)$ on ϵ. In practice the value of ϵ will be clear from other considerations, whenever we come across a continuous class UIR. Another point is that the generators $J_\alpha(s,\epsilon)$ seem to be invariant when the phase of $f_2(r)$ in (1.15) is changed relative to $f_1(r)$; in other words, they would all appear to, but actually do not, commute with the operator σ_3, which would be absurd since we are dealing with an irreducible representation. Again this is a deficiency in trying to identify a UIR C_q^ϵ by merely looking at the formal expressions for the generators, but can be taken care of appropriately (see below). In Ref. 6 the kernels describing the nonlocal actions of $\exp[i\mu J_0(s,\epsilon)]$ and $\exp[i\nu J_1(s,\epsilon)]$ have been listed and the ϵ dependences made explicit. We have equations of the form

$$\{\exp[i\zeta J_2(s,\epsilon)]f\}_j(r)=\exp(\zeta/2)f_j[r\exp(\zeta/2)],$$

$$[\{\exp(i\mu J_0(s,\epsilon))\text{ or }\exp(i\nu J_1(s,\epsilon))\}f]_j=\sum_{k=1}^{2}\int_0^\infty dr'\,r'\times\{L_{jk}^{(s,\epsilon)}(r,r';\mu)\text{ or }M_{jk}^{(s,\epsilon)}(r,r';\nu)\}f_k(r'),\quad j=1,2, \tag{1.18}$$

and the 2×2 matrix functions L, M of r, r' arising here can be found in Ref. 6. The automorphism τ is now implemented by the operator A acting as follows:

$$A=\sigma_1:\ A\begin{pmatrix} f_1(r)\\ f_2(r)\end{pmatrix}=\begin{pmatrix} f_2(r)\\ f_1(r)\end{pmatrix}. \tag{1.19}$$

Therefore, once the value of ϵ has been fixed by other means, we may recognize a UIR of the type C_q^ϵ when we find the generators to be of the form in Eq. (1.17) [and of course the space they act on to be of the form of $\mathcal{H}(s,\epsilon)$] and in addition if we are either able to show that the finite transformations have the form (1.18) or that τ is implemented in the manner of Eq. (1.19). [This last point takes care of the problem posed by the *formal* commutability of $J_\alpha(s,\epsilon)$ and σ_3.] It is now easy to choose the simultaneous eigenvectors of $J_2(s,\epsilon)$ and A so that they obey Eq. (1.7):

$$|s,\epsilon;p,a\rangle=\frac{1}{\sqrt{2\pi}}\begin{pmatrix}1\\ a\end{pmatrix}r^{2ip-1},\quad a=\pm 1. \tag{1.20}$$

With this, we have specified the standard forms that we shall adopt for the UIR's of $SU(1,1)$.

2. THE SPECIAL REPRESENTATIONS $\mathcal{D}^\pm$, $\mathcal{C}$

As stated in the Introduction, an important role is played in our analysis of the Clebsch–Gordan problem for $SU(1,1)$ by three special unitary representations of this group. One of them acts as a generating representation or source for all the discrete positive UIR's, another for all the negative ones, and the third for all the continuous UIR's. We will describe the properties of $\mathcal{D}^+$ first, $\mathcal{D}^-$ next, and $\mathcal{C}$ last.

Introduce the Hilbert space $\mathcal{H}(+)$ consisting of complex valued functions square-integrable over the two-dimensional plane. Elements of $\mathcal{H}(+)$ are written $f(x_1,x_2)$, with the norm given by

$$\|f\|^2=\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2\,|f(x_1,x_2)|^2. \tag{2.1}$$

In this space, we can set up two independent oscillator operators a_j and their Hermitian conjugates a_j^+ obeying the standard commutation rules

$$[a_j,a_k^+]=\delta_{jk},\quad [a_j,a_k]=[a_j^+,a_k^+]=0,\quad j,k=1,2. \tag{2.2}$$

These operators could be expressed in terms of x_j and $\partial/\partial x_j$ by

$$a_j=\frac{-i}{\sqrt{2}}\left(x_j+\frac{\partial}{\partial x_j}\right),\quad a_j^+=\frac{i}{\sqrt{2}}\left(x_j-\frac{\partial}{\partial x_j}\right). \tag{2.3}$$

We now define three operators $J_\alpha(+)$ as functions of the oscillator operators via

$$J_0(+)=\tfrac{1}{2}(a_j^+a_j+1),\quad J_1(+)=\tfrac{1}{4}(a_j^+a_j^++a_ja_j),\quad J_2(+)=(-i/4)(a_j^+a_j^+-a_ja_j). \tag{2.4}$$

A summation over a repeated index is understood. It is easy to check that these operators obey the commutation rules of $SU(1,1)$. On the other hand, they are explicitly Hermitian, so they generate a unitary representation of $SU(1,1)$ in the space $\mathcal{H}(+)$. This, by definition, is the representation $\mathcal{D}^+$.[15] Since $J_0(+)$ is positive definite, $\mathcal{D}^+$ must be a direct sum of UIR's of type D_k^+ alone. We now analyze $\mathcal{D}^+$.

The basic commutation relations (2.2), as well as the generators $J_\alpha(+)$ of $\mathcal{D}^+$, are invariant under the group of all real orthogonal transformations in two dimensions, acting on the basic variables in the following manner:

$$x_j\to O_{jk}x_k,\quad a_j\to O_{jk}a_k,\quad a_j^+\to O_{jk}a_k^+,\quad O^TO=1 \tag{2.5}$$

We have, therefore, a unitary representation of this group acting in $\mathcal{H}(+)$ and all the operators of this representation commute with the representation $\mathcal{D}^+$ of $SU(1,1)$. The full group of the matrices $\|O_{jk}\|$ consists of the identity component containing the matrices

$$\begin{Vmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{Vmatrix}, \quad 0 \le \alpha < 2\pi \tag{2.6}$$

and the component containing the matrix

$$\begin{Vmatrix} 1 & 0 \\ 0 & -1 \end{Vmatrix} \tag{2.7}$$

corresponding to the discrete transformation $x_1 \to x_1$, $x_2 \to -x_2$. The unitary operators representing the elements (2.6) on $\mathcal{H}(+)$ are generated using the Hermitian operator M_{12} given by

$$M_{12} = i(a_1^\dagger a_2 - a_2^\dagger a_1). \tag{2.8}$$

Let the discrete transformation (2.7) be represented by the unitary operator B, i.e., B acts on a function $f(x_1, x_2)$ as

$$[Bf](x_1, x_2) = f(x_1, -x_2). \tag{2.9}$$

The complete set of algebraic relations involving the generators of $\mathcal{D}^+$ on the one hand, and its symmetry operators, on the other, is

$$[J_\alpha(+), M_{12}] = 0, \quad BJ_\alpha(+)B^{-1} = J_\alpha(+),$$
$$BM_{12} = -M_{12}B, \quad B^2 = 1. \tag{2.10}$$

Now the Casimir operator for $\mathcal{D}^+$ can be easily calculated, and it becomes a simple function of M_{12}:

$$Q = (J_1(+))^2 + (J_2(+))^2 - (J_0(+))^2 = \tfrac{1}{4}(1 - M_{12}^2) = K(1-K),$$
$$K = \tfrac{1}{2}(1 + |M_{12}|). \tag{2.11}$$

We are now in a position to express $\mathcal{D}^+$ as a direct sum of UIR's of $SU(1,1)$. Let us introduce in place of x_j the polar variables r, φ via

$$x_1 = r\cos\varphi, \quad x_2 = r\sin\varphi, \quad 0 \le r < \infty, \quad 0 \le \varphi < 2\pi, \tag{2.12}$$

so that M_{12} becomes the operator $i\,\partial/\partial\varphi$. Breaking up $\mathcal{H}(+)$ into eigenspaces of M_{12} is accomplished by the Fourier expansion of the φ dependence of a general function $f(x_1, x_2)$:

$$f(x_j) = f(r, \varphi) = \sum_{m=-\infty}^{\infty} f_m(r)\frac{\exp(-im\varphi)}{\sqrt{2\pi}} \tag{2.13}$$

The mth term here is an eigenfunction of M_{12} with eigenvalue m, and by definition it is the component of f in the eigenspace $\mathcal{H}_m(+)$:

$$\mathcal{H}(+) = \sum_{m=-\infty}^{\infty} \mathcal{H}_m(+), \quad f_m(r)\exp(-im\varphi) \in \mathcal{H}_m(+),$$

$$\|f\|^2 = \sum_{m=0,\pm1\cdots} \int_0^\infty r\,dr\,|f_m(r)|^2. \tag{2.14}$$

[For simplicity, the direct sum sign $\oplus$ is omitted here.] Since B and M_{12} anticommute, the action of B on the eigenspaces of M_{12} is evidently

$$B\mathcal{H}_m(+) = \mathcal{H}_{-m}(+). \tag{2.15}$$

Every subspace $\mathcal{H}_m(+)$ is invariant under the generators $J_\alpha(+)$, and so under the action of the representation $\mathcal{D}^+$ of $SU(1,1)$. For given m, $\mathcal{H}_m(+)$ has the same structure as the space $\mathcal{H}(k,+)$ set up in the last section [recall that $\mathcal{H}(k,+)$ actually has no dependence on k]. $\mathcal{H}_m(+)$ consists of functions $f(r)$ with the norm (1.8). Making use of (2.3, 2.4, 2.12), each $J_\alpha(+)$ restricted to $\mathcal{H}_m(+)$ becomes a differential operator in r alone; it is found that

$$J_\alpha(+)\,|\text{ restricted to } \mathcal{H}_m(+) = J_\alpha((1+|m|)/2, +); \tag{2.16}$$

the operators on the right are the ones set up in Eq. (1.9) in the course of defining the standard forms for the UIR's D_k^+. Putting together all these facts, we conclude that the two subspaces $\mathcal{H}_m(+)$ and $\mathcal{H}_{-m}(+)$ both support the same UIR $D^+_{(1+|m|)/2}$ of $SU(1,1)$, and we have the direct sum decomposition of $\mathcal{D}^+$:

$$\mathcal{D}^+ = \sum_{m=-\infty}^{\infty} D^+_{(1+|m|)/2}. \tag{2.17}$$

The discrete positive UIR $D^+_{1/2}$ appears once, and the UIR's D_k^+ for $k = 1, 3/2, \cdots$ twice each.

The generating representation $\mathcal{D}^-$ for the negative discrete series is obtained from the above by obvious modifications. The space $\mathcal{H}(-)$ is defined in the same way as $\mathcal{H}(+)$, and there is no change in the operators a_j, $a_j^\dagger$ either. The generators $J_\alpha(-)$ of $\mathcal{D}^-$ are taken to be the transforms under τ of $J_\alpha(+)$:

$$J_0(-) = -J_0(+), \quad J_1(-) = -J_1(+), \quad J_2(-) = J_2(+). \tag{2.18}$$

There is no change in the symmetry group, it is again generated by M_{12} and B. The Casimir operator Q for $\mathcal{D}^-$ has the same expression in terms of M_{12} as previously, and the eigenspaces $\mathcal{H}_m(-)$ of M_{12} are also unaltered from the previous discussion. The necessary equations describing $\mathcal{H}(-)$, $\mathcal{D}^-$, and $J_\alpha(-)$ are

$$\mathcal{H}(-) = \sum_{m=-\infty}^{\infty} \mathcal{H}_m(-), \quad B\mathcal{H}_m(-) = \mathcal{H}_{-m}(-),$$

$$J_\alpha(-)\,|\text{ restricted to } \mathcal{H}_m(-) = J_\alpha((1+|m|)/2, -),$$

$$\mathcal{D}^- = \sum_{m=-\infty}^{\infty} D^-_{(1+|m|)/2}. \tag{2.19}$$

The standard forms $J_\alpha(k,-)$ for the UIR D_k^- are given in Eq. (1.13). The discrete negative UIR $D^-_{1/2}$ occurs once in $\mathcal{D}^-$, the UIR's D_k^- for $k = 1, 3/2, \cdots$ twice each.

Now we turn to the representation $\mathcal{C}$. Here, in contrast to the previous cases, the symmetry group will be a pseudo-orthogonal group so it will be necessary to use a suitable metric operator that relates upper to lower indices and conversely. We take the space $\mathcal{H}(\mathcal{C})$ of the representation $\mathcal{C}$ to be the same as $\mathcal{H}(\pm)$, and also define a_j, $a_j^\dagger$ exactly as before. But the generators $J_\alpha(\mathcal{C})$ will be

$$J_0(\mathcal{C}) = \tfrac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2),$$
$$J_1(\mathcal{C}) = \tfrac{1}{4}((a_1^\dagger)^2 - (a_2^\dagger)^2 + (a_1)^2 - (a_2)^2),$$
$$J_2(\mathcal{C}) = (-i/4)((a_1^\dagger)^2 + (a_2^\dagger)^2 - (a_1)^2 - (a_2)^2). \tag{2.20}$$

These are of course Hermitian, and they do obey the $SU(1,1)$ commutation rules. To make the symmetries of the present construction as clear as the symmetries of $\mathcal{D}^\pm$ were, let us define new basic operators and a metric tensor thus:

$$b_1 = a_1, \quad b_1^\dagger = a_1^\dagger, \quad b_2 = -a_2^\dagger, \quad b_2^\dagger = -a_2, \tag{2.21a}$$

$$g_{11} = +1, \quad g_{22} = -1, \quad g_{12} = g_{21} = 0. \tag{2.21b}$$

Then the basic relations (2.2) can be rewritten as

$$[b_j, b_k^+]=g_{jk}, \quad [b_j, b_k]=[b_j^+, b_k^+]=0; \tag{2.22}$$

the realizations of b_j in terms of x_j and $\partial/\partial x_j$ become

$$b_j=(-i/\sqrt{2})(x_j+\partial_j), \quad b_j^+=(i/\sqrt{2})(x_j-\partial_j),$$
$$\partial_j \equiv \frac{\partial}{\partial x^j}\cdot \tag{2.23}$$

If in (2.20) we substitute b_j in place of a_j appropriately, we then find

$$J_0(\mathcal{C})=\tfrac{1}{2}(g^{jk}b_j^+b_k+1),$$
$$J_1(\mathcal{C})=\tfrac{1}{4}g^{jk}(b_j^+b_k^++b_jb_k),$$
$$J_2(\mathcal{C})=(-i/4)g^{jk}(b_j^+b_k^+-b_jb_k). \tag{2.24}$$

Equations (2.22), (2.24) must be compared with Eqs. (2.2), (2.4), respectively. We see immediately that the basic commutation relations (2.22) and the generators $J_\alpha(\mathcal{C})$ are all invariant under the group of all real linear transformations which preserve the indefinite quadratic form

$$g^{jk}x_jx_k=x_1^2-x_2^2. \tag{2.25}$$

We have therefore a unitary representation of this group acting in $\mathcal{H}(\mathcal{C})$, and all the operators of this representation commute with the representation $\mathcal{C}$ of $SU(1,1)$. The full group of these matrices $\|O_j^k\|$ consists now of four distinct components. The identity component contains all the matrices of the form

$$\left\|\begin{matrix}\cosh\alpha & \sinh\alpha\\ \sinh\alpha & \cosh\alpha\end{matrix}\right\|, \quad -\infty<\alpha<\infty; \tag{2.26}$$

the second component contains the matrix

$$\left\|\begin{matrix}-1 & 0\\ 0 & -1\end{matrix}\right\| \tag{2.27}$$

corresponding to the transformation $x_j\to -x_j$, and all products of this matrix with the matrices (2.26); the third component is similarly generated by the matrix

$$\left\|\begin{matrix}1 & 0\\ 0 & -1\end{matrix}\right\| \tag{2.28}$$

corresponding to the transformation $x_1\to x_1$, $x_2\to -x_2$; and the fourth and last component is generated by the product of the above two matrices. The unitary operators representing the elements of the identity component, on $\mathcal{H}(\mathcal{C})$, are built up using the Hermitian generator S_{12} defined as

$$S_{12}=i(b_1^+b_2-b_2^+b_1)=i(a_1a_2-a_1^+a_2^+). \tag{2.29}$$

Let us write P and B for the unitary operators representing the discrete elements (2.27), (2.28), respectively; B is the same as before [cf., Eq. (2.9)], while

$$[Pf](x_j)=f(-x_j). \tag{2.30}$$

Then the full symmetry of the representation $\mathcal{C}$ of $SU(1,1)$ is expressed by

$$[J_\alpha(\mathcal{C}),S_{12}]=0, \quad BJ_\alpha(\mathcal{C})B^{-1}=PJ_\alpha(\mathcal{C})P^{-1}=J_\alpha(\mathcal{C}),$$
$$BS_{12}=-S_{12}B, \quad PS_{12}=S_{12}P, \quad PB=BP, \quad P^2=B^2=1. \tag{2.31}$$

If we compute the Casimir operator Q for $\mathcal{C}$, it becomes a function of S_{12}:

$$Q=(J_1(\mathcal{C}))^2+(J_2(\mathcal{C}))^2-(J_0(\mathcal{C}))^2=\tfrac{1}{4}+\tfrac{1}{4}(S_{12})^2. \tag{2.32}$$

Having analyzed the algebraic structure of the set of operators that commute with the representation $\mathcal{C}$ of $SU(1,1)$, we can now express $\mathcal{C}$ as a direct integral of continuous class UIR's of $SU(1,1)$. [That only such UIR's will appear is clear from the form of Q in (2.32).] Since P and S_{12} commute, we can decompose $\mathcal{H}(\mathcal{C})$ into simultaneous eigenspaces of these operators. Then, as shown in Ref. 6, the eigenspace with a definite value for S_{12} and a definite value for P carries a single UIR C_q^ϵ of $SU(1,1)$: The eigenvalue of S_{12} fixes q via (2.32), and $P=+1$ gives $\epsilon=0$, $P=-1$ gives $\epsilon=1/2$.[16] To break up $\mathcal{H}(\mathcal{C})$ into these eigenspaces, we must change from the x_j to hyperbolic-type variables; this requires dividing the x_1-x_2 plane into four regions. The new variables r, η are introduced in each region in this way:

$$|x_2|>|x_1|: \quad x_2=(\text{sign of } x_2)r\cosh\eta,$$
$$x_1=(\text{sign of } x_2)r\sinh\eta, \quad 0\le r<\infty, \quad -\infty<\eta<\infty;$$
$$|x_1|>|x_2|: \quad x_1=(\text{sign of } x_1)r\cosh\eta,$$
$$x_2=(\text{sign of } x_1)r\sinh\eta, \quad 0\le r<\infty, \quad -\infty<\eta<\infty. \tag{2.33}$$

Let the eigenspaces of P be written $\mathcal{H}_+(\mathcal{C})$ and $\mathcal{H}_-(\mathcal{C})$; these are made up of functions, respectively, even and odd under $x_j\to -x_j$. We may write for a general $f\in\mathcal{H}(\mathcal{C})$

$$f(x_j)=f_+(x_j)+f_-(x_j), \quad f_\pm(-x_j)=\pm f_\pm(x_j),$$
$$\|f\|^2=\|f_+\|^2+\|f_-\|^2=\int_{-\infty}^{\infty}dx_1\int_{-\infty}^{\infty}dx_2\,(|f_+(x_j)|^2+|f_-(x_j)|^2). \tag{2.34}$$

Within an eigenspace of P, a function $f_\pm$ is fully determined by its values in the region $x_2>|x_1|$ (which is half of the region $|x_2|>|x_1|$), and in the region $x_1>|x_2|$ (which is half of the region $|x_1|>|x_2|$). Denote these functions by $f_{\pm1}(r,\eta)$ and $f_{\pm2}(r,\eta)$, respectively; the $\pm$ refers to the eigenvalue of P, the 1 and 2 to $x_2>|x_1|$, $x_1>|x_2|$, respectively. So after splitting a general function $f\in\mathcal{H}(\mathcal{C})$ into its components $f_\pm$ in $\mathcal{H}_\pm(\mathcal{C})$ each of these components may be represented as a column vector with two components:

$$f_\pm=\begin{pmatrix}f_{\pm1}(r,\eta)\\ f_{\pm2}(r,\eta)\end{pmatrix},$$
$$\|f_\pm\|^2=2\int_0^\infty r\,dr\int_{-\infty}^{\infty}d\eta\,(|f_{\pm1}(r,\eta)|^2+|f_{\pm2}(r,\eta)|^2). \tag{2.35}$$

In both $\mathcal{H}_+(\mathcal{C})$ and $\mathcal{H}_-(\mathcal{C})$, $S_{12}=-i\,\partial/\partial\eta$. Next, to diagonalize S_{12}, the η dependences of $f_{\pm1}(r,\eta)$, $f_{\pm2}(r,\eta)$ must be represented by Fourier integrals:

$$\begin{pmatrix}f_{\pm1}(r,\eta)\\ f_{\pm2}(r,\eta)\end{pmatrix}=\int_{-\infty}^{\infty}ds\,\frac{\exp(2is\eta)}{\sqrt{\pi}}\begin{pmatrix}f_{\pm1,s}(r)\\ f_{\pm2,s}(r)\end{pmatrix},$$
$$\|f_\pm\|^2=2\int_{-\infty}^{\infty}ds\int_0^\infty r\,dr\,(|f_{\pm1,s}(r)|^2+|f_{\pm2,s}(r)|^2). \tag{2.36}$$

The integrand here, namely the column vector

$$\exp(2is\eta)\begin{pmatrix}f_{\pm1,s}(r)\\ f_{\pm2,s}(r)\end{pmatrix}, \tag{2.37}$$

is an eigenfunction of P and S_{12} with eigenvalues ±1, $2s$, respectively; and by definition (2.37) is the component of f in the eigenspace $\mathcal{H}_{\pm,2s}(\mathcal{C})$. We can write $\mathcal{H}(\mathcal{C})$ as

$$\mathcal{H}(\mathcal{C})=\mathcal{H}_+(\mathcal{C})+\mathcal{H}_-(\mathcal{C}),$$
$$\mathcal{H}_\pm(\mathcal{C})=\int_{-\infty}^{\infty} ds\ \mathcal{H}_{\pm,s}(\mathcal{C}), \tag{2.38}$$

thereby exhibiting the breakup into the simultaneous eigenspaces of P and S_{12}. The action of B is clearly analogous to Eq. (2.15):

$$B\ \mathcal{H}_{\pm,2s}(\mathcal{C})=\mathcal{H}_{\pm,-2s}(\mathcal{C}). \tag{2.39}$$

And on $\mathcal{H}_{\pm,2s}(\mathcal{C})$, the Casimir invariant Q reduces by virtue of Eq. (2.32) to multiplication by $(\frac{1}{4}+s^2)$.

Each subspace $\mathcal{H}_{\pm,2s}(\mathcal{C})$ is invariant under action of $J_\alpha(\mathcal{C})$ and so under the representation $\mathcal{C}$ of $SU(1,1)$. For a fixed choice of s and eigenvalue of P, this subspace has the same structure as the space $\mathcal{H}(s',\epsilon)$ set up in the last section [recall that $\mathcal{H}(s',\epsilon)$ actually had no dependence on s',ϵ]; it consists of pairs of functions $\{f_1(r),f_2(r)\}$, with the norm (1.16). Making use of Eqs. (2.23), (2.24), (2.33), each $J_\alpha(\mathcal{C})$ restricted to $\mathcal{H}_{\pm,2s}(\mathcal{C})$ becomes a matrix-cum-differential operator in r alone; it is found that

$$J_\alpha(\mathcal{C})\big|\ \text{restricted to}\ \mathcal{H}_{\pm,2s}(\mathcal{C})=J_\alpha(|s|,\epsilon). \tag{2.40}$$

The operators on the right are the ones set up in Eq. (1.17) while defining the standard forms for the UIR's C_q^ϵ. Putting together all these facts, we see that the two subspaces $\mathcal{H}_{+,2s}(\mathcal{C})$ and $\mathcal{H}_{+,-2s}(\mathcal{C})$ both support the same UIR $C^0_{1/4+s^2}$ of $SU(1,1)$; while $\mathcal{H}_{-,2s}(\mathcal{C})$ and $\mathcal{H}_{-,-2s}(\mathcal{C})$ both support the same UIR $C^{1/2}_{1/4+s^2}$. We thus have the direct integral decomposition of the representation $\mathcal{C}$:

$$\mathcal{C}=\int_{-\infty}^{\infty} ds\ C^0_{1/4+s^2}+\int_{-\infty}^{\infty} ds\ C^{1/2}_{1/4+s^2} \tag{2.41}$$

Each UIR C_q^ϵ appears with a multiplicity two in $\mathcal{C}$.

For the continuous class UIR's of $SU(1,1)$, one must investigate how the outer automorphism τ is implemented. Given the generators $J_\alpha(\mathcal{C})$ for the reducible representation $\mathcal{C}$, it is easy to construct a unitary operator $\mathcal{A}$ on $\mathcal{H}(\mathcal{C})$ which has the effect of implementing the mapping τ. We just take

$$[\mathcal{A}f](x_1,x_2)=f(x_2,x_1). \tag{2.42}$$

Then, using Eq. (2.20) for instance, we see easily that

$$\mathcal{A}\,J_{0,1}(\mathcal{C})\mathcal{A}^{-1}=-J_{0,1}(\mathcal{C}),\quad \mathcal{A}\,J_2(\mathcal{C})\,\mathcal{A}^{-1}=J_2(\mathcal{C}). \tag{2.43}$$

But we see equally easily that $\mathcal{A}$ commutes with both the symmetry operators S_{12} and P, while with B we get

$$\mathcal{A}\,B\,\mathcal{A}^{-1}=PB. \tag{2.44}$$

So in any case, the subspaces $\mathcal{H}_{\pm,2s}(\mathcal{C})$ are invariant under $\mathcal{A}$, and, in fact, if an element in $\mathcal{H}_{\pm,2s}(\mathcal{C})$ is written in the column vector form (2.37), $\mathcal{A}$ has the desired effect of interchanging upper and lower components. Thus, $\mathcal{A}$ leaves each UIR in the direct integral decomposition of $\mathcal{C}$ invariant, and within each UIR it has the form of the operator $\mathcal{A}$ of Eq. (1.19).[17] All these properties of the representation $\mathcal{C}$ will be needed when we consider the direct products of the form $D^+\otimes C$, $C\otimes C$.

The description of the representations $\mathcal{D}^\pm$, $\mathcal{C}$ that we have given overlaps partly with the work of Ref. 6; however, we have emphasized here the role of the symmetries of these constructions in performing the direct sum decomposition into irreducibles. It would be fairly evident by now how the two-dimensional rotational symmetries of $\mathcal{D}^\pm$, $\mathcal{C}$ get enlarged to four-dimensional ones when direct products like $\mathcal{D}^+\otimes\mathcal{D}^+$, $\mathcal{D}^+\otimes\mathcal{D}^-$, etc., are considered. We conclude this section by recalling the structures of the various Clebsch—Gordan series, and making some comments on them. Omitting the direct sum $\oplus$ symbol, the four essentially distinct series have these forms:

$$\text{(I)}\quad D_k^+\otimes D_{k'}^+=\sum_{k''=k+k',\,k+k'+1,\cdots} D^+_{k''},$$
$$k,k'=\tfrac{1}{2},1,\tfrac{3}{2},\cdots,$$

$$\text{(II)}\quad D_k^+\otimes D_{k'}^-=\theta(k-k'-1)\sum_{k''\geq 1\ \text{or}\ 3/2}^{k-k'} D^+_{k''}+\theta(k'-k-1)\sum_{k''\geq 1\ \text{or}\ 3/2}^{k'-k} D^-_{k''}+\int_0^\infty ds\ C^\epsilon_{1/4+s^2},$$

$k,k'=\frac{1}{2},1,\frac{3}{2},\cdots$, $\epsilon=0(\frac{1}{2})$ and $k''_{\min}=1(\frac{3}{2})$ if $k+k'=$ integer (half-odd integer);

$$\text{(III)}\quad D_k^+\otimes C^\epsilon_{1/4+s^2}=\sum_{k''\geq 1\ \text{or}\ 3/2}^{\infty} D^+_{k''}+\int_0^\infty ds'\ C^{\epsilon'}_{1/4+s'^2},$$

$k=\frac{1}{2},1,\cdots$, $\epsilon=0,\frac{1}{2}$, $0<s<\infty$, $\epsilon'=0(\frac{1}{2})$ and $k''_{\min}=1(\frac{3}{2})$ if $k+\epsilon=$ integer (half-odd integer);

$$\text{(IV)}\quad C^\epsilon_{1/4+s^2}\otimes C^{\epsilon'}_{1/4+s'^2}=\sum_{k''\geq 1\ \text{or}\ 3/2}^{\infty} D^+_{k''}+\sum_{k''\geq 1\ \text{or}\ 3/2}^{\infty} D^-_{k''}+2\int_0^\infty ds''\ C^{\epsilon''}_{1/4+s''^2},$$

$\epsilon,\epsilon'=0,\frac{1}{2}$, $0<s,s'<\infty$, $\epsilon''=0(\frac{1}{2})$ and $k''_{\min}=1(\frac{3}{2})$ if $\epsilon+\epsilon'=$ integer (half-odd integer).

Wherever there is a sum on k'', it is from a minimum to a maximum value in integer steps. The step function θ used in case (II) is defined thus: $\theta(x)=1$ for $x=0,\frac{1}{2},1,\frac{3}{2},\cdots$, and $=0$ for $x=-\frac{1}{2},-1,-\frac{3}{2},\cdots$. In cases I and III if on both sides of the given equations every D^+ is changed into a D^-, the resulting equations remain true. Now a very interesting aspect of these Clebsch—Gordan series is this: If we consider the direct product of any two UIR's of $SU(1,1)$, neither of which belongs to the continuous exceptional series, then in the decomposition of the product into UIR's the particular discrete terms $D^\pm_{1/2}$ will never make an appearance. It is well known that $D^\pm_{1/2}$ are to be distinguished from $D^\pm_k$ for $k\geq 1$ and C_q^ϵ for $q\geq\frac{1}{4}$ in another sense; in the regular representation of $SU(1,1)$, only the latter are present, both $D^\pm_{1/2}$ and the continuous exceptional UIR's are absent. We will show in papers II and IV of this sequence that it is the structure of the Plancherel formula of $SU(1,1)$ that is responsible for the absence of $D^\pm_{1/2}$ in the Clebsch—Gordan series (II) and (IV) above; the reason in the case of series (III) turns out to be a property of a particular representation of the group $O(3,1)$, as will be explained in paper III. The point to be noticed is the absence of $D^\pm_{1/2}$ in the decomposition of even those products in which one (or both) factors may itself be $D^\pm_{1/2}$. Another point to be noted is that in no series does the trivial identity representation of $SU(1,1)$ appear as a discrete summand.

3. C-G SERIES FOR THE PRODUCT $D^+ \times D^+$

Let us now take two representations of $SU(1,1)$ of the type $\mathcal{D}^+$, each in a space of the form $\mathcal{H}(+)$, and consider their direct product $\mathcal{D}^+\otimes\mathcal{D}^+$. The space of the total representation will be $\mathcal{H}=\mathcal{H}(+)\otimes\mathcal{H}(+)$, the variables of the first factor in the product will be numbered 1, 2, those of the second 3, 4. $\mathcal{H}$ then consists of functions $f(x_1,x_2,x_3,x_4)$ with

$$\|f\|^2=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dx_1\,dx_2\,dx_3\,dx_4\,|f(x_1,x_2,x_3,x_4)|^2. \tag{3.1}$$

We will use Greek subscripts $\mu,\nu,\cdots$ to go over the four values 1, 2, 3, 4; no metric tensor is needed since we will be dealing with the group $O(4)$. The four oscillator operators defined on $\mathcal{H}$ fulfill

$$[a_\mu,a_\nu^+]=\delta_{\mu\nu},\quad [a_\mu,a_\nu]=[a_\mu^+,a_\nu^+]=0,$$
$$a_\mu=(-i/\sqrt{2})(x_\mu+\partial_\mu),\quad a_\mu^+=(i/\sqrt{2})(x_\mu-\partial_\mu). \tag{3.2}$$

The generators of the first factor in the product $\mathcal{D}^+\otimes\mathcal{D}^+$ will involve just the variables numbered 1, 2 and will have the forms given in Eq. (2.4); we will write $J_\alpha(+,12)$ for them. Similarly, the generators of the second factor in the product are $J_\alpha(+,34)$ and the "total" generators for the product $\mathcal{D}^+\otimes\mathcal{D}^+$ will be

$$J_\alpha=J_\alpha(+,12)+J_\alpha(+,34). \tag{3.3}$$

We can express the J_α in terms of the a_μ, and then we find

$$J_0=\tfrac{1}{2}(a_\mu^+a_\mu+2),\quad J_1=\tfrac{1}{4}(a_\mu^+a_\mu^++a_\mu a_\mu),\quad J_2=(-i/4)(a_\mu^+a_\mu^+-a_\mu a_\mu). \tag{3.4}$$

In the summations over the repeated index μ, all four values are involved. We see immediately on inspection of Eqs. (3.2) and (3.4) that the basic commutation relations as well as the "total" generators J_α are invariant when the basic variables are subjected to any real linear orthogonal transformation in four dimensions:

$$x_\mu\to O_{\mu\nu}x_\nu,\quad a_\mu\to O_{\mu\nu}a_\nu,\quad a_\mu^+\to O_{\mu\nu}a_\nu^+,\quad O^TO=1. \tag{3.5}$$

These matrices constitute the full rotation group $O(4)$, and there is therefore a unitary representation of this group acting on $\mathcal{H}$, such that the corresponding unitary operators all commute with the operators of the representation $\mathcal{D}^+\otimes\mathcal{D}^+$ of $SU(1,1)$ which also acts on $\mathcal{H}$. For the present, it is enough to consider just the identity component of $O(4)$; its representation on $\mathcal{H}$ is clearly generated by the six generators

$$M_{\mu\nu}=i(a_\mu^+a_\nu-a_\nu^+a_\mu)=i(x_\mu\partial_\nu-x_\nu\partial_\mu). \tag{3.6}$$

[The $M_{\mu\nu}$ obey among themselves the $O(4)$ commutation relations.] The symmetry properties of the $SU(1,1)$ generators J_α are thus expressed by

$$[J_\alpha,M_{\mu\nu}]=0. \tag{3.7}$$

For the individual sets $J_\alpha(+,12)$ and $J_\alpha(+,34)$ we have only

$$[J_\alpha(+,12)\text{ or }J_\alpha(+,34),\,M_{12}\text{ or }M_{34}]=0. \tag{3.8}$$

[The discrete symmetries are not needed, as mentioned above.]

Let us establish next the connections between the various Casimir operators. For $SU(1,1)$, we have the Casimir operators Q_{12}, Q_{34} for the individual factors in the product $\mathcal{D}^+\otimes\mathcal{D}^+$, and then Q for the total. The first two are related to M_{12}, M_{34} via Eq. (2.11). There are two Casimir operators associated with the Lie algebra of the group $O(4)$, namely $M^2=M_{\mu\nu}M_{\mu\nu}$ and $\epsilon_{\mu\nu\lambda\sigma}M_{\mu\nu}M_{\lambda\sigma}$; but the particular form (3.6) of $M_{\mu\nu}$ that occurs in the present realization of $O(4)$ makes the second invariant vanish identically. This of course has the effect of restricting the types of UIR's of $O(4)$ appearing in $\mathcal{H}$.[18] Q can be now shown to essentially coincide with the nontrivial Casimir operator of $O(4)$. All in all, we have

$$Q_{12}=\tfrac{1}{4}(1-M_{12}^2),\quad Q_{34}=\tfrac{1}{4}(1-M_{34}^2),$$
$$Q=(J_1)^2+(J_2)^2-(J_0)^2=-\tfrac{1}{8}M_{\mu\nu}M_{\mu\nu}=-\tfrac{1}{8}M^2. \tag{3.9}$$

The direct product $\mathcal{D}^+\otimes\mathcal{D}^+$ contains within it the individual products of the form $D_k^+\otimes D_{k'}^+$ for all values of k and k'. We want to get at the C–G series for the latter, and then compute the C–G coefficients in the continuous basis. It is then clear that we must construct two types of bases for $\mathcal{H}$, an uncoupled basis and a coupled basis. In the uncoupled basis, we want the operators M_{12}, M_{34} (hence Q_{12}, Q_{34}), $J_2(+,12)$ and $J_2(+,34)$ to be simultaneously diagonal. Such basis vectors are direct products of basis vectors drawn one from each factor in a product of the form $D_k^+\otimes D_{k'}^+$. In the coupled basis, the simultaneously diagonal operators should be M_{12}, M_{34} (hence Q_{12}, Q_{34}), J_2 and M^2 (hence Q). By having M_{12} and M_{34} diagonal in both bases, we will be sure we are dealing with a single product $D_k^+\otimes D_{k'}^+$ and its reduction. The coupled basis vectors will belong to definite UIR's of the total $SU(1,1)$; at the same time they will be basis vectors for the UIR's of $O(4)$ in a definite form, namely a form in which M^2, M_{12} and M_{34} are diagonal. The point is that UIR's of $O(4)$ can be built up in more than one way, either "diagonalizing" a canonical $O(3)$ subgroup, or an $O(2)\otimes O(2)$ subgroup; what is needed here is the latter. By examining the allowed eigenvalues of M^2 while keeping those of M_{12} and M_{34} fixed, in a coupled basis vector, we will be able to read off the C–G series for a product $D_k^+\otimes D_{k'}^+$; by calculating the overlap between an uncoupled and a coupled basis vector, we will obtain the C–G coefficients.

In the place of the x_μ, let us introduce radial and angular variables by

$$x_1=r\cos(\beta/2)\cos\varphi,\quad x_2=r\cos(\beta/2)\sin\varphi,$$
$$x_3=r\sin(\beta/2)\cos\psi,\quad x_4=r\sin(\beta/2)\sin\psi,$$
$$0\le r<\infty,\ 0\le\beta\le\pi,\ 0\le\varphi,\ \psi\le 2\pi,$$
$$dx_1dx_2dx_3dx_4\equiv\tfrac{1}{4}r^3\,dr\,d\cos\beta\,d\varphi\,d\psi. \tag{3.10}$$

Then $M_{12}=i\,\partial/\partial\varphi$ and $M_{34}=i\,\partial/\partial\psi$. To pick up $D_k^+\otimes D_{k'}^+$, we choose (nonnegative) eigenvalues $(2k-1)$, $(2k'-1)$ for M_{12}, M_{34}, respectively. Then combining Eq. (1.12) with the analysis of the representation $\mathcal{D}^+$ given in Sec. 2, we can write the uncoupled basis vector Φ:

$$\Phi^{(k,+)\,(k',+)}_{p\qquad p'}=(1/\sqrt{\pi})\,(r\cos\beta/2)^{2ip-1}(1/\sqrt{2\pi})\,e^{-i(2k-1)\varphi}$$
$$\times(1/\sqrt{\pi})\,(r\sin\beta/2)^{2ip'-1}(1/\sqrt{2\pi})\,e^{-i(2k'-1)\psi},$$

$$M_{12}=2k-1,\quad M_{34}=2k'-1,\quad J_2(+,12)=p,\quad J_2(+,34)=p'. \tag{3.11}$$

This is normalized to a Kronecker delta in k as well as in k', and to a Dirac delta in p as well as in p'. [See Eq. (4.4).] Before putting down a coupled basis vector Ψ, we need to know the eigenfunctions of M^2, as well as what the generators J_α of $SU(1,1)$ look like when restricted to an eigenspace of M_{12}, M_{34}, and M^2. The $O(4)$ group has, locally, the same structure as $O(3)\otimes O(3)$, so we can split $M_{\mu\nu}$ into two independent (i.e., commuting) $O(3)$ Lie algebras. Let us call these L and R. We define them as

$$L_1=\tfrac{1}{2}(M_{32}+M_{14}),\quad L_2=\tfrac{1}{2}(M_{13}+M_{24}),\quad L_3=\tfrac{1}{2}(M_{21}+M_{34}),$$
$$R_1=\tfrac{1}{2}(M_{32}-M_{14}),\quad R_2=\tfrac{1}{2}(M_{13}-M_{24}),\quad R_3=\tfrac{1}{2}(M_{21}-M_{34}). \tag{3.12}$$

The $O(4)$-commutation relations among the $M_{\mu\nu}$ now appear as

$$[L_j,L_k]=i\epsilon_{jkl}L_l,\quad [R_j,R_k]=i\epsilon_{jkl}R_l,$$
$$[L_j,R_k]=0,\quad j,k,l=1,2,3. \tag{3.13}$$

The vanishing of the second Casimir operator of $O(4)$ implies that these two commuting $O(3)$ Lie algebras have the same Casimir operator; and this is essentially M^2. We find quite easily that

$$L^2=L_jL_j=R^2=R_jR_j=\tfrac{1}{8}M^2$$
$$=-\frac{\partial^2}{\partial\beta^2}-\cot\beta\frac{\partial}{\partial\beta}-\frac{1}{\sin^2\beta}\left(\frac{\partial^2}{\partial(\varphi+\psi)^2}+\frac{\partial^2}{\partial(\varphi-\psi)^2}-2\cos\beta\frac{\partial^2}{\partial(\varphi+\psi)\partial(\varphi-\psi)}\right).$$

For an eigenfunction of M_{12}, M_{34}, and M^2, the φ and ψ dependences are as in Eq. (3.11), while the β dependence is to be obtained by solving the eigenvalue equation for the differential operator above. The solutions to this equation are well known; they are the D functions of angular momentum theory.[19] This should be no surprise because these D functions are known to be the "spherical harmonics" on the unit sphere in four-dimensional Euclidean space. All in all, an eigenfunction of M_{12}, M_{34} and $Q=\frac{-1}{8}M^2$ with eigenvalues $2k-1$, $2k'-1$, and $k''(1-k'')$, respectively, turns out to be of the form

$$\frac{\exp[-i(2k-1)\varphi]}{\sqrt{2\pi}}\,\frac{\exp[-i(2k'-1)\psi]}{\sqrt{2\pi}}\left(\frac{2k''-1}{2}\right)^{1/2}\times d^{(k''-1)}_{k+k'-1,k-k'}(\beta)f(r) \tag{3.15}$$

and its norm is

$$\tfrac{1}{4}\int_0^\infty r^3dr\,|f(r)|^2. \tag{3.16}$$

In other words, the eigenspace of M_{12}, M_{34}, and M^2 with the stated eigenvalues consists of all functions (3.15) with the norm (3.16). Apart from the change in measure from $r\,dr$ to $\frac{1}{4}r^3dr$, such an eigenspace is seen to have the same form as the standard space $\mathcal{H}(k,+)$ in which the UIR D_k^+ was set up in Sec. 1. The next point is the form of J_α when restricted to this eigenspace. Apart from a similarity transformation to compensate for the changed measure, this form should be the standard one in Eq. (1.9). First we check that all dependence of J_α on the angular variables β, φ, ψ can be isolated in M^2 as we would expect; for J_0, for example, the steps are

$$J_0=1+\tfrac{1}{2}a_\mu^+a_\mu=\tfrac{1}{4}(x_\mu x_\mu-\partial_\mu\partial_\mu)=\tfrac{1}{4}(r^2-\Box^2),$$
$$\Box^2=\frac{1}{r^2}\left(x\cdot\partial\, x\cdot\partial+2x\cdot\partial-\frac{M^2}{2}\right),\quad x\cdot\partial=x_\mu\partial_\mu=r\frac{\partial}{\partial r},$$
$$J_0=\frac{1}{4}\left(-\frac{\partial^2}{\partial r^2}-\frac{3}{r}\frac{\partial}{\partial r}+r^2-\frac{4Q}{r^2}\right). \tag{3.17}$$

In a similar fashion, one can see that all the angular dependence of J_1 also can be isolated in M^2, while J_2 is already a purely "radial" operator.[20] Restriction of J_α to the subspace on which $Q=k''(1-k'')$ involves just substituting this value of Q in J_α; by following this with a suitable similarity transformation, we finally get

$$rJ_\alpha r^{-1}\mid Q=k''(1-k'')=J_\alpha(k'',+), \tag{3.18}$$

the operators on the right being given in Eq. (1.9). A further restriction to definite eigenvalues for M_{12} and M_{34} has no effect on Eq. (3 18).

The use of the $O(4)$ symmetry of the representation $\mathcal{D}^+\otimes\mathcal{D}^+$ of $SU(1,1)$ is now clear. The C–G series for $D_k^+\otimes D_{k'}^+$ is given by a knowledge of the possible eigenvalues of M^2 given those of M_{12} and M_{34}; in other words, it is determined by the knowledge of $O(4)$ spherical harmonics in the $O(2)\otimes O(2)$ basis. Since these $O(4)$ harmonics are just the D functions of angular momentum theory, we know by reference to Eq. (3.15) that the superscript on the d function must be greater than or equal to the magnitude of each subscript. Since any way both k and k' are $\geq\frac{1}{2}$, the C–G series for case (I) given in the previous section is now understood. Of course in the present case involving $D^+\otimes D^+$ there are more elementary ways of arriving at the C–G series, but our aim is to relate it to the $O(4)$ structure since this will generalize to all other cases. Next we have seen that if we split $\mathcal{H}$ into the eigenspaces of the "total" $SU(1,1)$ Casimir operator Q with various eigenvalues $k''(1-k'')$, then the restrictions of J_α to these eigenspaces are just the standard forms $J_\alpha(k'',+)$ developed in Sec. I (apart from a similarity transformation!). In a given eigenspace of Q, corresponding to some k'', the UIR $D_{k''}^+$ will appear many times, corresponding to the various possible products $D_k^+\otimes D_{k'}^+$ from which it could have originated. By next fixing the eigenvalues of M_{12} and M_{34} at $2k-1$, $2k'-1$, respectively, we pick up the UIR $D_{k''}^+$ contained in the particular product $D_k^+\otimes D_{k'}^+$. All these steps, suitably modified, will occur in the other types of direct products as well.

We conclude this section by writing down the coupled basis vector Ψ, whose construction is obvious by now. It is of the form (3.15), except that the "radial" dependence is determined by the eigenvalue of J_2:

$$\Psi^{(k,+)(k',+)(k'',+)}_{p''}=\frac{\exp[-i(2k-1)\varphi]}{\sqrt{2\pi}}\,\frac{\exp[-i(2k'-1)]\psi}{\sqrt{2\pi}}\times\left(\frac{2k''-1}{2}\right)^{1/2}\times d^{(k''-1)}_{k+k'-1,k-k'}(\beta)(2/\sqrt{\pi})\,r^{2ip''-2},$$

$$M_{12}=2k-1,\quad M_{34}=2k'-1,\quad Q=-\tfrac{1}{8}M^2=k''(1-k''),$$
$$J_2=p''. \tag{3.19}$$

This is normalized to Kronecker deltas in k, k', and k'', and to a Dirac delta in p'' [see Eq. (4.5)].

4. C-G COEFFICIENTS IN THE CONTINUOUS BASIS

In this section we will first set up a suitable notation for the $SU(1,1)$ Clebsch–Gordan coefficients in a continuous basis. Let us use the generic symbol $\mathcal{R}$ to denote any UIR of $SU(1,1)$ of interest, it could be either (k,η) or (s,ϵ). According to Eqs. (1.6), (1.14), (1.20), the vectors of the continuous basis in $\mathcal{R}$ can be written as

$$|\mathcal{R};p,a\rangle,\quad -\infty<p<\infty,\quad a=\pm; \tag{4.1}$$

p is the eigenvalue of $J_2(\mathcal{R})$; if $\mathcal{R}=(k,\eta)$, the additional label a is to be dropped, while if $\mathcal{R}=(s,\epsilon)$, it is to be retained and is the eigenvalue of the unitary operator A implementing the outer automorphism τ in $\mathcal{R}$. A glance at the four C–G series listed in Sec. 2 shows that there is one case, namely case (IV), in which the reduction of a direct product $\mathcal{R}\otimes\mathcal{R}'$ into a direct sum (integral) over various $\mathcal{R}''$ involves a multiplicity problem. A given UIR $\mathcal{R}''$ may occur twice in the reduction. Bearing this in mind, and also notation for basis states given in Eq. (4.1), it is easy to see that an adequate and unambiguous way of writing down a C–G coefficient in the continuous basis for the reduction of $\mathcal{R}\otimes\mathcal{R}'$ is this:

$$C(\mathcal{R}\mathcal{R}'\mathcal{R}''\gamma\,|\,pa\,p'b\,p''c); \tag{4.2}$$

pa are state labels within $\mathcal{R}$, $p'b$ within $\mathcal{R}'$, and $p''c$ within $\mathcal{R}''$. γ is the multiplicity label that distinguishes the two (possible) occurrences of $\mathcal{R}''$ in a given product $\mathcal{R}\otimes\mathcal{R}'$: It is needed only when all three UIR's are of continuous type. This C–G coefficient is to be computed as the scalar product between an uncoupled basis vector Φ and a coupled one, Ψ. In all our calculations, many distinct direct products are present at the same time in one large Hilbert space $\mathcal{H}$; we have seen this in the previous section. Now especially when the constituent UIR's $\mathcal{R}$ and $\mathcal{R}'$ involve one (or more) continuous class representations, one must be rather careful in relating a C–G coefficient to a scalar product of the form (Φ,Ψ). Let us first define the symbol $\delta(\mathcal{R}',\mathcal{R})$:

$$\begin{aligned}\delta(\mathcal{R}',\mathcal{R})&=\delta_{k'k}\,\delta_{\eta'\eta}\ \text{ if } \mathcal{R}=(k,\eta),\ \mathcal{R}'=(k',\eta'),\\ &=\delta_{\epsilon'\epsilon}\,\delta(s'-s)\ \text{ if } \mathcal{R}=(s,\epsilon),\ \mathcal{R}'=(s',\epsilon')\\ &=0 \text{ otherwise.}\end{aligned} \tag{4.3}$$

Whenever we construct uncoupled basis vectors Φ like that appearing in Eq. (3.11), they will obey the orthonormality condition

$$(\Phi^{\mathcal{R}''\ \mathcal{R}'''}_{p''c\ p'''d},\ \Phi^{\mathcal{R}\mathcal{R}'}_{pa\ p'b})=\delta(\mathcal{R}'',\mathcal{R})\,\delta(\mathcal{R}''',\mathcal{R}')\times\delta(p''-p)\delta(p'''-p')\,\delta_{ca}\,\delta_{db}. \tag{4.4}$$

Similarly, when we construct coupled vectors Ψ, they will obey

$$(\Psi^{\mathcal{R}''\mathcal{R}'''\ \mathcal{R}_2\gamma_2}_{p'b},\ \Psi^{\mathcal{R}\mathcal{R}'\ \mathcal{R}_1\gamma_1}_{pa})=\delta(\mathcal{R}'',\mathcal{R})\,\delta(\mathcal{R}''',\mathcal{R}')\times\delta(\mathcal{R}_2,\mathcal{R}_1)\,\delta_{\gamma_2\gamma_1}\,\delta(p'-p)\,\delta_{ba}. \tag{4.5}$$

The point we want to draw attention to is the presence of the first two delta functions on the right-hand sides of Eqs. (4.4) and (4.5), namely those involving the constituent UIR's in a direct product.[21] They are present because of the particular way we have solved the Clebsch–Gordan problem, namely dealing with all products of a given type (say $D^+\otimes D^+$) at once. The other factors on the right-hand sides of Eqs. (4.4) and (4.5) are standard and would be present in any treatment of the problem. For products of the type $D^+\otimes D^+$ or $D^+\otimes D^-$ the factors $\delta(\mathcal{R}'',\mathcal{R})\,\delta(\mathcal{R}''',\mathcal{R}')$ are quite harmless since they are finite; we can in fact choose $\mathcal{R}''=\mathcal{R}$ and $\mathcal{R}'''=\mathcal{R}'$ throughout. Keeping these facts in mind, we relate the C–G coefficient (4.2) to basis vectors Φ, Ψ in this way:

$$\left(\Phi^{\mathcal{R}_1\mathcal{R}'_1}_{pa\ p'b},\ \Psi^{\mathcal{R}\mathcal{R}'\ \mathcal{R}''\gamma}_{p''c}\right)=\delta(\mathcal{R}_1,\mathcal{R})\,\delta(\mathcal{R}'_1,\mathcal{R}')\times C(\mathcal{R}\mathcal{R}'\mathcal{R}''\gamma\,|\,pa\,p'b\,p''c). \tag{4.6}$$

Once the C–G coefficients have been extracted from the scalar products in this way, they become independent of the specific method we have used to handle the problem.

Conservation of J_2 implies that in the general C–G coefficient (4.2) there will always be a factor $\delta(p+p'-p'')$. So let us set

$$C(\mathcal{R}\mathcal{R}'\mathcal{R}''\gamma\,|\,pa\,p'b\,p''c)=\delta(p+p'-p'')\,\hat{C}(\mathcal{R}\mathcal{R}'\mathcal{R}''\gamma\,|\,pa\,p'b\,c) \tag{4.7}$$

Generally, only the values of $\hat{C}$ will be listed.

Since the orthonormality conditions for Φ and Ψ are specified in Eqs. (4.4) and (4.5), there are no ambiguities in writing down the orthogonality and completeness properties for the C–G coefficients. But we will omit the details. The notation and conventions set up above will be adequate to handle all the direct products we will treat. The multiplicity index γ will be relevant only in paper IV for the products $C\otimes C$, and its choice will be explained there. For the present we may drop it as well as the indices a, b, c.

The basis vectors given in Eqs. (3.11) and (3.19) have been constructed in accordance with the conditions in Eqs. (4.4) and (4.5). The C–G coefficient in a continuous basis, for the product $D^+_k\otimes D^+_{k'}\to D^+_{k''}$, can therefore be written as

$$\begin{aligned}C(k+\ k'+\ k''+\,|\,p\ p'\ p'')&=(\Phi^{(k+)\ (k'+)}_{p\ \ \ p'},\ \Psi^{(k+)(k'+)\ (k''+)}_{p''})\\ &=\left(\frac{2k''-1}{2\pi}\right)^{1/2}\delta(p+p'-p'')\int_0^{\pi}d\beta\left(\cos\frac{\beta}{2}\right)^{-2ip}\left(\sin\frac{\beta}{2}\right)^{-2ip'}\\ &\quad d^{(k''-1)}_{k+k'-1,\,k-k'}(\beta).\end{aligned} \tag{4.8}$$

The simple integrations over r, φ, and ψ have been carried out; the first of these produces the factor $\delta(p+p'-p'')$. In the evaluation of the β integral, let us for ease in writing set $j=k''-1$, $m=k+k'-1\geq n=k-k'$. We can use the formula[22] (valid for $m\geq n$)

$$d^{\,j}_{mn}(\beta)=\left(\frac{(j+m)!\,(j-n)!}{(j-m)!\,(j+n)!}\right)^{1/2}\frac{(\cos\beta/2)^{-m-n}(-\sin\beta/2)^{m-n}}{(m-n)!}\times{}_2F_1(j-n+1,\ -j-n;\ m-n+1;\ \sin^2\beta/2). \tag{4.9}$$

Substituting $t=\sin^2\beta/2$, we are in need of

$$\int_0^\pi d\beta \left(\cos\frac{\beta}{2}\right)^{-2ip}\left(\sin\frac{\beta}{2}\right)^{-2ip'} d^j_{mn}(\beta)$$

$$=\frac{(-1)^{m-n}}{(m-n)!}\left(\frac{(j+m)!(j-n)!}{(j-m)!(j+n)!}\right)^{1/2}\int_0^1 dt\; t^{-ip'+(m-n-1)/2}$$

$$\times(1-t)^{-ip-(m+n+1)/2}\,{}_2F_1(j-n+1,-j-n;\,m-n+1;t). \tag{4.10}$$

This can be evaluated using a formula that expresses an integral involving a generalized hypergeometric function of type ${}_pF_q$ in terms of ${}_{p+1}F_{q+1}$[23]; the t integral appearing on the right-hand side of (4.10) then has the value

$$[\Gamma(\tfrac{1}{2}(m-n+1)-ip')\,\Gamma(-\tfrac{1}{2}(m+n-1)-ip)/\Gamma(1-n-i(p+p'))]$$

$$\times{}_3F_2\left(\begin{matrix}j-n+1,-j-n,\tfrac{1}{2}(m-n+1)-ip';\\ m-n+1,1-n-i(p+p');\end{matrix}\;1\right).$$

Putting in the values of j, m, and n, and omitting the δ function present on the right-hand side in Eq. (4.8), we obtain the final form for $\hat{C}$ for the product $D^+_k\otimes D^+_{k'}\to D^+_{k''}$:

$$\hat{C}(k+k'+k''+|p\,p')=\frac{(-1)^{2k'-1}}{(2k'-1)!}\left(\frac{2k''-1}{2\pi}\right)^{1/2}$$

$$\times\left(\frac{(k'+k''+k-2)!(k'+k''-k-1)!}{(k''-k-k')!(k+k''-k'-1)!}\right)^{1/2}$$

$$\times\left(\frac{\Gamma(k'-ip')\,\Gamma(1-k-ip)}{\Gamma(k'+1-k-ip-ip')}\right)$$

$$\times{}_3F_2\left(\begin{matrix}k'+k''-k,k'+1-k-k'',k'-ip';\\ 2k',k'+1-k-ip-ip';\end{matrix}\;1\right). \tag{4.11}$$

5. C-G COEFFICIENTS FOR $D^-\times D^-$

The C—G series and C—G coefficients for the products $D^-\otimes D^-$ and $D^-\otimes C$ can be related to those for $D^+\otimes D^+$ and $D^+\otimes C$, respectively, by using the outer automorphism τ. In general, $\tau(\mathcal{R})$ will denote the UIR of $SU(1,1)$ that is obtained by acting on $\mathcal{R}$ with τ. So $\tau((k,\eta))=(k,-\eta)$ and $\tau((s,\epsilon))=(s,\epsilon)$. If we have the relation

$$\mathcal{R}\otimes\mathcal{R}'=\sum\mathcal{R}'', \tag{5.1}$$

certain special "values" of $\mathcal{R}''$ appearing on the right with corresponding multiplicities, then the relation

$$\tau(\mathcal{R})\otimes\tau(\mathcal{R}')=\sum\tau(\mathcal{R}'') \tag{5.2}$$

follows; again $\mathcal{R}''$ has the same values as in (5.1) with the same multiplicities. Applying this to the C—G series for $D^+\otimes D^+$ given in Sec. 2 [case (I)], we get

$$D^-_k\otimes D^-_{k'}=\sum_{k''=k+k',\,k+k'+1,\cdots} D^-_{k''},\quad k\text{ and }k'=\tfrac{1}{2},1,\tfrac{3}{2},\cdots. \tag{5.3}$$

To deal with the C—G coefficients, we remark that when a UIR D^+_k is converted into the UIR D^-_k with the help of τ, the generator J_2 is unaffected and neither is the choice of the continuous basis [see Eqs. (1.12), (1.14)]. In the UIR's C^ϵ_q, however, the eigenvalue a of the operator A implementing τ will occur. So we can easily see that the following general relation must be valid:

$$C(\tau(\mathcal{R})\,\tau(\mathcal{R}')\;\tau(\mathcal{R}'')\gamma\,|pa\;p'b\;p''c)$$
$$=abc\sum_{\gamma'}\alpha_{\gamma\gamma'}\;C(\mathcal{R}\mathcal{R}'\mathcal{R}''\,\gamma'\,|pa\;p'b\;p''c). \tag{5.4}$$

Here, $\alpha_{\gamma\gamma'}$ is a set of mixing coefficients possibly dependent on $\mathcal{R}$, $\mathcal{R}'$, $\mathcal{R}''$ but not on pa, etc. We shall use (5.4) only in those cases where no multiplicity label is necessary. Further, if any one of $\mathcal{R}$, $\mathcal{R}'$, or $\mathcal{R}''$ is a discrete class UIR, the appropriate one of the symbols a, b, c is to be dropped throughout. Using this relation in the present case, we easily get

$$C(k-k'-k''-|p\;p'\;p'')=C(k+k'+k''+|p\;p'\;p'') \tag{5.5}$$

and the same is then true for the related quantities $\hat{C}$.

6. SUMMARY

In this paper we have explained a new approach to understanding the structure of the Clebsch—Gordan series for the unitary representations of the noncompact group $SU(1,1)$, and have applied it in detail for the products of the types $D^+\otimes D^+$ and $D^-\otimes D^-$. We have also computed the Clebsch—Gordan coefficients for these cases in a continuous basis, and specified the orthonormality and completeness properties of these coefficients. In doing both these things, we have been led to a simple problem in the representation theory of the group $O(4)$. While the C—G series is not new, the C—G coefficients are new, and so is the relation of the former to the group $O(4)$.

We have also set up the basic notation and constructions that will be used in treating the remaining kinds of products.

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[16]The point is that eigenfunctions of $J_0(\mathscr{C})$ with integral eigenvalues have $P=+1$, those with half-odd integral eigenvalues have $P=-1$. These are consequences of the parity properties of harmonic oscillator eigenfunctions.

[17]The point is that if only Eq. (2.43) were known, then since $\mathcal{H}_{+,2s}$ and $\mathcal{H}_{+,-2s}$ (similarly $\mathcal{H}_{-,2s}$ and $\mathcal{H}_{-,-2s}$) support one and the the same UIR $C_q^0(C_q^{1/2})$, in principle $\mathscr{A}$ could have connected these two subspaces. But in fact this does not happen.

[18]The UIR's of $O(4)$ can be labeled (j_1, j_2), where j_1 and j_2 denote the constituent UIR's of the two commuting $O(3)$ groups of which $O(4)$ is (locally) the direct product. The vanishing of the second Casimir invariant of $O(4)$ means that only UIR's with $j_1 = j_2$ occur.

[19]See, for instance, A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton U. P., Princeton, N.J., 1960), Sec. 4.7.

[20]This isolation of the angular dependences of $J_{0,1}$ in M^2 is quite similar to the fact that the Hamiltonian for a nonrelativistic particle in a centrally symmetric potential $V(r)$, when expressed in spherical polar coordinates, involves partial derivatives with respect to the spherical polar angles θ, φ only via the operator of total angular momentum squared.

[21]Actually, Eqs. (4.4) and (4.5) are inadequate in the sense that in the decompositions of $\mathscr{D}^\pm$ and $\mathscr{C}$ into UIR's, each UIR that appears does so twice (except $D_{1/2}^\pm$), and this is to be kept track of. But just as in Eqs. (3.11) and (3.19) we agreed to choose nonnegative eigenvalues for M_{12}, M_{34}, this problem is not severe.

[22]We have combined Eq. (4.14) of M. E. Rose [*Elementary Theory of Angular Momentum* (Wiley, New York, 1963)] with Eq. (9.5.2) of N. N. Lebedev [*Special Functions and their Applications* (Prentice-Hall, Englewood Cliffs, N.J., 1965)].

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Clebsch–Gordan problem and coefficients for the three-dimensional Lorentz group in a continuous basis. II

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Following the approach of a previous paper, the Clebsch–Gordan problem for the group $SU(1,1)$ for products of the form $D^+ \otimes D^-$ is related to properties of the pseudo-orthogonal $O(2,2)$. A new understanding of the Clebsch–Gordan series for this case is achieved by analyzing the properties of $O(2,2)$ spherical harmonics. The Clebsch–Gordan coefficients in a continuous basis are also calculated.

INTRODUCTION

In a previous paper, referred to hereafter as I, we have described a new approach to the Clebsch—Gordan ($C—G$) problem for the unitary representations of the group $SU(1,1)$.[1] In this approach, the structure of the Clebsch—Gordan series in each of the four essentially distinct types of direct products gets determined by the properties of a suitable four-dimensional real orthogonal or pseudo-orthogonal group. At the same time this connection allows us to compute explicitly the Clebsch—Gordan coefficients in a continuous basis.

The method works with three special "generating" unitary representations $\mathcal{D}^+$, $\mathcal{D}^-$, and $\mathcal{C}$ of $SU(1,1)$, and exploits the symmetry properties of these representations and their direct products. In I, the product representation $\mathcal{D}^+ \otimes \mathcal{D}^+$ was analyzed and related to properties of the group $O(4)$ and its representations; in this way, both the C—G series and coefficients for products of the form $D_k^+ \otimes D_{k'}^+$ were obtained. In the present paper, the product representation $\mathcal{D}^+ \otimes \mathcal{D}^-$ will be similarly analyzed. The corresponding symmetry group will turn out to be $O(2,2)$, and the C—G series and coefficients for products of the form $D_k^+ \otimes D_{k'}^-$ will be determined by the properties of a special class of unitary irreducible representations (UIR's) of $O(2,2)$ set up in an $O(2) \otimes O(2)$ basis.

In Sec 1, we set up the unitary representation $\mathcal{D}^+ \otimes \mathcal{D}^-$ of $SU(1,1)$ and display its symmetry under the group $O(2,2)$. Section 2 is devoted to expressing the connection between $O(2,2)$ and $SU(1,1)$, as well as the action of $O(2,2)$ on real four-dimensional space, in a particularly convenient manner. Using the results of Sec. 2, we show in Sec. 3 how the problem of setting up $O(2,2)$ "spherical harmonics" reduces to knowing the structure of the regular representation of $SU(1,1)$; by this means the $O(2,2)$ harmonics are set up in the $O(2) \otimes O(2)$ basis. In Sec. 4 the Clebsch—Gordan series for a general product $D_k^+ \otimes D_{k'}^-$ is obtained from the properties of the $O(2,2)$ harmonics. Two types of bases for the space of the representation $\mathcal{D}^+ \otimes \mathcal{D}^-$ are constructed. With their help the C—G coefficients in a continuous basis are computed in Sec. 5. An important phase question associated with the occurrence of the UIR's (s,ϵ) in the product $D_k^+ \otimes D_{k'}^-$ is analyzed in the Appendix.

1. CONSTRUCTION AND SYMMETRIES OF THE REPRESENTATION $\mathcal{D}^+ \otimes \mathcal{D}^-$

Let us take two representations of $SU(1,1)$, one of type $\mathcal{D}^+$ in a Hilbert space $\mathcal{H}(+)$ and another of type D^- in $\mathcal{H}(-)$, and consider their direct product $\mathcal{D}^+ \otimes \mathcal{D}^-$.[2] The space of the total representation will be $\mathcal{H} = \mathcal{H}(+) \otimes \mathcal{H}(-)$: The variables of the first factor in the product will be numbered 1, 2, those of the second 3, 4. $\mathcal{H}$ then consists of functions $f(x_1, x_2, x_3, x_4)$ with

$$\|f\|^2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dx_1 dx_2 dx_3 dx_4 \, |f(x_1, x_2, x_3, x_4)|^2. \tag{1.1}$$

The four independent oscillator operators defined on $\mathcal{H}$ fulfill

$$[a_j, a_k^+] = \delta_{jk}, \quad [a_j, a_k] = [a_j^+, a_k^+] = 0,$$
$$a_j = \frac{-i}{\sqrt{2}}\left(x_j + \frac{\partial}{\partial x_j}\right), \quad a_j^+ = \frac{i}{\sqrt{2}}\left(x_j - \frac{\partial}{\partial x_j}\right),$$
$$j, k = 1, 2, 3, 4. \tag{1.2}$$

The generators of the first factor in the product representation $\mathcal{D}^+ \otimes \mathcal{D}^-$ will involve the variables numbered 1, 2 and will have the forms given in Eq. (I. 2. 4); we will write $J_\alpha(+, 12)$ for them. Similarly, the generators of the second factor in the product, written $J_\alpha(-, 34)$, have the forms given in Eq. (I. 2. 18). And the "total" generators for the product $\mathcal{D}^+ \otimes \mathcal{D}^-$ will be

$$J_\alpha = J_\alpha(+, 12) + J_\alpha(-, 34). \tag{1.3}$$

Written out in terms of a_j, a_j^+ the J_α have the forms

$$J_0 = \tfrac{1}{2}(a_1^+ a_1 + a_2^+ a_2 - a_3^+ a_3 - a_4^+ a_4),$$
$$J_1 = \tfrac{1}{4}(a_1^+ a_1^+ + a_2^+ a_2^+ + a_1 a_1 + a_2 a_2 - a_3^+ a_3^+ - a_4^+ a_4^+ - a_3 a_3 - a_4 a_4),$$
$$J_2 = (-i/4)(a_1^+ a_1^+ + a_2^+ a_2^+ + a_3^+ a_3^+ + a_4^+ a_4^+ - a_1 a_1 - a_2 a_2 - a_3 a_3 - a_4 a_4). \tag{1.4}$$

To make the symmetries of these generators more evident, let us define new basic operators and a metric tensor thus:

$$b_1 = a_1, \quad b_1^+ = a_1^+, \quad b_2 = a_2, \quad b_2^+ = a_2^+,$$
$$b_3 = -a_3^+, \quad b_3^+ = -a_3, \quad b_4 = -a_4^+, \quad b_4^+ = -a_4; \tag{1.5a}$$

$$g_{11} = g_{22} = +1, \quad g_{33} = g_{44} = -1, \quad g_{12} = g_{13} = \cdots = 0. \tag{1.5b}$$

Then the basic commutation relations (1.2) and the realizations of b and $b^\dagger$ become (greek indices henceforth go over 1, 2, 3, 4):

$$[b_\mu, b_\nu^\dagger] = g_{\mu\nu}, \quad [b_\mu, b_\nu] = [b_\mu^\dagger, b_\nu^\dagger] = 0,$$
$$b_\mu = (-i/\sqrt{2})(x_\mu + \partial_\mu), \quad b_\mu^+ = (i/\sqrt{2})(x_\mu - \partial_\mu), \quad \partial_\mu \equiv \frac{\partial}{\partial x^\mu}. \tag{1.6}$$

[Raising and lowering of indices $\mu, \nu, \cdots$ is to be done using $g_{\mu\nu}$.] The "total" generators J_α can be expressed in terms of b, b^+ and they then appear as

$$J_0 = \tfrac{1}{2}(g^{\mu\nu}b_\mu^+ b_\nu + 2), \quad J_1 = \tfrac{1}{4}g^{\mu\nu}(b_\mu^+ b_\nu^+ + b_\mu b_\nu),$$
$$J_2 = (-i/4)g^{\mu\nu}(b_\mu^+ b_\nu^+ - b_\mu b_\nu). \tag{1.7}$$

We see immediately that the basic commutation relations (1.6) and the generators J_α are all invariant under the group of all real linear transformations

$$x_\mu \to O_\mu{}^\nu x_\nu, \quad b_\mu \to O_\mu{}^\nu b_\nu, \quad b_\mu^+ \to O_\mu{}^\nu b_\nu^+. \tag{1.8}$$

which preserve the indefinite quadratic form

$$x\cdot x = x^\mu x_\mu = (x_1)^2 + (x_2)^2 - (x_3)^2 - (x_4)^2. \tag{1.9}$$

Such matrices constitute the full pseudo-orthogonal group $O(2,2)$. There is therefore a unitary representation of this group acting on $\mathcal{H}$, such that the corresponding unitary operators all commute with the operators of the representation $\mathcal{D}^+\otimes\mathcal{D}^-$ of $SU(1,1)$ which also acts on $\mathcal{H}$. For the present purpose, it is sufficient to consider just the component of $O(2,2)$ containing the identity; for simplicity we will write $O(2,2)$ for this component. Its representation on $\mathcal{H}$ is built up using the six Hermitian generators

$$M_{\mu\nu} = i(b_\mu^+ b_\nu - b_\nu^+ b_\mu) = i(x_\mu\partial_\nu - x_\nu\partial_\mu) \tag{1.10}$$

which obey the characteristic commutation relations

$$-i[M_{\mu\nu}, M_{\rho\sigma}] = g_{\nu\rho}M_{\mu\sigma} - g_{\mu\rho}M_{\nu\sigma} + g_{\nu\sigma}M_{\rho\mu} - g_{\mu\sigma}M_{\rho\nu}. \tag{1.11}$$

The symmetry properties of the $SU(1,1)$ generators J_α are thus expressed by

$$[J_\alpha, M_{\mu\nu}] = 0. \tag{1.12}$$

For the individual sets $J_\alpha(+,12)$ and $J_\alpha(-,34)$, we have only

$$[J_\alpha(+,12) \text{ or } J_\alpha(-,34),\ M_{12} \text{ or } M_{34}] = 0. \tag{1.13}$$

We establish next the connections between the various Casimir operators. For $SU(1,1)$, we have the Casimir operators Q_{12}, Q_{34} for the individual factors in the product $\mathcal{D}^+\otimes\mathcal{D}^-$, and then Q for the total. The first two are related to M_{12}, M_{34} via Eq. (I.2.11):

$$Q_{12} = \tfrac{1}{4}(1 - M_{12}^2), \quad Q_{34} = \tfrac{1}{4}(1 - M_{34}^2). \tag{1.14}$$

The Lie algebra of the group $O(2,2)$ possesses two Casimir operators, namely $M^2 = M^{\mu\nu}M_{\mu\nu}$ and $\epsilon_{\mu\nu\rho\sigma}M^{\mu\nu}M^{\rho\sigma}$. But the generators (1.10) for the representations of $O(2,2)$ of interest are such that the second invariant vanishes identically, thereby restricting the types of UIR's of $O(2,2)$ present in $\mathcal{H}$[3]. Q can now be shown to be essentially the nontrivial Casimir operator of $O(2,2)$:

$$Q = (J_1)^2 + (J_2)^2 - (J_0)^2 = -\tfrac{1}{8}M^{\mu\nu}M_{\mu\nu} = -\tfrac{1}{8}M^2. \tag{1.15}$$

On comparing the above discussion with Sec. 3 of I, the great similarity in the properties of $\mathcal{D}^+\otimes\mathcal{D}^+$ and $\mathcal{D}^+\otimes\mathcal{D}^-$ will be evident. It is just that the symmetry group $O(4)$ has been replaced throughout by $O(2,2)$. The differences in the two types of C–G series and C–G coefficients can therefore be attributed to this replacement.

The product $\mathcal{D}^+\otimes\mathcal{D}^-$ contains within it all products of the form $D_k^+\otimes D_{k'}^-$ for various values of k and k'.[4] We want to obtain the C–G series and coefficients for the latter. So we must construct two types of bases in $\mathcal{H}$, an uncoupled basis (Φ) and a coupled one (Ψ). The uncoupled basis vectors Φ will be simultaneous eigenvectors of the operators M_{12}, M_{34} (hence Q_{12}, Q_{34}), $J_2(+,12)$ and $J_2(-,34)$. Such basis vectors are direct products of basis vectors drawn one from each factor in a product of the form $D_k^+\otimes D_{k'}^-$. In the coupled basis, the simultaneously diagonal operators should be M_{12}, M_{34} (hence Q_{12}, Q_{34}), J_2, M^2 (hence Q), and where relevant the unitary operator that implements the outer automorphism τ of $SU(1,1)$. (This last because the continuous UIR's C_q^ϵ will be found to occur in the decomposition of any product $D_k^+\otimes D_{k'}^-$.) Having M_{12} and M_{34} diagonal in both bases ensures that we will be dealing with a single product $D_k^+\otimes D_{k'}^-$ and its reduction. The coupled basis vectors will belong to definite UIR's of the total $SU(1,1)$; at the same time they will be basis vectors for the UIR's of $O(2,2)$ in a definite form, namely a form in which the $O(2)\otimes O(2)$ subgroup (generated by M_{12} and M_{34}) is "diagonalized." The allowed eigenvalues of M^2, keeping those of M_{12} and M_{34} fixed, together with the forms of the generators J_α will determine the C–G series for a product $D_k^+\otimes D_{k'}^-$; the overlap between a Φ and a Ψ will yield the C–G coefficients.

Construction of the coupled basis vectors Ψ can be seen to involve the breaking up of $\mathcal{H}$ into simultaneous eigenspaces of M_{12}, M_{34}, and M^2. In other words, we are faced with the problem of setting up a complete set of "$O(2,2)$ spherical harmonics" in the real four-dimensional space R_4 endowed with the metric $g_{\mu\nu}$. This involves going over from the Cartesian variables x_μ of R_4 to new "radial" and "angular" variables. The transformations of $O(2,2)$ act on the angles alone. The unitary representation of $O(2,2)$ obtained by the action of this group on functions of the angles will yield, upon reduction, a complete set of "$O(2,2)$ spherical harmonics." The choice of the angle variables must be such that these harmonics are obtained in an $O(2)\otimes O(2)$ basis. We will develop all this in the next two sections by first relating the group $O(2,2)$ back to $SU(1,1)$, and then making use of the $SU(1,1)$ Plancherel formula as given by Bargmann.[5] We will conclude this section by putting the generators J_α of Eq. (1.7) into a new form. The purpose is to isolate all angle dependences of these operators in the operator M^2 (or Q). The steps are similar to those involved in Eq. (I.3.17), and yield

$$J_0 = \frac{1}{4}\left(x^2 - \frac{4Q}{x^2} - \frac{1}{x^2}(x\cdot\partial)^2 - \frac{2}{x^2}x\cdot\partial\right),$$
$$J_1 = -\frac{1}{4}\left(x^2 + \frac{4Q}{x^2} + \frac{1}{x^2}(x\cdot\partial)^2 + \frac{2}{x^2}x\cdot\partial\right),$$
$$J_2 = (-i/2)(x\cdot\partial + 2),$$
$$x^2 = x^\mu x_\mu, \quad x\cdot\partial = x^\mu\partial_\mu. \tag{1.16}$$

2. CONNECTION BETWEEN $O(2,2)$ AND $SU(1,1)$ AND CHOICE OF NEW VARIABLES

It is well known that locally the group $O(2,2)$ has the same structure as the direct product group $SU(1,1)\otimes SU(1,1)$, analogous to the relationship between $O(4)$ and $SU(2)\otimes SU(2)$. It is this fact that allows us to turn the construction of the "$O(2,2)$ spherical harmonics" into a problem involving the group $SU(1,1)$, and more especially the regular representation of $SU(1,1)$. We shall express the $O(2,2)$—$SU(1,1)\otimes SU(1,1)$ relationship in a particular way which will turn out to be suited to the choice of angular variables in R_4 as well.

We know that in the defining representation of $SU(1,1)$, each element g of this group corresponds to a complex 2×2 matrix in this fashion:

$$g=\begin{pmatrix}\alpha & \beta\\ \beta^* & \alpha^*\end{pmatrix}, \quad |\alpha|^2-|\beta|^2=1. \tag{2.1}$$

Let us split the complex numbers α, β into their real and imaginary parts by setting

$$\alpha=a_1-ia_2, \quad \beta=-a_3+ia_4. \tag{2.2}$$

[There is little danger of these real parameters $a_1\cdots a_4$ being mistaken for the annihilation operators used in the previous section.] Denote this quartet of real numbers by $\mathbf{a}$. Then elements of $SU(1,1)$ correspond one-to-one to quartets $\mathbf{a}$ obeying

$$a_1^2+a_2^2-a_3^2-a_4^2=1 \tag{2.3}$$

by the equation

$$g(\mathbf{a})=a_1-ia_2\sigma_3-a_3\sigma_1-a_4\sigma_2. \tag{2.4}$$

Consider the group multiplication law of $SU(1,1)$. The product $g(\mathbf{b})g(\mathbf{a})$ corresponds to a quartet of numbers $\mathbf{c}$ which are linear in both $\mathbf{b}$ and $\mathbf{a}$. In order to express the linearity in $\mathbf{a}$, we may write

$$g(\mathbf{b})g(\mathbf{a})=g(L(\mathbf{b})\mathbf{a}). \tag{2.5}$$

Here, on the right-hand side, $\mathbf{a}$ is thought of as a column vector with a_1, a_2, a_3, a_4 as entries, and $L(\mathbf{b})$ is a 4×4 real matrix that acts on $\mathbf{a}$ to give the quartet of real numbers corresponding to $g(\mathbf{b})g(\mathbf{a})$. The matrix elements of $L(\mathbf{b})$ are themselves linear in $\mathbf{b}$. Using the properties of the Pauli matrices, we get

$$L(\mathbf{b})=\begin{pmatrix} b_1 & -b_2 & b_3 & b_4\\ b_2 & b_1 & b_4 & -b_3\\ b_3 & b_4 & b_1 & -b_2\\ b_4 & -b_3 & b_2 & b_1\end{pmatrix}. \tag{2.6}$$

Either from the observation that along with $\mathbf{a}$, $L(\mathbf{b})\mathbf{a}$ must also obey Eq. (2.3), or by direct verification, it follows that $L(\mathbf{b})$ is an element of $O(2,2)$. From the defining Eq. (2.5) for $L(\mathbf{b})$ it follows that if $g(\mathbf{b})g(\mathbf{a})=g(\mathbf{c})$ is an equation holding among three elements of $SU(1,1)$, then $L(\mathbf{b})L(\mathbf{a})=L(\mathbf{c})$ as well.

In an analogous manner, another set of $O(2,2)$ transformations $R(\mathbf{a})$ can be defined by

$$g(\mathbf{b})g(\mathbf{a})^{-1}=g(R(\mathbf{a})\mathbf{b}),$$

$$R(\mathbf{a})=\begin{pmatrix} a_1 & a_2 & -a_3 & -a_4\\ -a_2 & a_1 & a_4 & -a_3\\ -a_3 & a_4 & a_1 & -a_2\\ -a_4 & -a_3 & a_2 & a_1\end{pmatrix}. \tag{2.7}$$

These too form a representation (nonunitary, of course) of $SU(1,1)$. And by comparing Eqs. (2.5) and (2.7) it can be seen that any matrix of type L will commute with any one of type R. All in all, then, corresponding to each $g\in SU(1,1)$ we have transformations $L(g)$, $R(g)\in O(2,2)$ such that

$$L(g')L(g)=L(g'g), \quad R(g')R(g)=R(g'g),$$
$$L(g')R(g)=R(g)L(g'). \tag{2.8}$$

These transformations $L(g)$, $R(g)$ together constitute the (identity component of the) group $O(2,2)$; in fact, the most general element of $O(2,2)$ is the product $L(g)R(g')$ for some $g, g'\in SU(1,1)$. Thus, we have shown that, locally at least, $O(2,2)$ has the same structure as $SU(1,1)\otimes SU(1,1)$.

The six generators $M_{\mu\nu}$ of $O(2,2)$ can also be separated into two commuting $SU(1,1)$ Lie algebras. If we define

$$L_0=\tfrac{1}{2}(M_{12}-M_{34}), \quad L_1=\tfrac{1}{2}(M_{23}+M_{14}), \quad L_2=\tfrac{1}{2}(M_{13}-M_{24}),$$
$$R_0=\tfrac{1}{2}(M_{12}+M_{34}), \quad R_1=\tfrac{1}{2}(M_{23}-M_{14}), \quad R_2=\tfrac{1}{2}(M_{13}+M_{24}), \tag{2.9}$$

then the L_α obey the $SU(1,1)$ commutation relations among themselves, the R_α also do so among themselves, while each L_α commutes with each R_β. The L_α are generators for the transformations $L(g)$ in $O(2,2)$, the R_α for $R(g)$. Since $O(2,2)\sim SU(1,1)\otimes SU(1,1)$, a general UIR of $O(2,2)$ consists of the direct product of two UIR's, one for each factor $SU(1,1)$ in the product. Thus we may denote it by $(\mathcal{R}_1,\mathcal{R}_2)$ where the operators L_α generate the UIR $\mathcal{R}_1$ of $SU(1,1)$, the operators R_α generate the UIR $\mathcal{R}_2$ of $SU(1,1)$ [$\mathcal{R}=(k,\eta)$ for the discrete series, (s,ϵ) for the continuous series]. Now we have to deal with the particular $O(2,2)$ representation which has the generators given in Eq. (1.10); and we have noted that in this case, the invariant $\epsilon_{\mu\nu\rho\sigma}M^{\mu\nu}M^{\rho\sigma}$ vanishes. The structure (1.10) for $M_{\mu\nu}$ has the consequence that the two commuting $SU(1,1)$ subgroups generated by L_α and R_α share the same Casimir operator. In fact, we have

$$L^2=(L_1)^2+(L_2)^2-(L_0)^2=R^2=(R_1)^2+(R_2)^2-(R_0)^2$$
$$=-\tfrac{1}{8}M^2. \tag{2.10}$$

Consistent with this, we will find that only two kinds of UIR's of $O(2,2)$ will appear in our analysis, namely $(\mathcal{R},\mathcal{R})$ and $(\mathcal{R},\tau(\mathcal{R}))$; $\mathcal{R}$ is a general UIR of $SU(1,1)$ and τ is the outer automorphism on $SU(1,1)$.

Now we shall deal with the action of $O(2,2)$ on the variables x_μ of R_4, and the choice of suitable angle variables. The whole of R_4 can be expressed as the union of two regions, V^+ in which $x^2>0$ and V^- in which $x^2<0$:

$$V^\pm:\ x^2\gtrless 0, \quad R_4=V^+\cup V^-. \tag{2.11}$$

[The lower-dimensional region $x^2=0$ is disregarded.] There is a natural mapping P that takes points in V^+ into V^- and vice versa[6]:

$$P:\ (x_1,x_2,x_3,x_4)\to(x_3,x_4,x_1,x_2). \tag{2.12}$$

So $(Px)^2=-x^2$. Under the action of $O(2,2)$, points in V^+ remain in V^+, those in V^- remain in V^-. In both cases, we define the radial coordinate r as $|x^2|^{1/2}$, i.e.,

$$x \in V^+: \ x^2 = r^2, \ 0 < r < \infty,$$
$$x \in V^-: \ x^2 = -r^2, \ 0 < r < \infty. \qquad (2.13)$$

Guided by the forms of Eqs. (2.3) (2.4) and (2.12), with each point $x \in R_4$, we associate an element $a(x) \in SU(1,1)$ by

$$a(x) = (1/r)(x_1 - ix_2\sigma_3 - x_3\sigma_1 - x_4\sigma_2) \ \text{ if } x \in V^+,$$
$$= (1/r)(x_3 - ix_4\sigma_3 - x_1\sigma_1 - x_2\sigma_2) \ \text{ if } x \in V^-. \qquad (2.14)$$

The definitions for the two regions $V^{\pm}$ are made so as to satisfy

$$a(Px) = a(x), \ \text{ any } x. \qquad (2.15)$$

It is clear that the element $a(x)$ in $SU(1,1)$ depends only on the "direction" of the point x in R_4, not on its radial coordinate r, since for any real number p we have

$$a(px) = a(x). \qquad (2.16)$$

We may now say that the various possible directions within V^+ are labelled one-to-one by the elements of $SU(1,1)$, and similarly within V^-. [It is obvious that in choosing all possible points x in V^+, $a(x)$ ranges over the whole of $SU(1,1)$; similarly for V^-.] Radial and angular type variables have to be introduced separately in V^+ and in V^-. We may think of the variable group element $a(x) \in SU(1,1)$ as being the (generalized) angle type "coordinate" in both V^+ and V^-. That is, in each region, we pass from the Cartesian coordinates x_μ to the radial and angular coordinates $(r, a(x))$ or (r, g), $g \in SU(1,1)$. Once a specific parametrization for the elements of the group $SU(1,1)$ is adopted, those three parameters will become three numerical angle type variables. Since we want to construct $O(2,2)$ spherical harmonics in an $O(2) \otimes O(2)$ basis, the appropriate parametrization of $SU(1,1)$ will be the one given by Bargmann.[7]

The manner in which a transformation of $O(2,2)$ rotates one direction in R_4 into another can now be expressed as follows:

$$a(L(g)x) = g a(x) \ \text{ for all } x,$$
$$a(R(g)x) = a(x)g^{-1} \ \text{ if } x \in V^+,$$
$$= a(x)\tau(g)^{-1} \ \text{ if } x \in V^-. \qquad (2.17)$$

We will leave the verification of this to the reader. [The action of τ on the element corresponding to the quartet (a_1, a_2, a_3, a_4) is to give the quartet $(a_1, -a_2, a_3, -a_4)$.]

In the Bargmann parametrization for $SU(1,1)$, a general element is specified by three coordinates μ, ζ, μ' by writing the matrix (2.1) as the product

$$\begin{pmatrix} e^{i\mu/2} & 0 \\ 0 & e^{-i\mu/2} \end{pmatrix} \begin{pmatrix} \cosh\zeta/2 & \sinh\zeta/2 \\ \sinh\zeta/2 & \cosh\zeta/2 \end{pmatrix} \begin{pmatrix} e^{i\mu'/2} & 0 \\ 0 & e^{-i\mu'/2} \end{pmatrix}. \qquad (2.18)$$

The ranges for these parameters are $0 \le \mu \le 2\pi$, $0 \le \zeta < \infty$, $0 \le \mu' \le 4\pi$. In a general representation of $SU(1,1)$, the element (2.18) is represented by $\exp(i\mu J_0)\exp(i\zeta J_2)\exp(i\mu' J_0)$. By equating the element $a(x)$ to (2.18), we get the equations relating x_μ to the new variables in V^+ and V^-:

$$V^+: \ x_1 = r\cosh\frac{\zeta}{2}\cos\mu_+, \quad x_2 = -r\cosh\frac{\zeta}{2}\sin\mu_+,$$
$$x_3 = -r\sinh\frac{\zeta}{2}\cos\mu_-, \quad x_4 = -r\sinh\frac{\zeta}{2}\sin\mu_-; \qquad (2.19a)$$
$$V^-: \ x_1 = -r\sinh\frac{\zeta}{2}\cos\mu_-, \quad x_2 = -r\sinh\frac{\zeta}{2}\sin\mu_-,$$
$$x_3 = r\cosh\frac{\zeta}{2}\cos\mu_+, \quad x_4 = -r\cosh\frac{\zeta}{2}\sin\mu_+;$$
$$\mu_\pm = \frac{1}{2}(\mu' \pm \mu). \qquad (2.19b)$$

We can split the Hilbert space $\mathcal{H}$ into two subspaces $\mathcal{H}_\pm$ corresponding to functions that vanish in $V^\mp$, respectively. A general function f in $\mathcal{H}$ can be written as a pair of functions f_-, f_+ giving the values of f in V^- and V^+, respectively. Each of these is in the first instance a function of r and a variable element g of $SU(1,1)$, $f_\mp(r;g)$; and on using the parameters μ, ζ, μ' for g, each becomes a function of r, μ, ζ, and μ'. The Jacobian for the transformation is easily computed; it is the same in both V^- and V^+, and we get

$$dx_1dx_2dx_3dx_4 = 2\pi^2 r^3 dr da(x),$$
$$da(x) = \tfrac{1}{2} d\cosh\zeta (d\mu/2\pi)(d\mu'/4\pi). \qquad (2.20)$$

Here, $da(x)$ is the invariant volume element on $SU(1,1)$ as defined by Bargmann. The structure of $\mathcal{H}$ then appears thus[8]:

$$f(x) \in \mathcal{H} \Rightarrow f = \begin{pmatrix} f_-(r;\mu\zeta\mu') \\ f_+(r;\mu\zeta\mu') \end{pmatrix}, \quad 0 \le r, \zeta < \infty, 0 \le \mu, \mu'/2 \le 2\pi,$$
$$\|f\|^2 = \int_0^\infty 2\pi^2 r^3 \, dr \int_{SU(1,1)} da(x)(|f_+(r;\mu\zeta\mu')|^2 + |f_-(r;\mu\zeta\mu')|^2). \qquad (2.21)$$

$\mathcal{H}_+(\mathcal{H}_-)$ consists of vectors which have vanishing $f_-(f_+)$.

The $O(2,2)$ transformations, and so the generators $M_{\mu\nu}$, leave $\mathcal{H}_+$ and $\mathcal{H}_-$ invariant. Each $M_{\mu\nu}$ can be represented on each of $\mathcal{H}_+$ and $\mathcal{H}_-$ as a partial differential operator in the "angles" μ, ζ and μ'. We are particularly interested in M_{12} and M_{34}, and they have these forms:

$$\mathcal{H}_-: \ M_{12} = i\left(\frac{\partial}{\partial\mu'} - \frac{\partial}{\partial\mu}\right), \quad M_{34} = i\left(\frac{\partial}{\partial\mu'} + \frac{\partial}{\partial\mu}\right), \qquad (2.22)$$
$$\mathcal{H}_+: \ M_{12} = -i\left(\frac{\partial}{\partial\mu'} + \frac{\partial}{\partial\mu}\right), \quad M_{34} = -i\left(\frac{\partial}{\partial\mu'} - \frac{\partial}{\partial\mu}\right).$$

Quite generally, the expressions for $M_{12}, M_{23}, M_{31}, M_{14}, M_{24}$, and M_{34} in $\mathcal{H}_-$ coincide with those for $-M_{34}, M_{14}, M_{31}, M_{23}, M_{24}$ and $-M_{12}$, respectively in $\mathcal{H}_+$. Therefore, the operator M^2 has the same appearance in $\mathcal{H}_-$ and $\mathcal{H}_+$. But we shall not need to deal with it directly.

3. THE $O(2,2)$ SPHERICAL HARMONICS

Complete sets of $O(2,2)$ spherical harmonics in both V^- and V^+ will be built up via the Plancherel formula for $SU(1,1)$.[5] Let us recall this formula. It states that every square-integrable function on $SU(1,1)$, $f(g)$, can be expanded in terms of the representation matrices $\mathcal{D}^{(\mathcal{R})}_{mn}(g)$ of the principal series of UIR's of $SU(1,1)$ as follows:

$$f(g) = \int d\mathcal{R}\,\mu(\mathcal{R}) \sum_{mn} \tilde{f}_{nm}(\mathcal{R}) \mathcal{D}^{(\mathcal{R})}_{mn}(g). \qquad (3.1)$$

Here, the process of "integrating" a function $\tilde{f}(\mathcal{R})$ over the set of relevant UIR's of $SU(1,1)$ is defined as

$$\int d\mathcal{R}\, \tilde{f}(\mathcal{R}) \equiv \sum_{k=1,3/2,\cdots} \sum_{\eta=\pm} \tilde{f}(k,\eta) + \sum_{\epsilon=0,1/2} \int_0^\infty ds\, \tilde{f}(s,\epsilon)\,. \tag{3.2}$$

The weight function $\mu(\mathcal{R})$ is given by

$$\begin{aligned} \mu(\mathcal{R}) &= (2k-1)^{1/2} \quad \text{if } \mathcal{R}=(k,\eta) \\ &= (2s/\coth\pi s)^{1/2} \quad \text{if } \mathcal{R}=(s,0) \\ &= (2s/\tanh\pi s)^{1/2} \quad \text{if } \mathcal{R}=(s,1/2). \end{aligned} \tag{3.3}$$

The coefficients $\tilde{f}_{nm}(\mathcal{R})$ that appear in the expansion are given by

$$\tilde{f}_{nm}(\mathcal{R}) = \mu(\mathcal{R}) \int dg\, \mathcal{D}^{(\mathcal{R})}_{mn}(g)^* f(g), \tag{3.4}$$

and the Plancherel theorem is the statement

$$\int dg\, |f(g)|^2 = \int d\mathcal{R} \sum_{mn} |\tilde{f}_{nm}(\mathcal{R})|^2. \tag{3.5}$$

The invariant volume element dg has already been specified in Eq. (2.20), using the Bargmann parametrization. We can define a generalized Kronecker symbol $\delta(\mathcal{R},\mathcal{R}')$ that is appropriate to the definition (3.2) of integration with respect to $\mathcal{R}$ [see Eq. (I.4.3)]; using it, we easily establish the orthonormality properties of the matrices $\mathcal{D}^{(\mathcal{R})}_{mn}(g)$:

$$\int dg\, \mathcal{D}^{(\mathcal{R})}_{mn}(g)^* \mathcal{D}^{(\mathcal{R}')}_{m'n'}(g) = \delta(\mathcal{R}',\mathcal{R})\delta_{m'm}\delta_{n'n}/\mu(\mathcal{R}')\mu(\mathcal{R}). \tag{3.6}$$

In all the above, the $\mathcal{D}^{(\mathcal{R})}_{mn}(g)$ were the representation matrices for the UIR's of $SU(1,1)$ in the basis wherein J_0 is diagonal. These functions have been given by Bargmann. With the coordinates μ, ζ, μ' for $SU(1,1)$, we have

$$\mathcal{D}^{(\mathcal{R})}_{mn}(\mu,\zeta,\mu') = \exp(im\mu + in\mu')\, d^{(\mathcal{R})}_{mn}(\zeta). \tag{3.7}$$

A relation that we will need is the behavior of these functions under the automorphism τ of $SU(1,1)$. This is given by

$$\mathcal{D}^{(\mathcal{R})}_{mn}(\tau(g)) = (-1)^{m-n} \mathcal{D}^{\tau(\mathcal{R})}_{-m,-n}(g). \tag{3.8}$$

The expressions for the "little-d" functions $d^{(\mathcal{R})}_{mn}(\zeta)$ will be presented when needed.

Let us now consider the question of setting up $O(2,2)$ spherical harmonics in the region V^+. What we need is a complete set of functions of the "angle variables" $a(x)$ which are bases for UIR's of $O(2,2)$, and in terms of which we may expand the "angular dependence" [i.e., dependence on $a(x)$] of a function $f_+(x_\mu) = f_+(r, a(x))$ defined in V^+. On the basis of Eqs. (2.17) and (3.1), we can see that such a set of functions is given by

$$\mathcal{Y}^{+(\mathcal{R})}_{(mn)}(x) = \mathcal{D}^{(\mathcal{R})}_{mn}(a(x)), \quad x \in V^+. \tag{3.9}$$

$\mathcal{R}$ goes over just those UIR's of $SU(1,1)$ that appear in the Plancherel formula; it is like the "l" in the ordinary three-dimensional spherical harmonics $Y^l_m(\theta,\phi)$, while the role of m in the latter is played now by the composite index (mn).[9] We can determine the UIR of $O(2,2)$ carried by the harmonics $\mathcal{Y}^{+(\mathcal{R})}_{(mn)}(x)$ for fixed $\mathcal{R}$ by using Eq. (2.17) and the group composition laws for the $\mathcal{D}$ matrices:

$$\mathcal{Y}^{+(\mathcal{R})}_{(mn)}(L(g)R(g')x) = \sum_{m'n'} \mathcal{D}^{(\mathcal{R})}_{mm'}(g)\mathcal{D}^{(\mathcal{R})}_{nn'}(g')^* \mathcal{Y}^{+(\mathcal{R})}_{(m'n')}(x), \quad x\in V^+. \tag{3.10}$$

Now the matrices $\mathcal{D}^{(\mathcal{R})}(g)^*$ give the UIR complex conjugate to $\mathcal{R}$, and this in turn is just the UIR $\tau(\mathcal{R})$. We can then say that for fixed $\mathcal{R}$ and $x\in V^+$, the harmonics $\mathcal{Y}^{+(\mathcal{R})}_{(mn)}(x)$ carry the UIR $(\mathcal{R}, \tau(\mathcal{R}))$ of $O(2,2)$. The spectrum of UIR's of $O(2,2)$ present in $\mathcal{H}_+$ is then

$$\mathcal{H}_+:\ (k+,k-),\ (k-,k+),\ (s\epsilon, s\epsilon),\ k=1,3/2,\cdots,\quad \epsilon=0,1/2,\quad 0\le s<\infty. \tag{3.11}$$

Any function $f_+(r;a(x))$ in $\mathcal{H}_+$ can be expanded as

$$f_+(r;a(x)) = \int d\mathcal{R}\, \mu(\mathcal{R}) \sum_{mn} f^{(\mathcal{R})}_{+,nm}(r) \mathcal{Y}^{+(\mathcal{R})}_{(mn)}(x),$$
$$f^{(\mathcal{R})}_{+,nm}(r) = \mu(\mathcal{R}) \int da(x)\, \mathcal{Y}^{+(\mathcal{R})}_{(mn)}(x)^* f_+(r;a(x)), \tag{3.12}$$

with

$$\|f_+\|^2 = \int_0^\infty 2\pi^2 r^3\, dr \int d\mathcal{R} \sum_{mn} |f^{(\mathcal{R})}_{+,nm}(r)|^2. \tag{3.13}$$

In particular, if we have two functions $f(r)\mathcal{Y}^{+(\mathcal{R})}_{(mn)}(x)$ and $f'(r)\mathcal{Y}^{+(\mathcal{R}')}_{(m'n')}(x)$ in $\mathcal{H}_+$, their scalar product will be

$$(f',f) = \frac{\delta(\mathcal{R}',\mathcal{R})\delta_{m'm}\delta_{n'n}}{\mu(\mathcal{R}')\mu(\mathcal{R})} \int_0^\infty 2\pi^2 r^3\, dr\, f'(r)^* f(r). \tag{3.14}$$

The spectrum of UIR's of $O(2,2)$ occurring in $\mathcal{H}_-$ differs from that in $\mathcal{H}_+$, and this will have important consequences for the reduction of the representation $\mathcal{D}^+ \otimes \mathcal{D}^-$ of $SU(1,1)$. To start with, let us define

$$\bar{\mathcal{Y}}^{(\mathcal{R})}_{(mn)}(x) = \mathcal{D}^{(\mathcal{R})}_{mn}(a(x)), \quad x\in V^-. \tag{3.15}$$

Then under the $O(2,2)$ transformation $L(g)R(g')$, instead of Eq. (3.10) we now have

$$\bar{\mathcal{Y}}^{(\mathcal{R})}_{(mn)}(L(g)R(g')x) = \sum_{m'n'} \mathcal{D}^{(\mathcal{R})}_{mm'}(g)\mathcal{D}^{(\mathcal{R})}_{nn'}(\tau(g'))^* \bar{\mathcal{Y}}^{(\mathcal{R})}_{(m'n')}(x),\quad x\in V^-. \tag{3.16}$$

On taking account of Eq. (3.8), we see that now for fixed $\mathcal{R}$ we have the UIR $(\mathcal{R},\mathcal{R})$ of $O(2,2)$. If $\mathcal{R}$ is a discrete UIR of $SU(1,1)$, this is not equivalent to $(\mathcal{R}, \tau(\mathcal{R}))$, while if $\mathcal{R}$ is in the continuous class, it is equivalent to $(\mathcal{R}, \tau(\mathcal{R}))$. The spectrum of UIR's of $O(2,2)$ occurring in $\mathcal{H}_-$, is therefore this:

$$\mathcal{H}_-:\ (k+,k+),\ (k-,k-),\ (s\epsilon,s\epsilon),\quad k=1,3/2,\cdots,\quad \epsilon=0,1/2,\quad 0\le s<\infty. \tag{3.17}$$

Now the UIR $(s\epsilon, s\epsilon)$ is present in both $\mathcal{H}_+$ and $\mathcal{H}_-$, and it is therefore useful to choose the corresponding spherical harmonics in the two cases so that the transformation laws under $O(2,2)$ are not merely equivalent but identical. Comparing Eq. (3.16) with Eqs. (3.8) and (3.10), we are led to the following final choice of $O(2,2)$ spherical harmonics in the region V^-[10]:

$$\mathcal{Y}^{-(\mathcal{R})}_{(mn)}(x) = (-1)^{n-\epsilon}\mathcal{D}^{(\mathcal{R})}_{m,-n}(a(x)), \quad x\in V^-. \tag{3.18}$$

$\epsilon=0$ or $\frac{1}{2}$ according as n is integral or half-odd integral. Then, for $\mathcal{R}=(s,\epsilon)$ we have, uniformly;

$$\mathcal{Y}^{\pm(\mathcal{R})}_{(mn)}(L(g)R(g')x) = \sum_{m'n'} \mathcal{D}^{(\mathcal{R})}_{mm'}(g)\mathcal{D}^{(\mathcal{R})}_{nn'}(g')^* \mathcal{Y}^{\pm(\mathcal{R})}_{(m'n')}(x). \tag{3.19}$$

The analogs to Eqs. (3.12) and (3.13) in the case of a function $f_-(x)$ belonging to $\mathcal{H}_-$ are as follows:

$$f_-(r;a(x)) = \int d\mathcal{R}\, \mu(\mathcal{R}) \sum_{mn} f^{(\mathcal{R})}_{-,nm}(r) \mathcal{Y}^{-(\mathcal{R})}_{(mn)}(x),$$

$$f_{-,nm}^{(\mathcal{R})}(r)=\mu(\mathcal{R})\int da(x)\mathcal{Y}_{(mn)}^{-(\mathcal{R})}(x)^{*}f_{-}(r;a(x)),$$
$$\|f_{-}\|^{2}=\int_{0}^{\infty}2\pi^{2}r^{3}\,dr\int d\mathcal{R}\sum_{mn}|f_{-,nm}^{(\mathcal{R})}(r)|^{2};\tag{3.20}$$

and the scalar product of two elements $f(r)\mathcal{Y}_{(mn)}^{-(\mathcal{R})}(x)$ and $f'(r)\mathcal{Y}_{(m'n')}^{-(\mathcal{R}')}(x)$ in $\mathcal{H}_{-}$ will be of exactly the same form as in Eq. (3.14).

The definitions given in Eqs. (3.9) and (3.18) for $\mathcal{Y}_{(mn)}^{+(\mathcal{R})}(x)$ and $\mathcal{Y}_{(mn)}^{-(\mathcal{R})}(x)$, respectively, constitute a full solution to the problem of setting up the $O(2,2)$ spherical harmonics in an $O(2)\otimes O(2)$ basis. Taking account of the differences in the forms of M_{12}, M_{34} in $\mathcal{H}_{-}$ and in $\mathcal{H}_{+}$ as expressed by Eq. (2.22), and also the differences between Eqs. (3.9) and (3.18), we see that we have uniformly

$$M_{12}\mathcal{Y}_{(mn)}^{\pm(\mathcal{R})}(x)=(m+n)\mathcal{Y}_{(mn)}^{\pm(\mathcal{R})}(x),$$
$$M_{34}\mathcal{Y}_{(mn)}^{\pm(\mathcal{R})}(x)=(n-m)\mathcal{Y}_{(mn)}^{\pm(\mathcal{R})}(x).\tag{3.21}$$

We now have adequate information to write down the general forms of vectors in $\mathcal{H}$ that are eigenvectors of M_{12}, M_{34} and also belong to definite UIR's of $O(2,2)$. While M_{12} as defined in (1.10) coincides with the operator used in I in the analysis of the representation $\mathcal{D}^{+}$ of $SU(1,1)$, M_{34} is the negative of that used there in the analysis of the representation $\mathcal{D}^{-}$. To pick out the particular product $D_{k}^{+}\otimes D_{k'}^{-}$ in $\mathcal{D}^{+}\otimes\mathcal{D}^{-}$ (which incidentally is present four times unless k and/or k' is $\frac{1}{2}$), it is convenient to choose the eigenvalues $(2k-1)$ and $(1-2k')$ for M_{12}, M_{34}, respectively. (The former is nonnegative, the latter nonpositive.) For such values of M_{12} and M_{34}, not all the UIR's of $O(2,2)$ listed in Eqs. (3.11) and (3.17) can appear. Specifically, from (3.21) we have $m=k+k'-1\geq 0$, so the UIR's $(k''-,k''+)$ in $\mathcal{H}_{+}$ and $(k''-,k''-)$ in $\mathcal{H}_{-}$ will not show up. Given the eigenvalues for M_{12}, M_{34} as above, an element in $\mathcal{H}$ belonging to the UIR $(k''+,k''+)$ of $O(2,2)$ must lie within $\mathcal{H}_{-}$; in the notation of Eq. (2.21) it must have the form

$$f_{-}(r)\mu(k'')(-1)^{k'-k+\epsilon}\begin{pmatrix}\mathcal{D}_{k+k'-1,k'-k}^{(k''+)}(\mu\zeta\mu')\\0\end{pmatrix},\tag{3.22}$$

and its norm will be

$$\int_{0}^{\infty}2\pi^{2}r^{3}|f_{-}(r)|^{2}\,dr.\tag{3.23}$$

If on the other hand it is to belong to the UIR $(k''+,k''-)$, it must lie in $\mathcal{H}_{+}$ and have the form

$$f_{+}(r)\mu(k'')\begin{pmatrix}0\\\mathcal{D}_{k+k'-1,k-k'}^{(k''+)}(\mu\zeta\mu')\end{pmatrix};\tag{3.24}$$

its norm will be

$$\int_{0}^{\infty}2\pi^{2}r^{3}|f_{+}(r)|^{2}\,dr.\tag{3.25}$$

Both vectors (3.22) and (3.24) possess the eigenvalue $k''(1-k'')$ with respect to the total $SU(1,1)$ Casimir operator Q; the former vector will exist only if $k'\geq k+1$, the latter only if $k\geq k'+1$. This is because in the Plancherel formula for $SU(1,1)$ the two UIR's $D_{1/2}^{\pm}$ are absent, so in the above we must have $k''\geq 1$.

The third type of vector we are interested in belongs to the UIR $(s\epsilon,s\epsilon)$ of $O(2,2)$ (and of course has $M_{12}=2k-1$, $M_{34}=1-2k'$). Since this UIR of $O(2,2)$ is present in both $\mathcal{H}_{+}$ and $\mathcal{H}_{-}$, such a vector involves two radial functions and has the general form:

$$\mu(s,\epsilon)\begin{pmatrix}f_{-}(r)(-1)^{k'-k+\epsilon}\exp(i\varphi(s,\epsilon))\mathcal{D}_{k+k'-1,k'-k}^{(s,\epsilon)}(\mu\zeta\mu')\\f_{+}(r)\qquad\mathcal{D}_{k+k'-1,k-k'}^{(s,\epsilon)}(\mu\zeta\mu')\end{pmatrix}.\tag{3.26}$$

The purpose of the phase factor $\varphi(s,\epsilon)$ is to ensure that when the vector (3.26) is acted upon by the operators of the representation $\mathcal{D}^{+}\otimes\mathcal{D}^{-}$ of $SU(1,1)$, the changes brought about in $f_{-}(r)$ and $f_{+}(r)$ will have the standard forms explained in I and characteristic of the UIR (s,ϵ) of $SU(1,1)$. It has been evaluated in the Appendix and turns out to be $\varphi(s,0)=2\varphi(s,\frac{1}{2})=\pi$. It is evident that the vector (3.26) possesses the eigenvalue $\frac{1}{4}+s^{2}$ with respect to Q. If we take another vector of the form (3.26) but with the replacements $f_{\mp}(r)\to f_{\mp}'(r)$, $s\to s'$, $\epsilon\to\epsilon'$, then the scalar product of this vector with (3.26) will be

$$\delta(s'-s)\delta_{\epsilon'\epsilon}\int_{0}^{\infty}2\pi^{2}r^{3}(f_{-}'(r)^{*}f_{-}(r)+f_{+}'(r)^{*}f_{+}(r))\,dr.\tag{3.27}$$

This is the analog of Eqs. (3.23) and (3.25) and has to be stated in this way because s is a continuous variable. Of course, all the three equations (3.23), (3.25), (3.27) are consequences of Eq. (3.6).

4. C-G SERIES FOR THE PRODUCTS $D^{+}\otimes D^{-}$

We know that the generators J_{α} of the representation $\mathcal{D}^{+}\otimes\mathcal{D}^{-}$ of $SU(1,1)$, commute with the transformations of $O(2,2)$. Let us consider the action of a finite $SU(1,1)$ transformation on a vector of the form (3.22). This vector will preserve its property of being an eigenvector of M_{12}, M_{34} and of belonging to the UIR $(k''+,k''+)$ of $O(2,2)$; in other words, under the action of $SU(1,1)$ the sole change will be in the radial function $f_{-}(r)$. Stated yet another way, the subspace of $\mathcal{H}$ containing all vectors of the form (3.22) for all possible $f_{-}(r)$ is invariant under $\mathcal{D}^{+}\otimes\mathcal{D}^{-}$; and the restrictions of J_{α} to this subspace yield purely radial differential operators that act on $f_{-}(r)$. These radial operators are easy to get, since we may use Eq. (1.16) and the facts that in considering vectors like (3.22) we may set $Q=k''(1-k'')$, $x^{2}=-r^{2}$. In this way we find

$$rJ_{\alpha}r^{-1}\Big|_{\substack{M_{12}=2k-1\\M_{34}=1-2k'\\(k''+,k''+)}}=J_{\alpha}(k'',-).\tag{4.1}$$

The operators on the right are the ones defined in Eq. (I.1.13) in setting up the UIR's D^{-} in a standard form. The similarity transformation needed on the left before achieving the standard form is to compensate for the fact that the measure in the radial integration in (3.23) is $r^{3}\,dr$ unlike the measure $r\,dr$ in Eq. (I.1.8). Therefore, the subspace of $\mathcal{H}$ under consideration carries the UIR $D_{k''}^{-}$ of $SU(1,1)$, in the standard form. This UIR occurs in the decomposition of the particular product $D_{k}^{+}\otimes D_{k'}^{-}$ within $\mathcal{D}^{+}\otimes\mathcal{D}^{-}$, going with the choices $M_{12}=(2k-1)$, $M_{34}=(1-2k')$. Since this subspace in $\mathcal{H}$ exists only when $k'\geq k+1$, we draw the conclusion that $D_{k}^{+}\otimes D_{k'}^{-}$ contains $D_{k''}^{-}$ only if $k'\geq k+1$ and $k''\leq k'-k$. In any case, $k''\geq 1$, so all in all $1\leq k''\leq k'-k$ is the condition for $D_{k''}^{-}$ to occur in $D_{k}^{+}\otimes D_{k'}^{-}$.

In a similar fashion, the restriction of J_{α} to the subspace of vectors of the form (3.24) gives operators in the standard form for the UIR $D_{k''}^{+}$:

$$rJ_\alpha r^{-1}\Big|_{\substack{M_{12}=2k-1\\ M_{34}=1-2k'\\ (k''+,k''-)}} = J_\alpha(k'',+). \tag{4.2}$$

In this case, we substituted $x^2=r^2$ and $Q=k''(1-k'')$ in (1.16); the operators $J_\alpha(k'',+)$ are given in Eq. (I.1.9). This subspace of $\mathcal{H}$ carries the UIR $D^+_{k''}$, and since it exists only when $k \geq k'+1$, we see that the product $D^+_k \otimes D^-_{k'}$ contains $D^+_{k''}$ under the conditions $1 \leq k'' \leq k-k'$.

Finally, the restriction of J_α to the subspace of vectors (3.26) will yield differential operators in r which are simultaneously 2×2 matrices; purely formally we find

$$rJ_\alpha r^{-1}\big|_{M_{12}=2k-1,M_{34}=1-2k',(s\epsilon,s\epsilon)} = J_\alpha(s,\epsilon), \tag{4.3}$$

where the standard operators on the right appear in Eq. (I.1.17). The existence of the present subspace places no conditions on k and k'; ϵ just gets determined by $k+k'$ in the natural way. Of course, establishing Eq. (4.3) is not enough to guarantee that we have found the UIR (s,ϵ) of $SU(1,1)$ in the standard form in the subspace of $\mathcal{H}$ made up of the vectors (3.26). But it is shown in the Appendix, by considering the finite transformation $\exp(i\mu J_0)$ and its action on the vector (3.26), that this is indeed the case. We can then draw the conclusion that within this subspace of $\mathcal{H}$ the outer automorphism τ of $SU(1,1)$ is implemented by the operation of interchanging $f_-(r)$ and $f_+(r)$.

From all these considerations, the structure of the C–G series,

$$D^+_k\otimes D^-_{k'} = \theta(k-k'-1)\sum_{k''\geq 1\,\text{or}\,3/2}^{k-k'} D^+_{k''} + \theta(k'-k-1)\sum_{k''\geq 1\,\text{or}\,3/2}^{k'-k} D^-_{k''} + \int_0^\infty ds\, C^\epsilon_{1/4+s^2}, \tag{4.4}$$

$k, k' = \frac{1}{2}, 1, \frac{3}{2}, \cdots$, $\epsilon = 0(\frac{1}{2})$ and $k''_{\min} = 1(\frac{3}{2})$ if $k+k'=$ integer (half-odd integer)

may be inferred. Here, $\theta(x)=1$ for $x=0,\frac{1}{2},1,\frac{3}{2},\cdots$ and $=0$ for $x=-\frac{1}{2},-1,-\frac{3}{2},\cdots$. We see that the structure of this series is determined by the spectrum of $O(2,2)$ representations in an $O(2)\otimes O(2)$ basis, present in $\mathcal{H}$.

We conclude this section with the construction of the uncoupled and coupled basis vectors for $\mathcal{H}$. Suppose we had used radial and polar variables separately for the pairs x_1x_2 and x_3x_4, namely, set $x_1+ix_2=\rho\exp(i\varphi)$, $x_3+ix_4=\rho'\exp(i\varphi')$. Then, on the basis of our analysis of $\mathcal{D}^\pm$ in Sec. 2 of I, as well as Eq. (I.1.12) and (I.1.14), apart from numerical factors an uncoupled basis vector would be

$$\exp[-i(2k-1)\varphi](\rho)^{2ip-1}\exp[i(1-2k')\varphi'](\rho')^{2ip'-1}. \tag{4.5}$$

This is an eigenvector of M_{12}, $J_2(+,12)$, M_{34}, $J_2(-,34)$ with eigenvalues $(2k-1)$, p, $(1-2k')$, p', respectively. It is a basis vector for the product $D^+_k\otimes D^-_{k'}$. To express this vector in the form of Eq. (2.21), we must relate ρ, φ, ρ', φ' to r, μ, ζ, μ' in V^+ and in V^-. Comparing with Eq. (2.19) we get

$$V^+:\ \rho=r\cosh\zeta/2,\quad \varphi=-\mu_+,\quad \rho'=r\sinh\zeta/2,\quad \varphi'=\pi+\mu_-,$$
$$V^-:\ \rho=r\sinh\zeta/2,\quad \varphi=\pi+\mu_-,\quad \rho'=r\cosh\zeta/2,\quad \varphi'=-\mu_+. \tag{4.6}$$

Then the properly normalized uncoupled basis vector Φ is

$$\Phi^{(k+)(k'-)}_{p\ \ p'} = [r^{2i(p+p')-2}/2\pi^2]\exp[i(k+k'-1)\mu] \times\begin{pmatrix}(-1)^{2k-1}(\sinh\zeta/2)^{2ip-1}(\cosh\zeta/2)^{2ip'-1}\exp[i(k'-k)\mu'] \\ (-1)^{2k'-1}(\cosh\zeta/2)^{2ip-1}(\sinh\zeta/2)^{2ip'-1}\exp[i(k-k')\mu']\end{pmatrix}. \tag{4.7}$$

These vectors obey

$$(\Phi^{(k_1+)(k_1'-)}_{p_1\ \ p_1'}, \Phi^{(k+)(k'-)}_{p\ \ p'}) = \delta_{k_1k}\delta_{k_1'k'}\delta(p_1-p)\delta(p_1'-p'). \tag{4.8}$$

[We are restricting ourselves to nonnegative eigenvalues for M_{12} and nonpositive ones for M_{34} throughout.]

For the coupled basis vectors Ψ in all three cases, namely (3.22), (3.24), (3.26), the radial dependences are determined by the fact that we want J_2 to be diagonal. In addition, in the case of (3.26), the ratio of f_- to f_+ is given by the eigenvalue a of the operator A implementing the automorphism τ. The vectors Ψ and their normalizations follows:

$$\Psi^{(k+)(k'-)(k''+)}_{p''} = \frac{1}{\pi}\left(\frac{2k''-1}{2\pi}\right)^{1/2} r^{2ip''-2} \times\begin{pmatrix}0\\ \mathcal{D}^{(k''+)}_{k+k'-1,k-k'}(\mu\zeta\mu')\end{pmatrix},\quad k-k'\geq k''\geq 1; \tag{4.9a}$$

$$\Psi^{(k+)(k'-)(k''-)}_{p''} = \frac{1}{\pi}\left(\frac{2k''-1}{2\pi}\right)^{1/2}(-1)^{k'-k+\epsilon} r^{2ip''-2} \times\begin{pmatrix}\mathcal{D}^{(k''+)}_{k+k'-1,k'-k}(\mu\zeta\mu')\\ 0\end{pmatrix},\quad k'-k\geq k''\geq 1; \tag{4.9b}$$

$$\Psi^{(k+)(k'-)(s\epsilon)}_{p''a} = \frac{\mu(s,\epsilon)}{2\pi\sqrt{\pi}} r^{2ip''-2} \times\begin{pmatrix}(-1)^{-k'+k+\epsilon}\exp[i\varphi(s,\epsilon)]\mathcal{D}^{(s,\epsilon)}_{k+k'-1,k'-k}(\mu\zeta\mu')\\ a\mathcal{D}^{(s,\epsilon)}_{k+k'-1,k-k'}(\mu\zeta\mu')\end{pmatrix}. \tag{4.9c}$$

Vectors Ψ of distinct types are orthogonal. [In any case, types (a) and (b) do not exist simultaneously.] For the rest

$$(\Psi^{(k_1+)(k_1'-)(k_1''+)}_{p_1''}, \Psi^{(k+)(k'-)(k''+)}_{p''}) = \delta_{k_1k}\delta_{k_1'k'}\delta_{k_1''k''}\delta(p_1''-p''),$$
$$(\Psi^{(k_1+)(k_1'-)(k_1''-)}_{p_1''}, \Psi^{(k+)(k'-)(k''-)}_{p''}) = \delta_{k_1k}\delta_{k_1'k'}\delta_{k_1''k''}\delta(p_1''-p''),$$
$$(\Psi^{(k_1+)(k_1'-)(s_1\epsilon_1)}_{p_1''a_1}, \Psi^{(k+)(k'-)(s\epsilon)}_{p_1''a}) = \delta_{k_1k}\delta_{k_1'k'}\delta(s_1-s)\delta(p_1''-p'') \times\delta_{\epsilon_1\epsilon}\delta_{a_1a}. \tag{4.10}$$

These results are essentially consequences of Eq. (3.6). The normalization conditions (4.8), (4.10) agree with the convention expressed in Eqs. (I.4.4) and (I.4.5).

5. C–G COEFFICIENTS IN A CONTINUOUS BASIS

There are three types of C–G coefficients to be calculated, namely $C(k+k'-\mathcal{R}\,|pp'p''a)$ for $\mathcal{R}=(k''+)$, $(k''-)$ and (s,ϵ). These three coefficients are the scalar products of the uncoupled basis vector Φ in Eq. (4.7) with the coupled ones Ψ in (4.9a, b, c), respectively. The factor $\delta(p+p'-p'')$ will always be present, its coefficients in the three cases, written $\hat{C}(k+k'-\mathcal{R}\,|pp'a)$ will be computed.

From Eqs. (4.7) and (4.9a) we get

$$\hat{C}(k+k'-k''+|pp')=(-1)^{2k'-1}\left(\frac{2k''-1}{2\pi}\right)^{1/2}\times\int_0^\infty d\zeta(\cosh\zeta/2)^{-2ip}(\sinh\zeta/2)^{-2ip'}d^{(k''+)}_{k+k'-1,k-k'}(\zeta). \quad (5.1)$$

In arriving at this result, the trivial integrations over μ, μ', and r have been carried out; the r integration gives us the factor $\delta(p+p'-p'')$ and on dropping it we get the quantity $\hat{C}$. Now the "little-d" function in (5.1) is given by Bargmann; it is the matrix element of the finite $SU(1,1)$ transformation $\exp(i\zeta J_2)$ between eigenstates of J_0 with eigenvalues $k+k'-1$ and $k-k'$, in the UIR $(k''+)$ of $SU(1,1)$. It can be expressed in terms of the hypergeometric function as[11]:

$$d^{(k''+)}_{mn}(\zeta)=\frac{1}{(m-n)!}\left(\frac{(m-k'')!(m+k''-1)!}{(n-k'')!(n+k''-1)!}\right)^{1/2}\times(\cosh\zeta/2)^{-m-n}(\sinh\zeta/2)^{m-n}\times{}_2F_1(k''-n,1-k''-n;1+m-n;-\sinh^2\zeta/2),$$
$$m=k+k'-1\geq n=k-k'\geq 1. \quad (5.2)$$

Instead of using this directly in (5.1), it is convenient to change the argument of the ${}_2F_1$ function to $\tanh^2\zeta/2$ using the transformation[12]

$${}_2F_1(k''-n,1-k''-n;1+m-n;-\sinh^2\zeta/2)=(\cosh\zeta/2)^{2n-2k''}{}_2F_1(k''-n,k''+m;1+m-n;\tanh^2\zeta/2). \quad (5.3)$$

Then, on further substituting $\tanh^2\zeta/2=t$, the ζ integration in (5.1) reduces to the evaluation of

$$\int_0^1 dt\ t^{k'-1-ip'}(1-t)^{k''+ip+ip'-1}{}_2F_1(k''-n,k''+m;1+m-n;t). \quad (5.4)$$

This can be done, the result being essentially a generalized hypergeometric function of the variety ${}_3F_2$; the value of the integral is[13]

$$\frac{\Gamma(k'-ip')\Gamma(k''+ip+ip')}{\Gamma(k'+k''+ip)}\times{}_3F_2\left(\begin{matrix}k''+k'-k,k''+k'+k-1,k'-ip';1\\2k',k'+k''+ip;\end{matrix}\right). \quad (5.5)$$

Putting all the pieces together, the final expression for the $\hat{C}$ coefficient for the product $D^+_k\otimes D^-_{k'}\to D^+_{k''}$ has the appearance

$$\hat{C}(k+k'-k'+|pp')=(-1)^{2k'-1}\left(\frac{2k'-1}{2\pi}\right)^{1/2}\frac{1}{(2k'-1)!}\times\left(\frac{(k+k'-k''-1)!(k+k'+k''-2)!}{(k-k'-k'')!(k+k''-k'-1)!}\right)^{1/2}\times\frac{\Gamma(k'-ip')\Gamma(k''+ip+ip')}{\Gamma(k'+k''+ip)}\times{}_3F_2\left(\begin{matrix}k''+k'-k,k'+k'+k-1,k'-ip';1\\2k',k'+k''+ip;\end{matrix}\right). \quad (5.6)$$

In a similar fashion, the $\hat{C}$ coefficient for the case $D^+_k\otimes D^-_{k'}\to D^-_{k''}$ turns out to be

$$\hat{C}(k+k'-k''-|pp')=(-1)^{2k-1}\left(\frac{2k''-1}{2\pi}\right)^{1/2}\frac{1}{(2k-1)!}\times\left(\frac{(k+k'-k''-1)!(k+k'+k''-2)!}{(k'-k-k'')!(k'+k''-k-1)!}\right)^{1/2}\times\frac{\Gamma(k-ip)\Gamma(k''+ip+ip')}{\Gamma(k+k''+ip')}\times{}_3F_2\left(\begin{matrix}k''+k-k',k''+k+k'-1,k-ip;1\\2k,k+k''+ip;\end{matrix}\right). \quad (5.7)$$

The expressions in (5.6) and (5.7) should be compared to that in Eq. (I.4.11) corresponding to the case $D^+_k\otimes D^+_{k'}\to D^+_{k''}$. In all three cases, the final result consists of just a single term, that being the ${}_3F_2$ function. In all other kinds of products, the $\hat{C}$ coefficients turn out to involve two or more ${}_3F_2$ functions.

The last case to be treated is $D^+_k\otimes D^-_{k'}\to C^\epsilon_q$. Now using Eqs. (4.7) and (4.9c), doing the trivial r, μ, μ' integrations and dropping the factor $\delta(p+p'-p'')$, we arrive at

$$\hat{C}(k+k'-s\epsilon|pp'a)=-\frac{\mu(s,\epsilon)}{2\sqrt{\pi}}\int_0^\infty d\zeta[\exp\{i\varphi(s,\epsilon)\}(-1)^{k+k'-\epsilon}\times(\cosh\zeta/2)^{-2ip'}(\sinh\zeta/2)^{-2ip}d^{(s,\epsilon)}_{k+k'-1,k'-k}(\zeta)+a(-1)^{2k'}\times(\cosh\zeta/2)^{-2ip}(\sinh\zeta/2)^{-2ip'}d^{(s,\epsilon)}_{k+k'-1,k-k'}(\zeta)]. \quad (5.8)$$

Now, these d functions are the matrix elements of $\exp(i\zeta J_2)$ in the $O(2)$ basis, in the UIR C^ϵ_q, $q=\frac{1}{4}+s^2$. They are given by[11]

$$d^{(s,\epsilon)}_{mn}(\zeta)=\frac{1}{(m-n)!}\left(\frac{\Gamma(m+\frac{1}{2}+is)\Gamma(m+\frac{1}{2}-is)}{\Gamma(n+\frac{1}{2}+is)\Gamma(n+\frac{1}{2}-is)}\right)^{1/2}\times(\cosh\zeta/2)^{-m-n}(\sinh\zeta/2)^{m-n}{}_2F_1(\tfrac{1}{2}-n+is,\tfrac{1}{2}-n-is;1+m-n;-\sinh^2\zeta/2),\quad m=k+k'-1\geq n=\pm(k'-k). \quad (5.9)$$

It is again preferable to have $\tanh^2\zeta/2$ as the argument of the ${}_2F_1$ function, and this is achieved using[12]

$${}_2F_1(\tfrac{1}{2}-n+is,\tfrac{1}{2}-n-is;1+m-n;-\sinh^2\zeta/2)=(\cosh\zeta/2)^{2n-2is-1}{}_2F_1(\tfrac{1}{2}-n+is,\tfrac{1}{2}+m+is;1+m-n;\tanh^2\zeta/2) \quad (5.10)$$

which is the same as Eq. (5.3) with k'' replaced by $\frac{1}{2}+is$. Then (5.8) becomes

$$\hat{C}(k+k'-s\epsilon|pp'a)=-\frac{\mu(s,\epsilon)}{2\sqrt{\pi}}[(-1)^{k+k'-\epsilon}\exp\{i\varphi(s,\epsilon)\}\times I(kp,k'p';s)+(-1)^{2k'}aI(k'p',kp;s)],$$

$$I(k'p',kp;s)=\frac{1}{(2k'-1)!}\left(\frac{\Gamma(k+k'-\frac{1}{2}+is)\Gamma(k+k'-\frac{1}{2}-is)}{\Gamma(k-k'+\frac{1}{2}+is)\Gamma(k-k'+\frac{1}{2}-is)}\right)^{1/2}\times\int_0^\infty d\zeta(\cosh^2\zeta/2)^{-k'-i(p+s)}(\sinh^2\zeta/2)^{k'-ip'-1/2}\times{}_2F_1(\tfrac{1}{2}+is+k'-k,-\tfrac{1}{2}+is+k+k';2k';\tanh^2\zeta/2). \quad (5.11)$$

The substitution $\tanh^2\zeta/2=t$ puts the ζ integral in the form

$$\int_0^1 dt\ t^{k'-ip'-1}(1-t)^{-1/2+i(p'+p+s)}{}_2F_1(\tfrac{1}{2}+is+k'-k,-\tfrac{1}{2}+is+k+k';2k';t). \quad (5.12)$$

This is the same integral as appears in (5.4) but with the change $k''\to\frac{1}{2}+is$ (and with $m=k+k'-1$, $n=k-k'$). Likewise its value is given by setting $k''\to\frac{1}{2}+is$ in (5.5). All in all, then, the C–G coefficient in the present case is given by Eq. (5.11) with the value of $I(k'p',kp;s)$ being

$$I(k'p',kp;s)=\frac{1}{(2k'-1)!}\left(\frac{\Gamma(k+k'-\frac{1}{2}+is)\Gamma(k+k'-\frac{1}{2}-is)}{\Gamma(k-k'+\frac{1}{2}+is)\Gamma(k-k'+\frac{1}{2}-is)}\right)^{1/2}$$
$$\times\frac{\Gamma(k'-ip')\Gamma(\frac{1}{2}+i(p+p'+s))}{\Gamma(\frac{1}{2}+k'+i(p+s))}$$
$$\times{}_3F_2\left(\begin{matrix}k'-k+\frac{1}{2}+is,\ k'+k-\frac{1}{2}+is,\ k'-ip';1\\ 2k',\ k'+\frac{1}{2}+i(p+s);\end{matrix}\right). \quad (5.13)$$

In contrast to the purely discrete case, we see then that these C—G coefficients are sums of two terms, each involving the generalized hypergeometric function ${}_3F_2$.

6. SUMMARY

Following the approach of the previous paper, we have related the Clebsch—Gordan problem of $SU(1,1)$ for products of the type $D_k^+\otimes D_{k'}^-$ to the properties of the "spherical harmonics" for the group $O(2,2)$, and thus we have understood in a new way the form of the C—G series in this case. Luckily, the properties of these spherical harmonics could be gleaned from properties of $SU(1,1)$ itself, since locally $O(2,2)$ has the structure $SU(1,1)\otimes SU(1,1)$. The C—G coefficients for such products in a continuous basis have been computed and again are expressible in terms of the ${}_3F_2$ function. For the purely discrete cases, $D^+\otimes D^-\to D^\pm$ the C—G coefficient is just a single term, but in the case $D^+\otimes D^-\to C$ there are two terms. The fact that the two UIR's $D_{1/2}^\pm$ are never contained in a product of the form $D_k^+\otimes D_{k'}^-$ for any values of k and k' whatsoever, including the values $\frac{1}{2}$, is reunderstood in a satisfying manner: it is because these two UIR's are absent in the $SU(1,1)$ Plancherel formula, so we have no "$O(2,2)$ spherical harmonics" corresponding to them.

APPENDIX

We shall explain here the need for the phase $\varphi(s,\epsilon)$ occurring in Eq. (3.26), and then determine it. We have explained in Sec. 1 of I the manner in which the UIR C_q^ϵ of $SU(1,1)$ could be set up in a Hilbert space consisting of pairs of functions $f_1(r), f_2(r)$; the forms for the scalar product and the generators $J_\alpha(s,\epsilon)$ are in Eqs. (I.1.16) and (I.1.17). However, as noted there, the expressions for the generators are purely formal; they must either be supplemented by precise statements about their domains, or alternatively one could directly write down the actions of finite group elements. For example, we have

$$h=\exp[itJ_0(s,\epsilon)]f:$$
$$h_j(r)=\sum_{k=1}^{2}\int_0^\infty dr'\,r'L_{jk}^{(s,\epsilon)}(r,r';t)f_k(r'). \quad (A1)$$

The $L_{jk}^{(s,\epsilon)}$ are known, and the value of $L_{12}^{(s,\epsilon)}$, which is all we will need is[14]:

$$L_{12}^{(s,\epsilon)}(r,r';t)=\frac{-1}{\pi\sin t/2}\exp[(i/2)(r^2-r'^2)\cot t/2]$$
$$\times(\exp[\pi s]+\tilde{\epsilon}\exp[-\pi s])$$
$$\times K_{2is}(rr'/\sin t/2). \quad (A2)$$

(The $\tilde{\epsilon}$ on the right has values ±1 according as $\epsilon=0,\frac{1}{2}$).

Now consider the representations of the groups $SU(1,1)$ and $O(2,2)$ which were both defined in Sec. 1 to act on the Hilbert space $\mathcal{H}$ and which had the property of commuting with one another. By analyzing the $O(2,2)$ representation, we were able to define appropriate "spherical harmonics" in the two regions V^+, V^- of R_4; they served the purpose of fully reducing the representations of $O(2,2)$ occurring in $\mathcal{H}_-$ and $\mathcal{H}_+$, respectively. We are interested in the occurrences of the UIR $(s\epsilon, s\epsilon)$ of $O(2,2)$ in $\mathcal{H}_-$ as well as in $\mathcal{H}_+$. By means of the definitions of $\mathcal{Y}_{(mn)}^{+(\mathcal{R})}(x)$ in Eq. (3.9) and $\mathcal{Y}_{(mn)}^{-(\mathcal{R})}(x)$ in Eq. (3.18), we were able to ensure the complete identity of their transformation laws under $O(2,2)$, for the case $\mathcal{R}=(s,\epsilon)$; this fact is stated in Eq. (3.19). For any set of constants C_{mn}, and for a fixed (s,ϵ), let us consider an element f in $\mathcal{H}$ of the form

$$f=\begin{pmatrix}f_-(r)\,e^{i\varphi(s,\epsilon)}\sum_{mn}C_{mn}\mathcal{Y}_{(mn)}^{-(s,\epsilon)}(x)\\ f_+(r)\qquad\sum_{mn}C_{mn}\mathcal{Y}_{(mn)}^{+(s,\epsilon)}(x)\end{pmatrix}$$
$$=\begin{pmatrix}f_-(r)\,e^{i\varphi(s,\epsilon)}\sum_{mn}C_{mn}(-1)^{n+\epsilon}\mathcal{D}_{m,-n}^{(s\epsilon)}(a(x))\\ f_+(r)\qquad\sum_{mn}C_{mn}\mathcal{D}_{mn}^{(s\epsilon)}(a(x))\end{pmatrix}. \quad (A3)$$

Now the transformations of $O(2,2)$ can in no way "distinguish" between the upper and lower components of such an f since they are constructed in exactly the same way from functions having identical $O(2,2)$ transformation laws. On the other hand, since the transformations of the representation $\mathcal{D}^+\otimes\mathcal{D}^-$ of $SU(1,1)$ commute with $O(2,2)$, they can in no way alter the $O(2,2)$ structure of an element f in $\mathcal{H}$. So for example if $h=\exp[itJ_0]f$, where f is the above vector and J_0 is one of the generators of $\mathcal{D}^+\otimes\mathcal{D}^-$, then h must be of *exactly the same form* as f, with the *same* set of coefficients C_{mn}; the only change can be a replacement of $f_\mp(r)$ by two new radial functions $h_\mp(r)$. We have here essentially the UIR C_q^ϵ of $SU(1,1)$ acting on the pairs of radial functions $f_\mp(r)$. We must now choose the phase $\varphi(s,\epsilon)$ in such a way that the relations that express $h_\mp(r)$ in terms of $f_\mp(r)$ are in exactly the standard form corresponding to the UIR C_q^ϵ, namely, Eq. (A1). The point is that the only freedom we have is in the choice of this phase, and it should be possible to choose it so as to achieve the above purpose.

To fix $\varphi(s,\epsilon)$, it is clearly enough to obtain the connection between $h_-(r)$ and $f_+(r)$, and arrange matters so that precisely the kernel (A2) is required. We must of course get the connection between h_- and f_+ by some global means; this is quite easy since J_0 involves just harmonic oscillator Hamiltonians. In four-dimensional Cartesian variables, we have [cf. Eq. (1.7)][15]

$$J_0=\tfrac{1}{4}(x^\mu x_\mu-\partial^\mu\partial_\mu),$$
$$[\exp(itJ_0)f](x)\equiv h(x;t)=\int d^4x'\,L(x,x';t)f(x'),$$
$$L(x,x';t)=(2\pi\sin t/2)^{-2}\exp[-i((x^2+x'^2)\cos t/2$$
$$-2x\cdot x')/2\sin t/2] \quad (A4)$$

Now suppose $f(x')$ vanishes when $x'\in V^-$, while we want to evaluate $h(x;t)$ for $x\in V^-$. Then we must change variable from x'^μ to r', $\mu_\pm'$, ζ' according to Eq. (2.19a) and from x^μ to r, $\mu_\pm$, ζ according to Eq. (2.19b), and rewrite Eq. (A4). Now the invariants have the values

$$x^2 = -r^2, \quad x'^2 = +r'^2,$$
$$x\cdot x' = rr'(\cosh\zeta/2\sinh\zeta'/2\cos(\mu_+ + \mu'_-) - \sinh\frac{\zeta}{2}$$
$$\times\cosh\frac{\zeta'}{2}\cos(\mu_- + \mu'_+)). \quad \text{(A5)}$$

Writing $h_-(r;\mu\zeta\mu')$ for $h(x)$ when $x\in V^-$, (A4) becomes

$$h_-(r;\mu\zeta\mu') = (2\pi\sin t/2)^{-2}\int_0^\infty 2\pi^2 r'^3 dr' \int_1^\infty \tfrac{1}{2}d\cosh\zeta'$$
$$\times\int_0^{2\pi}\frac{d\mu'_+}{2\pi}\int_0^{2\pi}\frac{d\mu'_-}{2\pi}\exp[(i/2)(r^2 - r'^2)\cot t/2]$$
$$\times\exp\left[i\frac{rr'}{\sin t/2}\left(\cosh\frac{\zeta}{2}\sinh\frac{\zeta'}{2}\times\cos(\mu_+ + \mu'_-) - \sinh\frac{\zeta}{2}\right.\right.$$
$$\left.\left.\times\cosh\frac{\zeta'}{2}\cos(\mu'_+ + \mu_-)\right)\right]f_+(r';\mu''\zeta'\mu'''), \quad \mu'_\pm$$
$$= \tfrac{1}{2}(\mu''' \pm \mu''). \quad \text{(A6)}$$

Let us now put in for f_+ an expression like the second element in the column vector (A3), namely,

$$f_+(r';\mu''\zeta'\mu''') = f_+(r')\sum_{mn} C_{mn}\exp[im\mu'' + in\mu''']d_{mn}^{(s,\epsilon)}(\zeta'). \quad \text{(A7)}$$

Then the integrations over $\mu'_\pm$ can be explicitly carried out using

$$\int_0^{2\pi} d\varphi\,\exp[i(a\cos\varphi \pm m\varphi)] = 2\pi\exp[im\pi/2]J_m(a), \quad \text{(A8)}$$

$J_m(a)$ being the ordinary Bessel function. One then finds

$$h_-(r;\mu\zeta\mu') = (2\sin t/2)^{-2}\sum_{mn} C_{mn}\exp[im\mu]$$
$$\times\exp[-in(\mu' + \pi)]$$
$$\times\int_0^\infty dr' r'^3 f_+(r')\exp[(i/2)(r^2 - r'^2)\cot t/2]\int_1^\infty d\cosh\zeta'$$
$$\times d_{mn}^{(s\epsilon)}(\zeta')J_{m+n}(\alpha)J_{m-n}(\beta),$$
$$\alpha = rr'\sinh\zeta/2\cosh\zeta'/2\Big/\sin t/2, \quad \beta = rr'\cosh\zeta/2$$
$$\times\sinh\zeta'/2\sin t/2. \quad \text{(A9)}$$

The phase $\varphi(s,\epsilon)$ must now be chosen so that this has just the form of the first element in the column vector (A3) and the kernel with which $f_+(r')$ is being integrated is precisely $L_{12}^{(s,\epsilon)}(r, r';t)$ (except for the change in measure $r\,dr$ to $r^3 dr$). That is, for appropriate choice of $\varphi(s,\epsilon)$, the right-hand side of (A9) must coincide with

$$\exp[i\varphi(s,\epsilon)]\sum_{mn} C_{mn}(-1)^{n+\epsilon}\exp[i\mu m]\exp[-i\mu' n]d_{m,-n}^{(s,\epsilon)}(\zeta)\frac{1}{r}$$
$$\times\int_0^\infty r' dr' \times L_{12}^{(s,\epsilon)}(r, r';t)r' f_+(r'). \quad \text{(A10)}$$

Since both C_{mn} and $f_+(r')$ are arbitrary, $\varphi(s,\epsilon)$ is to be determined from the following equality:

$$\int_1^\infty d\cosh\zeta' d_{mn}^{(s,\epsilon)}(\zeta')J_{m+n}(\alpha)J_{m-n}(\beta)$$
$$= \exp[i\varphi(s,\epsilon)]\exp[i\pi(2n + 1 + \epsilon)]\frac{4\sin t/2}{\pi rr'}d_{m,-n}^{(s,\epsilon)}(\zeta)$$
$$\times(e^{\pi s} + \tilde{\epsilon}\,e^{-\pi s})\times K_{2is}(rr'/\sin t/2). \quad \text{(A11)}$$

This is to be valid for all rr', ζ, t, m, and n. For each (s,ϵ), by making particularly simple choices of m, n we can determine $\varphi(s,\epsilon)$.

Take first the case $\epsilon = 0$, when $\tilde{\epsilon} = +1$. It is then simplest to choose $m = n = 0$, and also set $\zeta = 0$. Using, as a particular case of Eq. (5.9),

$$d_{00}^{(s,0)}(\zeta') = F(\tfrac{1}{2} - is,\ \tfrac{1}{2} + is;\ 1;\ -\sinh^2\zeta'/2), \quad \text{(A12)}$$

and also writing u for the combination $rr'/\sin t/2$, (A11) simplifies to

$$\int_1^\infty d\cosh\zeta' F(\tfrac{1}{2} - is,\ \tfrac{1}{2} + is;\ 1;\ -\sinh^2\zeta'/2)J_0(u\sinh\zeta'/2)$$
$$= \{-\exp[i\varphi(s,0)]\}\frac{8\cosh\pi s}{\pi u}K_{2is}(u). \quad \text{(A13)}$$

But the left-hand side is a known integral,[16] and its value happens to be just what multiplies the factor $\{-\exp[i\varphi(s,0)]\}$ on the right; hence we conclude $\varphi(s,0) = \pi$.

Next, when $\epsilon = \frac{1}{2}$ and $\tilde{\epsilon} = -1$, choose $m = -n = \frac{1}{2}$, $\zeta = 0$. In place of (A12), now we use

$$d_{1/2,-1/2}^{(s,1/2)}(\zeta') = -s\sinh(\zeta'/2)F(1 - is,\ 1 + is;\ 2;$$
$$-\sinh^2\zeta'/2). \quad \text{(A14)}$$

Then (A11) simplifies to

$$\int_1^\infty d\cosh\zeta' F(1 - is,\ 1 + is;\ 2;\ -\sinh^2\zeta'/2)(\sinh\zeta'/2)J_1$$
$$\times(u\sinh\zeta'/2)$$
$$= \exp[i(\varphi(s,\tfrac{1}{2}) - \pi/2)]\frac{8\sinh\pi s}{\pi us}K_{2is}(u). \quad \text{(A15)}$$

Once again the left-hand side is a known integral, and its value coincides with the right-hand side save for the first factor.[16] This then yields $\varphi(s,\frac{1}{2}) = \pi/2$, so $\varphi(s,\epsilon)$ is fully determined.

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[1] B. Radhakrishnan and N. Mukunda, J. Math. Phys. 15, 000 (1974). The notation of this paper will be followed in the present work.

[2] These representations and their properties are given in Sec. 2, Ref. 1.

[3] The nature of this restriction is explained in the next section.

[4] Actually, each such product appears four times since each D_k^+ occurs twice in $\mathcal{D}^+$ and each D_k^- twice in $\mathcal{D}^-$, except for the cases $k = k' = \frac{1}{2}$.

[5] V. Bargmann, Ann. Math. 48, 568 (1947), especially Secs. 12 and 13.

[6] The transformation P does not commute with the transformations of $O(2,2)$. Specifically, we have $PL(g)P^{-1} = L(g)$ but $PR(g)P^{-1} = R(\tau(g))$.

[7] Reference 5, p. 595.

[8]For a reason that will be clear later, we prefer to list f_- first, f_+ second. It is so that the UIR C_q^ϵ encountered in the reduction of $D_k^+ \otimes D_{k'}^-$ be obtained in the standard form of I.

[9]This statement is not quite correct; the superscript $\mathcal{R}$ does not denote a UIR of $O(2,2)$, that is to be denoted by $(\mathcal{R}, \mathcal{R})$ or $(\mathcal{R}, \tau(\mathcal{R}))$ which becomes cumbersome to write.

[10]Comparing Eqs. (3.9) and (3.18), we see that if $\mathcal{R} = (k, \eta)$, the ranges of m, n are $\pm(k, k+1, \cdots)$ for $\mathcal{Y}^{+(\mathcal{R})}_{\{mn\}}(x)$ according as $\eta = \pm$, while in the case of $\mathcal{Y}^{-(\mathcal{R})}_{\{mn\}}(x)$ the ranges of m and $-n$ are $\pm(k, k+1, \cdots)$.

[11]Reference 5, p. 628.

[12]N. N. Lebedev, *Special Functions and their Applications* (Prentice-Hall, Englewood Cliffs, N. J., 1965), Eq. (9.5.2).

[13]I. S. Gradshtyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1965), p. 849, formula (7.512.5).

[14]N. Mukunda and B. Radhakrishman, J. Math. Phys. 14, 254 (1973). K here is the MacDonald function.

[15]We have used a result in R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965), p. 63.

[16]*Bateman Manuscript Project, Tables of Integral Transforms*, edited by A. Erdelyi (McGraw-Hill, New York, 1954), Vol. 2, p. 81, formula 8.17(3). Note that the conditions on the parameters that are given in this reference are those that follow from naive power-counting, disregarding the oscillatory behavior of the Bessel function at infinity. A similar comment applies to our use of the formula quoted in Ref. 13.

C^*-algebraic formalism for coarse graining. I. General theory*†

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Bernouilli's principle of insufficient reason is formulated in a noncommutative C^*-algebraic generalization of probability theory. This idea is developed here for general quantum systems, and a simple illustration of it is given. Subsequent papers in this series will deal with more sophisticated models.

INTRODUCTION

This paper, the first in a series, is organized in the following manner. In Sec. 1 we present the general formalism we want to propose. Section 2 is an outlook, in which we examine some of the possible applications of this formalism. Section 3 contains a most simple illustration of the ideas put forward in Sec. 1.

1. THE GENERAL FORMALISM

Various generalizations of the related concepts of coarse graining *a priori* probability and conditional expectation from classical probability theory to the noncommutative probability theory of quantum mechanics have appeared in the literature for the past twenty years.[1-3] However, the continuity of the one-particle momentum spectrum in infinitely extended quantum systems renders their momentum coarse graining at once physically desirable and beyond the scope of these papers. The present paper offers a general formalism which allows, in particular, a proper definition of the momentum coarse-graining operation. This specific application will be discussed in details in subsequent papers in this series, for we want to concentrate here on the general formalism. For illustrative purposes, however, we include in the present paper a very simple model which we treat in accordance with our formalism.

A C^*-algebraic[4] framing of the probabilistic concepts referred to above has been suggested by one of us (GGE). Recalling the main points, let $\mathfrak{A}$ be the C^*-algebra (with unit) of observables of a physical system Σ, and let $\mathfrak{S}$ denote the set of states on $\mathfrak{A}$. By necessity or by choice an incomplete set of observables $\mathcal{P}$, assumed to be a C^*-subalgebra (with unit) of $\mathfrak{A}$, is selected for experimental observation. The experimental determination, through $\mathcal{P}$, of a state ρ_0 of Σ provides then only partial information about the state of the system; this information is summarized by the restriction $\hat{\rho}_0$ of ρ_0 to $\mathcal{P}$. The question now is whether a rational choice for ρ_0 can be made based on the known information given by $\hat{\rho}_0$, or, equivalently, whether a "best bet" for the remaining expectation values can be placed. To answer this question, one must choose among the nonempty (2.10.1 of Ref. 5) subset $E\hat{\rho}_0 \subseteq \mathfrak{S}$ of all extensions of $\hat{\rho}_0$ to $\mathfrak{A}$. The states $\rho \in E\hat{\rho}_0$, which by definition have the same restriction to $\mathcal{P}$, are termed $\mathcal{P}$-equivalent.

Our criterion for choosing the bettor's extension $\bar{\hat{\rho}}_0$ of $\hat{\rho}_0$ is a refinement of Bernoulli's "principle of insufficient reason." In the physical models considered below there exists a symmetry group G of automorphisms of $\mathfrak{A}$, which is conjugate to $\mathcal{P}$ in the sense that $\mathcal{P}$ is the set of all G-invariant elements of $\mathfrak{A}$, $\mathcal{P} \equiv \mathfrak{A}^G$. The existence of the conjugate pair $(\mathcal{P}, G)$ is expected on physical grounds: An observed effect E is experimentally shown to depend upon $\mathcal{P}$ only by demonstrating that transformation by G does not affect the result. Considering $\mathcal{P}$ to be the momentum observables of a one-particle system in free space and G to be the group of space translations illustrates this point. Now, since G acts trivially on $\mathcal{P}$, one possesses "insufficient reason," on the basis of the determination of $\hat{\rho}_0$, to favor the assignment to $\langle \bar{\hat{\rho}}_0 : S\rangle$ of any value different from that assigned to $\langle \bar{\hat{\rho}}_0 : gS\rangle$ for any $S \in \mathfrak{A}$ or any $g \in G$. Therefore, the bettor's extension must be G-invariant. If there should exist a unique G-invariant extension of $\hat{\rho}_0$ to $\mathfrak{A}$, it is then the "best bet" for ρ_0. It is important to realize at this point that the question of whether or not the odds warrant betting at all is not considered here. In applications to generalized master equations,[6] this question must be resolved by detailed analysis of the "interference term." We shall seek, therefore, to establish that the following property holds for some models Σ to be considered below.

Property C: Let $(\mathfrak{A}, \mathcal{P}, G)$ be defined as above. Then, each state $\hat{\rho}$ on $\mathcal{P}$ admits exactly one G-invariant extension to $\mathfrak{A}$.

When this property C is established for a model Σ, one can define, as we shall presently see: the *a priori* probability assignment conditional upon $\mathcal{P}$; the $\mathcal{P}$-coarse graining map; and, with other mild restrictions (Lemma 1.5), the $\mathcal{P}$-conditional expectation.

The a priori probability assignment conditional upon $\mathcal{P}$: Suppose that Σ possesses property C. Denote by $\mathcal{E}^*(\hat{\omega}|\mathcal{P})$ the unique G-invariant extension to $\mathfrak{A}$ of the state $\hat{\omega}$ on $\mathcal{P}$. The map $\mathcal{E}^*(\cdot|\mathcal{P}):\mathfrak{S}(\mathcal{P}) \to \mathfrak{S}^G$, of the set $\mathfrak{S}(\mathcal{P})$ of all states on $\mathcal{P}$ into the set $\mathfrak{S}^G$ of all G-invariant states on $\mathfrak{A}$, is an affine bijection called the *a priori* probability assignment conditional upon $\mathcal{P}$.

The $\mathcal{P}$-coarse graining operator: Let ω be any state on $\mathfrak{A}$ and denote by $\hat{\omega}$ its restriction on $\mathcal{P}$. The mapping $\mathcal{D}(\cdot|\mathcal{P}) : \mathfrak{S} \to \mathfrak{S}^G$, defined by $\mathcal{D}(\omega|\mathcal{P}) = \mathcal{E}^*(\hat{\omega}|\mathcal{P})$ is an affine surjection called the $\mathcal{P}$-coarse graining operator. For each $\omega \in \mathfrak{S}$, $\mathcal{E}^*(\hat{\omega}|\mathcal{P})$ is the maximal "coarsening" of ω which preserves the $\mathcal{P}$-information content of ω, and it is the "best bet" for ω based upon the partial information obtainable by observation of $\mathcal{P}$ only.

The $\mathcal{P}$-conditional expectation: The term "$\mathcal{P}$-conditional expectation" shall be reserved for a map $\mathcal{E}(\cdot|\mathcal{P}) : \mathfrak{A} \to \mathcal{P}$ whose dual coincides on $\mathfrak{S}(\mathcal{P})$ with $\mathcal{E}^*(\cdot|\mathcal{P})$

and which possesses the following properties:

(i) $\mathcal{E}(\lambda S+\gamma T|\mathcal{P})=\lambda\mathcal{E}(S|\mathcal{P})+\gamma\mathcal{E}(T|\mathcal{P})\ \forall S, T\in\mathfrak{A}, \forall\lambda,\gamma\in\mathbb{C}$,

(ii) $\mathcal{E}(S^*S|\mathcal{P})\geq 0\ \forall\ S\in\mathfrak{A}$,

(iii) $\mathcal{E}(1|\mathcal{P})=1$,

(iv) $\mathcal{E}(S\mathcal{E}(T|\mathcal{P})|\mathcal{P})=\mathcal{E}(S|\mathcal{P})\ \mathcal{E}(T|\mathcal{P})\ \forall S, T\in\mathfrak{A}$,
$\mathcal{E}(\mathcal{E}(T|\mathcal{P})S|\mathcal{P})=\mathcal{E}(T|\mathcal{P})\ \mathcal{E}(S|\mathcal{P})$.

It would be consistent with Halmos' nomenclature[7] to call our $\mathcal{P}$-coarse graining operator a $\mathcal{P}$-conditional expectation. However, we prefer to follow here Umegaki's notation.[1]

We shall prove in Theorem 1.6 that if G is amenable[8] and if $(\mathfrak{A}, G)$ admits at least one faithful (for $\mathfrak{A}$), covariant representation, Property C ensures existence of $\mathcal{E}(\cdot|\mathcal{P})$; uniqueness is inherent to its definition.

We first examine some of the consequences of amenability of G.

1.1 *Lemma*: Let G be a topological group, let $\mathfrak{A}$ be a C^*-algebra with unit, and let $\alpha: G\to\mathrm{Aut}\,\mathfrak{A}$ be a strongly continuous homomorphism of G into the automorphism group of $\mathfrak{A}$. Denote by $\mathfrak{A}^G$ (resp. $\mathfrak{A}^{*G}$) the set of all G-invariant elements of $\mathfrak{A}$ (resp. $\mathfrak{A}^*$). Let η be a mean on CB(G). Then,

(a) For each continuous linear form ϕ on $\mathfrak{A}$, the mapping $\eta^*\phi:\mathfrak{A}\to\mathbb{C}$, defined by $\langle\eta^*\phi:S\rangle=\eta\langle\phi:\alpha_{(\cdot)}S\rangle\ \forall\ S\in\mathfrak{A}$, is also a continuous linear form on $\mathfrak{A}$.

(b) The mapping $\eta^*:\mathfrak{A}^*\to\mathfrak{A}^*$ defined in (a) enjoys the following properties:

(0) $\eta^*(\lambda\phi+\gamma\psi)=\lambda\eta^*\phi+\gamma\eta^*\psi\ \forall\ \phi,\ \psi\in\mathfrak{A}^*, \forall\lambda,\ \gamma\in\mathbb{C}$;

(i) $\|\eta\phi\|\leq\|\phi\|\ \forall\ \phi\in\mathfrak{A}^*$;

(ii) $\phi\geq 0\Rightarrow\eta^*\phi\geq 0\ \forall\phi\in\mathfrak{A}^*$;

(iii) $\langle\eta^*\phi:1\rangle=\langle\phi:1\rangle\ \forall\ \phi\in\mathfrak{A}^*$;

(iv) $\eta^*\phi\circ S=\eta^*(\phi\circ S)$,
$S\circ\eta^*\phi=\eta^*(S\circ\phi),\ \forall S\in\mathfrak{A}^G, \forall\phi\in\mathfrak{A}^*$;

(v) $\eta^*\phi\in\mathrm{Co}\{\alpha_g^*\phi\,|\,g\in G\}^{-w^*}\ \forall\ \phi\in\mathfrak{A}^*$;

(vi) if η is an invariant mean, then $\alpha_g^*\eta^*\phi=\eta^*\alpha_g^*\phi=\eta^*\phi\ \forall g\in G, \forall\phi\in\mathfrak{A}^*$, and η^* is a parallel projector.

The proof of this result is analogous to that used by Radin.[9]

1.2 *Corollary*: Let G be an amenable topological group. Then, there exists at least one G-invariant extension of each state $\hat{\rho}$ on $\mathfrak{A}^G\equiv\mathcal{P}$.

Proof: Notice first that $E\hat{\rho}$ is a convex, w^*-closed, G-stable, nonempty subset of $\mathfrak{S}$. Let η be any invariant mean on CB(G), and let $\psi\in E\hat{\rho}$. Then, by (v) $\eta^*\psi\in\mathrm{Co}\{\alpha_g^*\psi\,|\,g\in G\}^{-w^*}\subseteq E\hat{\rho}$, and by (vi) $\eta^*\psi$ is G-invariant. To sum up, amenability of G in a model system Σ assures existence of a G-invariant extension to $\mathfrak{A}$ of each state of $\mathcal{P}$, i.e., guarantees the existence part of Property C. Uniqueness remains to be proven independently.

Property C is rather stringent, as illustrated by the following result.

1.3 *Corollary*: For any state $\hat{\rho}$ on $\mathcal{P}$, let $M=\cap_{\psi\in E\hat{\rho}}\mathrm{Co}\{\alpha_g^*\psi\,|\,g\in G\}^{-w^*}$. When G is amenable, the following conditions are equivalent:

(i) $\mathfrak{S}^G\cap E\hat{\rho}$ contains exactly one point;

(ii) M is not empty.

Proof: From Cor. 1.2 we have already that $\mathfrak{S}\cap E\hat{\rho}$ is not empty. For the present corollary it is therefore sufficient to prove that $\psi\neq\phi$ both in $\mathfrak{S}^G\cap E\hat{\rho}$ occurs exactly when M is empty, but this follows immediately from the proof of Cor. 1.2 and from the construction of M.

1.4 *Lemma*: Let G be a topological group, let $\mathcal{N}$ be a von Neumann algebra acting on a Hilbert space $\mathcal{H}$, and let $\alpha: G\to\mathrm{Aut}\mathcal{N}$ be a strongly continuous homomorphism of G into the automorphism group of $\mathcal{N}$. Denote by $\mathcal{N}^G$ the set of all G-invariant elements of $\mathcal{N}$. Let η be a mean on CB(G). Then,

(a) For each $S\in\mathcal{N}$, the mapping $\eta^b S:\mathcal{N}_*\to\mathbb{C}$, defined by $\langle\phi:\eta^b S\rangle=\eta\langle\phi:\alpha_{(\cdot)}S\rangle\ \forall\phi\in\mathcal{N}_*$ is a continuous linear form on $\mathcal{N}_*$, and therefore defines an element of $\mathcal{N}$.

The mapping $\eta^b:\mathcal{N}\to\mathcal{N}$ defined in (a) enjoys the following properties:

(0) $\eta^b(\lambda S+\gamma T)=\lambda\eta^b S+\gamma\eta^b T\ \ \forall\lambda,\gamma\in\mathbb{C}, \forall S, T\in\mathcal{N}$;

(i) $\|\eta^b S\|\leq\|S\|\ \ \forall S\in\mathcal{N}$;

(ii) $\eta^b(S^*S)\geq 0\ \ \forall S\in\mathcal{N}$;

(iii) $\eta^b(1)=1$;

(iv) $\eta^b(ST)=\eta^b S\cdot T\ \ \forall S\in\mathcal{N}, \forall T\in\mathcal{N}^G$,
$\eta^b(TS)=T\eta^b S$;

(v) $\eta^b S\in\mathrm{Co}\{\alpha_g S\,|\,g\in G\}^{-\mathrm{ultraweak}}$;

(vi) If η is an invariant mean, then

$\eta^b S=\alpha_g\eta^b S=\eta^b\alpha_g S\ \forall g\in G, \forall S\in\mathcal{N}$, and η^b is a G-invariant, $\mathcal{N}^G$-conditional expectation in the sense of Umegaki.[1] The proof is analogous to that presented on p. 180 of Ref. 10.

1.5 *Lemma*: With the assumptions and notation of Lemma 1.4, suppose further that (i) η is an invariant mean, (ii) there exists a C^*-subalgebra (with unit) $\mathfrak{A}$ of $\mathcal{N}$ which is stable under the action of G, and (iii) there exists precisely one G-invariant extension to $\mathfrak{A}$ of each state $\hat{\omega}$ on $\mathcal{P}\equiv\mathfrak{A}^G$. Then:

(a) For each $S\in\mathfrak{A}$, $\eta^b S$ is the unique G-invariant element of $\mathrm{Co}\{\alpha_g S\,|\,g\in G\}^{-\mathcal{N}}$;

(b) $\eta^b\mathfrak{A}=\mathcal{P}$, and $(\eta^b|_{\mathfrak{A}})^*\ \hat{\rho}=\mathcal{E}^*(\hat{\rho}|\mathcal{P})\ \forall\hat{\rho}\in\mathfrak{S}(\mathcal{P})$.

Proof: (*ad*a) Let η be an invariant mean on CB(G) and let $\eta^*:\mathcal{N}^*\to\mathcal{N}^*$ be defined as in Lemma 1.1, and $\eta^b:\mathcal{N}\to\mathcal{N}^G$ as in Lemma 1.4. Now let ϕ be an arbitrary state on $\mathcal{N}$. Then, by virtue of Lemmas 1.1 (iii, iv, vi) and 1.4 (iii, iv, vi), $\phi\circ\eta^b|_{\mathfrak{A}}$ and $\eta^*\phi|_{\mathfrak{A}}$ are two G-invariant states on $\mathfrak{A}$ whose restriction to $\mathcal{P}$ is $\widehat{\phi|_{\mathfrak{A}}}$. From the uniqueness assumption of the present lemma,

$$\phi\circ\eta^b|_{\mathfrak{A}}=\eta^*\phi|_{\mathfrak{A}}=\mathcal{E}^*(\widehat{\phi|_{\mathfrak{A}}}\,|\mathcal{P}). \tag{1.1}$$

Now let $\{M_\beta\}_{\beta\in I}$ be a net of discrete means convergent in the w^*-topology of CB(G)* to η.[8] Then,[11] for ϕ on $\mathcal{N}$,

$$\eta^*\phi=\sigma(\mathcal{N}^*,\mathcal{N})-\lim_{\beta\in I}M_\beta^*\phi. \tag{1.2}$$

Therefore, for each $S \in \mathfrak{A}$ Eqs. (1.1) and 1.2) imply

$$\langle \eta^* \phi : S\rangle = \lim_{B\in I}\langle \phi : M_B^b S\rangle = \langle \phi : \eta^b S\rangle. \tag{1.3}$$

It follows by linearity and the arbitrariness of ϕ that

$$\eta^b S = \sigma(\mathcal{N}, \mathcal{N}^*) - \lim_{B\in I} M_B^b S \quad \forall S \in \mathfrak{A}. \tag{1.4}$$

Thus, for each $S = \mathfrak{A}$, $\eta^b S \in \mathrm{Co}\{\alpha_g S \mid g \in G\}^{-\mathrm{weak}} = \mathrm{Co}\{\alpha_g S \mid g \in G\}^{-N}$ by Mazur's theorem (V. 3.13 of Ref. 12). Suppose now that $\bar{S} \neq \bar{S}'$ are two G-invariant elements of $\mathrm{Co}\{\alpha_g S \mid g \in G\}^{-N}$. Choose a state ϕ on $\mathcal{N}$ such that $\langle \phi : \bar{S}\rangle \neq \langle \phi : \bar{S}'\rangle$. By G-invariance of η and by continuity $\langle \eta^*\phi : T\rangle = \langle \eta^* \phi : S\rangle\ \forall T \in \mathrm{Co}\{\alpha_g S \mid g \in G\}^{-N}$. Thus, we have the contradiction: $\langle \phi : \bar{S}\rangle = \langle \eta^*\phi : \bar{S}\rangle = \langle \eta^*\phi : \bar{S}'\rangle = \langle \phi : \bar{S}'\rangle$. This proves (a).

(adb) That $\eta^b \mathfrak{A} = \mathcal{P}$ follows from (a) and the stability of $\mathfrak{A}$ under G. The second assertion then follows from Eq. (1.1).

The following result then follows immediately from the above lemma.

1.6 *Theorem*: Let $(\mathfrak{A}, \mathcal{P}, G)$ be the triple formed by a C^*-algebra $\mathfrak{A}$ (with unit), a C^*-subalgebra (with unit) $\mathcal{P}$ of $\mathfrak{A}$, and a continuous group G of automorphisms of $\mathfrak{A}$ such that $\mathcal{P}$ is the set of G-invariant elements of $\mathfrak{A}$. Suppose further that

(i) G is amenable,

(ii) $(\mathfrak{A}, \mathcal{P}, G)$ satisfies Property C,

(iii) $\exists$ a covariant representation $(\pi(\mathfrak{A}), U_\pi(G))$ of $(\mathfrak{A}, G)$ in the set of all bounded operators $B(\mathcal{H})$ on some Hilbert space $\mathcal{H}$ such that $\pi : \mathfrak{A} \to B(\mathcal{H})$ is faithful.

Then, the $\mathcal{P}$-conditional expectation $\mathcal{E}(\cdot \mid \mathcal{P}) : \mathfrak{A} \to \mathcal{P}$ is defined and unique.

Actually, in applications of this theorem to various models it is often sufficient to establish a weakened form of Property C; we establish the existence of a unique G-invariant extension of each state defined on some $P \subseteq \mathfrak{A}^G$ instead of on $\mathfrak{A}^G$ itself. When G is amenable, this weakening is of no consequence as seen from the following result.

1.7 *Proposition*: Let $(\mathfrak{A}, \mathcal{P}, G)$ be the triple formed by a C^*-algebra $\mathfrak{A}$, a C^*-subalgebra (with unit) $\mathcal{P}$ of $\mathfrak{A}$, and a continuous group G of automorphisms of $\mathfrak{A}$ such that $\mathcal{P} \subseteq \mathfrak{A}^G$. Suppose further that

(i) G is amenable,

(ii) each state on $\mathcal{P}$ admits a unique G-invariant extension to $\mathfrak{A}$.

Then, $\mathcal{P} = \mathfrak{A}^G$.

Proof: Suppose that $\mathcal{P} \neq \mathfrak{A}^G$. Then, by 11.3.1 of Ref. 5, there exist states $\psi \neq \psi'$ on $\mathfrak{A}^G$ such that $\langle \psi : S\rangle = \langle \psi' : S\rangle$ $\forall S \in \mathcal{P}$. Thus, by hypothesis (i) and Cor. 1.2 there exist G-invariant extensions $\bar{\psi}$ and $\bar{\psi}'$ of ψ and ψ', respectively, to $\mathfrak{A}$. By construction $\langle \psi : S\rangle = \langle \psi' : S\rangle$ $\forall S \in \mathcal{P}$, and $\bar{\psi} \neq \bar{\psi}'$. This contradicts hypothesis (ii). Hence $\mathcal{P} = \mathfrak{A}^G$.

2. OUTLOOK

The interest of the results presented in Sec. 1 is that the conditions under which they are valid are satisfied in models of physical relevance. Our principal motivation was indeed to develop a formalism in which the momentum coarse graining of infinitely extended quantum systems can be properly defined so that applications to nonequilibrium statistical mechanics can be envisaged.

In particular, one of us has shown[4] that, in the heretofore available formalism, the generalized master equation (GME) for momentum observables of quantum systems in finite volume[13] cannot have the semigroup or Markoff property without being trivial. On the other hand, we have shown with a dissipative model[14] that this no-go result must be bypassed for at least one infinitely extended quantum system. Many other authors (cf. Ref. 6) have indeed emphasized the necessity of continuity of the one-particle momentum spectrum for explanation of dissipation at the macroscopic level of quantum mechanics.

The advantage of our C^*-algebraic formulation is demonstrated by its ability to describe the momentum coarse graining of infinitely extended quantum systems, whereas the continuity of the one-particle momentum spectrum was an essential obstacle (cf, Ref. 2, Prop. 5, and Ref. 3, Cor. 3.1) in doing so within the framework provided by the previous von Neumann algebraic formulations.

As an illustration of the physical content of the mathematical structure analyzed in Sec. 1, we establish in the next section that Property C is satisfied for momentum coarse graining of multiparticle quantum systems in free space and demonstrate that the $\mathcal{P}$-coarse graining operator may be heuristically identified with the "diagonal part operator with respect to the basis of plane waves."

This shows in a most simple example that the considerations presented in this paper do make contact with the physical world. More complicated situations will be discussed along these lines in subsequent papers[15,16] in this series.

3. MOMENTUM COARSE GRAINING OF MULTIPARTICLE QUANTUM SYSTEMS IN FREE SPACE

Let Σ be a quantum mechanical system constituted by a single particle confined to move on the configuration space $\mathbb{R}$. We first describe this system in the C^*-algebraic language of the introduction and show that it possesses Property C, where $\mathcal{P}$ is the C^*-algebra of momentum observables and where G is the group of space translations. We further show that the additional conditions of Theorem 1.6 are satisfied so that all the terms defined in the introduction (i.e., coarse graining, *a priori* probability assignment, and conditional expectation) have unambiguous meaning for this model.

Let $\mathcal{H} \equiv \mathcal{L}^2(\mathbb{R})$ be the Hilbert space of all square integrable functions on the real line $\mathbb{R}$. Denote by $\mathcal{S}(\mathbb{R})$ the set of all infinitely differentiable, complex-valued functions on $\mathbb{R}$ for which

$$\lim_{|x|\to\infty} x^N \frac{d^M f}{dx^M}(x) = 0 \quad \forall N, M \in \mathbb{Z}^+. \tag{3.1}$$

Let P and Q be the momentum and position operators defined on $\mathcal{S}(\mathbb{R})$ by

$$\left.\begin{aligned}(Qf)(x)&=xf(x)\\(Pf)(x)&=-i\frac{df}{dx}(x)\end{aligned}\right\}\ \forall f\in\mathcal{S}(\mathbb{R}).\tag{3.2}$$

Since P and Q are each essentially self-adjoint on $\mathcal{S}(\mathbb{R})$, Eqs. (1.2) define P and Q as self-adjoint operators on $\mathcal{L}^2(\mathbb{R})$. P and Q generate via Stone's theorem strongly continuous one-parameter unitary groups on $\mathcal{L}^2(\mathbb{R})$:

$$\begin{aligned}U(a)&=\exp(-iaP)\quad\forall a\in\mathbb{R},\\V(b)&=\exp(-ibQ)\quad\forall b\in\mathbb{R}.\end{aligned}\tag{3.3}$$

$U(a)$ and $V(b)$ satisfy the Weyl form of the canonical commutation relations (CCR's).

$$U(a)\,V(b)=V(b)\,U(a)\exp(iab)\quad\forall a,b\in\mathbb{R}.\tag{3.4}$$

The C^*-algebra $\mathfrak{A}$ generated in $\mathcal{B}(\mathcal{L}^2(\mathbb{R}))$ by $\{U(a)\,V(b)\,|\,a,\ b\in\mathbb{R}\}$ describes the momentum and position observables of a particle on the configuration space $\mathbb{R}$. The C^*-subalgebra $\mathcal{P}$ generated by $\{U(a)\,|\,a\in\mathbb{R}\}$ describes the momentum observables. The group G, conjugate to $\mathcal{P}$, is identified with the group of space translations. This group is represented in the automorphism group of $\mathcal{B}(\mathcal{L}^2(\mathbb{R}))$ by a strongly continuous homomorphism α defined by

$$\alpha_aS\equiv U(a)\,S\,U(-a)\quad\forall a\in\mathbb{R},\forall S\in\mathcal{B}(\mathcal{L}^2(\mathbb{R})).\tag{3.5}$$

For each $a\in\mathbb{R}$, α_a restricts to an automorphism of $\mathfrak{A}$.

We now recall a result identifying the translationally invariant states on $\mathfrak{A}$.

3.1 *Lemma*: Let ω be a G-invariant state on $\mathfrak{A}$ and denote by $\hat{\omega}$ its restriction to $\mathcal{P}$. Then, $\langle\omega:U(a)\,V(b)\rangle=\delta_{b,0}\langle\hat{\omega}:U(a)\rangle\ \forall\,a,b\in\mathbb{R}$.

Proof: See p. 232 in Ref. 10.

Since $\mathfrak{A}_0\equiv\mathcal{L}\{U(a)\ V(b)\,|\,a,\ b\in\mathbb{R}\}$ is a dense linear subset of $\mathfrak{A}$, Lemma 3.1 implies, by linearity and continuity, uniqueness of any G-invariant extension of $\hat{\omega}$. This, with amenability of G (Cor. 1.2), gives the following:

3.2 *Proposition*: Let $(\mathfrak{A},\mathcal{P},G)$ be as above. For each state $\hat{\omega}$ on $\mathcal{P}$, there exists precisely one G-invariant extension to $\mathfrak{A}$. This established Property C.

We now investigate the momentum coarse graining of the normal states on $\mathcal{B}(\mathcal{L}^2(\mathbb{R}))$, heuristically identifying $\mathcal{D}(\cdot\,|\,\mathcal{P})$ with the "diagonal part operator with respect to the basis of plane waves."

The mapping $j:\mathcal{L}^\infty(\mathbb{R})\to\mathcal{B}(\mathcal{L}^2(\mathbb{R}))$ of the set of all essentially bounded functions on $\mathbb{R}$ into $\mathcal{B}(\mathcal{L}^2(\mathbb{R}))$, defined by

$$j(f)=\int_{\mathbb{R}}f(k)\,dE_k,\tag{3.6}$$

where dE is the spectral measure associated with the momentum operator P, is (see Ref. 17, 1.7.3 Th. 2) a C^*- and W^*-isomorphism of $\mathcal{L}^\infty(\mathbb{R})$ onto the maximal Abelian von Neumann algebra to which P is affiliated. Let $e_a\in\mathcal{L}^\infty(\mathbb{R})$ denote $\exp[-ia(\cdot)]$. Since

$$j(e_a)=\int_{\mathbb{R}}\exp(-iak)\,dE_k=\exp(-iaP)=U(a)\quad\forall a\in\mathbb{R},\tag{3.7}$$

j establishes a C^*-isomorphism of AP($\mathbb{R}$), the space of almost periodic functions, onto the C^*-algebra $\mathcal{P}$.

Now let χ_{k_0} be the state on AP($\mathbb{R}$) defined by evaluation at k_0: $\langle\chi_{k_0}:f\rangle=f(k_0)\ \forall f\in\text{AP}(\mathbb{R})$. $\hat{k}_0\equiv j^{*-1}\chi_{k_0}$ is therefore a state on $\mathcal{P}$ defined by continuous linear extension from

$$\langle\hat{k}_0:U(a)\rangle=\exp(-iak_0)\ \forall\,a\in\mathbb{R}.\tag{3.8}$$

Now define $\bar{k}_0\equiv\mathcal{E}^*(\hat{k}_0\,|\,\mathcal{P})$. Since $\bar{k}_0$ is translation invariant, dispersion free on $\mathcal{P}$ and satisfies $\langle\bar{k}_0:\exp(-iPa)\rangle=\exp(-ik_0a)$, $\bar{k}_0$ is interpreted as the plane wave state with wave vector k_0.

3.3 *Proposition*: Let ρ be a density matrix whose Fourier transform has continuous symmetric kernel $\mathcal{F}\rho\mathcal{F}^{-1}(k,k')$ with compact support on

$$\mathbb{R}^2[\text{i.e., }\mathcal{F}\rho f(k)=\int dk'\,\mathcal{F}\rho\mathcal{F}^{-1}(k,k')\,\mathcal{F}f(k')].$$

Then

$$\langle D(\rho\,|\,\mathcal{P}):S\rangle=\int_{\mathbb{R}}dk\,\mathcal{F}\rho\mathcal{F}^{-1}(k,k)\langle\bar{k}:S\rangle\quad\forall S\in\mathfrak{A}.$$

Proof: We first prove that the right-hand side actually defines a state on $\mathfrak{A}$. Since $\mathcal{F}\rho\mathcal{F}^{-1}(k,k)\geq 0$, and since $\int dk\,\mathcal{F}\rho\mathcal{F}^{-1}(k,k)=1$, it suffices to show that the function $\langle\bar{k}:S\rangle$ is measurable for each $S\in\mathfrak{A}$, but this follows from

$$\langle\bar{k}:S\rangle=\langle\bar{0}:V(-k)\,SV(k)\rangle\quad\forall k\in\mathbb{R}.\tag{3.9}$$

and the fact that this is a continuous function of k. Therefore, the right-hand side defines a state on $\mathfrak{A}$. To prove equality, of the rhs with lhs of the conclusion, it is sufficient by Proposition 3.2, to prove that ρ agrees with the right-hand side when restricted to $\mathcal{P}$. It clearly suffices to show that

$$\langle\rho:U(a)\rangle=\int_{\mathbb{R}}dk\,\mathcal{F}\rho\mathcal{F}^{-1}(k,k)\exp(-ika)\quad\forall a\in\mathbb{R}.\tag{3.10}$$

On the other hand $\mathcal{F}\rho\mathcal{F}^{-1}(k,k')=\sum_i\lambda_i\phi_i^*(k)\,\phi_i(k')$, where $\{\phi_i\}_{i\in\mathbb{Z}^+}$ is an orthonormal basis of $\mathcal{L}^2(\mathbb{R})$ and the sum is uniformly convergent by Mercer's theorem.[18] Therefore,

$$\begin{aligned}\langle\rho:\ U(a)\rangle&\\=&\sum_j\int dk\,dk'\left(\sum_i\lambda_i\phi_i^*(k')\,\phi_i(k)\right)\phi_j(k')\exp(-iak)\,\phi_j(k)\\=&\sum_j\lambda_j\int dk\exp(-iak)\,\phi_j^*(k)\phi_j(k)\\=&\int\mathcal{F}\rho\mathcal{F}^{-1}(k,k)\exp(-iak)\,dk,\end{aligned}\tag{3.11}$$

where Mercer's theorem has been used to interchange the sums and integrals. This proves (3.10) and the proposition.

The previous results show the coarse graining operator $D(\cdot\,|\,\mathcal{P}):\mathfrak{S}\to\mathfrak{S}^G$ sends, under the assumptions of the proposition, the density matrix ρ into its diagonal part with respect to the "basis" of plane waves. $D(\rho\,|\,\mathcal{P})$ is however no longer a density matrix. Indeed, there are no translation invariant density matrices on $\mathcal{L}^2(\mathbb{R})$.[19]

Now let ρ be any density matrix on $\mathcal{B}(\mathcal{H})$. Since the restriction $\hat{\rho}$ of ρ to $\mathcal{P}$ is ultraweakly continuous, it admits a unique ultraweakly continuous extension to $\mathcal{P}''=j\mathcal{L}^\infty(\mathbb{R})$. There exists, therefore, a unique $\mathcal{L}^1$-distribution function $f_{\hat{\rho}}$ such that $f_{\hat{\rho}}(k)\geq 0$, $\int f_{\hat{\rho}}(k)\,dk=1$ and

$$\hat{\rho}=j^{*-1}f_{\hat{\rho}}\tag{3.12}$$

or, equivalently,

$$\langle\hat{\rho} : S\rangle = \int f_{\hat{\rho}}(k)\,(j^{-1}S)(k)\,dk \quad \forall S \in \mathcal{P}. \tag{3.13}$$

Therefore, by Proposition 1.2,

$$\langle D(\rho \,|\, \mathcal{P}) : T\rangle = \int f_{\hat{\rho}}(k)\langle \bar{k} : T\rangle\, dk. \tag{3.14}$$

By virtue of Proposition 3.3, $f_{\hat{\rho}}(k)$ may be interpreted as the "diagonal part" $\mathcal{F}\rho\mathcal{F}(k,k')$.

Denote by $\mathfrak{S}^N$ the set of all density matrices on $\mathcal{B}(\mathcal{L}^2(\mathbb{R}))$. It is readily established that the mapping $j^* \circ \mathcal{E}^*(\cdot \,|\, \mathcal{P})^{-1}$ is an affine bijection of the "diagonal" density matrices $\mathcal{D}(\mathfrak{S}^N \,|\, \mathcal{P})$ onto the set of all $\mathcal{L}^1$-distribution functions. This fact has been used[20] by one of us (JCW) to rederive by traditional methods the Pauli-type master equation for the model of Ref. 14.

In closing this section, we want to add that a straightforward change of notation suffices to generalize the preceeding considerations to N-particle quantum systems on the configuration space $\mathbb{R}^M$. The case of an infinite number of degrees of freedom might be treated analogously provided that the test function space is complete.

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C^*-algebraic formalism for coarse graining. II. Momentum coarse graining for Fermi systems in finite volume*†

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The general C^*-algebraic formalism developed by the authors for the coarse-graining operations in quantum statistical mechanics is shown to be applicable to the case of a Fermi system confined in a finite volume.

INTRODUCTION

In a previous paper[1] the present authors proposed a noncommutative extension of Bernouilli's principle of insufficient reason as a possible approach to the problems concerned with the definition and uses of the various notions of coarse graining in quantum statistical mechanics. A certain "Property C" had to be satisfied for this extension to be most fruitful. The present paper shows that this condition is satisfied for a Fermi system confined in a finite volume; this is done in Sec. 2. Section 3 contains a comparison of our C^*-algebraic approach with the W^*-algebraic approach suggested by the work of Kovács and Szücs.[2] Section 1 fixes our notation for Fermi systems.

1. BASIC FACTS ABOUT FERMI SYSTEMS

Let $\mathfrak{H}$ be the Hilbert space of one-particle wavefunctions for a Fermi system Σ. Denote by $\otimes_{i=1}^{N}\mathfrak{H}_i$ the N-fold tensor product of copies of $\mathfrak{H}$. The permutation group of N elements, $\mathcal{S}_N$, admits of a unitary representation, $U:\mathcal{S}_N\to\mathcal{B}(\otimes_{i=1}^{N}\mathfrak{H}_i)$ where for each $\rho\in\mathcal{S}_N$, U_ρ is defined by continuous linear extension from

$$U_\rho\bigotimes_{i=1}^{N} f_i \equiv \bigotimes_{i=1}^{N} f_{\rho(i)}.$$

Denote by A the projection $(N!)^{-1}\sum_{\rho\in\mathcal{S}_N}(-1)^{\sigma(\rho)}U_\rho$ of $\otimes_{i=1}^{N}\mathfrak{H}_i$ onto its antisymmetric subspace.

Let $\mathcal{H}_F(\mathfrak{H})$ be the antisymmetric Fock space constructed over $\mathfrak{H}$; i.e.,

$$\mathcal{H}_F(\mathfrak{H})=\sum_{N=0}^{\infty}\otimes\mathcal{H}^N \tag{1.1}$$

where

$$\mathcal{H}^N=\begin{cases}\mathbf{C} \text{ if} & \text{if } N=0\\ A\bigotimes_{i=1}^{N}\mathfrak{H}_i & \text{if } N\geq 1\end{cases}$$

The creation operator $a^*(f)$ [resp. destruction operator $a(f)$ for a fermion with wavefunction $f\in\mathfrak{H}$ is defined on $\mathcal{H}_F(\mathfrak{H})$ by

$$[a^*(f)\Phi]^{N+1}=(\sqrt{N+1})^{-1}A(f\otimes\Phi^N)\quad\forall N\in\mathbf{Z}^+,\forall\Phi\in\mathcal{H}_F(\mathfrak{H}) \tag{1.2}$$

[resp. $a(f)=a^*(f)^*$].

These operators satisfy the canonical anticommutation relations (CAR's)

$$[a(f),a(g)]_+=0,\quad [a(f),a^*(g)]_+=(f,g)\quad\forall f,g\in\mathfrak{H}. \tag{1.3}$$

The mapping $a^*:\mathfrak{H}\to\mathcal{B}(\mathcal{H}_F(\mathfrak{H}))$ is linear and satisfies

$$\|a^*(f)\|\leq\|f\|_{\mathfrak{H}}. \tag{1.4}$$

The C^*-algebra $\mathfrak{A}(\mathfrak{H})$ of the CAR is the C^*-subalgebra of $\mathcal{B}(\mathcal{H}_F(\mathfrak{H}))$ generated by $\{a^*(f)\mid f\in\mathfrak{H}\}$.

The group of all one-particle symmetries of the Fermi system Σ is obtained by extension[3] to automorphisms of $\mathfrak{A}(\mathfrak{H})$ of the group of unitary operators on $\mathfrak{H}$. Let in fact, V be an arbitrary unitary operator on $\mathfrak{H}$. We define $\tilde{V}$ on $\mathcal{B}(\mathcal{H}_F(\mathfrak{H}))$ by

$$(\tilde{V}\Phi)^N=\begin{cases}\bigotimes_{i=1}^{N}V_i\Phi^N & \text{for } N\geq 1,\ \forall\Phi\in\mathcal{H}_F(\mathfrak{H}),\\ \Phi & \text{for } N=0.\end{cases} \tag{1.5}$$

Evidently, the mapping $\sim:\mathcal{U}(\mathfrak{H})\to\mathcal{B}(\mathcal{H}_F(\mathfrak{H}))$ is a unitary representation of the unitary group $\mathcal{U}(\mathfrak{H})$ in $\mathcal{B}(\mathcal{H}_F(\mathfrak{H}))$. Denote by $\alpha:\mathcal{U}(\mathfrak{H})\to\mathrm{Aut}\mathcal{B}(\mathcal{H}_F(\mathfrak{H}))$ the homomorphism of $\mathcal{U}(\mathfrak{H})$ into the automorphism group of $\mathcal{B}(\mathcal{H}_F(\mathfrak{H}))$ defined for each $V\in\mathcal{U}(\mathfrak{H})$ by

$$\alpha_V S=\tilde{V}S\tilde{V}^*\quad\forall S\in\mathcal{B}(\mathcal{H}_F(\mathfrak{H})). \tag{1.6}$$

Since $\alpha_V a(f)=a(Vf)$ $\forall f\in\mathfrak{H}$, $\forall V\in\mathcal{U}(\mathfrak{H})$, α_V restricts to an automorphism of $\mathfrak{A}(\mathfrak{H})$ for each $V\in\mathcal{U}(\mathfrak{H})$.

A state of the Fermi system Σ is a positive, normalized, linear functional on the C^*-algebra $\mathfrak{A}(\mathfrak{H})$. Denote the set of all states by $\mathfrak{S}(\mathfrak{H})$. By virtue of the CAR [Eq. (1.3)] a state ω on $\mathfrak{A}(\mathfrak{H})$ is determined, by linearity and by continuity, by its n-point correlation functions:

$$\begin{aligned}&W_{N,M}(f_1,\ldots,f_N;g_1,\ldots,g_M)\\ &\quad\equiv\langle\omega:a^*(f_N)\cdots a^*(f_1)a(g_1)\cdots a(g_M)\rangle\\ &\quad\forall N,M\in\mathbf{Z}^+,\forall\{f_i\}_{i=1}^{N},\ \{g_j\}_{j=1}^{M}\subseteq\mathfrak{H}.\end{aligned} \tag{1.7}$$

We shall, in particular, be interested in the set of gauge invariant generalized free states on $\mathfrak{A}(\mathfrak{H})$.

1.1 *Definition*: Let $G_0(\mathfrak{H})=\{\exp(i\phi)1\mid 0\leq\phi\leq 2\pi\}\subset\mathcal{U}(\mathfrak{H})$ denote the gauge group of $\mathfrak{H}$. $G_0(\mathfrak{H})$ is represented in $\mathrm{Aut}\mathfrak{A}(\mathfrak{H})$ by the extension map.

Remark: A state $\omega\in\mathfrak{S}(\mathfrak{H})$ is gauge invariant if and only if $W_{N,M}=0$ for $N\neq M$.

1.2 *Definition*[4]: A state ω_s is a gauge invariant generalized free state on $\mathfrak{A}(\mathfrak{H})$ if the n-point correlation functions have the form

$$W^S_{N,M}(f_1,\ldots,f_N;g_1,\ldots,g_M)=N!\,\delta_{M,N}\left(\bigotimes_{i=1}^{N}g_i,\ \bigotimes_{i=1}^{N}S_iA\bigotimes_{i=1}^{N}f_i\right)\quad\forall\{f_i\}_{i=1}^{N},\ \{g_j\}_{j=1}^{M}\subset\mathfrak{H},$$

where $S=S_i$ is a linear operator on $\mathfrak{H}$ satisfying $0\leq S\leq 1$.

2. MOMENTUM COARSE GRAINING OF FERMI SYSTEMS IN FINITE VOLUME

We specialize the formalism of the preceeding section to a Fermi system Σ confined to an N-dimensional torus. For the sake of notational simplicity we consider explicitly only the particular case of the unit circle S^1. The Hilbert space $\mathfrak{H}$ of one-particle wavefunction is then $\mathcal{L}^2(S^1)$ and the appropriate fermion algebra is $\mathfrak{A}(\mathcal{L}^2(S^1)) \equiv \mathfrak{A}$. Denoting by $\mathcal{P}$ the C^*-algebra of second quantized momentum observables and by G the group of generalized space translations, we shall prove in this section (Proposition 2.2 below) that the central "property C" postulated in Ref. 1 is satisfied for the specific situation characterized by the triple $(\mathfrak{A}, \mathcal{P}, G)$ considered in the present paper.

The C^*-algebra of second-quantized momentum observables is defined as follows. Let P be the generator of space translations on $\mathcal{L}^2(S^1)$. Denote by $\{P_k \mid k \in \mathbf{Z}\}$ the one-dimensional eigenprojectors of P and by $\{f_k \mid k \in \mathbf{Z}\}$ the corresponding orthonormal basis of $\mathcal{L}^2(S^1)$. Let $\mathcal{P}_1$ be the maximally Abelian von Neumann subalgebra of $\mathcal{B}(\mathfrak{H})$ to which P is affiliated. Since $\mathcal{P}_1$ is generated by $\{P_k \mid k \in \mathbf{Z}\}$, there exists, for each $S \in \mathcal{P}_1$, a unique $f_s \in \mathcal{L}^\infty(\mathbf{Z})$ such that

$$S = \sum_{k \in \mathbf{Z}} f_s(k)\, P_k. \tag{2.1}$$

Since the second-quantization map $\sim : \mathcal{B}(\mathfrak{H}) \to \mathcal{B}(\mathcal{H}_F(\mathfrak{H}))$ sends S to $\tilde{S} = \sum_{k \in \mathbf{Z}} f_s(k) N_k$, where $N_k \equiv a_k^* a_k \equiv a^*(f_k) a(f_k)$, it is natural to define the C^*-algebra $\mathcal{P}$ of second-quantized momentum observables $U\{\mathbf{1}\}$ to be the C^*-subalgebra of $\mathfrak{A}$ generated by $\{N_k \mid k \in \mathbf{Z}\}$.

It is furthermore natural to define the group G of symmetries conjugate to $\mathcal{P}$ by extension of the unitary group G of $\mathcal{P}_1$.

We now establish a result identifying the G-invariant states on $\mathfrak{A}$.

2.1 *Lemma*: Let ω be a G-invariant state on $\mathfrak{A}$ and denote by $\hat{\omega}$ its restriction to $\mathcal{P}$. Then, for all $\{f_i\}_{i=1}^N$, $\{g_j\}_{j=1}^M \subset \mathcal{L}^2(S^1)$ and for all $N, M \in \mathbf{Z}^+$

$$W_{N,M}(f_1, \ldots, f_N; g_1, \ldots, g_M) = \delta_{M,N}\, N! \left(\bigotimes_{i=1}^N \tilde{g}_i,\ K_{\hat{\omega}}^N A \bigotimes_{i=1}^N \tilde{f}_i \right)$$

where $K_{\hat{\omega}}^N(k_1, \ldots, k_N) \equiv \langle \hat{\omega} : N_{k_1} \cdots N_{k_N} \rangle$ is a symmetric multiplication operator on $\otimes_{j=1}^N \mathcal{L}^2(\mathbf{Z})_j$ and where $\sim$ denotes Fourier transform.

Proof: Let ω be any state on $\mathfrak{A}$ and let $V = \sum_{k \in \mathbf{Z}} \times \exp[i f_v(k)] P_k \in G$. Then,

$$\langle \omega : \alpha_V(a_{j_N}^* \cdots a_{j_1}^* a_{k_1} \cdots a_{k_M}) \rangle = \langle \omega : a_{j_N}^* \cdots a_{j_1}^* a_{k_1} \cdots a_{k_M} \rangle$$

$$\times \exp\{-i[f(k_1) + \cdots + f(k_M) - f(j_1) \cdots - f(j_N)]\}$$

$$\forall \{k_i\}_{i=1}^M,\ \{j_l\}_{l=1}^N \subset \mathbf{Z},\ \forall N, M \in \mathbf{Z}^+. \tag{2.2}$$

The assumptions that ω is G-invariant places restrictive conditions on the set of correlation functions referred to in Eq. (2.2) If $\langle \omega : a_{j_N}^* \cdots a_{j_1}^* a_{k_1} \cdots a_{k_M} \rangle \neq 0$, then $j_i \neq j_i'$, $1 \leq i \neq i' \leq N$, and $k_l \neq k_{l'}$ for $1 \leq l \neq l' \leq M$. Now if for some $1 \leq i \leq N$ there existed no $1 \leq l \leq M$ such that $j_i = k_l$ we would have upon choosing $f_{j_i}(k) = \pi \delta_{k, j_i}$ the following contradiction:

$$\langle \omega : a_{j_N}^* \cdots a_{j_1}^* a_{k_1} \cdots a_{k_M} \rangle = -\langle \omega : a_{j_N}^* \cdots a_{j_1}^* a_{k_1} \cdots a_{k_M} \rangle. \tag{2.3}$$

The conclusion is that the correlation functions vanish unless the two sets $\{j_i\}_{i=1}$ and $\{k_l\}_{l=1}^M$ are identical and unless $j_i \neq j_i'$ for $1 \leq i \neq i' \leq N$. Moreover, in this case

$$\langle \omega : a_{j_N}^* \cdots a_{j_1}^* a_{k_1} \cdots a_{k_N} \rangle = (-i)^{\sigma(p)} \langle \omega : N_{j_1} \cdots N_{j_N} \rangle, \tag{2.4}$$

where $p \in S_N$ is the unique permutation such that $j_i = k_{p^{-1}i}$. Hence, if ω is a G-invariant state, then

$$\langle \omega : a_{j_N}^* \cdots a_{j_1}^* a_{k_1} \cdots a_{k_M} \rangle = (\otimes \tilde{f}_{k_i},\ K_{\hat{\omega}}^N A \otimes \tilde{f}_{j_i})\, \delta_{M,N} N! \tag{2.5}$$

where $K_{\hat{\omega}}^N$ is the multiplication operator, $K_{\hat{\omega}}^N(k_1, \ldots, k_N) = \langle \hat{\omega} : N_{k_1} \cdots N_{k_N} \rangle$.

By sesquilinearity and continuity, we have, for all $\{f_i\}_{i=1}^N$, $\{g_j\}_{j=1}^M \subset \mathcal{L}^2(S^1)$,

$$W_{N,M}(f_1, \ldots, f_N; g_1, \ldots, g_M) = \delta_{M,N} N!\ (\bigotimes_{i=1}^N \tilde{g}_i, K_{\hat{\omega}}^N A \bigotimes_{i=1}^N \tilde{f}_i). \tag{2.6}$$

Since any state on $\mathfrak{A}$ is determined by its n-point functions, the preceeding lemma together with corollary 1.2 in Ref. 1 establishes Property C for the present model, namely:

2.2 *Proposition*: Let $\mathfrak{A}$ be the CAR C^*-algebra $\mathfrak{A}(\mathcal{L}^2(S^1))$, $\mathcal{P}$ be the C^*-algebra of second quantized momentum observables, and G be the group of generalized translations. Then for every state $\hat{\omega}$ on $\mathcal{P}$ there exists exactly one G-invariant extension of $\hat{\omega}$ to $\mathfrak{A}$.

3. COMPARISON WITH OTHER APPROACHES

The aim of this section is to compare our C^*-algebraic approach to coarse graining with the von-Neumann-algebraic approach suggested by the work of Kovács and Szücs.[2] In order for the latter to be at all applicable to the present model we first must check that $\mathfrak{A}'' = \mathcal{B}(\mathcal{H}_F)$ is G-finite.

Denote by Γ the family of all finite subsets γ of $\mathbf{Z}$. Let $N(\gamma)$ denote the number of elements of γ. In each subset γ we impose an arbitrary but fixed ordering $\gamma = \{k_i\}_{i=1}^{N(\gamma)}$; we define the corresponding antisymmetrized product of normal modes Φ_γ,

$$\Phi_\gamma^M = \delta_{M,N(\gamma)} [N(\gamma)!]^{1/2} A \bigotimes_{i=1}^{N(\gamma)} f_{k_i},$$
$$\Phi_\phi^M = \delta_{M,0} \tag{3.1}$$

It is well known that $\{\Phi_\gamma\}_{\gamma \in \Gamma}$ composes an orthonormal basis of H_F. For each $\gamma \in \Gamma$, denote by P_γ the projector onto the one-dimensional subspace spanned by Φ_γ.

Now, for any $V \in G$, let $f_V : \mathbf{Z} \to \mathbb{R}$ be so that $V = \sum_K \exp[i f_v(k)] P_k$. It is easily seen that $\tilde{V} \Phi_\gamma = \Pi_{l=1}^{N(\gamma)} \times \exp[i f_v(k_l)] \Phi_\gamma$, where $\gamma = \{K_1, \ldots, K_{N(\gamma)}\}$. Therefore, the state whose density matrix is P_γ is G-invariant. Furthermore, since the support of P_γ in $\mathcal{B}(H_F)$ is just P_γ and since $\sum_{\gamma \in \Gamma} P_\gamma = 1$, $\mathcal{B}(H_F)$ is a G-finite von Neumann algebra.[2] Let $T \to T^G$ be the corresponding G-canonical map.

We can now exhibit the relations between the two approaches. Indeed, since T^G is the unique G-invariant element of $\mathrm{Co}\{\alpha_V T \mid V \in G\}^{-\mathrm{ultraweak}}$ $\forall T \in \mathcal{B}(\mathcal{H}_F)$, and since since by Lemma 1.5 in Ref. 1 $\mathcal{E}(T \mid \mathcal{P}) \in \mathrm{Co}\{\alpha_V T \mid V \in G\}^{-N}$ $\forall T \in \mathfrak{A}$, we have that $\mathcal{E}(T \mid \mathcal{P}) = T^G$ $\forall T \in \mathfrak{A}$. Since $T \to T^G$ is normal, it follows from this and the weak operator density of $\mathfrak{A}$ in $\mathcal{B}(\mathcal{H}_F)$ that the G-canonical map is the unique normal extension of $\mathcal{E}(\cdot \mid \mathcal{P})$ to $\mathcal{B}(\mathcal{H}_F)$. This implies in particular that, for every ultraweakly continuous state ρ on $\mathfrak{A} \subset \mathcal{B}(\mathcal{H}_F)$, $D(\rho \mid \mathcal{P})$ is also ultraweakly continuous. Further, (Cor 4.1 of Ref. 2 each normal state $\hat{\rho}$ on $\mathcal{B}(\mathcal{H}_F)^G$ admits a unique normal, G-invariant extension to $\mathcal{B}(\mathcal{H}_F)$ which, by virtue of Property C, must agree with $\mathcal{E}^*(\hat{\rho} \mid \mathcal{P})$ on $\mathfrak{A}$. Thus, every aspect of our C^*-algebraic formulation has its von Neumann algebraic counterpart for this model, and the two formulations are equivalent provided that only normal states on $\mathcal{B}(\mathcal{H}_F)$ are considered.

The fact that our C^*-algebraic formulation is not limited, in more general cases as well, by this restriction could be used to sharpen some heuristic features often[5] alluded to in the physical literature.

In the literature of nonequilibrium statistical mechanics, $D(\cdot \mid \mathcal{P})$ is called the diagonal part operator with respect to the basis of antisymmetrized products of "normal modes" since, as the reader may easily verify, for any density matrix ρ we have

$$D(\rho \mid \mathcal{P}) = \sum_{\gamma \in \Gamma} (Tr\, \rho P_\gamma) P_\gamma. \tag{3.2}$$

$D(\cdot \mid \mathcal{P})$ is commonly used to derive the generalized master equation (GME) for a mechanical system of fermions in finite volume. We suggest that the C^*-algebraic formulation of momentum-coarse graining can accomplish van Hove's aim[5] when he restricts the GME, for purposes of taking the thermodynamic limit, to his loosely defined "smooth observables." This point of view is supported by the fact that the C^*-algebraic formulation admits a generalization for a Fermi system in infinite free space[6] whereas the von Neumann-algebraic formulation does not.

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C^*-algebraic formalism for coarse graining. III. Momentum coarse graining for Fermi systems in infinite free space*†

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The C^*-algebraic formalism developed by the authors for the coarse-graining operations in quantum statistical mechanics is adapted to the case of an infinite Fermi system in free space.

INTRODUCTION

The present paper is the third in a series in which we propose a C^*-algebraic formalism for coarse graining. Our motivation is to obtain a mathematically well-defined theory which would incorporate the following two features: (a) It should transpose to quantum mechanics the familiar Bernouilli principle of insufficient reason, basic to classical probability theory, and (b) it should provide a way to treat physical situations such as momentum coarse graining, which escaped from the scope of previous theories.[1–3] Part (a) has been discussed in the first paper[4] of this series, whereas a first step in achieving part (b) has been described in a second paper.[5] The aim of the present paper is to extend the results previously obtained[5] to the case of infinite Fermi systems in free space. For sake of conciseness, we use freely in this paper the definition and notations used in our previous[4,5] papers.

We shall thus consider in the present paper a Fermi system in the N-dimensional free space R^N. For the sake of notational simplicity we specialize to the case $N=1$, the generalization to arbitrary N being straight forward. Let $\mathfrak{A} = \mathcal{L}^2(\mathbb{R})$ be the Hilbert space of one-particle wavefunctions and denote by $\mathfrak{H} = \mathfrak{A}(\mathcal{L}^2(\mathbb{R}))$ the corresponding fermion algebra. For the basic facts and notation concerning Fermi systems, the reader is referred to Sec. 1 of our previous paper.[5] Let P and Q, respectively, denote the one-particle momentum and position operators. In particular P is realized here as the self-adjoint operator associated with the multiplication operator defined on $\mathcal{S}(\mathbb{R})$ in $\mathcal{L}^2(\mathbb{R})$ by $(P\Psi)(x) = x\Psi(x)$. The obvious obstacle in extending directly to the present case the considerations developed previously,[5] when Σ is confined to a finite volume, is that the one-particle momentum observable P now has continuous spectrum, thus making it necessary to resort to a limiting procedure to define the C^*-algebra $\mathcal{P}$ of second quantized momentum observables. Yet the choice of the group of $\mathcal{P}$-trivial symmetries is still clear. Let indeed G be the unitary group of the maximally Abelian sub-von Neumann algebra of $\mathcal{B}(\mathcal{L}^2(\mathbb{R}))$ to which the one-particle momentum is affiliated. To be specific, we define for every essentially bounded function $S \in \mathcal{L}^\infty(\mathbb{R}^N)$ on $\mathbb{R}^N$ the bounded operator T_S on $\mathcal{L}^2(\mathbb{R}^N)$ by

$$(T_S f)(x_1, \ldots, x_N) = S(x_1, \ldots, x_N) f(x_1, \ldots, x_N) \quad \forall f \in \mathcal{L}^2(\mathbb{R}^N).$$

The mapping $S \to T_S$ is a W^*- and C^*-isomorphism of $\mathcal{L}^\infty(\mathbb{R}^N)$ onto the maximal Abelian von Neumann algebra of "diagonalizable operators" on $\mathcal{L}^2(\mathbb{R}^N)$.[6] Hereafter we shall simply write S for T_S (whether S is meant as an operator or an essentially bounded function will be clear from the context). Consequently the von Neumann algebra of "diagonalizable operators" on $\mathcal{L}^2(\mathbb{R}^N)$ will be identified with $\mathcal{L}^\infty(\mathbb{R}^N)$. For $N=1$, $\mathcal{L}^\infty(\mathbb{R}^N)$ is the maximal Abelian von Neumann subalgebra of $\mathcal{B}(\mathcal{L}^2(\mathbb{R}))$ to which the one-particle momentum operator is affiliated. The unitary group G of this algebra is represented in $\mathrm{Aut}\,\mathfrak{A}$ by the natural extension described for instance in Sec. 1 of Ref. 5. Similarly the group of momentum translations is given by a strongly continuous, one-parameter automorphism group on $\mathfrak{A}$, $\{\alpha_b \equiv \alpha_{V_b} | V_b = \exp(-iQb)\ \forall b \in \mathbb{R}\}$. We now outline the argument to be presented in this section.

In Sec. 1, we introduce the approximate, operator-valued, momentum correlation densities and use them for the definition of the set $\mathfrak{S}^{\mathcal{P}}$ of momentum-measurable states and of the notion of momentum equivalence. Once again amenability of G implies existence of at least one G-invariant state in each equivalence class.

In Sec. 2, we characterize (Theorem 2.10) the n-point correlation functions of an arbitrary G-invariant state on $\mathfrak{A}$, and thereby obtain the principal tool of this investigation.

In Sec. 3, we use the characterization of Sec. 2 to establish two lines of inquiry. On the one hand, we establish (Theorem 3.3) existence and uniqueness of a G-invariant state in each $\mathcal{P}$-equivalence class. In line with the argument presented in Ref. 4, we then define the $\mathcal{P}$-coarse grained representative of a class to be its G-invariant state, thus defining the $\mathcal{P}$-coarse graining operator $D(\cdot\,|\mathcal{P})$. On the other hand, we define (Theorems 3.7 and 3.8) a von Neumann algebra $\mathcal{P}_\omega'' \subset \pi_\omega(\mathfrak{A})''$ acting on the GNS representation space $\mathcal{H}_\omega$ associated to an arbitrary G-invariant state ω on $\mathfrak{A}$. We then investigate momentum-coarse graining on the island $\mathfrak{S}_\omega$ of normal states on $\pi_\omega(\mathfrak{A})''$. In particular, we show (Prop. 3.10) that normal states ψ on $\pi_\omega(\mathfrak{A})''$ are $\mathcal{P}$-equivalent if and only if they have the same restriction $R_\omega\psi$ to $\mathcal{P}_\omega''$. Moreover, Prop. 3.11 establishes that every normal state $\hat{\psi}$ on $\mathcal{P}_\omega''$ admits a unique, normal G-invariant extension $\mathcal{E}_\omega(\hat{\psi}|\mathcal{P})_*$ to $\pi_\omega(\mathfrak{A})''$ and, further, that $D(\psi|\mathcal{P}) = \mathcal{E}_\omega(R_\omega\psi|\mathcal{P})_*$ for all $\psi \in \mathfrak{S}_\omega$. Finally, Theorem 3.13 establishes the existence of a normal, G-invariant, $\mathcal{P}_\omega''$-conditional expectation $\mathcal{E}_\omega(\cdot\,|\mathcal{P})$ on $\pi_\omega(\mathfrak{A})''$ to which $\mathcal{E}_\omega(\cdot\,|\mathcal{P})_*$ is dual.

In Sec. 4, we prove, using $\mathcal{P}^{\pi}_{\omega}$ as a tool, that the set of all G-invariant states $\mathfrak{S}^G$ on $\mathfrak{A}$ is a (Choquet) simplex. Denoting by $\mathcal{S}$ the set of all extreme points of $\mathfrak{S}^G$, we show that $\mathcal{S}$ coincides with the set of all space translation and gauge invariant generalized free states on $\mathfrak{A}$. We call the reader's attention to the sharp ergodic Theorem 4.1, and to the last remark in that section, which indicates how and why our C^*-algebraic formalism goes further than the usual von Neumann-algebraic formalism, thus sustaining our last conclusion in Ref. 5.

In Sec. 5, we define the C^*-algebra $\mathcal{P}$ of second-quantized momentum observables as the set of all continuous functions on the compact (Prop. 5.1) phase space $\mathcal{S}$. We prove (Theorem 5.2) that $\mathcal{S}$ is homeomorphic to the compact space $\mathcal{L}^{\infty}(\mathbb{R})^+_1$ of all essentially bounded functions F on $\mathbb{R}$ such that $0 \leqslant F \leqslant 1$. For each $\omega \in \mathcal{S}$, the corresponding function F_ω is interpreted as the momentum number density of the state ω on the Fermi system considered. Once $\mathcal{P}$ is defined, we can recover, in only slightly modified form, the structure described in Ref. 4: (i) There exists a generalized conditional expectation $\mathcal{E}(\cdot \mid \mathcal{P})$ mapping $\mathfrak{A}$ into $\mathcal{P}$; (ii) each $\mathcal{P}$-measurable state admits (Theorem 5.12) a unique generalized restriction to $\mathcal{P}$; (iii) each state $\mathcal{P}$ admits (Theorem 5.13) a unique G-invariant extension $\mathcal{E}(\psi \mid \mathcal{P})^*$ to $\mathfrak{A}$ with $\mathcal{E}(\cdot \mid \mathcal{P})^*$ dual to $\mathcal{E}(\cdot \mid \mathcal{P})$. Finally, we discuss the implementability of $\mathcal{E}(\cdot \mid \mathcal{P})$, thus making contact (Theorem 5.16) with $\mathcal{E}_\omega(\cdot \mid \mathcal{P})$ defined in Sec. 3.

1. $\mathcal{P}$-MEASURABLE STATES

The purpose of this subsection is to introduce the second-quantized momentum observables in a language appropriate to our investigation. We first define the approximate, operator-valued, momentum correlation densities $K^N_\delta(x_1, \ldots, x_N)$; we then indicate suitable circumstances under which sharp correlation densities are obtainable by taking the limit $\delta \to 0$.

For each interval $\delta = [-\delta/2, \delta/2]$, denote by χ_δ the characteristic function of δ and let $\Delta_{x_0} = \chi_\delta(x - x_0)/\delta^{1/2}$ ($\Delta_0 \equiv \Delta$). Since the automorphism group $\{\alpha_x \mid x \in \mathbb{R}\}$ of momentum translations is strongly continuous, the operator-valued function

$$K^N_\delta(x_1, \ldots, x_N) \equiv \alpha_{x_N}(a^*(\Delta)) \cdots \alpha_{x_1}(a^*(\Delta)a(\Delta)) \cdots \alpha_{x_N}(a(\Delta)) \quad \text{on } \mathbb{R}^N$$

is strongly continuous. Let $K(\mathbb{R})$ be the space of continuous functions with compact support. Bochner's theorem[7] ensures that, for every $f_i, g_i \in K(\mathbb{R})$, $i = 1, \ldots, N$, N finite, the integral

$$K^N_\delta(f_1, \ldots, f_N; g_1, \ldots, g_N) \equiv \int_{\mathbb{R}^N} d^N x \prod_{i=1}^N f_i(x_i)\bar{g}_i(x_i) \times K^N_\delta(x_1, \ldots, x_N)$$

exists as a norm convergent limit of a sequence of simple functions. Therefore,

$$\{K^N_\delta(f_1, \ldots, f_N; g_1, \ldots, g_N) \mid f_i, g_i \in K(\mathbb{R});\ i = 1, \ldots, N; N \text{ finite}\} \subset \mathfrak{A}.$$

Let us now give a heuristic motivation for what we want to achieve. If the following limits were to exist, we would expect them to satisfy

$$\lim_{\delta \to 0} K^N_\delta(x_1, \ldots, x_N) = \begin{cases} N_{x_1} \cdots N_{x_N}, & \text{if } i \neq j \text{ implies } x_i \neq x_j \text{ for all } i, j = 1, \ldots, N, \\ 0, & \text{otherwise.} \end{cases}$$

We would therefore interpret these limiting observables as the second-quantized momentum correlations generating $\mathcal{P}$. It would then be natural to generalize the notion of restriction of a continuous linear form to $\mathcal{P}$ by computing

$$\hat{\psi}(x_1, \ldots, x_N) \equiv \lim_{\delta \to 0} \langle \psi : K^N_\delta(x_1, \ldots, x_N) \rangle.$$

We will therefore define the set $\mathfrak{S}^{\mathcal{P}}$ of all the states on $\mathfrak{A}$ for which the idealization $\delta \to 0$ makes sense. We show in Lemma 3.6 that this set is indeed quite large.

1.1 *Definition*: A continuous linear form ψ on $\mathfrak{A}$ is said to be $\mathcal{P}$-measurable if, for each $N \in \mathbb{Z}^+$ and for arbitrary but fixed $\{f_i\}^N_{i=1}$ and $\{g_i\}^N_{i=1} \subset K(\mathbb{R})$

$$\forall \epsilon > 0 \quad \exists \delta_\epsilon \quad \ni \delta, \delta' < \delta_\epsilon$$
$$\Rightarrow |\langle \psi : \alpha_V\{K^N_\delta(f_1, \ldots, f_N; g_1, \ldots, g_N)\} - \alpha_{V'}\{K^N_{\delta'}(f_1, \ldots, f_N; g_1, \ldots, g_N)\}\rangle| < \epsilon,$$

independent of V or $V' \in G$.

Denote by $\mathfrak{A}^{*\mathcal{P}}$ the set of all $\mathcal{P}$-measurable continuous linear forms on $\mathfrak{A}$ and by $\mathfrak{S}^{\mathcal{P}}$ the set of all states in $\mathfrak{A}^{*\mathcal{P}}$.

1.2 *Definition*: For each $\psi \in \mathfrak{A}^{*\mathcal{P}}$, the restriction $\hat{\psi}$ of ψ to $\mathcal{P}$ is the form $\hat{\psi}$ defined as

$$\hat{\psi}^N(f_1, \ldots, f_N; g_1, \ldots, g_N) = \lim_{\delta \to 0} \langle \psi : K^N_\delta(f_1, \ldots, f_N; g_1, \ldots, g_N) \rangle$$

for all $N \in \mathbb{Z}^+$, and all $\{f_i\}^N_{i=1}$, $\{g_i\}^N_{i=1} \subset K(\mathbb{R})$. Two states ψ and ψ' on $\mathfrak{A}$ are said to be $\mathcal{P}$-equivalent (which we denote by $\psi \approx \psi'$) if their restrictions to $\mathcal{P}$ coincide.

Remarks: (i) $\mathcal{P}$ itself will only be defined later on in this section (see Sec. 5), but its definition is clearly not a prerequisite for the above definition. (ii) The relation $\approx$ on $\mathfrak{S}^{\mathcal{P}}$ is clearly an equivalence relation.

1.3 *Proposition*: $\mathfrak{A}^{*\mathcal{P}}$ is a norm-closed, G-stable, linear subspace of $\mathfrak{A}^*$.

Proof: $\mathfrak{A}^{*\mathcal{P}}$ is clearly a G-stable, linear manifold. To show that $\mathfrak{A}^{*\mathcal{P}}$ is norm closed, choose a Cauchy sequence $\{\psi_M\}_{M \in \mathbb{Z}^+} \subset \mathfrak{A}^{*\mathcal{P}}$ convergent to ψ, say. Clearly,

$$\begin{aligned} &|\langle \psi : \alpha_V\{K^N_\delta(f_1, \ldots, f_N; g_1, \ldots, g_N)\} - \alpha_{V'}\{K^N_{\delta'}(f_1, \ldots, f_N; g_1, \ldots, g_N)\}\rangle| \\ &\leqslant |\langle \psi_M : \alpha_V\{K^N(f_1, \ldots, f_N; g_1, \ldots, g_N)\} - \alpha_{V'}\{K^N_{\delta'}(f_1, \ldots, f_N; g_1, \ldots, g_N)\}\rangle| \\ &\quad + 2\|\psi - \psi_M\| \prod_{i=1}^N \|f_i\|_2 \|g_i\|_2. \end{aligned} \tag{1.1}$$

Now, for any $\epsilon > 0$,

$$\exists M_\epsilon \ni M \geqslant M_\epsilon \Rightarrow \|\psi - \psi_M\| \prod_{i=1}^N \|f_i\|_2 \|g_i\|_2 < \epsilon.$$

Since $\psi_{M_\epsilon} \in \mathfrak{A}^{*\mathcal{P}}$, there exist $\delta_{M_\epsilon, \epsilon/2}$ such that

$$\delta, \delta' < \delta_{M_\epsilon, \epsilon/2} \Rightarrow |\langle \psi_{M_\epsilon} : \alpha_V\{K^N_\delta(f_1, \ldots, f_N; g_1, \ldots, g_N)\}$$

$$- \alpha_{V'}\{K_\delta^N,(f_1,\ldots,f_N;\, g_1,\ldots,g_N)\}\rangle \big| < \epsilon/2.$$

These remarks, together with Eq. (1.1), imply that $\psi \in \mathfrak{A}^{*\mathcal{P}}$.

With a view toward establishing Property C, we prove the following:

1.4 *Proposition*: Let $\psi \in \mathfrak{S}^{\mathcal{P}}$ and $\phi \in \mathrm{Co}\{\alpha_V{}^*\psi \mid V \in G\}^{-w*}$. Then $\phi \in \mathfrak{S}^{\mathcal{P}}$ and $\phi \approx \psi$.

Proof: There exists[8] a net $\{M_\beta\}_{\beta \in I}$ of discrete means on CB(G) such that w^*-lim $M_\beta{}^*\psi = \phi$. By virtue of the hypothesis that $\psi \in \mathfrak{S}^{\mathcal{P}}$, we have, for fixed $\{f_i\}_{i=1}^N$, $\{g_i\}_{i=1}^N \subset K(\mathrm{R})$,

$$\forall \epsilon > 0 \quad \exists \delta_\epsilon > 0 \quad \ni \delta, \delta' < \delta_\epsilon \Rightarrow$$

$$\big|\langle M_\beta{}^*\psi : \alpha_V\{K_\delta^N(f_1,\ldots,f_N;\, g_1,\ldots,g_N)\}$$
$$- \alpha_{V'}\{K_{\delta'}^N(f_1,\ldots,f_N;\, g_1,\ldots,g_N\}\rangle \big| < \epsilon, \tag{1.2}$$

independent of $\beta \in I$ or of V or $V' \in G$. By continuity, the same is true for ϕ replacing $M_\beta{}^*\psi$. Hence $\phi \in \mathfrak{S}^{\mathcal{P}}$. Similarly,

$$\forall \epsilon > 0 \quad \exists \delta_\epsilon \quad \ni \delta < \delta_\epsilon$$

$$\big|\langle M_\beta{}^*\psi : K_\delta^N(f_1,\ldots,f_N;\, g_1,\ldots,g_N)\rangle$$
$$- \hat{\psi}^N(f_1,\ldots,f_N;\, g_1,\ldots,g_N)\big| < \epsilon, \tag{1.3}$$

independent of $\beta \in I$. By continuity the same is true with $M_\beta{}^*\psi$ replaced by ϕ. Thus $\phi \approx \psi$.

1.5 *Corollary*: There exists at least one G-invariant state in each $\mathcal{P}$-equivalence class.

Proof: Choose ψ from an arbitrary $\mathcal{P}$-equivalence class. Since G is amenable, there exists (Lemma 1.1 in Ref. 4) a G-invariant state $\phi \in \mathrm{Co}\{\alpha_V{}^*\psi \mid V \in G\}^{-w*}$. By Prop. 1.4, $\phi \approx \psi$.

To establish uniqueness, and hence the central "Property C" of Ref. 4, we must investigate the set of G-invariant states. This will be done in the next sections (see in particular Theorem 3.3).

2. THE DIAGONAL FORM OF THE G-INVARIANT STATES

The principal result of this section is Theorem 2.10 where the form of the n-point correlation functions of a G-invariant state is characterized. Comparison of this result with Lemma 2.1 in Ref. 5 and its subsequent interpretation demonstrates that the set of G-invariant states provides a mathematically consistent definition for what one would heuristically refer to as the set of states which are diagonal with respect to the basis of antisymmetrized products of plane waves. Unless explicitly given, the proofs pertaining to results of this section will be found in Appendix A.

2.1 *Definition*: Consider the dense linear manifold in $\mathcal{L}^2(\mathrm{R}^N)$ consisting of all finite linear combinations of the form

$$f = \sum_{j=1}^{J} \lambda_j' \bigotimes_{m=1}^{N} X_m^j \quad \forall J \in \mathrm{Z}^+,\ \forall \{\lambda_j\}_{j=1}^J \subseteq \mathrm{C}$$

and $\{X_m^j\}_{m=1,\ldots,N}^{j=1,\ldots,J}$ are characteristic functions of Lebesgue measurable subsets of R with finite measure. Denote this set by $\mathcal{L}_0^2(\mathrm{R}^N)$.

The (N,N)-point correlation functions $W_{N,N}$ of a state ω on $\mathfrak{A}$ were defined in formula (1.7) in Ref. 5. The following lemma shows that any such function extends by linearity to a positive, sesquilinear form on $\mathcal{L}_0^2(\mathrm{R}^N)$.

2.2 *Lemma*: Let ω be a state on $\mathfrak{A}$. For each pair $f,\ g \in \mathcal{L}_0^2(\mathrm{R}^N)$, that is

$$f = \sum_{j=1}^{J} \lambda_j \Big(\bigotimes_{m=1}^{N} X_m^j\Big), \quad g = \sum_{k=1}^{K} \gamma_k \Big(\bigotimes_{m=1}^{N} Y_m^k\Big)$$

form

$$\sum_{j=1}^{J}\sum_{k=1}^{K} \lambda_j \bar{\gamma}_k\, W_{N,N}(X_1^j,\ldots,X_N^j;\, Y_1^k,\ldots,Y_N^k) \equiv W_N^0(f,g). \tag{2.1}$$

This expression depends on f, g only, not on the particular decomposition used. We have

(i) $W_N^0(\lambda f_1 + f_2,\ \gamma g_1 + g_2) = \lambda\bar{\gamma} W_N^0(f_1,g_1) + \lambda W_N^0(f_1,g_2) + \bar{\gamma} W_N^0(f_2,g_1) + W_N^0(f_2,g_2)$ $\quad \forall f_1,f_2,g_1,g_2 \in \mathcal{L}_0^2(\mathrm{R}^N),\ \forall \lambda,\gamma \in \mathrm{C}$

(ii) $W_N^0(f,f) \ge 0 \quad \forall f \in \mathcal{L}_0^2(\mathrm{R}^N)$.

We furthermore notice that the extension W_N^0 of the (N,N)-point correlation function of a G-invariant state on $\mathfrak{A}$ is continuous; specifically:

2.3 *Lemma*: Let ω be a G-invariant state on $\mathfrak{A}$. Then

$$|W_N^0(f,g)| \le N!\, \|f\|_2 \|g\|_2 \qquad \forall f,\ g \in \mathcal{L}_0^2(\mathrm{R}^N).$$

As a consequence of this lemma we obtain by continuity that for every G-invariant state ω on $\mathfrak{A}$, the (N,N)-point correlation functions define uniquely a continuous, positive, sesquilinear form W_N over $\mathcal{L}^2(\mathrm{R}^N)$ whose restriction to $\mathcal{L}_0^2(\mathrm{R}^N)$ is W_N^0.

2.4 *Lemma*: Let ω be a G-invariant state on $\mathfrak{A}$, and let W_N be the corresponding continuous, positive, sesquilinear form over $\mathcal{L}^2(\mathrm{R}^N)$. There exists a unique bounded linear operator $B_\omega^N \in \mathcal{B}(\mathcal{L}^2(\mathrm{R}^N))$ such that $W_N(f,g) = (g, B_\omega^N f)\ \forall f, g \in \mathcal{L}^2(\mathrm{R}^N)$. Moreover,

(i) $\quad W_{NN}(f_1,\ldots,f_N; g_1,\ldots,g_N) = W_N\Big(\bigotimes_{m=1}^N f_m,\ \bigotimes_{m=1}^N g_m\Big)$ $\quad \forall \{f_m\}_{m=1}^N,\ \{g\}_{m=1}^N \subset \mathcal{L}^2(\mathrm{R})$,

(ii) $\quad 0 \le B_\omega^N \le N!$,

(iii) $\quad [B_\omega^N,\ U_p] = 0 \quad \forall p \in \mathcal{S}_N$.

Proof: The existence and uniqueness of B_ω^N as well as (ii) follows directly from Riesz theorem (i) follows from the sesquilinearity and continuity of the W_{NN}.

To prove (iii), it suffices to prove that

$$\Big(\bigotimes_{m=1}^N g_m,\ U_p^* B_\omega^N U_p \bigotimes_{m=1}^N f_m\Big) = \Big(\bigotimes_{m=1}^N g_m,\ B_\omega^N \bigotimes_{m=1}^N f_m\Big)$$

$$\forall \{f_m\},\ \{g_m\} \subset \mathcal{L}^2(\mathrm{R})$$

since the linear span of $\{\otimes_{m=1}^N f_m \mid f_m \in \mathcal{L}^2(\mathrm{R})\}$ is dense in $\mathcal{L}^2(\mathrm{R}^N)$ and since B_ω^N is bounded and linear.

By use of (i) and the anticommutation relations we have

$$\Big(\bigotimes_{m=1}^N g_m,\ U_p^* B_\omega^N U_p \bigotimes_{m=1}^N f_m\Big) = \Big(\bigotimes_{m=1}^N g_{p(m)},\ B_\omega^N \bigotimes_{m=1}^N f_{p(m)}\Big)$$

$$= W_{NN}(f_{p(1)}, \ldots, f_{p(N)}; g_{p(1)}, \ldots, g_{p(N)})$$
$$= (-1)^{2\sigma(p)} W_{NN}(f_1, \ldots, f_N; g_1, \ldots, g_N)$$
$$= \left(\bigotimes_{m=1}^{N} g_m,\ B_\omega^N \bigotimes_{m=1}^{N} f_m\right).$$

This completes the proof of the lemma.

2.5 *Notation*: We have seen in Lemma 2.4, that for each G-invariant state ω on $\mathfrak{A}$, and each $N \in \mathbb{Z}^+$ there exists a unique continuous sesquilinear extension W_N to $\mathcal{L}^2(\mathbb{R}^N)$ of the (N,N)-point correlation functions W_{NN} defined by ω. Denote by $\{W_N\}_{N\in \mathbb{Z}^+}$ the set of all such extensions. Denote by $\{B_\omega^N\}_{N\in \mathbb{Z}^+}$ the set of corresponding bounded, symmetric, positive, linear operators.

We begin our investigation of the family $\{B_\omega^N\}_{N\in \mathbb{Z}^+}$ of bounded operators associated to a G-invariant state ω with the following statement:

2.6 *Lemma*: Let B_ω^N be the bounded operator on $\mathcal{L}^2(\mathbb{R}^N)$ associated by Lemma 2.4 with a G-invariant state ω on $\mathfrak{A}$. Choose a family $\{Y_m\}_{m=1}^N$ of disjoint measurable subsets of R. Denote by $\{P_m\}_{m=1}^N$ the corresponding family of orthogonal projections in $\mathcal{L}^\infty(\mathbb{R})$ [i.e., $P_m f(x) = Y_m(x) f(x)\ \forall f \in \mathcal{L}^2(\mathbb{R})$]. Let $P_y = \otimes_{m=1}^N P_m$ be the projection on $\mathcal{L}^2(\mathbb{R}^N)$ associated with the measurable rectangle $Y \equiv Y_1 \times \cdots \times Y_N$ in $\mathbb{R}^N$. Then

$$P_y B_\omega^N P_y \in \mathcal{L}^\infty(\mathbb{R}^N).$$

We now patch together the $P_y B_\omega^N P_y$:

2.7 *Lemma*: Let $P^N = \{P_y \mid Y = Y_1 \times \cdots \times Y_N;\ Y_i$ measurable; $Y_i \cap Y_{i'} = \emptyset,\ i \neq i'\}$. Denote by Γ the directed set of all finite subsets of P^N, ordered by inclusion. For each $\gamma \in \Gamma$, define $P(\gamma) = \mathrm{lub}\{P \mid P \in \gamma\}$. Then the net $\{P(\gamma)\}_{\gamma\in\Gamma}$ converges to 1 in the weak operator topology.

For the purposes of the next lemma we make the following definition. Let $\gamma = \{P_{y_i}\}_{i=1}^{N(\gamma)} \in \Gamma$. A set of projectors $\{P_k\}_{k=1}^{k}$ will be said to be a disjunction of γ in $\mathcal{L}^\infty(\mathbb{R}^N)$ if

(a) $\{P_k\}_{k=1}^K \subset \mathcal{L}^\infty(\mathbb{R}^N)$,

(b) $P_k P_{k'} = 0, \quad 1 \leq k \neq k' \leq K$,

(c) For each $1 \leq k \leq K$, there exists an $1 \leq i \leq N(\gamma)$ such that $P_k \subset P_{y_i}$,

(d) $P(\gamma) = \sum_{k=1}^{K} P_k$.

We remark that there exist many disjunctions of γ in $\mathcal{L}^\infty(\mathbb{R}^N)$. We, however, have:

2.8 *Lemma*: Let B_ω^N be the bounded operator on $\mathcal{L}^2(\mathbb{R}^N)$ associated with a G-invariant state ω on $\mathfrak{A}$. Choose $\gamma \in \Gamma$ and let $\{P_k\}_{k=1}^K$ be a disjunction of γ in $\mathcal{L}^\infty(\mathbb{R}^N)$. Then, $F_\omega^N(\gamma) \equiv \sum_{k=1}^K P_k B_\omega^N P_k$ depends on γ only, and not on the particular disjunction chosen to define it. Moreover,

(i) $F_\omega^N(\gamma) \in \mathcal{L}^\infty(\mathbb{R}^N)$,

(ii) $0 \leq F_\omega^N(\gamma) \leq 1$,

(iii) $\gamma \subset \gamma' \Rightarrow F_\omega^N(\gamma) = P(\gamma) F_\omega^N(\gamma')$,

(iv) $\gamma \subset \gamma' \Rightarrow F_\omega^N(\gamma) \leq F_\omega^N(\gamma')$.

We now patch together the $F_\omega^N(\gamma)$:

2.9 *Lemma*: Let $\{F_\omega^N(\gamma)\}_{\gamma\in\Gamma}$ be the net in $\mathcal{L}^\infty(\mathbb{R}^N)$ defined in Lemma 2.8 for an arbitrary G-invariant state ω on $\mathfrak{A}$. Then $\{F_\omega^N(\gamma)\}_{\gamma\in\Gamma}$ converges in the weak operator topology on $B(\mathcal{L}^2(\mathbb{R}^N))$ to an operator $F_\omega^N \in \mathcal{L}^\infty(\mathbb{R}^N)$. Moreover,

(i) F_ω^N is the unique operator in $\mathcal{L}^\infty(\mathbb{R}^N)$ such that
$$F_\omega^N P = P B_\omega^N P \quad \forall\ P \in P^N,$$

(ii) $N!\, F_\omega^N A = B_\omega^N$,

(iii) $0 \leq F_\omega^N \leq 1$,

(iv) $[F_\omega^N, U_p] = 0\ \forall\ p \in \mathcal{S}_N$.

We are now equipped to give a sharp characterization of the n-point correlation functions of a G-invariant state.

2.10 *Theorem*: Let ω be a G-invariant state on $\mathfrak{A}$. There exists a unique family $\{F_\omega^N\}_{N\in \mathbb{Z}^+}$ such that

(i) $$W_{NM}(f_1, \ldots, f_N; g_1, \ldots, g_M) = \delta_{M,N} N! \left(\bigotimes_{m=1}^{M} g_m,\ F_\omega^N A \bigotimes_{m=1}^{N} f_m\right) \quad \forall \{f_n\}_{n=1}^N,\ \{g_m\}_{m=1}^M \subset \mathcal{L}^2(\mathbb{R}).$$

(ii) $F_\omega^N \in \mathcal{L}^\infty(\mathbb{R}^N) \quad \forall\ N \in \mathbb{Z}^+$.

Conversely, if ω is a state on $\mathfrak{A}$ and if there exists a family $\{F_\omega^N\}_{N\in \mathbb{Z}^+}$ satisfying (i) and (ii), then ω is G-invariant, and

(a) $0 \leq F_\omega^N \leq 1 \quad \forall\ N \in \mathbb{Z}^+$,

(b) $[U_p, F_\omega^N] = 0 \quad \forall\ p \in \mathcal{S}_N$.

Proof: Assume that ω is G-invariant. Since the gauge group is contained in G, ω is gauge invariant. Existence is given by Lemmas 2.4 and 2.9 and the fact that ω is gauge invariant. To prove uniqueness, let $\bar{F}_\omega^N$, F_ω^N satisfy (i), (ii) above. From Lemma 2.4, $N!\,\bar{F}_\omega^N A = B_\omega^N$. Choose $P \in P^N$. Then

$$P B_\omega^N P = N!\, P \bar{F}_\omega^N A\, P = P \bar{F}_\omega^N \left(\sum_{p\in \mathcal{S}_N} (-1)^{\sigma(p)} U_p\right) P$$
$$= \sum_{p\in \mathcal{S}_N} (-1)^{\sigma(p)} P\, \bar{F}^N U_p P U_p^* U_p$$
$$= \sum_{p\in \mathcal{S}_N} (-1)^{\sigma(p)} P U_p P U_p^*\ \bar{F}_\omega^N\ U_p \quad \text{by (ii)}$$
$$= P \bar{F}_\omega^N \quad \text{since } P \in P^N.$$

Similarly $P B_\omega^N P = P F_\omega^N$. Lemma 2.9 (i) gives $\bar{F}_\omega^N = F_\omega^N$. This proves uniqueness. The converse part of the theorem is obvious. For (a) and (b), see Lemma 2.9 (iii) and (iv). This completes the proof of the theorem.

2.11 *Corollary*: Let ω be a G-invariant state on $\mathfrak{A}$. Then ω is a generalized free state iff $F_\omega^N = \otimes_{m=1}^N F_{\omega,m}^1$ for all $N \in \mathbb{Z}^+$.

Proof: If ω is quasi free, $\bar{F}_\omega^N = \otimes_{m=1}^N F_{\omega,m}^1$ satisfies (i) and (ii) of the theorem. Hence $F_\omega^N = \otimes_{m=1}^N F_{\omega,m}^1$. The converse is obvious.

3. MOMENTUM OBSERVABLES AND COARSE GRAINING

Unless explicitly given here the proofs for results of this subsection will be found in Appendix B.

3.1 *Definition*: Let ω be a G-invariant state on $\mathfrak{A}$, and let $\{F_\omega^N\}_{N\in Z^+}$ be the essentially bounded functions associated to ω by Theorem 2.10. For each $M,N\in Z^+$ and for $\{f_i^\circ\}_{i=1}^M$, $\{g_i^\circ\}_{i=1}^M\subset K(\mathbb{R})$, define $F_\omega^{N,M}(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)\in\mathcal{L}^\infty(\mathbb{R}^N)$ by

$$F_\omega^{N,M}(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)(x_1,\ldots,x_N)$$
$$\equiv\int_{\mathbb{R}^M}dx_{N+1}\cdots dx_{N+M}\prod_{j=1}^M f_j^\circ(x_{N+j})\bar g_j^\circ(x_{N+j})F^{N+M}(x_1,\ldots,x_N,\ldots,x_{N+M})$$

Clearly,

$$\text{ess sup}\,|F_\omega^{N,M}(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)|\le\prod_{j=1}^M\|f_j^\circ\|_2\|g_j^\circ\|_2.$$

We remark that since the F_ω^N are symmetric, the labeling in this definition is not critical and the $F_\omega^{N,M}$ are also symmetric.

The relation between the associated functions $F_\omega^{N,M}$ of a G-invariant state ω and its sharp momentum-correlation densities is described in the following lemma:

3.2 *Lemma*: Let ω be a G-invariant state on $\mathfrak{A}$, $\{F_\omega^{N,M}\}_{N,M\in Z^+}$ be the associated family of essentially bounded functions. Let

$$\{f_i\}_{i=1}^N,\ \{g_i\}_{i=1}^N,\ \{f_j^\circ\}_{j=1}^M\{g_j^\circ\}_{j=1}^M\subset K(\mathbb{R}),\quad V\in G.$$

(i) $\lim_{\delta\to0}\langle\omega:a^*(f_N)\cdots a^*(f_1)\,\alpha_V\{K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)\}\times a(g_1)\cdots a(g_N)\rangle$
$$=N!\Big(\bigotimes_{i=1}^N g_i,F_\omega^{N,M}(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)A\bigotimes_{i=1}^N f_i\Big).$$

(ii) The convergence of (i) is uniform in $V\in G$.

Remark: In view of the uses to which we intend to put this lemma, it might be appropriate to point out here that the special case $N=0$ reads:

$$\lim_{\delta\to0}\langle\omega:\alpha_V\{K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)\}\rangle$$
$$=F_\omega^{0,M}(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)$$
$$\equiv\int_{\mathbb{R}^M}d^Mx\prod_{j=1}^M f_j^\circ(x_j)\bar g_j^\circ(x_j)F_\omega^M(x_1,\ldots,x_M).$$

The existence of the $\mathcal{P}$-coarse graining operator is now established:

3.3 *Theorem*: Every G-invariant state on $\mathfrak{A}$ is $\mathcal{P}$-measurable and there exists precisely one G-invariant state in each $\mathcal{P}$-equivalence class. For each $\psi\in\mathfrak{S}^{\mathcal{P}}$, denote by $D(\psi|\mathcal{P})$ the unique G-invariant state $\mathcal{P}$-equivalent to ψ. $D(\cdot\,|\,\mathcal{P}):\mathfrak{S}^{\mathcal{P}}\to\mathfrak{S}^G$, called the $\mathcal{P}$-coarse graining operator, is an affine surjection.

Proof: The special case $N=0$ of Lemma 3.2 establishes that $\mathfrak{S}^G\subset\mathfrak{S}^{\mathcal{P}}$. Theorem 2.10 then guarantees uniqueness. Existence was proven in Corollary 1.5. The remainder is obvious.

Now let ω be a G-invariant state on $\mathfrak{A}$ and let $(\Pi_\omega,\mathcal{H}_\omega,\mathcal{U}_\omega,\Omega)$ denote the GNS covariant representation of $(\mathfrak{A},G)$ associated with ω. Denote by $\mathfrak{A}_\omega^*$ the set of all continuous linear forms on $\mathfrak{A}$ which are ultraweakly continuous on $\Pi_\omega(\mathfrak{A})\subset\mathcal{B}(\mathcal{H}_\omega)$ and by P_ω(resp. $\mathfrak{S}_\omega$) those which are, moreover, positive (resp. states). For each $\psi\in\mathfrak{A}_\omega^*$, denote by $\bar\psi$ its ultraweakly continuous extension to $\Pi_\omega(\mathfrak{A})''$. Denote by P_ω^G (resp. $\mathfrak{S}_\omega^G$) the set of G-invariant elements of P_ω(resp. $\mathfrak{S}_\omega$).

3.4 *Lemma*: Let $\{f\}$, $\{f_i^\circ\}_{i=1}^M$, $\{g_i^\circ\}_{i=1}^M\subset K(\mathbb{R})$. Let λ be a continuous linear form on $\mathfrak{A}$. The following are equivalent:

(i) $\langle\lambda:a^\natural(f)\alpha_V\{K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)\}\rangle$ converges uniformly in G as $\delta\to0$ to a limit which is independent of $V\in G$.

(ii) $\langle\lambda:\alpha_V\{K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)\}a^\natural(f)\rangle$ converges uniformly in G as $\delta\to0$ to a limit which is independent of $V\in G$.

Moreover, when these limits exist they are equal.

We now prove the more general result:

3.5 *Lemma*: Let ω be a G-invariant state on $\mathfrak{A}$. Let $\{f_i\}_{i=1}^N$, $\{g_i\}_{i=1}^N$, $\{f_i^\circ\}_{i=1}^M$, $\{g_i^\circ\}_{i=1}^M\subset K(\mathbb{R})$. Let $\{h_i\}_{i=1}^{2N}$ be an arbitrary ordering of $\{f_i\}_{i=1}^N\cup\{g_i\}_{i=1}^N$. Define

$$a(h_i)\equiv\begin{cases}a^*(h_i)&\text{if } h_i\in\{f_i\}_{i=1}^N,\\ a(h_i)&\text{if } h_i\in\{g_i\}_{i=1}^N,\end{cases}$$

Then, for arbitrary $1\le j\le 2N$,

$$\langle\omega:a^\natural(h_1)\cdots a^\natural(h_j)\alpha_V\{K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)\}\times a^\natural(h_{j+1})\cdots a^\natural(h_{2N})\rangle$$

converges as $\delta\to0$ to a limit which is independent of $V\in G$. Moreover, the convergence is uniform in G.

Proof: Formally commuting the $a^\natural(h_j)$ with $\alpha_VK_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)$ the problem is reduced to the case given by Lemma 3.2. Commuting back by Lemma 3.4 gives the following result.

3.6 *Lemma*: $\mathfrak{A}_\omega^*\subset\mathfrak{A}^{*\mathcal{P}}$.

Proof: Denote by

$$\mathcal{H}_\omega^\circ=\{\Pi_\omega(a^\natural(h_1)\cdots a^\natural(h_N))\Omega\,|\,N\in Z^+,\ \{h_i\}_{i=1}^N\subset K(\mathbb{R})\}$$

and by

$$\mathfrak{A}_\omega^{*\circ}=\{W_{\psi,\Phi}\circ\Pi_\omega\,|\,\psi,\Phi\in\mathcal{H}_\omega^\circ\}.$$

By gauge invariance of ω and Lemma 3.5, $\mathfrak{A}_\omega^{*\circ}\subset\mathfrak{A}^{*\mathcal{P}}$. By Proposition 1.3, $\mathcal{L}(\mathfrak{A}_\omega^{*\circ})^{-N}\subset\mathfrak{A}^{*\mathcal{P}}$, and by cyclicity of Ω, $\mathcal{L}(\mathfrak{A}_\omega^{*\circ})^{-N}=\mathfrak{A}_\omega^*$.

3.7 *Theorem*: Let ω be a G-invariant state on $\mathfrak{A}$, and let $(\Pi_\omega,\mathcal{U}_\omega,\mathcal{H}_\omega,\Omega)$ be the cyclic, covariant representation of $(\mathfrak{A},G)$ associated via the GNS construction to ω. Let $\mathcal{Z}_\omega=\Pi_\omega(\mathfrak{A})''\cap\Pi_\omega(\mathfrak{A})'$. Then:

(i) $\Pi_\omega(K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots g_M^\circ))$ converges in the weak (resp. ultraweak) topology of $B(H_\omega)$ as $\delta\to0$ to an operator $K_\omega^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots g_M^\circ)\in\mathcal{B}(\mathcal{H}_\omega)$ $\forall\{f_i^\circ\}_{i=1}^M$, $\{g_i^\circ\}_{i=1}^M\subset K(\mathbb{R})$.

(ii) $K_\omega^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)\in\mathcal{Z}_\omega\cap\{\mathcal{U}_\omega(G)\}'$.

(iii) The convergence of $\mathcal{U}_\omega(V)^*\Pi_\omega(K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ))\mathcal{U}_\omega(V)$ to $K_\omega^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots g_M^\circ)$ as $\delta\to0$ is uniform in $V\in G$ in the weak operator and in the ultraweak operator topologies.

(iv) $K_\omega^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)=\Pi_{i=1}^M K_\omega^1(f_i^\circ;g_i^\circ)$.

Proof: Since

$$\|\Pi_\omega(K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ))\|\le\prod_{j=1}^M\|f_j^\circ\|_2\|g_j^\circ\|_2$$

and since the weak operator and ultraweak topologies coincide on bounded sets, it is sufficient to prove our statements for the weak operator topology.

Since for each $\delta > 0$, the sesquilinear form

$$(\psi, \Phi) \to (\psi, \Pi_\omega(K_\delta^M(f_1^\circ, \dots, f_M^\circ; g_1^\circ, \dots g_M^\circ))\Phi)$$

from $\mathcal{H}_\omega \times \mathcal{H}_\omega$ to C is bounded by $\Pi_{i=1}^M \|f_i^\circ\|_2 \|g_i^\circ\|_2$, its limit, which exists by Lemma 3.6, is bounded as well. Riesz' theorem then gives (i). (ii) follows from Lemmas 3.4 and 3.6. (iii) follows from Lemma 3.6. Now we prove (iv). It is sufficient to prove that

$$(\psi, K_\omega^M(f_1^\circ, \dots, f_M^\circ; g_1^\circ, \dots, g_M^\circ)\Phi) = \left(\psi, \prod_{j=1}^M K_\omega^1(f_j^\circ; g_j^\circ)\Phi\right) \quad \forall \Phi, \psi \in \mathcal{H}_\omega^\circ.$$

However, since $K_\omega^N(f_1^\circ, \dots, f_M^\circ; g_1^\circ, \dots, g_M^\circ) \in \mathcal{Z}_\omega \cap \{\mathcal{U}_\omega(G)\}'$ and since ω is gauge invariant, it suffices to show the result for

$$\psi = \Pi_\omega\{a(f_1) \cdots a(f_N)\}\Omega \quad \forall \{f_j\}_{j=1}^N, \ \{g_j\}_{j=1}^N \subset K(\mathbb{R}),$$
$$\Phi = \Pi_\omega\{a(g_1) \cdots a(g_N)\}\Omega.$$

We prove the result by induction. It is trivially true for $M = 1$. Assume

$$K_\omega^{M-1}(f_1^\circ, \dots, f_{M-1}^\circ\ g_1^\circ, \dots, g_{M-1}^\circ) = \prod_{j=1}^{M-1} K_\omega^1(f_j^\circ; g_j^\circ).$$

We will show that

$$K_\omega^M(f_1^\circ, \dots, f_M^\circ; g_1^\circ, \dots, g_M^\circ) = K_\omega^{M-1}(f_1^\circ, \dots, f_{M-1}^\circ; g_1^\circ, \dots, g_{M-1}^\circ) K_\omega^1(f_M^\circ; g_M^\circ).$$

In fact

$$\begin{aligned}(\psi, K_\omega^1(f_M^\circ; g_M^\circ) & K_\omega^{M-1}(f_1^\circ, \dots, f_{M-1}^\circ; g_1^\circ, \dots, g_{M-1}^\circ)\Phi) \\ &= \lim_{\delta \to 0} (\psi, \Pi_\omega\{K_\delta^1(f_M^\circ; g_M^\circ)\} K_\omega^{M-1}(f_1^\circ, \dots, f_{M-1}^\circ; g_1^\circ, \dots g_{M-1}^\circ)\Phi) \\ &= \lim_{\delta \to 0} \Big(\psi, [\textstyle\int dx\, f_M^\circ(x) \bar{g}_M^\circ(x) \Pi_\omega\{a(\Delta_x) a(\Delta_x)\}] \\ &\qquad \times K_\omega^{M-1}(f_1^\circ, \dots, f_{M-1}^\circ; g_1^\circ, \dots, g_{M-1}^\circ)\Phi\Big),\end{aligned}$$

where, due to continuity of Π_ω, the integral converges as a norm limit of simple functions on $B(\mathcal{H}_\omega)$. Since K_ω^{M-1} is bounded, we have

$$= \lim_{\delta \to 0} \int dx\, f_M^\circ(x) \bar{g}_M^\circ(x)$$

$$\times (\psi, \Pi_\omega\{a^*(\Delta_x) a(\Delta_x)\} K_\omega^{M-1}(f_1^\circ, \dots, f_{M-1}^\circ; g_1^\circ, \dots, g_{M-1}^\circ)\Phi).$$

Since $K_\omega^{M-1} \in \mathcal{Z}_\omega$, we have

$$= \lim_{\delta \to 0} \int dx\, f_M^\circ(x)\, \bar{g}_M^\circ(x)$$
$$\times (\Pi_\omega\{a(\Delta_x) \cdots a(f_N)\}\Omega,\ K_\omega^{M-1}(f_1^\circ, \dots, f_{M-1}^\circ; g_1^\circ, \dots, g_{M-1}^\circ)$$
$$\times \Pi_\omega\{a(\Delta_x) \cdots a(g_N)\}\Omega).$$

And, by Lemma 3.2,

$$= \lim_{\delta \to 0} (N+1)! \int dx\, f_M^\circ(x) g_M^\circ(x) \times \left(\Delta_x \bigotimes_{j=1}^N g_j,\ F_\omega^{N+1, M-1}(f_1^\circ, \dots, f_{M-1}^\circ; g_1^\circ, \dots, g_{M-1}^\circ) A \times \Delta_x \bigotimes_{j=1}^N f_j\right).$$

And, by the argument of Lemma 3.2,

$$= N! \left(\bigotimes_{j=1}^N g_j,\ F_\omega^{N,M}(f_1^\circ, \dots, f_M^\circ; g_1^\circ, \dots, g_M^\circ) A \bigotimes_{j=1}^N f_j\right)$$

$$= (\psi, K_\omega^M(f_1^\circ, \dots, f_M^\circ; g_1^\circ, \dots, g_M^\circ)\Phi).$$

This completes the proof of (iv).

The heuristic remarks made in the beginning of Sec. 1, embodied as they now are in the $K_\omega(f,g)$, provide the motivation for the following definition.

3.8 *Definition*: Let $\mathcal{P}_\omega$ denote the C^*-algebra generated by $\{K_\omega^1(f,g) \mid f, g \in K(\mathbb{R})\}$, where $K^1(f,g)$ are the elements of $\mathcal{Z}_\omega \cap \{\mathcal{U}_\omega(G)\}'$ defined in Theorem 3.7. $\mathcal{P}_\omega''$ is called the von Neumann algebra of momentum observables attached to the G-invariant state ω on $\mathfrak{A}$.

In the next theorem we show in which sense $\mathcal{P}_\omega''$ is naturally associated with a number density on the momentum space R.

3.9 *Theorem*: Let ω be a G-invariant state on $\mathfrak{A}$, $\mathcal{P}_\omega''$ the von Neumann algebra of momentum observables associated with ω. Consider the mapping $K_\omega^1: K(\mathbb{R}) \times K(\mathbb{R}) \to \mathcal{B}(\mathcal{H}_\omega)$ defined $K_\omega^1(f \times g) \equiv K_\omega^1(f, g)$. Then:

(i) $K_\omega^1: K(\mathbb{R}) \times K(\mathbb{R}) \to \mathcal{B}(\mathcal{H}_\omega)$ admits a unique extension to a norm-continuous, operator-valued, positive, sesquilinear form over $\mathcal{L}^2(\mathbb{R})$.

(ii) $K_\omega^1(f;g) \in \mathcal{P}_\omega \quad \forall f, g \in \mathcal{L}^2(\mathbb{R})$

(iii) $K_\omega^1(Vf; Vg) = K_\omega^1(f, g) \quad \forall f, g \in \mathcal{L}^2(\mathbb{R}), \quad \forall V \in G.$

(iv) There exists a unique operator-valued, weak-operator measurable function $K_\omega(x)$ such that

$$K_\omega(f, g) = \int_{\mathbb{R}} dx\, f(x) \bar{g}(x) K_\omega(x).$$

Moreover,

$$\left.\begin{array}{l}\text{(a) } 0 \le K_\omega(x) \le 1 \\ \text{(b) } K_\omega(x) \in \mathcal{P}_\omega''\end{array}\right\} \text{ a.e.} - dx.$$

Proof:

(adi) We first remark that for each $\delta > 0, f_1, f_2, g_1, g_2 \in K(\mathbb{R}),\ \lambda, \gamma \in \mathbb{C}$.

$$\begin{aligned}(1)\ \Pi_\omega\{K_\delta^1(f_1 + \lambda f_2; g_1 + \gamma g_2)\} &= \Pi_\omega\{K_\delta^1(f_1, g_1)\} \\ &\quad + \bar{\gamma}\Pi_\omega\{K_\delta^1(f_1, g_2)\} \\ &\quad + \lambda\Pi_\omega\{K_\delta^1(f_2; g_1)\} \\ &\quad + \lambda\bar{\gamma}\Pi_\omega\{K_\delta^1(f_2; g_2)\},\end{aligned}$$

(2) $\|\Pi_\omega(K_\delta^1(f_1, g_1))\| \le \|f_1\|_2 \|g_1\|_2$,

(3) $\Pi_\omega\{K_\delta^1(Vf; Vg)\} = \Pi_\omega\{K_\delta^1(f; g)\}$,

(4) $\Pi_\omega(K_\delta^1(f; f)) \ge 0$.

Therefore, $K_\omega^1(f; g) = \omega - \lim_{\delta \to 0} \Pi_\omega\{K_\delta^1(f; g)\}$ enjoys all these four properties.

(i) and (iii) then follow trivially from the continuity of K_ω^1 over the dense subset $K(\mathbb{R})$ of $\mathcal{L}^2(\mathbb{R})$. (ii) is immediate since, for $f, g \in \mathcal{L}^2(\mathbb{R})$, $K_\omega^1(f; g)$ is the limit of a norm convergent sequence in $\mathcal{P}_\omega$ which is, a fortiori, norm closed. We now prove (iv). For each $\psi, \Phi \in H_\omega$, Riesz' theorem defines a unique bounded operator $N_\omega(\psi, \Phi) \in \mathcal{B}(\mathcal{L}^2(\mathbb{R}))$ such that

$$(g, N_\omega(\psi; \Phi)f) = (\psi, K_\omega^1(f; g)\Phi).$$

The invariance (iii) implies that $N_\omega(\Phi; \psi)$ commutes with the maximal Abelian von Neumann algebra $\mathcal{L}^\infty(\mathbb{R})$. Hence $N_\omega(\psi; \Phi) \in \mathcal{L}^\infty(\mathbb{R})$ and there exists an a.e. unique essentially bounded function $N_\omega(\psi; \Phi)(x)$ such that

$$N_\omega(\psi;\Phi)\,h(x)=N_\omega(\psi;\Phi)\,(x)\,h(x)\text{a. e.}\forall \qquad h\in \mathcal{L}^2(\mathbb{R}).$$

Now

$$\operatorname{ess\,sup}|N_\omega(\psi,\Phi)(x)| = \sup|(g, N_\omega(\psi;\Phi)f)|,\quad \|f\|_2=1,\quad \|g\|_2=1,$$

$$=\sup|(\psi, K^1_\omega(f,g)\Phi)| \le \|\psi\|\,\|\Phi\|,\quad \|f\|_2=1,\quad \|g\|_2=1,$$

Moreover, since $N_\omega(\psi,\Phi)$ is clearly a positive sesquilinear operator-valued form on $B(H_\omega)$, $N_\omega(\psi,\Phi)(x)$ is a positive, and by the previous remark, continuous, sesquilinear form for a. e. $x\in\mathbb{R}$. Hence, again by Riesz' theorem, there exists an almost everywhere unique, bounded, weak operator-measurable density $K'_\omega(x)$ such that $(\psi, K_\omega(x)\Phi)=N_\omega(\psi,\Phi)(x)$ a. e. $-dx$. It is clear, by construction, that $0\le K(x)\le 1$ a. e. and that

$$K^1_\omega(f;g)=\int_{\mathbb{R}} K_\omega(x)f(x)\bar{g}(x)\,dx.$$

To prove b, let $T\in \mathcal{P}'_\omega$; then

$$(\psi,[T,K^1_\omega(f,g)]\Phi)=\int_{\mathbb{R}}(\psi,[T,K_\omega(x)]\Phi)\quad f(x)\bar{g}(x)dx=0.$$

Thus $K_\omega(x)\in \mathcal{P}''_\omega$ a. e. $-dx$. This completes the proof of the theorem.

To sum up, we have shown that, in the representation associated with any G-invariant state ω, one may define a number density operator $K_\omega(x)$ on the one-particle momentum space of the Fermi system. In the center $\mathcal{Z}_\omega$ of the representation canonically associated with ω, we have isolated the algebra of momentum observables $\mathcal{P}''_\omega$, it is the von Neumann algebra "generated" by the number density operator referred to above. We shall see in the next subsection that $\mathcal{P}''_\omega$ is rich in information about the state ω.

The following proposition establishes the role of $\mathcal{P}''_\omega$ in connection with the concept of $\mathcal{P}$-equivalence introduced in 1.2.

3.10 *Proposition*: Let ω be a G-invariant state on $\mathfrak{A}$. For each $\psi\in P_\omega$ denote by $R_\omega\tilde{\psi}$ the restriction of $\tilde{\psi}$ to $\mathcal{P}''_\omega$. The two states ψ and $\psi'\in\mathfrak{S}_\omega$ are $\mathcal{P}$-equivalent if and only if $R_\omega\tilde{\psi}=R_\omega\tilde{\psi}'$.

Proof: By Theorem 3.7, for each $\psi\in P_\omega$ we have

$$\hat{\psi}^M(f_1,\ldots,f_M;g_1,\ldots,g_M)\equiv\lim_{\delta\to 0}\langle\psi:K^M_\delta(f_1,\ldots,f_M;g_1,\ldots,g_M)\rangle$$
$$=\langle\tilde{\psi}:K^M_\omega(f_1,\ldots,f_M;g_1,\ldots,g_M)\rangle$$
$$=\langle R_\omega\tilde{\psi}:K^M_\omega(f_1,\ldots,f_M;g_1,\ldots,g_M)\rangle$$
$$\forall\{f_i\}^M_{i=1},\ \{g_i\}^M_{i=1}\subset K(\mathbb{R}).$$

Therefore, if $\psi\approx\psi'$, we have, by the ultraweak density of the linear span of the $\{K^M_\omega\}$ in $\mathcal{P}''_\omega$ and the ultraweak continuity of $R_\omega\tilde{\psi}$ and $R_\omega\tilde{\psi}'$, that $R_\omega\tilde{\psi}'=R_\omega\tilde{\psi}$. The converse is immediate.

We are now ready for the next step outlined in the introduction, namely, the assignment of a $\mathcal{P}''_\omega$-*a priori* probability. We shall also indicate its relation with the $\mathcal{P}$-coarse graining operator, defined in Theorem 3.3 and now restricted to $\mathfrak{S}_\omega$.

3.11 *Proposition*: Let ω be a G-invariant state on $\mathfrak{A}$. Let E_ω be the projector on $\mathcal{H}_\omega$ defined by $E_\omega\mathcal{H}_\omega=[\mathcal{P}_\omega\Omega]^-$. Then:

(i) For each $S\in\Pi_\omega(\mathfrak{A})''$, there exists a unique $\bar{S}\in\mathcal{P}''_\omega\ni E_\omega SE_\omega=E_\omega\bar{S}$.

(ii) For each $\psi\in P_\omega$ denote by $R_\omega\tilde{\psi}$ the restriction of $\tilde{\psi}$ to $\mathcal{P}''_\omega$. The mapping $R_\omega:P^G_\omega\to\{\mathcal{P}_\omega\}^+_*$ is an order isomorphism. Denote its inverse by $\mathcal{E}_\omega(\cdot\mid\mathcal{P})_*$. $\mathcal{E}_\omega(\cdot\mid\mathcal{P})_*$ is called the $\mathcal{P}''_\omega$-*a priori* probability assignment.

(iii) For each $\phi\in\{\mathcal{P}''_\omega\}^+_*$, there exists a vector $\xi\in E_\omega\mathcal{H}_\omega\ni\mathcal{E}_\omega(\phi\mid\mathcal{P})_*=W_{\xi,\xi}\circ\Pi_\omega$.

(iv) $D(\psi\mid\mathcal{P})=\mathcal{E}_\omega(R_\omega\tilde{\psi}\mid\mathcal{P})_*\in\mathfrak{S}^G_\omega\quad\forall\psi\in\mathfrak{S}_\omega$.

Proof: (adi): Since $E_\omega\{[E_\omega SE_\omega,T]\}E_\omega=0\,\forall S\in\mathcal{P}''_\omega$ by Theorem 3.7 (ii) and since $E_\omega\in\mathcal{P}'_\omega$, $E_\omega SE_\omega$ commutes with the maximally Abelian von Neumann subalgebra (see Cor. 2, p. 89 in Ref. 6) $\mathcal{P}''_\omega|_{E_\omega}$ of $\mathcal{B}(E_\omega\mathcal{H}_\omega)$, therefore, there exists $\bar{S}\in\mathcal{P}''_\omega$ such that $E_\omega SE_\omega=E_\omega\bar{S}$. However, since the central support of E_ω in $\mathcal{P}''_\omega$ is the projector upon $[\mathcal{P}'_\omega\mathcal{P}_\omega\Omega]\supset[\Pi_\omega(\mathfrak{A})\Omega]^-=\mathcal{H}_\omega$, the mapping $\mathcal{P}''_\omega\to\mathcal{P}''_\omega|_{E_\omega}$ is an isomorphism (Prop. 2, p. 19, of Ref. 6). Hence $\bar{S}$ is unique.

(adii) R_ω is clearly order preserving. Injectivity: It clearly suffices to show that $\mathcal{P}''_\omega$ separates $\mathfrak{S}^G_\omega$. This is immediate from proposition 3.10 and Theorem 3.3.

Surjectivity and (iii): We have seen that the mapping $P:\mathcal{P}''_\omega\to\mathcal{P}''_\omega|_{E_\omega}$ is an isomorphism. Consequently, the dual map gives a positive linear bijection P^*: $(\mathcal{P}''_\omega|_{E_\omega})^+_*\to\{\mathcal{P}_\omega\}^+_*$. Let ϕ be a positive normal form on $\mathcal{P}''_\omega$. Since all the normal forms on the maximally Abelian von Neumann algebra $\mathcal{P}''_\omega|_{E_\omega}$ are vector forms (see, for instance, exercise 4, p. 120, in Ref. 6), there exists a $\xi\in E_\omega\mathcal{H}_\omega$ such that $(\xi,S\xi)=\langle(P^*)^{-1}\phi:S\rangle=\langle\phi:P^{-1}S\rangle\,\forall S\in\mathcal{P}''_\omega|_{E_\omega}$. Suppose that $T(\in\mathcal{P}''_\omega)=P^{-1}S$. Then, $(\xi,T\xi)=(\xi,E_\omega T\xi)=(\xi,S\xi)=\langle\phi:P^{-1}S\rangle=\langle\phi:T\rangle$. Clearly, the vector form $\omega_{\xi;\xi}\circ\Pi_\omega\in P^G_\omega$ and its restriction to $\mathcal{P}''_\omega$ is ϕ.

(iv) Since $\psi\approx D(\psi\mid\mathcal{P})$ and by Prop. 3.10 $\mathcal{E}_\omega(R_\omega\psi\mid\mathcal{P})_*\approx\psi$, and since both are G-invariant, equality follows from Theorem 3.3.

Our final task in fulfilling the program of the introduction is to define the $\mathcal{P}''_\omega$-conditional expectation, and this can now be done:

3.12 *Definition*: Let ω be a G-invariant state on $\mathfrak{A}$. For each $S\in\Pi_\omega(\mathfrak{A})''$, let $\mathcal{E}_\omega(S\mid\mathcal{P})$ denote the unique element of $\mathcal{P}''_\omega$ such that $E_\omega S\,E_\omega=\mathcal{E}_\omega(S\mid\mathcal{P})E_\omega$. $\mathcal{E}_\omega(\cdot\mid\mathcal{P})$: $\Pi_\omega(\mathfrak{A})''\to\mathcal{P}''_\omega$ is called the $\mathcal{P}''_\omega$-conditional expectation on $\Pi_\omega(\mathfrak{A})''$.

We now establish that the $\mathcal{P}''_\omega$-*a priori* probability assignment is dual to the $\mathcal{P}''_\omega$-conditional expectation, and we detail the properties of $\mathcal{E}_\omega(\cdot\mid\mathcal{P})$.

3.13 *Theorem*: Let ω be a G-invariant state on $\mathfrak{A}$ and $\mathcal{E}_\omega(\cdot\mid\mathcal{P}):\Pi_\omega(\mathfrak{A})''\to\mathcal{P}''_\omega$ be as above. Then,

(i) $\mathcal{E}_\omega(\lambda S+\gamma T\mid\mathcal{P})=\lambda\mathcal{E}_\omega(S\mid\mathcal{P})+\gamma\mathcal{E}_\omega(T\mid\mathcal{P})\quad\forall\lambda,\gamma\in\mathbb{C},\quad\forall S,T\in\Pi_\omega(\mathfrak{A})''$,

(ii) $\mathcal{E}_\omega(1\mid\mathcal{P})=1$,

(iii) $\mathcal{E}_\omega(S\mathcal{E}_\omega(T\mid\mathcal{P})\mid\mathcal{P})=\mathcal{E}_\omega(S\mid\mathcal{P})\mathcal{E}_\omega(T\mid\mathcal{P})\quad\forall S,T\in\Pi_\omega(\mathfrak{A})''$,

(iv) $\mathcal{E}_\omega(S^*S\mid\mathcal{P})\ge 0\quad\forall S\in\Pi_\omega(\mathfrak{A})''$,

(v) $\|\mathcal{E}_\omega(S\mid\mathcal{P})\|\le\|S\|$

$\forall S \in \Pi_\omega(\mathfrak{A})''$ and $\mathcal{E}_\omega(\cdot\,|\mathcal{P})$ is normal.

(vi) $\mathcal{E}_\omega(\mathcal{U}_{\omega(V)} S \mathcal{U}^*_{\omega(V)}\,|\mathcal{P}) = \mathcal{E}_\omega(S|\mathcal{P}) \quad \forall S \in \Pi_\omega(\mathbf{V})'', \quad \forall V \in G.$

(vii) $\langle \psi : \mathcal{E}_\omega(S|\mathcal{P})\rangle = \langle \mathcal{E}_\omega(\psi|\mathcal{P})_* : S\rangle \quad \forall S \in \Pi_\omega(\mathfrak{A})'', \quad \forall \psi \in (\mathcal{P}_\omega)^+_*$

Proof: Properties (i)—(vi) are immediate from the definition.

(ad vii) Since $\psi \circ \mathcal{E}_\omega(\cdot\,|\mathcal{P})$ and $\mathcal{E}_\omega(\psi|\mathcal{P})_* \in P^G_\omega$ have the same restriction to $\mathcal{P}''_\omega$, they are identical by Proposition 3.11 (ii).

3.14 Corollary:

(i) $\mathcal{E}_\omega(a^*(f_N)\cdots a^*(f_1)a(g_1)\cdots a(g_M)\,|\mathcal{P})$
$$= \delta_{M,N} \sum_{p \in \mathcal{S}_N} (-1)^{\sigma(p)} \prod_{i=1}^N K_\omega(f_i; g_{p(i)})$$
$\forall \{f_i\}_{i=1}^N,\ \{g_i\}_{i=1}^M \subset K(\mathrm{R}).$

(ii) $\mathcal{E}_\omega(\Pi_\omega(\mathfrak{A})\,|\mathcal{P}) \subset \mathcal{P}_\omega$ (not only $\mathcal{P}''_\omega$).

Proof: (ad i) Follows from Theorem 3.13 (vii), G-invariance of $\mathcal{E}_\omega(\psi|\mathcal{P})_*$, Theorem 3.7 (i) and (iv), and Theorem 2.10.

(ad ii) Follows from (i) and linearity and continuity of $\mathcal{E}_\omega(\cdot\,|\mathcal{P})$.

4. G-ERGODIC STATES AND THE GEOMETRIC STRUCTURE OF G^G

The principal aim of this section is to prove that $\mathfrak{S}^G$ is a (Choquet) simplex whose extreme points coincide with the set of all translation invariant, gauge invariant generalized free states.

4.1 *Proposition*: Let ω be a G-invariant state on $\mathfrak{A}$, and let E_ω be the projector onto the closed subspace $[\mathcal{P}_\omega\Omega]^-$. The following are equivalent:

(0) $\mathcal{P}''_\omega = \{\lambda I\,|\,\lambda \in \mathrm{C}\}$,

(1) E_ω is one dimensional,

(2) ω is extremal G-invariant,

(3) ω is a factor state (i.e., $\mathcal{Z}_\omega = \{\lambda I\,|\,\lambda \in \mathrm{C}\}$)

(4) ω is a generalized free state.

Proof: (0)$\Rightarrow$(1): trivial.

(1)$\Rightarrow$(0): If E_ω is one dimensional, then $\mathcal{P}''_\omega|_{E_\omega} = \{\mathrm{C}I\}|_{E_\omega}$. But since the map $\mathcal{P}''_\omega \to \mathcal{P}''_\omega|_{E_\omega}$ is an isomorphism [cf. proof of Prop. 3.11 (i)], this implies that $\mathcal{P}''_\omega = \{\mathrm{C}I\}$.

(i)$\Rightarrow$(2): ψ G-invariant and dominated by ϕ would imply $\psi \in P^G_\omega$.[9] By Prop. 3.11 (iii) and (i), this implies $\psi = \phi$.

(2)$\Rightarrow$(1): If ω is extremal, we have

$$(\Omega, S\Pi_\omega(T)\Omega) = (\Omega, \Pi_\omega(T)\Omega)$$
$$\forall T \in \mathfrak{A}, \quad \forall S \in \mathcal{P}''_\omega \quad 0 \leq S, \text{ and } (\Omega, S\Omega) = 1.$$

Hence due to the density of $\{\Pi_\omega(T)\Omega\,|\,T \in \mathfrak{A}\}$ in $\mathcal{H}_\omega$, $S\Omega = \Omega$. Since every operator $S \in \mathcal{P}''_\omega$ may be written as a linear combination of positive elements of $\mathcal{P}''_\omega$, $\exists\, \lambda_s \in \mathrm{C} \ni S\Omega = \lambda_s\Omega \ \forall S \in \mathcal{P}''_\omega$. Therefore E_ω is one dimensional.

(3)$\Rightarrow$(0): Since $\mathcal{P}''_\omega \subset \mathcal{Z}_\omega$ (Theorem 3.7).

(4)$\Rightarrow$(3): This follows from the result of Dell'Antonio[10] and Rideau.[11]

It remains to show (0)$\Rightarrow$(4): Let $\mathcal{P}''_\omega = \{\mathrm{C}I\}$. Then by Lemma 3.2, Theorem 3.7 (i) and (iv), and assumption (0), we have

$$\left(\bigotimes_{i=1}^M g_i^\circ,\ F^M_\omega \bigotimes_{i=1}^M f_i^\circ\right) = \langle \tilde{\omega} : K^M_\omega(f_1^\circ, \ldots, f_M^\circ; g_1^\circ, \ldots, g_M^\circ)\rangle$$
$$= \langle \tilde{\omega} : \prod_{i=1}^M K^1_\omega(f_i; g_i)\rangle$$
$$= \prod_{i=1}^M \langle \tilde{\omega} : K^1_\omega(f_i; g_i)\rangle$$
$$= \left(\bigotimes_{i=1}^M g_i^\circ,\ \bigotimes_{i=1}^M F^1_{\omega,i} \bigotimes_{i=1}^M f_i^\circ\right)$$
$$\forall \{f_i^\circ\}_{i=1}^M,\ \{g_i^\circ\}_{i=1}^M \subset K(\mathbf{R}).$$

Thus $F^M_\omega = \otimes_{i=1}^M F^1_{\omega,i}$ for all $M \in \mathrm{Z}^+$ and, by Corollary 2.11, ω is a generalized free state. This completes the proof of the proposition.

4.2 *Theorem*: The set of all G-invariant states $\mathfrak{S}^G$ is a simplex whose extreme points coincide with the set of space translation and gauge invariant generalized free states on $\mathfrak{A}$.

Proof: The proof that $\mathfrak{S}^G$ is a simplex is done along classical lines. It must be proven that the cone P^G of G-invariant positive linear forms on $\mathfrak{A}$ is a lattice (cf. p. 218 of Ref. 9) i.e., that all $\phi_1, \phi_2 \in P^G$ have a unique l.u.b., $\phi_1 \vee \phi_2$, and g.l.b. $\phi_1 \wedge \phi_2$). As ϕ_1, ϕ_2 are dominated by the G-invariant state $(\langle \phi_1 + \phi_2 : I\rangle)^{-1}(\phi_1 + \phi_2) \equiv \omega$ and hence are ultraweakly continuous on $\pi_\omega(\mathfrak{A})$, it suffices to show that P^G_ω is a lattice. This is the case since P^G_ω is order isomorphic to the set of positive normal forms on the Abelian von Neumann algebra $\mathcal{P}''_\omega$ by Proposition 3.11 (ii).

The characterization of extreme points follows from Proposition 4.1, and the result of Balslev and Verbeure.[12]

Remark: Consider the Fock representation of $\mathfrak{A}$, (π_F, H_F, Ω_F). Since π_F is irreducible $\pi_F(\mathfrak{A})'' = B(\mathcal{H}_F)$; E_F is one dimensional; $\mathcal{P}''_\omega = \{\mathrm{C}I\}$; and $\mathfrak{S}^G_F = \{\omega_F\}$. Let $f \geq 0 \in \mathcal{L}^\infty(\mathrm{R})$ and define $(A_f\Phi)^N = 0, N \neq 1$; $f\Phi^1, N = 1$. Clearly, $A_f \in \pi_F(\mathfrak{A})'' \cap \mathcal{U}_F(G)'$, yet $\langle \tilde{\omega}_F : A_f\rangle = 0$ so that $\pi_F(\mathfrak{A})''$ is not G-finite. This remark should be contrasted with Kovács and Szücs'[13] assumptions which are thus too restrictive from the physical problem considered here.

5. THE C^*-ALGEBRA OF SECOND QUANTIZED MOMENTUM OBSERVABLES P AND THE P-CONDITIONAL EXPECTATION

5.1 *Proposition*: The set $\mathcal{S}$ of extremal G-invariant states is a w^*-closed (hence compact) subset of $\mathfrak{S}$.

Proof: By proposition 4.1, $\mathcal{S}$ is the intersection of the w^*-closed set $\mathfrak{S}^G$ with the w^*-closed[14] set of gauge invariant generalized free states.

Theorem 2.10 defines for each G-invariant generalized free state ω a unique operator $F_\omega \in \mathcal{L}^\infty(\mathbb{R})$ such that

$\langle\omega : a^*(f)\, a(g)\rangle = (g, F_\omega f) \quad \forall f, g \in \mathcal{L}^2(\mathrm{R})$.

5.2 *Theorem*: The mapping $\tau : \omega \to F_\omega$ of $(\mathcal{S}, \sigma(\mathcal{S}, \mathfrak{A}))$ to $(\mathcal{L}^\infty(\mathrm{R})_1^+, \sigma(\mathcal{L}^\infty(\mathrm{R})_1^+, \mathcal{L}^1(\mathrm{R}))$ is a homeomorphism.

Proof: τ is clearly injective.

τ is surjective by the construction of Araki and Wyss[15] and Theorem 2.10.

τ is continuous. In fact, let $\{\omega_\alpha\}_{\alpha\in I}$ be a net in $\mathcal{S}$, convergent in the w^*-topology to ω, say. Then

$$\lim_{\alpha\in I}\langle\omega_\alpha : a^*(f)a(g)\rangle = \lim_{\alpha\in I}(g, F_{\omega_\alpha} f) = (g, F_\omega f) \quad \forall f, g \in \mathcal{L}^2(\mathbb{R}).$$

Therefore τ is continuous. τ is a homeomorphism since any continuous bijection of a compact space onto a Hausdorff space is a homeomorphism.[16] This proves the theorem.

Proposition 5.1 defines a classical phase space $\mathcal{S}$ which we shall interpret below as the spectrum of the C^*-algebra of momentum observables. Theorem 5.2 gives a physical description of $\mathcal{S}$. To see this, we recall (3.9):

$$\langle\tilde{\omega} : K_\omega(f, g)\rangle = \int_{\mathrm{R}} f(x)\bar{g}(x)F_\omega(x)dx = \int f(x)\bar{g}(x)\langle\tilde{\omega} : K_\omega(x)\rangle dx;$$

therefore

$$F_\omega(x) = \langle\tilde{\omega} : K_\omega(x)\rangle \quad \text{a.e.} - dx$$

Therefore, $F_\omega(x)$ is the number density on the one-particle momentum spectrum of the state ω of the Fermi system.

5.3 *Definition*: (i) Denote by $\mathcal{P}$ the C^*-algebra of all complex-valued, continuous functions on the compact Hausdorff space $(\mathcal{S}, \sigma(\mathcal{S}, \mathfrak{A}))$.

(ii) For each pair $f, g \in \mathcal{L}^2(\mathbb{R})$, define $K(f, g) \in \mathcal{P}$ by $K(f,g)[\psi] = \langle\psi : a^*(f)\, a(g)\rangle \quad \forall \psi \in \mathcal{S}$

5.4 *Remark*: $K(f, g)[\psi] \equiv \langle\psi : a^*(f)a(g)\rangle = (g, F_\psi f) = \langle\tilde{\psi} : K_\psi(f, g)\rangle$, where the last equality results from Theorem 3.7 (i) and Lemma 3.2.

5.5 *Theorem*: Define $\mathcal{E}(\cdot\,|\mathcal{P}) : \mathcal{C}(\mathfrak{S}) \to \mathcal{P}$ by

$$\mathcal{E}(T\,|\,\mathcal{P})[\psi] \equiv \langle\psi : T\rangle \quad \forall\psi \in \mathcal{S}, \quad \forall T \in \mathcal{C}(\mathfrak{S}).$$

Then, $\mathcal{E}(\cdot\,|\mathcal{P})$ enjoys the following properties:

(i) $\mathcal{E}(\lambda S + \gamma T\,|\,\mathcal{P}) = \lambda\mathcal{E}(S\,|\,\mathcal{P}) + \gamma\mathcal{E}(T\,|\,\mathcal{P})$ $\quad \forall\lambda, \gamma \in \mathrm{C}, \quad \forall S, T \in C(\mathfrak{S})$.

(ii) $\mathcal{E}(T^*T\,|\,\mathcal{P}) \geq 0 \qquad T \in C(\mathfrak{S})$.

(iii) $\mathcal{E}(1\,|\,\mathcal{P}) = 1$.

(iv) $\mathcal{E}(\alpha_V S\,|\,\mathcal{P}) = \mathcal{E}(S\,|\,\mathcal{P}) \quad \forall V \in G, \quad S \in \mathfrak{A}$.

(v) $\|\mathcal{E}(S\,|\,\mathcal{P})\| \leq \|S\| \quad \forall S \in \mathfrak{A}$.

The proof is immediate.

The following lemmas aim toward proving that $\mathcal{E}(\mathfrak{A} : \mathcal{P})^{-N} = \mathcal{P}$. (Proposition 5.8).

5.6 *Lemma*. Denote by $\mathcal{P}_0$ the sub*-algebra of $\mathcal{P}$ generated by $\{K(f,g)\,|\, f, g \in K(\mathrm{R})\} \cup 1$. Then $\mathcal{P}_0$ is norm dense in $\mathcal{P}$.

Proof: It suffices, by the Stone–Weierstrass theorem, to show that $\mathcal{P}_0$ separates $\mathcal{S}$. To that end, let $\phi \neq \psi \in \mathcal{S}$. By Theorem 5.2, $F_\phi \neq F_\psi$. Hence, there exists $f, g \in K(\mathrm{R}) \ni 0 \neq (g, (F\phi - F\psi)f) = K(f, g)[\phi] - K(f, g)[\psi]$. This proves the lemma.

5.7 *Lemma*: Let $\{f_i\}_{i=1}^N$, $\{g_i\}_{i=1}^N \subset K(\mathrm{R})$. Then,

$$\text{w-}\lim_{M\to\infty} \mathcal{E}(K_{1/M}^N(f_1, \ldots, f_N; g_1, \ldots, g_M)\,|\,\mathcal{P}) = \prod_{i=1}^N K(f_i; g_i).$$

Proof: For each $\psi \in \mathcal{S}$ we have, by Theorem 3.7 (i) and (iv), Theorem 4.1, and Remark 5.4.

$$\lim_{M\to\infty} \mathcal{E}(K_{1/M}(f_1, \ldots, f_N; g_1, \ldots, g_N)\,|\,\mathcal{P})[\psi] = \lim_{M\to\infty}\langle\psi : K_{1/M}(f_1, \ldots, f_N; g_1, \ldots, g_N)\rangle = \langle\tilde{\psi} : \prod_{i=1}^N K_\psi(f_i; g_i)\rangle = \prod_{i=1}^N \langle\tilde{\psi} : K_\psi(f_i; g_i)\rangle = \prod_{i=1}^N K(f_i; g_i)[\psi].$$

Therefore, the bounded sequence $\{\mathcal{E}(K_{1/M}^N(f_1, \ldots, f_N; g_1, \ldots, g_N)\,|\,\mathcal{P})\}_{M\in\mathbb{Z}^+}$ converges pointwise to the continuous function $\prod_{i=1}^N K(f_i; g_i)$. From Ref. 17, Theorem 6.11 and its Corollary 6.12, we get the weak convergence.

5.8 *Proposition*: $\mathcal{E}(\mathfrak{A}\,|\,\mathcal{P})^{-N} = \mathcal{P}$

Proof: $\mathcal{E}(\mathfrak{A}\,|\,\mathcal{P})$ is clearly a convex subset of $\mathcal{P}$, weakly dense by Lemmas 5.6 and 5.7. By virtue of Mazur's theorem (V.3.13 of Ref. 17) $\mathcal{E}(\mathfrak{A}\,|\,\mathcal{P})$ is also norm dense.

We remark that $\mathcal{E}(\;\,|\,\mathcal{P}) : \;\to \mathcal{P}$ may be viewed as a generalized conditional expectation. Indeed, there exists, by 5.16 (taking direct sums if necessary), a Hilbert space which supports faithful *-representations Π and $\hat{\Pi}$ of $\mathfrak{A}$ and $\mathcal{P}$, respectively, such that $\mathcal{E}(\;\,|\,\mathcal{P})$ is implemented by a normal conditional expectation of $\Pi(\mathfrak{A})''$ onto $\hat{\Pi}(\mathcal{P})''$. Query: Is $\mathcal{E}(\mathfrak{A}\,|\,\mathcal{P}) = \mathcal{P}$?

The following lemmas aim toward showing how each $\mathcal{P}$-equivalence class is associated to a unique state on $\mathcal{P}$ and toward defining the *a priori* probability assignment conditional upon $\mathcal{P}$ (Theorem 5.13).

Denote by $\mathcal{B}(\mathfrak{S})$ (resp. $\mathcal{B}(\mathcal{S})$) the σ-ring of Borel sets of $\mathfrak{S}$ (resp. $\mathcal{S}$). Since $\mathcal{S}$ is w^*-closed (Prop. 5.1), the σ-ring $\mathcal{B}(\mathfrak{S}) \cap \mathcal{S} = \{\Delta \cap \mathcal{S}\,|\,\Delta \in \mathcal{B}(\mathfrak{S})\}$ is a sub-σ-ring of $\mathcal{B}(\mathfrak{S})$ and isomorphic to $\mathcal{B}(\mathcal{S})$. Therefore, if μ is a regular measure on $(\mathfrak{S}, \mathcal{B}(\mathfrak{S}))$, its restriction μ^R (cf. III. 8, Ref. 17) with respect to $\mathcal{B}(\mathfrak{S}) \cap \mathcal{S}$ defines by Riesz representation theorem a continuous linear form on $\mathcal{P}$.

Now, since $\mathfrak{S}^G$ is a (Choquet) simplex (Theorem 4.2) there exists (p. 218, Ref. 9) for each state $\omega \in \mathfrak{S}^G$ a unique, normalized, positive regular measure μ_ω on $\mathfrak{S}$ such that

(a) $\langle\omega : A\rangle = \int_{\mathfrak{S}}\langle\phi : A\rangle\, d\mu_\omega(\phi) \qquad \forall A \in \mathfrak{A}$.

(b) μ_ω is concentrated on $\mathcal{S}$.

Thus, μ_ω^R defines a state on $\mathcal{P}$.

5.9 *Definition*: Let ω be a G-invariant state on $\mathfrak{A}$, μ_ω the measure on $\mathfrak{S}$ associated to ω by Choquet's theorem, and let μ_ω^R denote its relativization with respect to $\mathcal{B}(\mathfrak{S}) \cap \mathcal{S}$. Denote by $R\omega$ the state on $\mathcal{P}$ defined by $R\omega : f\rangle = \int_{\mathcal{S}}\langle\phi : f\rangle\, d\mu_\omega^R(\phi) \;\forall f \in \mathcal{P}$.

5.10 *Remark*: Evidently,

$$\langle \omega : A\rangle = \int_{\mathfrak{S}} \langle \phi : A\rangle \, d\mu_\omega(\phi) = \int_{\mathcal{S}} \langle \phi : \mathcal{E}(A\,|\,\mathcal{P})\rangle \, d\mu_\omega^R(\phi)$$
$$\equiv \langle R\omega : \mathcal{E}(A\,|\,\mathcal{P})\rangle \qquad \forall A \in \mathfrak{A}; \quad \forall \omega \in \mathfrak{S}^G.$$

5.11 *Lemma*: Let ω be a G-invariant state on $\mathfrak{A}$, and let $\{f_i\}_{i=1}^N$, $\{g_i\}_{i=1}^N \subset K(\mathbb{R})$. Then,

$$\langle \tilde{\omega} : K_\omega^N(f_1, \dots, f_N; g_1, \dots, g_N)\rangle = \Big\langle R\omega : \prod_{i=1}^N K(f_i; g_i)\Big\rangle$$

Proof: By Remark 5.10 and Lemma 5.7, we have

$$\langle \tilde{\omega} : K_\omega^N(f_1, \dots, f_N; g_1, \dots, g_N)\rangle$$
$$= \lim_{M\to\infty} \langle \omega : K_{1/M}^N(f_1, \dots, f_N; g_1, \dots, g_N)\rangle$$
$$= \lim_{M\to\infty} \langle R\omega : \mathcal{E}(K_{1/M}^N(f_1, \dots, f_N; g_1, \dots, g_N))\rangle$$
$$= \langle R\omega : \prod_{i=1}^N K(f_i; g_i)\rangle.$$

The next theorem identifies the "restriction" of a $\mathcal{P}$-measurable state to $\mathcal{P}$.

5.12 *Theorem*: Let ψ be an arbitrary $\mathcal{P}$-measurable state.

There exists a unique state $\hat{\psi}$ on $\mathcal{P}$, such that

$$\hat{\psi}^N(f_1, \dots, f_N; g_1, \dots, g_N) = \Big\langle \hat{\psi} \prod_{i=1}^N K(f_i; g_i)\Big\rangle$$
$$\forall N \in \mathbb{Z}^+,$$
$$\forall \{f_i\}_{i=1}^N, \{g_i\}_{i=1}^N \subset K(\mathbb{R})$$

Proof: By virtue of Theorem 3.3, there exists a G-invariant state $\mathcal{P}$-equivalent to ψ. Existence then follows by Lemma 5.11. Uniqueness follows by linearity and continuity from Lemma 5.6. The next theorem gives existence of a unique G-invariant "extension" to $\mathfrak{A}$ of every state on $\mathcal{P}$ and thus defines the *a priori* probability assignment conditional upon $\mathcal{P}$.

5.13 *Theorem*: Let $\hat{\psi}$ be a state on $\mathcal{P}$. There exists a unique G-invariant extension $\bar{\hat{\psi}}$ of $\hat{\psi}$ to $\mathfrak{A}$ (i.e., $\hat{\bar{\hat{\psi}}} = \hat{\psi}$.) Denote by $\mathcal{E}^*(\cdot\,|\,\mathcal{P}) : \mathfrak{S}(\mathcal{P}) \to \mathfrak{S}^G$, the mapping defined by $\mathcal{E}^*(\hat{\psi}\,|\,\mathcal{P}) = \bar{\hat{\psi}}\ \forall \hat{\psi} \in \mathfrak{S}(\mathcal{P})$. Then,

$$\langle \mathcal{E}^*(\hat{\psi}\,|\,\mathcal{P}) : A\rangle = \langle \hat{\psi} : \mathcal{E}(A\,|\,\mathcal{P})\rangle \quad \forall A \in \mathfrak{A}, \quad \hat{\psi} \in \mathfrak{S}(\mathcal{P}).$$

Proof: *Existence*: Define $\bar{\hat{\psi}} \equiv \hat{\psi} \circ \mathcal{E}(\cdot\,|\,\mathcal{P})$. By Theorem 5.5, $\bar{\hat{\psi}}$ is a G-invariant state on $\mathfrak{A}$. Since $\bar{\hat{\psi}}$ is G-invariant, $\hat{\bar{\hat{\psi}}} = R\bar{\hat{\psi}}$ (see proof of 5.12). By 3.10, $\langle \bar{\hat{\psi}} : A\rangle = \langle R\bar{\hat{\psi}} : \mathcal{E}(A\,|\,\mathcal{P})\rangle\ \forall A \in \mathfrak{A}$. Thus,

$$\langle \hat{\psi} : \mathcal{E}(A\,|\,\mathcal{P})\rangle \equiv \langle \bar{\hat{\psi}} : A\rangle = \langle R\bar{\hat{\psi}} : \mathcal{E}(A\,|\,\mathcal{P})\rangle$$
$$= \langle \hat{\bar{\hat{\psi}}} : \mathcal{E}(A\,|\,\mathcal{P})\rangle \quad \forall A \in \mathfrak{A}$$

Hence, by 5.8, $\hat{\psi} = \hat{\bar{\hat{\psi}}}$.

Uniqueness follows from Theorem 3.3. The last assertion follows from the existence argument. Finally, we discuss the implementability of $\mathcal{E}(\cdot\,|\,\mathcal{P})$.

5.14 *Lemma* Let ω be a G-invariant state on $\mathfrak{A}$, $(\pi_\omega, H_\omega, \Omega)$ the GNS triple associated to ω, and let E_ω be as in 3.11. Let

$$q = \lambda_0 + \sum_{N=1}^M \sum_{i=1}^{I_N} \lambda_i \prod_{j=1}^N K(f_j^i; g_j^i) \in \mathcal{P}_0$$

where $M, N, I_N \in \mathbb{Z}^+$ and $\{f_j^i\}, \{g_j^i\} \subset K(\mathbb{R})$.

The expression

$$E_\omega\{\lambda_0 + \sum_{N=1}^M \sum_{i=1}^{I_N} \lambda_i \prod_{j=1}^N K_\omega(f_j^i; g_j^i)\} \equiv \hat{\Pi}_\omega^\circ(q)$$

depends on q only, not the particular decomposition used to define it.

Proof: Choose $\xi \in E_\omega H_\omega$ and compute;

$$(*) \quad \langle \omega_{\xi,\xi} : \lambda_0 1 + \sum_{N=1}^M \sum_{i=1}^{I_N} \lambda_i \prod_{j=1}^N K_\omega(f_j^i; g_j^i)\rangle$$
$$= \langle R(\omega_{\xi,\xi} \circ \Pi_\omega) : q\rangle, \quad \text{by Lemma 5.11.}$$

Independence follows by polarization.

5.15 *Lemma*: The mapping $q \to \hat{\pi}_\omega^\circ(q)$ of $\mathcal{P}_0$ into $B(E_\omega H_\omega)$ admits a unique extension to a^*-representation of $\mathcal{P}$.

Proof: Clearly,

(1) $\hat{\Pi}_\omega^\circ(\lambda S + \gamma T) = \lambda \hat{\Pi}_\omega^\circ(S) + \gamma \hat{\Pi}_\omega^\circ(T) \quad \forall \lambda, \gamma \in \mathbb{C}, \ \forall S, T \in \mathcal{P}_0,$

(2) $\hat{\Pi}_\omega^\circ(ST) = \Pi_\omega^\circ(S)\Pi_\omega^\circ(T) \quad \forall S, T \in \mathcal{P}_0,$

(3) $\hat{\Pi}_\omega^\circ(K(f;g)^*) = \hat{\Pi}_\omega^\circ(K(g;f)) = E_\omega K_\omega(g;f)$
$= \hat{\Pi}_\omega^\circ(K(f;g))^* \quad \forall f, g \in K(\mathbb{R}),$

(4) $$\|\Pi_\omega^\circ(S)\|^2 = \sup_{\substack{\xi \in E_\omega H_\omega \\ \|\xi\|=1}} \langle \omega_{\xi,\xi} : \hat{\Pi}_\omega^\circ(S^*S)\rangle$$
$$= \sup_{\substack{\xi \in E_\omega H_\omega \\ \|\xi\|=1}} \langle R(\omega_{\xi,\xi} \circ \Pi_\omega) : S^*S\rangle \le \|S\|^2$$
$$\forall S \in \mathcal{P}_0.$$

The result then follows by continuity.

5.16 *Theorem*: Let ω be a G-invariant state on $\mathfrak{A}$, let $(H_\omega, \pi_\omega, \Omega)$ be the GNS triple associated to ω, let $\mathcal{P}_\omega$ be as in definition 3.8, let $\mathcal{E}_\omega(\cdot\,|\,\mathcal{P})$ be as in definition 3.12. Then:

(i) The mapping $K(f;g) \to K_\omega(f;g)\ \forall f, g \in K(\mathbb{R})$ admits a unique extension to a representation $\hat{\pi}_\omega$ of $\mathcal{P}$ in $B(H_\omega)$.

(ii) $\pi_\omega(\mathcal{P}) = \mathcal{P}_\omega$

(iii) $\hat{\Pi}_\omega \circ \mathcal{E}(\cdot\,|\,\mathcal{P}) = \mathcal{E}_\omega(\cdot\,|\,\mathcal{P}) \circ \Pi_\omega$

Proof: (adi) Since $\mathcal{P}_\omega \to \mathcal{P}_\omega|_{E_\omega}$ is an isomorphism (cf. proof of Prop. 3.11) the existence of the extension of assertion (i) follows from Lemma 5.15. Uniqueness is trivial.

(adii) It is clear that $\hat{\pi}_\omega(\mathcal{P})$ is norm dense in $\mathcal{P}_\omega$. Since $\hat{\pi}_\omega(\mathcal{P})$ is closed, (ii) follows.

(adiii) It suffices to show that $E_\omega \hat{\Pi}_\omega \circ \mathcal{E}(\cdot\,|\,\mathcal{P}) = E_\omega \mathcal{E}_\omega(\cdot\,|\,\mathcal{P}) \circ \Pi_\omega$. By polarization it suffices to show that, for each $\xi \in E_\omega H_\omega$,

$$\langle \omega_{\xi,\xi} : \hat{\Pi}_\omega(\mathcal{E}(A\,|\,\mathcal{P}))\rangle = \langle \omega_{\xi,\xi} : \mathcal{E}_\omega(\Pi_\omega(A)\,|\,\mathcal{P})\rangle \quad \forall A \in \mathfrak{A}$$

By virtue of remark 5.10, we have

$$\langle \omega_{\xi,\xi} : \mathcal{E}_\omega(\Pi_\omega(A)\,|\,\mathcal{P})\rangle = \langle \omega_{\xi,\xi} : E_\omega \Pi_\omega(A) E_\omega\rangle$$
$$= \langle \omega_{\xi,\xi} : \Pi_\omega(A)\rangle = \langle R(\omega_{\xi,\xi} \circ \Pi_\omega) : \mathcal{E}(A\,|\,\mathcal{P})\rangle.$$

Further, by continuous linear extension from Equation

(*) of Lemma 5.14, it follows that $\langle R(\omega_{\xi,\xi}\circ \Pi_\omega\rangle : \mathcal{E}(A\mid p)\rangle = \langle \omega_{\xi,\xi}: \hat{\Pi}_\omega(\mathcal{E}(A\mid p))\rangle$.

This proves the theorem.

APPENDIX A: PROOFS FOR SEC. 2

Proof of lemma 2.2

We first prove independence of decomposition. Due to linearity of $W_N^\circ(f;g)$, it suffices to consider the two cases, $f=0$ and/or $g=0$. Since taking the complex conjugate of Eq. (2.1) interchanges f and g, it suffices to choose $g=0$ and show that each addend of $\sum_j$ in Eq. (2.1) vanishes. Choose a finite family $\{Z_l\}_{l=1}^L$ of characteristic functions of disjoint measurable subsets of R with finite measure such that

$$Y_m^k = \sum_{l=1}^L {}^l\gamma_m^k\, Z_l, \quad 1\le k\le K,\ 1\le m\le N,\ {}^l\gamma_m^k=0 \text{ or } 1. \tag{A1}$$

Substitution into Eq. (2.1) yields

$$\begin{aligned} g&=\sum_{k=1}^K \gamma_k \bigotimes_{m=1}^N \left(\sum_{l=1}^L {}^l\gamma_m^k Z_l\right)\\ &=\sum_{k=1}^K \gamma_k \sum_{l_1,\dots,l_N=1}^L \prod_{m=1}^N {}^{l_m}\gamma_m^k \bigotimes_{m=1}^N Z_{l_m}\\ &=\sum_{l_1,\dots,l_N=1}^L \sum_{k=1}^K \gamma_k \prod_{m=1}^N {}^{l_m}\gamma_m^k \bigotimes_{m=1}^N Z_{l_m}=0. \end{aligned} \tag{A2}$$

Since $Z_l Z_{l'}=0$ for $l\ne l'$, the vectors $\otimes_{m=1}^N Z_{l_m}$ are orthogonal for distinct n-tuples $(l_1,\dots,l_N)$. Taking the scalar product with $\otimes_{m=1}^N Z_{l_m}$ for fixed $(l_1,\dots,l_N)$ yields

$$\sum_{k=1}^K \gamma_k \prod_{m=1}^N {}^{l_m}\gamma_m^k=0 \quad \forall \{l_m\}_{m=1}^N \tag{A3}$$

Consider for fixed $1\le j\le J$ the corresponding addend in Eq. (2.1). We show it vanishes when $g=0$:

$$\begin{aligned} &\sum_{k=1}^K \bar\gamma_k\, W_{N,N}(X_1^j,\dots,X_N^j;Y_1^k,\dots,Y_N^k)\\ &=\sum_{k=1}^K \bar\gamma_k W_{N,N}\left(X_1^j,\dots,X_N^j;\sum_{l=1}^L {}^l\gamma_1^k Z_l,\dots,\sum_{l=1}^L {}^l\gamma_N^k Z_l\right)\\ &=\sum_{k=1}^K \bar\gamma_k \sum_{l_1,\dots,l_N=1}^L \prod_{m=1}^N {}^{l_m}\gamma_m^k\ W_{N,N}(X_1^j,\dots,X_N^j;Z_{l_1},\dots,Z_{l_N})\\ &=\sum_{l_1,\dots,l_N=1}^L\left(\sum_{k=1}^K \bar\gamma_k \prod_{m=1}^N {}^{l_m}\gamma_m^k\right) W_{N,N}(X_1^j,\dots,X_N^j:Z_{l_1},\dots,Z_{l_N})\\ &=0 \quad \text{by (A3)}. \end{aligned} \tag{A4}$$

This proves independence. Property (i) is immediate. To prove (ii), choose $f=\sum_{j=1}^J \lambda_j(\otimes_{m=1}^N X_m^j)$. Define $A(f) =\sum_{j=1}^J \bar\lambda_j\, a(X_1^j)\cdots a(X_N^j)$. Evidently, $W_{NN}^\circ(f,f) =\langle\omega: A(f)^*A(f)\rangle\ge 0$. This proves the lemma.

Proof of lemma 2.3

By virtue of Schwartz' inequality, $|W_N^\circ(f,g)|\le W_N^\circ(f,f)^{1/2}\,W_N^\circ(g,g)^{1/2}$, it suffices to prove that $W_N^\circ(f,f)\le N!\,\|f\|_2^2\ \forall f\in \mathcal{L}_0^2(\mathrm{R}^N)$.

We simplify as in Lemma 2.2. Choose a finite family $\{X_l\}_{l=1}^L$, of characteristic functions of disjoint measurable subsets of R with finite measure such that

$$f=\sum_{l_1,\dots,l_N=1}^L \lambda_{l_1,\dots,l_N} \bigotimes_{m=1}^N X_{l_m},\quad \{\lambda_{l_1,\dots,l_N}\}_{l_1,\dots,l_N=1}^L\subset \mathbf{C}$$

[compare (A2)].

Clearly,

$$W_N^\circ(f,f)=\sum_{\substack{l_1,\dots,l_N=1\\ j_1,\dots,j_N=1}}^L \lambda_{j_1,\dots,j_N}\,\bar\lambda_{l_1,\dots,l_N}\,W_{N,N}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N}). \tag{A5}$$

We investigate $W_{N,N}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N})$. Notice that since the $\{X_l\}_{l=1}^L$ are mutually orthogonal one has, by straightforward application of the anticommutation relations, $W_{N,N}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N})=0$ if either $X_{j_m}=X_{j_{m'}}$ or $X_{l_m}=X_{l_{m'}}$ for $1\le m\ne m'\le N$. Moreover, $W_{N,N}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N})=0$ if $\{X_{j_m}\}_{m=1}^N\ne\{X_{l_m}\}_{m=1}^N$ due to G-invariance. Indeed, assume the converse:

(i) $W_{NN}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N})\ne 0$,

(ii) For some $0\le m\le N$ there exists no $1\le m'\le N \quad j_m=l_{m'}$.

Assumption (i) implies that $X_{j_m}X_{j_{m'}}=0$, $1\le m\ne m'\le N$, while assumption (ii) implies that $X_{j_m}X_{l_{m'}}=0$, $1\le m'\le N$. Choose $V=\exp(i\pi X_{j_m})\in G$. Since ω is G-invariant we have

$$\begin{aligned} &W_{NN}(X_{j_1},\dots,X_{j_N};X_{l_N},\dots,X_{l_N})\\ &\equiv\langle\omega: a^*(X_{j_N})\cdots a^*(X_{j_1})\,a(X_{l_1})\cdots a(X_{l_N})\rangle\\ &=\langle\alpha_V^*\omega: a^*(X_{j_N})\cdots a^*(X_{j_1})\,a(X_{l_1})\cdots a(X_{l_N})\rangle\\ &=\langle\omega: a^*(X_{j_N})\cdots a^*(e^{i\pi}X_{j_m})\cdots a^*(X_{j_1})a(X_{l_1})\cdots a(X_{l_N})\rangle\\ &=-W_{NN}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N}), \end{aligned}$$

contradicting hypothesis (i). Therefore

$$W_{NN}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N})=0 \quad \text{if } \{X_{j_m}\}_{m=1}^N \ne \{X_{l_m}\}_{m=1}^N.$$

In the event that $W_{NN}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N})\ne 0$, there exists a unique permutation $p\in \mathcal{S}_N$ such that $j_m =l_{p(m)} \quad 1\le m\le N$. Moreover,

$$\begin{aligned} &W_{NN}(X_{j_1},\dots,X_{j_N};X_{l_1},\dots,X_{l_N})\\ &=(-1)^{\sigma(p)}\,W_{NN}(X_{j_1},\dots,X_{j_N};X_{j_1},\dots,X_{j_N}). \end{aligned}$$

Define the symmetric operator F_ω° on $\mathcal{L}^2(\mathrm{R}^N)$ by

$$F_\omega^\circ\equiv\sum_{i_1,\dots,i_N=1}^L\left(\prod_{m=1}^N \|X_1\|_2^2\right)^{-1} W_{NN}(X_{i_1},\dots,X_{i_N};X_{i_1},\dots,X_{i_N}) \times \bigotimes_{m=1}^N P_{i_m}, \tag{A6}$$

where P_{i_m} is the projector on $\mathcal{L}^2(\mathrm{R})$ associated to the characteristic function X_{i_m}. Since $0\le W_{NN}(X_{i_1},\dots,X_{i_N};X_{i_1},\dots,X_{i_N})\le \prod_{m=1}^N\|X_{i_m}\|_2^2$, $0\le F_\omega^\circ\le 1$. We compute $N!\,(\otimes_{m=1}^N X_{l_m}, F_\omega^\circ A\otimes_{m=1}^N X_{j_m})$:

$$N!\sum_{i_1,\dots,i_N=1}^L\left(\prod_{m=1}^N\|X_{i_m}\|_2^2\right)^{-1} W_{NN}(X_{i_1},\dots,X_{i_N};X_{i_1},\dots,X_{i_N}) \times\left(\bigotimes_{m=1}^N X_{l_m},\ \bigotimes_{m=1}^N P_{i_m}A\bigotimes_{m=1}^N X_{j_m}\right)$$

$$=\left(\prod_{m=1}^{N}\|X_{j_m}\|_2^2\right)^{-1} W_{NN}(X_{j_1},\ldots,X_{j_N};X_{j_1},\ldots,X_{j_N})$$

$$\times\sum_{p\in S_N}(-1)^{\sigma(p)}\prod_{m=1}^{N}(X_{l_m},X_{j_{p(m)}})$$

$$=\begin{cases}0 & \text{if } l_m=l_{m'},\ 1\le m\ne m'\le N\\ 0 & \text{if } \{X_{j_m}\}_{m=1}^N\ne\{X_{l_m}\}_{m=1}^N\\ (-1)^{\sigma(p)}W_{NN}(X_{j_1},\ldots,X_{j_N};X_{j_1},\ldots,X_{j_N})\end{cases}$$

where $l_m=j_{j_{p(m)}}$, $1\le m\le N$, otherwise.

Collecting these results, we have

$$W_{NN}(X_{j_1},\ldots,X_{j_N};X_{l_1},\ldots,X_{l_N})=N!\left(\bigotimes_{m=1}^N X_{l_m}, F_\omega^\circ A\bigotimes_{m=1}^N X_{j_m}\right) \tag{A7}$$

Substituting of this result into Eq. (A5), we have

$$W_N^\circ(f,f)=N!(f,F_\omega^\circ Af)=N!(f,AF_\omega^\circ Af)\le N!\ \|f\|_2^2 \tag{A8}$$

This completes the proof of the lemma.

Proof of lemma 2.6

It suffices to prove that $P_yB_\omega^NP_y\in \mathcal{L}^\infty(\mathbb{R}^N)'$ since the von Neumann algebra, $\mathcal{L}^\infty(\mathbb{R}^N)$, is a maximal Abelian subalgebra of $B(\mathcal{L}^2(\mathbb{R}^N))$. Moreover,

$$\mathcal{L}^\infty(\mathbb{R}^N)=\left\{\bigotimes_{m=1}^N f_m\,|\,\{f_m\}_{m=1}^N\subset\mathcal{L}^\infty(\mathbb{R})\right\}''$$
$$=\left\{\bigotimes_{m=1}^N V_m\,|\,\{V_m\}_{m=1}^N\subset G\right\}'$$

It therefore suffices to prove that

$$[P_yB_\omega^NP_y,\bigotimes_{m=1}^N V_m]=0\quad\forall\{V_m\}_{m=1}^N\subset G.$$

Since the linear span of $\{\otimes_{m=1}^N f_m\,|\,\{f_m\}_{m=1}^N\subset\mathcal{L}^2(\mathbb{R})\}$ is dense in $\mathcal{L}^2(\mathbb{R}^N)$, it suffices to show

$$\left(\bigotimes_{m=1}^N h_m,\left\{\bigotimes_{m=1}^N V_m^*P_yB_\omega^NP_y\bigotimes_{m=1}^N V_m-P_yB_\omega^NP_y\right\}\bigotimes_{m=1}^N f_m\right)=0$$
$$\forall\{f_m\},\ \{h_m\}\subset\mathcal{L}^2(\mathbb{R}),\ \forall\{V_m\}\subset G. \tag{A9}$$

In fact,

$$\left(\bigotimes_{m=1}^N h_m,\bigotimes_{m=1}^N V_m^*\bigotimes_{m=1}^N P_m B_\omega^N\bigotimes_{m=1}^N P_m\bigotimes_{m=1}^N V_m\bigotimes_{m=1}^N f_m\right)$$
$$=\left(\bigotimes_{m=1}^N V_mP_mh_m, B_\omega^N\bigotimes_{m=1}^N V_mP_mf_m\right)=\left(\bigotimes_{m=1}^N VP_mh_m, B_\omega^N\bigotimes_{m=1}^N VP_mf_m\right)$$
$$\left[\text{where } V\equiv\sum_{m=1}^N P_mV_m+\left(1-\sum_{n=1}^N P_m\right)\in G\right]$$
$$=W_{NN}(VP_1f_1,\ldots,VP_Nf_N;VP_1h_1,\ldots,VP_Nh_N)$$
$$=W_{NN}(P_1f_1,\ldots,P_Nf_N;P_1h_1,\ldots,P_Nh_N)$$
$$=\left(\bigotimes_{m=1}^N h_m,P_yB_\omega^NP_y\bigotimes_{m=1}^N f_m\right).$$

This proves (A9) and the lemma.

Proof of lemma 2.7

Since $\{P(\gamma)\}_{\gamma\in\Gamma}$ forms an increasing bounded filter in the von Neumann algebra $\mathcal{L}^\infty(\mathbb{R}^N)$, it converges in the weak[6] operator topology of $B(\mathcal{L}^2(\mathbb{R}^N))$ to its least upper bound $\overline{P}$.

Since $P(\gamma)P(\gamma')=P(\gamma)$ for $\gamma\subset\gamma'$, $P(\gamma)\overline{P}$ $=$ w-op $\lim_{\gamma'\in\Gamma}P(\gamma)P(\gamma')=P(\gamma)$. Thus $\overline{P}^2$ $=$ w-op $\lim_{\gamma\in\Gamma}P(\gamma)\overline{P}=$ w-op $\lim_{\gamma\in\Gamma}\overline{P}(\gamma)=\overline{P}$. Moreover, since $\overline{P}^*=$ w-op $\lim_{\gamma\in\Gamma}P(\gamma)^*=\overline{P}$, $\overline{P}$ is a projector in $\mathcal{L}^\infty(\mathbb{R}^N)$. To prove that $\overline{P}=1$, first notice that $1=P_{\mathbb{R}^N-\mathbb{D}^N}$, where $\mathbb{D}^N=\{X\in\mathbb{R}^N|X_i=X_{i'}$, for some $1\le i\ne i'\le N\}$, since $\mathbb{D}^N$ is a set of measure zero. But it is clear that $\mathbb{R}^N-\mathbb{D}^N=\cup\{y=y_1\times\cdots\times y_N\,|\,y_i\cap y_{i'}=\phi;\ y_i$ measurable; $\forall 1\le i\ne i'\le N\}$.

Thus $\overline{P}\supset P_{\mathbb{R}^N-\mathbb{D}^N}=1$. This completes the proof of the lemma.

Proof of lemma 2.8

Choose two disjunctions $\{P_k\}_{k=1}^K$, $\{O_j\}_{j=1}^J$ of γ in $\mathcal{L}^\infty(\mathbb{R}^N)$. Notice that $P_kB_\omega^NP_k, O_jB_\omega^NO_j\in\mathcal{L}^\infty(\mathbb{R}^N)$. Indeed, if $P_k\subset P_{y_i}\in\gamma$, say, $P_kB_\omega^NP_k=P_kP_{y_i}B_\omega^NP_{y_i}P_k\in\mathcal{L}^\infty(\mathbb{R}^N)$. Thus,

$$\sum_k P_kB_\omega^NP_k=P(\gamma)\sum_k P_kB_\omega^NP_k$$
$$=\sum_k\sum_j P_kO_jB_\omega^NO_jP_k$$
$$=P(\gamma)\sum_j O_jB_\omega^NO_j=\sum_j O_jB_\omega^NO_j.$$

This proves independence of the chosen disjunction.

(adi) $P_kB_\omega^NP_k\in\mathcal{L}^\infty(\mathbb{R}^N)$ $\forall 1\le k\le K$.

(adii) We first remark that $\|PB_\omega^NP\|\le 1$ $\forall P\in P^N$. Indeed, it suffices to prove that

$$|(f,PB_\omega^NPf)|\le\|f\|_2^2\quad\forall f\in\mathcal{L}_0^2(\mathbb{R}^N).$$

Since $Pf\in\mathcal{L}_0^2(\mathbb{R}^N)$, there exists by the explicit construction of Eqs. (A6) and (A7) an operator $0\le F_\omega^\circ\le 1$ on $\mathcal{L}^2(\mathbb{R}^N)$ such that

$$|(f,PB_\omega^NPf)|=N!\,|(f,PF_\omega^\circ APf)|.$$

By construction $PF_\omega^\circ=F_\omega^\circ P$; therefore

$$|(f,PB_\omega^NPf)|=|(f,F_\omega^\circ Pf)|\le\|f\|_2^2.$$

Thus,

$$0\le\sum_k P_kB_\omega^NP_k\le\sum_k P_k\le 1.$$

(adiii). Let $\gamma\subset\gamma'$ and let $\{P_k\}_{k=1}^K$ be a disjunction of γ' in $\mathcal{L}^\infty(\mathbb{R}^N)$. Then $P(\gamma)F_\omega^N(\gamma')=P(\gamma)\sum_k P_kB_\omega^NP_k$ $=\sum_k P(\gamma)P_kB_\omega^NP_kP(\gamma)=F_\omega^N(\gamma)$ since $\{P_kP(\gamma)\}_{k=1}^K$ is a disjunction of γ.

(adiv) $F_\omega^N(\gamma')-F_\omega^N(\gamma)=[1-P(\gamma)]F_\omega^N(\gamma')[1-P(\gamma)]\ge 0.$

Proof of lemma 2.9

By Lemma 2.8 (iv) $\{F_\omega^N(\gamma)\}_{\gamma\in\Gamma}$ is an increasing, bounded filter in $\mathcal{L}^\infty(\mathbb{R}^N)$ and therefore converges in the weak operator topology of $B(\mathcal{L}^2(\mathbb{R}^N))$ to its least upper bound F_ω^N. Since $\mathcal{L}^\infty(\mathbb{R}^N)$ is weakly closed, $F_\omega^N\in\mathcal{L}^\infty(\mathbb{R}^N)$.

(adi) Suppose that $\overline{F}_\omega^N\in\mathcal{L}^\infty(\mathbb{R}^N)$ is such that $\overline{F}_\omega^NP$ $=PB_\omega^NP$ $\forall P\in P^N$. Choose $\gamma\in\Gamma$ and let $\{P_k\}_{k=1}^K$ be a disjunction of γ in $\mathcal{L}^\infty(\mathbb{R}^N)$. Then $\overline{F}_\omega^NP_k=P\,F_\omega^N(\gamma)P_k$. Indeed suppose that $P_k\subset P\in\gamma$. It follows that

$$\overline{F}_\omega^NP_k=\overline{F}_\omega^NPP_k=P_kPB_\omega^NPP_k=P_kB_\omega^NP_k=P_kF_\omega^N(\gamma).$$

Thus,

$$\overline{F}_\omega^NP(\gamma)=\sum_k\overline{F}_\omega^NP_k=\sum_k F_\omega^N(\gamma)P_k=F_\omega^N(\gamma)$$

$$= \text{w-op} \lim_{\gamma' \in \Gamma} P(\gamma) F_\omega^N(\gamma') = P(\gamma) F_\omega^N.$$

Hence

$$\bar{F}_\omega^N = \text{w-op} \lim_{\gamma' \in \Gamma} P(\gamma) \bar{F}_\omega^N = \text{w-op} \lim_{\gamma' \in \Gamma} F_\omega^N P(\gamma) = F_\omega^N.$$

This proves uniqueness.

(adii) Consider the operator $N!\, F_\omega^N A - B_\omega^N$ on $\mathcal{L}^2(\mathbb{R}^N)$. Since $\mathcal{L}_0^2(\mathbb{R}^N)$ is dense in $\mathcal{L}^2(\mathbb{R}^N)$, it suffices to show that

$$(h, (N!\, F_\omega^N A - B_\omega^N) f) = 0 \;\forall f, h \in \mathcal{L}_0^2(\mathbb{R}^N).$$

By virtue of the decomposition (A3), it suffices to show that if $\{X_k\}_{k=1}^K$ is a disjoint family of measurable sets with finite measure, then

$$\left(\bigotimes_{i=1}^N X_{k_i}, N!\, F_\omega^N A \bigotimes_{i=1}^N X_{k_i'}\right) = \left(\bigotimes_{i=1}^N X_{k_i}, B_\omega^N \bigotimes_{i=1}^N X_{k_i'}\right).$$

The left member vanishes by inspection if $\{k_i\} \neq \{k_i'\}$, while the right vanishes by the invariance argument of Lemma 2.3. On the other hand, both sides vanish if $k_i = k_{i'}$ for $1 \le i \neq i' \le N$ by antisymmetry. It remains to be shown that

$$\left(\bigotimes_{i=1}^N X_{k_i}, N!\, F_\omega^N A \bigotimes_{i=1}^N X_{k_i}\right) = \left(\bigotimes_{i=1}^N X_{k_i}, B_\omega^N \bigotimes_{i=1}^N X_{k_i}\right)$$

since the other permutations follow trivially. But, this last equation is true by part (i) of this lemma and the fact that $F_\omega^N \in \mathcal{L}^\infty(\mathbb{R}^N)$.

(adiii) The intersection $B(\mathcal{L}^2(\mathbb{R}^N))_1 \cap B(\mathcal{L}^2(\mathbb{R}^N))_+$ is closed in the weak operator topology of $B(\mathcal{L}^2(\mathbb{R}))$.

(adiv) Choose $p \in \mathcal{S}_N$. Clearly $\mathcal{U}_p^* F_\omega^N \mathcal{U}_p \in \mathcal{L}^\infty(\mathbb{R}^N)$. For each $P \in P^N$, $\mathcal{U}_p^* P \mathcal{U}_p \in P^N$. Therefore

$$\begin{aligned}\mathcal{U}_p F_\omega^N \mathcal{U}_p P &= \mathcal{U}_p^* F_\omega^N (\mathcal{U}_p P \mathcal{U}_p^*) \mathcal{U}_p \\ &= \mathcal{U}_p^* (\mathcal{U}_p P \mathcal{U}_p^*) B_\omega^N (\mathcal{U}_p P \mathcal{U}_p^*) \mathcal{U}_p \\ &= P B_\omega^N P.\end{aligned}$$

Hence, by the uniqueness of F_ω^N, $U_p^* F_\omega^N U_p = F_\omega^N \;\forall p \in S_N$. This completes the proof of the lemma.

APPENDIX B: PROOFS FOR SEC. 3

Proof of lemma 3.2

(adi)

$$\begin{aligned}&\langle \omega : a^*(f_N) \cdots a^*(f_1)\, \alpha_V[K_\delta^M(f_1^\circ, \ldots, f_M^\circ; g_1^\circ, \ldots, g_M^\circ)]\, a(g_1) \cdots a(g_N)\rangle \\ &= \int_{\mathbb{R}^M} d^M x \left(\prod_{j=1}^M f_j^\circ(x_j) \bar{g}_j^\circ(x_j)\right) \\ &\quad \times \langle \omega : a^*(f_N) \cdots a^*(f_1)\, a^*(V\Delta_{x_M}) \cdots a^*(V\Delta_{x_1}) a(V\Delta_{x_1}) \\ &\quad \times a(V\Delta_{x_M}) a(g_1) \cdots a(g_N)\rangle \\ &= \int_{\mathbb{R}^M} d^M x \left(\prod_{j=1}^M f_j^\circ(x_j) \bar{g}_j^\circ(x_j)\right) (N+M)! \\ &\quad \times \left(\bigotimes_{j=1}^M V\Delta_{x_j} \bigotimes_{j=M+1}^{M+N} g_j,\; F_\omega^{N+M} A \bigotimes_{j=1}^M V\Delta_{x_j} \bigotimes_{j=M+1}^{N+M} f_j\right) \\ &= \sum_{p \in \mathcal{S}_{N+M}} (-1)^{\sigma(p)} \int_{\mathbb{R}^M} d^M x \left(\prod_{j=1}^M f_j^\circ(x_j) \bar{g}_j^\circ(x_j)\right) \\ &\quad \times \left(\bigotimes_{j=1}^M V\Delta_{x_j} \bigotimes_{j=N+1}^{N+M} g_j,\; F_\omega^{N+M} \mathcal{U}_p \bigotimes_{j=1}^M V\Delta_{x_j} \bigotimes_{j=M+1}^{N+M} f_j\right),\end{aligned}$$

where we have relabeled with $j \to j+M$. This expression splits into a sum over permutations of three types:

Type 1: $p(j) = j$, $1 \le j \le M$;

Type 2: $p(j) \le M$ for some $j \ge M+1$;

Type 3: $j \le M \Rightarrow p(j) \le M$ but $p(j) \neq j$ for $1 \le j \le M$.

First consider a type-1 permutation characterized by $p \in \mathcal{S}_N$:

$$\begin{aligned}&(-1)^{\sigma(p)} \int_{\mathbb{R}^M} d^M x \left(\prod_{j=1}^M f_j^\circ(x_j) \bar{g}_j^\circ(x_j)\right) \\ &\quad \left(\left(\bigotimes_{j=1}^M V_j \otimes 1^N\right) \bigotimes_{j=1}^M \Delta_{x_j} \bigotimes_{j=M+1}^{M+N} g_j,\right. \\ &\quad \left. F_\omega^{N+M} \left(\bigotimes_{j=1}^M V_j \otimes 1^N\right) \bigotimes_{j=1}^M \Delta_{x_j} \bigotimes_{j=M+1}^{N+M} f_{p(j)}\right) \\ &= (-1)^{\sigma(p)} \int_{\mathbb{R}^M} d^M x \left(\prod_{j=1}^M f_j^\circ(x_j) \bar{g}_j^\circ(x_j)\right) \\ &\quad \times \left(\bigotimes_{j=1}^M \Delta_{x_j} \bigotimes_{j=M+1}^{M+N} g_j,\; F_\omega^{N+M} \bigotimes_{j=1}^M \Delta_{x_j} \bigotimes_{j=M+1}^{M+N} f_{p(j)}\right) \\ &= (-1)^{\sigma(p)} \int_{\mathbb{R}^M} d^M x \left(\prod_{j=1}^M f_j^\circ(x_j) \bar{g}_j^\circ(x_j)\right) \\ &\quad \times \left(\bigotimes_{j=1}^M \Delta_{x_j},\; F_\omega^{M,N}(f_{p(1)}, \ldots, f_{p(N)}; g_1, \ldots, g_N) \bigotimes_{j=1}^M \Delta_{x_j}\right) \\ &= (-1)^{\sigma(p)} \int_{\mathbb{R}^{2M}} d^M x\, d^M y \left\{\prod_{j=1}^M f_j^\circ(X_j) \bar{g}_j^\circ(X_j) \Delta^2(y_j - x_j)\right\} \\ &\quad \times F_\omega^{M,N}(f_{p(1)}, \ldots, f_{p(N)}; g_1, \ldots, g_N)(y_1, \ldots, y_N).\end{aligned}$$

Changing variables $x_j' = x_j$, $y_j' = y_j - x_j$ and changing the order of integration by Fubini's theorem, one obtains

$$\begin{aligned}&= (-1)^{\sigma(p)} \int_{\mathbb{R}_M} d^M y' \prod_{j=1}^M \Delta^2(y_i) \\ &\quad \times \left(\bigotimes_{j=1}^M f_j^\circ \bar{g}_j^\circ \circ F_\omega^{N,M}(f_{p(1)}, \ldots, f_{p(N)}; g_1, \ldots, g_N)\right) \\ &\quad (-y_1', \ldots, -y_M'),\end{aligned}$$

where $\circ$ denotes convolution.

Since the second term in the integrand is a continuous function on $\mathbb{R}^M$, the expression converges as $\delta \to 0$ to

$$\begin{aligned}&(-1)^{\sigma(p)} \left(\bigotimes_{j=1}^M f_j^\circ \bar{g}_j^\circ \circ F_\omega^{N,M}(f_{p(1)}, \ldots, f_{p(N)}; g_1, \ldots, g_N)\right. \\ &\quad \left.(0, 0, \ldots, 0)\right) \\ &= (-1)^{\sigma(p)} \left(\bigotimes_{j=1}^M g_j^\circ,\; F_\omega^{N,M}(f_{p(1)}, \ldots, f_{p(N)}; g_1, \ldots, g_N) \bigotimes_{j=1}^M f_j^\circ\right) \\ &= (-1)^{\sigma(p)} \left(\bigotimes_{j=1}^N g_j,\; F_\omega^{M,N}(f_1^\circ, \ldots, f_M^\circ; g_1^\circ, \ldots, g_M^\circ) \bigotimes_{j=1}^N f_{p(j)}\right)\end{aligned}$$

since F^{N+M} is symmetric.

Now consider type-2 permutations. We will show they converge to zero as $\delta \to 0$ uniformly in V. We consider for the sake of notation the special, but typical, case

$$p(M+1) = 1, \quad p(1) = M+1, \quad p(j) = j \quad \forall j \neq 1 \text{ or } M+1.$$

We have

$$\left|\int_{\mathbb{R}^M} d^Mx \prod_{j=1}^{M} f_j^\circ(x_j)\bar{g}_j^\circ(x_j)\left(\bigotimes_{j=1}^{M} V\Delta_{x_j}\bigotimes_{j=M+1}^{M+N} g_j, F_\omega^{N+M} f_{M+1}\right.\right.$$

$$\left.\left.\bigotimes_{j=2}^{M} V\Delta_{x_j}\otimes V\Delta_{x_1}\bigotimes_{j=M+2}^{M+N} f_j\right)\right|$$

$$=\left|\int_{\mathbb{R}^2} dx_1\,dy\, f_1^\circ(x_1)\bar{g}_1^\circ(x_1)(\overline{V\Delta}_{x_1})(y)f_1(y)\right.$$

$$\times\int_{\mathbb{R}^{M-1}} dx_2\cdots dx_M\, f_2^\circ(x_2)\bar{g}_2^\circ(x_2)\cdots f_M^\circ(x_M)\bar{g}_M^\circ(x_M)$$

$$\times F_\omega^{1,N+M-1}(V\Delta_{x_2},\ \ldots,\ V\Delta_{x_M},\ V\Delta_{x_1},\ \ f_2,\ldots,f_N;$$

$$\left.\times V\Delta_{x_2},\ldots,V\Delta_{x_M},g_1,\ldots,g_N)(y)\right|$$

$$\leq \|f_2^\circ\|_2\|g_2^\circ\|_2\cdots\|f_M^\circ\|_2\|g_M^\circ\|_2\|g_1\|_2\cdots\|g_N\|_2\|f_2\|_2\cdots\|f_N\|_2$$

$$\times\int_{\mathbb{R}^2} dx dy\,|f_1^\circ|(X)\,|\bar{g}_1^\circ|(X)\,|V\Delta_{x_1}|(y)|\,f_1|\,(y).$$

Since $V\in\mathcal{L}^\infty(\mathbb{R})$, $|V\Delta_X|(y)=\Delta_X(y)=\Delta_0(y-x)$ a. e. $-dx$

Finally, calling λ the (V and δ independent) constant preceding the last integral, we have

$$\equiv\lambda\delta^{1/2}\int|f_1^\circ|(x)\,|g_1^\circ|(x)\int dy\,|f_1|(y)\chi_\delta(y-x)/\delta$$

$$\leq\lambda\delta^{1/2}\|f_1^\circ\|_2\|g_1^\circ\|_2\,\|f_1\circ\chi_\delta/\delta\|_\infty$$

$$\leq\lambda\delta^{1/2}\|f_1^\circ\|\,\|g_1^\circ\|\,\|f_1\|_\infty.$$

Thus as $\delta\to 0$, terms of type 2 converge to zero, uniformly in $V\in G$.

Now consider type-3 terms. Again we consider for the sake of notational simplicity a special but typical case:

$$p(1)=2,\quad p(2)=1,\quad p(j)=j\quad \forall j\neq 1 \text{ or } 2.$$

We have

$$\left|\int_{\mathbb{R}^M} d^Mx\prod_{j=1}^{M} f_j^\circ(x_j)\bar{g}_j^\circ\ \left(\bigotimes_{j=1}^{M} V\Delta_{x_j}\bigotimes_{j=M+1}^{M+N} g_j,\right.\right.$$

$$\left.\left.F_\omega^{N+M}\,V\Delta_{x_2}\otimes V\Delta_{x_1}\bigotimes_{j=2}^{M} V\Delta_{x_j}\bigotimes_{j=M+1}^{M+N} f_j\right)\right|$$

$$=\left|\int_{\mathbb{R}^3} dy\,dx_1dx_2 f_1^\circ(x_1)\bar{g}_1^\circ(x_1)f_2^\circ(x_2)\bar{g}_2^\circ(x_2)\right.$$

$$\times(\overline{V\Delta}_{x_1})|(y)(V\Delta_{x_2})(y)$$

$$\times\int_{\mathbb{R}^{M-2}} dx_3\cdots dx_M\prod_{j=3}^{M} f_j^\circ(x_j)\,\bar{g}_j^\circ(x_j)$$

$$\left.\times F_\omega^{1,N+M-1}(V\Delta_{x_1},\ V\Delta_{x_2},f_N;\ V\Delta_{x_2},\ldots,g_N)(y)\right|$$

$$\leq\prod_{j=3}^{M}\|f_j^\circ\|_2\|g_j^\circ\|_2\prod_{i=1}^{N}\|f_i\|_2\|g_i\|_2$$

$$\times\int_{\mathbb{R}^3} dy\,dx_1dx_2\,|f_1^\circ|(x_1)\,|g_1^\circ|(x_1)\,|f_2^\circ|(x_2)\,|g_2^\circ|(x_2)$$

$$\times\Delta(y-x_1)\,\Delta(y-x_2)$$

$$\leq\lambda\int_{\mathbb{R}^2} dx_1dx_2\,|f_1^\circ|(x_1)\,|g_1^\circ|(x_1)\,|f_2^\circ|(x_2)\,|g_2^\circ|(x_2)$$

$$\times\chi_\delta(x_1-x_2)$$

$$\leq\delta\lambda\int dx_2\,|f_2^\circ|(x_2)\,|g_2^\circ|(x_2)\int dx_1\,|f_1^\circ|(x_1)\,|g_1^\circ|(x_1)$$

$$\times\chi_\delta(x_1-x_2)/\delta$$

$$\leq\delta\lambda\|f_2^\circ\|_2\,\|g_2^\circ\|_2\,\|\,|f_1^\circ g_1^\circ|\circ\chi_\delta/\delta\|_\infty$$

$$\leq\delta\lambda\,\|f_2^\circ\|_2\,\|g_2^\circ\|_2\,\|f_1^\circ\|_\infty\,\|g_1^\circ\|_\infty.$$

Thus expressions of type 3 converge to zero as $\delta\to 0$ uniformly in $V\in G$.

Collecting these results, we have

$$\lim_{\delta\to 0}\langle\omega: a^*(f_N)\cdots a^*(f_1)\,\alpha_V[K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)]$$

$$\times a(g_1)\cdots a(g_N)\rangle$$

$$=\sum_{p\in S_N}(-1)^{\sigma(p)}\left(\bigotimes_{j=1}^{N} g_j,\ F_\omega^{N,M}(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)\bigotimes_{j=1}^{N} f_{p(j)}\right)$$

$$=N!\left(\bigotimes_{j=1}^{N} g_j,\ F_\omega^{N,M}(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_M^\circ)A\bigotimes_{j=1}^{N} f_j\right),$$

which proves (i). Moreover, since the first expression is a *finite* sum of terms uniformly convergent in $V\in G$, this limit is reached uniformly in $V\in G$. This completes the proof of the lemma.

Proof of lemma 3.4

We prove the result for $a^\natural(f)=a(f)$; the argument for $a^*(f)$ is similar. Since λ is continuous and linear, we have

$$\langle\lambda: a(f)\alpha_V[K_\delta^M(f_1^\circ,\ldots,f_M^\circ;g_1^\circ,\ldots,g_N^\circ)]\rangle$$

$$=\int_{\mathbb{R}^M} d^Mx\prod_{j=1}^{M} f_j^\circ(x_j)\bar{g}_j^\circ(x_j)$$

$$\langle\lambda: a(f)\,a^*(V\Delta_{x_M})\cdots a^*(V\Delta_{x_1})a(V\Delta_{x_1})\cdots a(V\Delta_{x_M})\rangle$$

$$=\int_{\mathbb{R}^M} d^Mx\prod_{j=1}^{M} f_j^\circ(x_j)\bar{g}_j^\circ(x_j)$$

$$\Big\{\langle\lambda: a^*(V\Delta_{x_M})\cdots a^*(V\Delta_{x_1})a(V\Delta_{x_1})\cdots a(V\Delta_{x_M})a(f)\rangle$$

$$+\sum_{i=1}^{M}(-1)^{N+i}(f,\ V\Delta_{x_i})$$

$$\langle\lambda: a^*(V\Delta_{x_M})\cdots a^*(\not{V}\Delta_{x_i})\cdots a^*(V\Delta_{x_1})a(V\Delta_{x_1})\cdots a(V\Delta_{x_M})\rangle\Big\}$$

by use of the anticommutation relations. The lemma will be proven if we can show that the commutation terms converge to zero uniformly in $V\in G$. We consider the term $i=1$ without loss of generality:

$$\left|\int_{\mathbb{R}} dx_1 f_1^\circ(x_1)\bar{g}_1^\circ(x_1)(\overline{V\Delta_{x_1}, f})\ \int_{\mathbb{R}^{M-1}} dx_2\cdots dx_M\prod_{j=2}^{M} f_j^\circ(x_j)g_j^\circ(x_j)\right.$$

$$\left.\times\langle\lambda: a^*(V\Delta_{x_M})\cdots a^*(V\Delta_{x_1})a(V\Delta_{x_1})\cdots a(V\Delta_{x_M})\rangle\right|$$

$$\leq\|\lambda\|\prod_{j=2}^{M}\|f_j^\circ\|_2\|g_j^\circ\|_2\int_{\mathbb{R}^2} dx\,dy\,|f_1^\circ|(x)\,|g_1^\circ|(x)\,\Delta(y-x)\,|f|(y)$$

$$\leq\|\lambda\|\prod_{j=1}^{M}\|f_j^\circ\|_2\,\|g_j^\circ\|_2\,\|f\circ\chi_\delta/\delta^{1/2}\|_\infty$$

$$\leq \|\lambda\| \prod_{j=1}^{M} \|f_j^\circ\|_2 \|g_j^\circ\|_2 \|f\|_\infty \delta^{1/2}.$$

Therefore the commutation terms converge to zero uniformly in $V \in G$. This proves the lemma.

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Time-independent multichannel scattering theory for charged particles*

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Rigorous derivations are given of two time-independent formulas for the multichannel scattering operator for nonrelativistic charged particle systems. The derivations are based on Dollard's time-dependent theory and use techniques of spectral integration. The formulas involve a complex power of the resolvent operator, in contrast to short-range formulas. Bilateral Laplace transforms are used to derive a generalized multichannel resolvent equation and to prove existence and uniqueness of the solution. The formulas are applied to recover the well-known two-body Coulomb scattering amplitude.

I. INTRODUCTION

A substantial body of literature (see Refs. 1–6 and references cited therein) exists on how to employ the Faddeev–Yakubovskiĭ[7,8] equations to study the scattering of systems of charged particles. Most papers on the subject have been restricted to situations in which there are at most two charged bodies in the open channels. In such situations the asymptotic effects of the long-range Coulomb interaction can be treated exactly, thus avoiding the principal complication of the problem. Attempts to treat more general processes have not been satisfactory.[1–3]

Remarkably, none of these papers seriously pursues the question of whether the time-independent scattering theory represented by the Faddeev–Yakubovskiĭ equations is appropriate for charged particles. This is especially noteworthy in the face of evidence to the contrary.

For example, when the interactions have short range, the time-independent theory is justified on the basis of the physically more transparent time-dependent theory (see Ref. 9 and references cited therein). For some reason such a procedure has not been repeated for multichannel scattering involving Coulomb interactions. This omission is especially remarkable, since inclusion of Coulomb effects is known[10–12] to require modifications of the time-dependent short-range theory. One would expect the time-independent theory to require similar modifications.

There is also evidence from relativistic theory. Recent work[13–15] demonstrates that the relativistic propagator for "free" charged particles is a momentum-dependent complex power of the usual free propagator. Such complex powers do not appear in the multiple scattering expansions[16] corresponding to the Faddeev–Yakubovskiĭ equations.

Even in the thoroughly studied two-body Coulomb problem one finds evidence that the basic equation, the Lippmann–Schwinger equation, needs modification. Calculations based on this equation are plagued by divergences,[5,17–19] which are usually absorbed into conveniently ill-defined normalization factors. Statements abound[18–20] that the transition amplitude defined by the Lippmann-Schwinger equation vanishes, or at least is not unitary. Yet such statements are known[10–12] to be false for the two-body Coulomb amplitude.

In this paper we propose to take this evidence seriously and to reinvestigate the foundations of the time-independent scattering theory for charged particles. We begin in Sec. II by recalling the essential elements of the well-established multichannel time-dependent theory of Dollard.[10–12]. This formulation was chosen, instead of alternative ones,[21–24] because of its similarity to the familiar short-range theory. The theory is then recast in a more convenient two-Hilbert space setting. In Sec. III two time-independent formulas for the multichannel scattering operator S are derived with the aid of techniques of spectral integration.[9] It turns out that these time-independent formulas involve a complex power of the resolvent of the Hamiltonian. This is in marked contrast to the standard short-range theory where the resolvent appears only to the first power. An elementary theory for complex powers of the resolvent operators is developed in Sec. IV. Specifically, bilateral Laplace transforms are used to derive a generalized multichannel resolvent equation and to prove existence and uniqueness of the solution. The formulas of Secs. III and IV reduce, in the absence of Coulomb interactions, to familiar short-range formulas. We turn to the two-body problem in Sec. V to demonstrate that the well-known Coulomb scattering amplitude is recovered from our formulas in a straightforward, albeit tedious, way. The calculation is rigorous and no divergences need to be explained away. Concluding remarks are found in Sec. VI.

II. TIME-DEPENDENT FORMULATION

In Dollard's formulation[10–12] of time-dependent multichannel scattering one contemplates a system of N distinguishable spinless charged particles interacting via Coulomb-like potentials. Asymptotically the particles are in a particular channel β which consists of an arrangement of the particles into n, $2 \le n \le N$, clusters, each of which is in a specific quantum mechanical bound state. The basic assumptions of the theory are the following, collectively called assumption (D).

Assumption D:

D1. The total Hamiltonian H is of the form $H = H_0$

$+ V + V_c$, where H_0 denotes the free Hamiltonian, V the short-range potentials, and V_c the potentials for the Coulomb interactions. The operator H is self-adjoint with domain $\mathcal{D}_H$ in a separable Hilbert space $\mathcal{H}$.

D2. The "distorted" free channel Hamiltonians $H_\beta(t)$ are of the form $H_\beta(t) = H_\beta t + \alpha\,\epsilon(t) H'_\beta(t)$, where the H_β are the free channel Hamiltonians and the $H'_\beta(t)$ represent the "anomalous" behavior. The symbol α denotes the fine structure constant, and $\epsilon(t)$ is equal to $+1$ for $t > 0$ and equal to -1 for $t < 0$. The $H'_\beta(t)$ are of the form $H'_\beta(t) = F_\beta \ln|t| + A_\beta$ for certain time-independent operators F_β and A_β [cf. Eq. (71) of Ref. 11]. The $H_\beta(t)$ and $H'_\beta(t)$ are, for any t, self-adjoint operators with domains in separable Hilbert spaces $\mathcal{H}_\beta \subset \mathcal{H}$ and with absolutely continuous spectra. The Hilbert space $\mathcal{H}_0$, corresponding to a clustering with only one particle per cluster, is the entire space $\mathcal{H}$.

D3. The "modified" channel wave operators

$$\Omega_\pm^{(\beta)} \equiv \operatorname*{s-lim}_{t\to\pm\infty} e^{iHt} e^{-iH_\beta(t)} P_\beta \tag{2.1}$$

exist on $\mathcal{H}$ for all channels β, where P_β are the orthogonal projections of $\mathcal{H}$ onto $\mathcal{H}_\beta$. If the channels β and γ have the same clustering but possibly different bound states, then

$$P_\beta P_\gamma = \delta_{\beta\gamma} P_\beta, \tag{2.2}$$

where $\delta_{\beta\gamma}$ is the Kronecker delta function. The orthogonal projections $E_\pm^{(\beta)}$ of $\mathcal{H}$ onto the ranges of $\Omega_\pm^{(\beta)}$ satisfy

$$E_\pm^{(\beta)} E_\pm^{(\gamma)} = \delta_{\beta\gamma} E_\pm^{(\beta)} \tag{2.3}$$

for all channels β and γ.

In order to work most efficiently with the multichannel problem, it is desirable to place the theory in a two-Hilbert space setting. Proceeding as in the short-range case[9] one defines the direct sum Hilbert space $\mathcal{H}' \equiv \oplus_\beta \mathcal{H}_\beta$ and the bounded injection operator $J: \mathcal{H}' \to \mathcal{H}$ by $J \oplus_\beta \phi_\beta \equiv \Sigma_\beta \phi_\beta$. Then the adjoint of J is $J^*\psi = \oplus_\beta P_\beta \psi$. Define the multichannel "distorted" Hamiltonian $H_D(t)$ for $\Phi \equiv \oplus_\beta \phi_\beta$ in its domain $\mathcal{D}(H_D(t)) \subset \mathcal{H}'$ by

$$H_D(t)\Phi \equiv \oplus_\beta H_\beta(t) \phi_\beta. \tag{2.4}$$

The decomposition of $H_\beta(t)$ in Assumption D2 implies the decomposition

$$H_D(t) = H' t + \alpha\,\epsilon(t) H'_D(t), \tag{2.5}$$

where $H'\Phi \equiv \oplus_\beta H_\beta \phi_\beta$ and $H'_D(t)\Phi \equiv \oplus_\beta H'_\beta(t)\phi_\beta$. Furthermore, the time-dependent part of the operator $H'_D(t)$ may be isolated by a decomposition of the form

$$H'_D(t) = F \ln|t| + A. \tag{2.6}$$

The operators H', F, and A are all self-adjoint and commute with each other on properly restricted (dense) domains.[10-12] The "modified" multichannel wave operators $\Omega_\pm: \mathcal{H}' \to \mathcal{H}$ are defined by

$$\Omega_\pm \Phi \equiv \Sigma_\beta \Omega_\pm^{(\beta)} \phi_\beta, \tag{2.7}$$

and the multichannel scattering operator $S: \mathcal{H}' \to \mathcal{H}'$ by

$$S \equiv \Omega_+^* \Omega_-. \tag{2.8}$$

The properties of this two-Hilbert space formulation that are important for this paper are contained in the following proposition.

Proposition: Let Assumption (D) be true. Then the following statements are valid.

(1) The wave operators $\Omega_\pm$ defined by Eq. (2.7) satisfy

$$\Omega_\pm = \operatorname*{s-lim}_{t\to\pm\infty} e^{iHt} J e^{-iH_D(t)}, \tag{2.9}$$

and the adjoint wave operators $\Omega_\pm^*: \mathcal{H} \to \mathcal{H}'$ have the representations

$$\Omega_\pm^* = \operatorname*{w-lim}_{t\to\pm\infty} e^{iH_D(t)} J^* e^{-iHt}. \tag{2.10}$$

In addition, the wave operators satisfy the equations

$$\Omega_\pm^* \Omega_\pm = I \quad \text{and} \quad \Omega_\pm \Omega_\pm^* = E_\pm, \tag{2.11}$$

where I is the identify on $\mathcal{H}'$ and $E_\pm \equiv \Sigma_\beta E_\pm^{(\beta)}$.

(2) The scattering operator S defined by Eq. (2.8) satisfies

$$S = \operatorname*{w-lim}_{t\to\infty} e^{iH_D(t)} J^* e^{-2iHt} J e^{iH_D(t)}. \tag{2.12}$$

As in the short-range case, the weak limits in Eqs. (2.10) and (2.12) may not, in general, be replaced by strong limits.

Proof: The propositions follow from the corresponding single channel properties in essentially the same way as the short-range analogs.[9] QED

III. TRANSITION TO TIME-INDEPENDENT THEORY

A. Lemmata

Lemma 1: Suppose the following statements are true.

(i) There exists a strongly measurable, essentially bounded[25] mapping $f: \mathbf{R}^+ \to \mathcal{H}$, where $\mathbf{R}^+$ is the (open) positive real line and $\mathcal{H}$ is a Hilbert space, such that

$$f_\infty \equiv \lim_{t\to\infty} f(t) \tag{3.1}$$

exists.

(ii) There exists $\epsilon_0 > 0$ and a measurable function $k: (0, \epsilon_0] \times \mathbf{R}^+ \to \mathbf{R}^+$ that for each ϵ in $(0, \epsilon_0]$ is integrable with respect to t on $\mathbf{R}^+$. Moreover, the conditions

$$\lim_{\epsilon\to 0^+} \int_0^\infty dt k(\epsilon, t) = 1, \tag{3.2}$$

$$\lim_{\epsilon\to 0^+} \int_0^T dt k(\epsilon, t) = 0 \tag{3.3}$$

are satisfied for all T, $0 < T < \infty$.

Then, the vector

$$K_\epsilon f \equiv \int_0^\infty dt k(\epsilon, t) f(t) \tag{3.4}$$

is well defined (in $\mathcal{H}$) for all ϵ in $(0, \epsilon_0]$, and

$$f_\infty = \lim_{\epsilon\to 0^+} K_\epsilon f. \tag{3.5}$$

Proof: The integrability (for fixed ϵ) of $k(\epsilon, t)$ and the measurability and boundedness of f imply the existence of the Bochner integral $K_\epsilon f$ (Theorem 3.7.4 of Ref. 26). To prove Eq. (3.5), consider

$$K_\epsilon f - f_\infty = \int_0^\infty dt k(\epsilon, t)[f(t) - f_\infty] + f_\infty \left\{ \int_0^\infty dt k(\epsilon, t) - 1 \right\}. \tag{3.6}$$

The second term on the right in Eq. (3.6) vanishes in the limit $\epsilon\to 0^+$ by virtue of the assumed boundedness of f_∞ and by Eq. (3.2). It remains to prove that the first term also goes to zero. Let $\delta > 0$ be given and let $\|\cdot\|$ denote the norm on $\mathcal{H}$. Then, Eq. (3.1) implies the existence of $T > 0$ such that $\|f(t)-f_\infty\| < (\delta/2)$ for $t \geq T$. For $t < T$ the bound $\|f(t)-f_\infty\| \leq 2f_0 < \infty$, where f_0 is the essential supremum of $\|f(t)\|$, is valid. The inequality

$$\|\int_0^\infty dtk(\epsilon, t)[f(t)-f_\infty]\| < (\delta/2)\int_T^\infty dtk(\epsilon, t) + 2f_0\int_0^T dtk(\epsilon, t) \tag{3.7}$$

follows. It is clear from Eqs. (3.2) and (3.3) that there exists $\epsilon_1\in(0, \epsilon_0]$ such that the right side of Eq. (3.7) is less than δ if $\epsilon < \epsilon_1$. Since δ was arbitrary this proves that the first term on the right of Eq. (3.6) also vanishes in the limit $\epsilon\to 0^+$ and hence that Eq. (3.5) is true. QED

Lemma 2: Assume the following.

(i) Spectral families $E_\lambda^{(1)}$ and $E_\lambda^{(2)}$ are defined on respective separable Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$.

(ii) There is a family of essentially bounded[25] linear operators $B_t: \mathcal{H}_1\to\mathcal{H}_2$ that are labeled by a parameter t that varies over a (finite or infinite) interval Δ of the real line.

(iii) There exists on $\Delta\times\Lambda$, where Λ is an interval (finite or infinite) of the real line, a measurable complex-valued function $u(t, \lambda)$.

(iv) There is a real-valued Lebesgue integrable function $v(t)$ defined on Δ with the property that $|u(t, \lambda)| \leq v(t)$ for almost all $t\in\Delta$, $\lambda\in\Lambda$. Then the following statements are true.

(1) Suppose that the integral $\int_\Lambda u(t, \lambda)dE_\lambda^{(1)}\phi$ exists for almost all $t\in\Delta$ and all $\phi\in\mathcal{H}_1$. Then the existence for some $\psi\in\mathcal{H}_1$ of one of the integrals

$$\int_\Delta dtB_t(\int_\Lambda u(t, \lambda)dE_\lambda^{(1)}\psi) \quad\text{or}\quad \int_\Lambda(\int_\Delta dtB_t u(t, \lambda))dE_\lambda^{(1)}\psi \tag{3.8}$$

implies the existence of the other and their equality.

(2) Suppose that the integral $\int_\Lambda u(t, \lambda)dE_\lambda^{(2)}\phi$ exists for almost all $t\in\Delta$ and all $\phi\in\mathcal{H}_2$. Then the existence for some $\psi\in\mathcal{H}_1$ of one of the integrals

$$\int_\Delta dt(\int_\Lambda u(t, \lambda)dE_\lambda^{(2)})B_t\psi \quad\text{or}\quad \int_\Lambda dE_\lambda^{(2)}(\int_\Delta dt u(t, \lambda)B_t\psi) \tag{3.9}$$

implies the existence of the other and their equality.

Remark: Lemma 2 is but a minor modification of previously published results[9] and hence will not be proved here. The modification is necessary because $H_D(t)$ is not defined at $t=0$.

Lemma 3: Assume the following:

(i) A spectral family $E_\lambda^{(1)}$ defines a self-adjoint linear operator $H_1=\int\lambda dE_\lambda^{(1)}$ with domain $\mathcal{D}(H_1)$ dense in a separable Hilbert space $\mathcal{H}_1$.

(ii) A family of (possibly unbounded) linear operators U_λ is defined on $\mathcal{D}(U_\lambda)\subset H_1$ and has range in a separable Hilbert space $\mathcal{H}_2$. The labeling parameter λ varies over an interval Λ, finite or infinite, of the real line $\mathbf{R}$. At each point $\lambda\in\Lambda$ the domain $\mathcal{D}(U_\lambda)$ contains $\mathcal{D}(H_1)$, and for each finite subset $K\subset\Lambda$ there exists a nonnegative integer m and constants $b_k=b_k(K)$, $k=1,\ldots,m$, such that for all $\lambda\in K$ the inequality

$$\|U_\lambda\Phi\|_2 \leq \sum_{k=0}^m b_k\|H_1^k\Phi\|_1 \tag{3.10}$$

holds for each $\phi\in\mathcal{D}(H_1^m)$. By convention $H_1^0\Phi\equiv\Phi$. In Eq. (3.10) the subscripts 1 and 2 indicate that the norms are to be taken in the spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

(iii) There is a complex-valued function $w(\eta, \lambda)$ defined on $\mathbf{R}\times\Lambda$ such that the integral

$$w(H_1, \lambda)\phi \equiv \int_{\mathbf{R}} w(\eta, \lambda)dE_\eta^{(1)}\phi \tag{3.11}$$

exists for all $\lambda\in\Lambda$ and all $\phi\in\mathcal{D}(H_1)$. For every finite subset $K\subset\Lambda$ there are nonnegative constants $L=L(K)$ and $\gamma=\gamma(K)$, with $\gamma>\frac{1}{2}$, such that the inequality

$$|w(\eta, \lambda)-w(\eta', \lambda)| \leq L|\eta-\eta'|^\gamma \tag{3.12}$$

holds for all $\eta, \eta', \lambda\in K$.

Then, the existence for some $\psi\in\mathcal{H}_1$ of one of the spectral integrals,

$$\int_\Lambda U_\lambda w(H_1, \lambda)dE_\lambda^{(1)}\psi \quad\text{or}\quad \int_\Lambda U_\lambda w(\lambda, \lambda)dE_\lambda^{(1)}\psi, \tag{3.13}$$

implies the existence of the other and their equality. Further, if $\psi\in\mathcal{H}_2$ belongs to $\mathcal{D}(U_\lambda^*)$ for all $\lambda\in\Lambda$, the existence of one of the spectral integrals,

$$\int_\Lambda dE_\lambda^{(1)}w^*(H_1, \lambda)U^*\psi \quad\text{or}\quad \int_\Lambda dE_\lambda^{(1)}w^*(\lambda, \lambda)U_\lambda^*\psi, \tag{3.14}$$

implies the existence of the other and their equality.

Proof: The proof of a similar previous result applies with the exception that inequalities (3.10) through (3.12) of Ref. 9 are to be replaced by the following:

$$\|\Gamma_\pi\psi\|_2 \leq \sum_i\sum_{k=0}^m b_k\|H_1^k B_i\psi\|_1, \tag{3.15}$$

$$\leq L\sum_{k=0}^m b_k\sum_i|\lambda_i-\lambda_{i-1}|^\gamma\|H_1^m E^{(1)}(\Lambda_i)\psi\|_1, \tag{3.16}$$

$$\leq L|\pi|^{\gamma-1/2}(b-a)^{1/2}\sum_{k=0}^m b_k\|H_1^k E^{(1)}((a, b])\psi\|_1. \tag{3.17}$$

B. The scattering operator

In this subsection time-independent formulas for the multichannel scattering operator $S=\Omega_+^*\Omega_-$ are given.

The first formula is a multichannel Coulomb analog of a short-range result that was discovered for individual channels by Hunziker. (See Theorem 3 of Ref. 9.)

Theorem 1: Let Assumption (D) be true. Then the scattering operator S has on $\mathcal{H}'$ the representation

$$S=\operatorname*{w-lim}_{\epsilon\to 0^+}[\epsilon^\gamma/\Gamma(\gamma)]e^{i\alpha A}\int_\lambda dE_\lambda'\int_\mu\int_\sigma dF_\sigma\int_\tau L(\gamma+ia[\sigma+\tau], [\lambda+\mu+i\epsilon]/2)dF_\tau dE_\mu' e^{i\alpha A}. \tag{3.18}$$

Here γ is any positive number, and $\Gamma(\cdot)$ is the gamma function. The operator $L(\nu, z)$ is defined, for complex ν and z, by

$$L(\nu, z) \equiv (i/2)^\nu\Gamma(\nu)J^*(z-H)^{-\nu}J. \tag{3.19}$$

The integral in Eq. (3.18) is a repeated spectral integral which may be evaluated in any order of integration.

Proof: Define

$$C_t \equiv e^{i\alpha H_D'(t)} J^* e^{-2iHt} J e^{i\alpha H_D'(t)}. \quad (3.20)$$

The operator C_t is strongly measurable and bounded in norm by $\|J\|^2$. Thus for $\Phi \in \mathcal{H}'$, $\epsilon > 0$, and $x \in \mathbf{R} \equiv (-\infty, \infty)$ the Bochner integrals

$$Q_\epsilon \Phi = \int_0^\infty dt e^{-\epsilon t} t^{\gamma-1} e^{iH't} C_t e^{iH't} \Phi, \quad (3.21)$$

$$\tilde{C}(x)\Phi \equiv \int_0^\infty dt e^{i(x+i\epsilon)t} t^{\gamma-1} C_t \Phi \quad (3.22)$$

both exist and define bounded linear operators Q_ϵ and $\tilde{C}(x)$, respectively (Theorem 3.8.1 of Ref. 26.) The properties of C_t, the fact that H' commutes with $H_D'(t)$ on a dense subset of $\mathcal{H}'$, and Lemma 1 with $k(\epsilon, t) = [\epsilon^\gamma/\Gamma(\gamma)] t^{\gamma-1} e^{-\epsilon t}$, $\gamma > 0$, imply that the asymptotic limit of Eq. (2.12) may be replaced by an Abelian limit to obtain

$$S = \operatorname*{w-lim}_{\epsilon \to 0^+} [\epsilon^\gamma/\Gamma(\gamma)] Q_\epsilon. \quad (3.23)$$

The limit S is independent of γ. Now replace the factors $e^{iH't}$ in Eq. (3.21) with their spectral representations, and use Lemma 2 to interchange the order of the t-integration with the spectral integrations (cf. the proof of Theorem 3 in Ref. 9). The result is

$$Q_\epsilon \Phi = \int_\lambda dE_\lambda' \int_\mu \tilde{C}(\lambda + \mu) dE_\mu' \Phi, \quad (3.24)$$

where $\tilde{C}$ is defined by Eq. (3.22).

It remains to compute $\tilde{C}$. Recall that A commutes with F on a dense subset of $\mathcal{H}'$. Then, by Eqs. (2.6), (3.20), and (3.22), and by the boundedness of $K \equiv e^{i\alpha A}$,

$$\tilde{C}(x)\Phi = K \int_0^\infty dt e^{i(x+i\epsilon)t} t^{\gamma-1} e^{i\alpha F \ln t} J^* e^{-2iHt} J e^{i\alpha F \ln t} K \Phi. \quad (3.25)$$

Replacing the factors $e^{i\alpha F \ln t}$ in Eq. (3.25) by their spectral representations and using Lemma 2 to interchange the order of the t-integration with the spectral integrations yields

$$\tilde{C}(x)\Phi = K \int_\sigma dF_\sigma \int_\tau L(\nu, (x + i\epsilon)/2) dF_\tau K \Phi, \quad (3.26)$$

where $\nu = \gamma + i\alpha(\sigma + \tau)$ and

$$L(\nu, z) \equiv \int_0^\infty dt t^{\nu-1} e^{2izt} J^* e^{-2iHt} J. \quad (3.27)$$

In order to find a formula for $L(\nu, z)$, first take the bounded operators J and J^* outside of the integrand in Eq. (3.27). Second, replace the factor e^{-2iHt} by its spectral representation. Third, use Lemma 2 to interchange the order of spectral and t-integration. This gives

$$L(\nu, z) = J^* \int_\eta dE_\eta^H D(\nu, z, \eta) J, \quad (3.28)$$

where $E_\eta^H (-\infty < \eta < \infty)$ is the spectral family for H. The function $D(\nu, z, \eta)$ is defined by

$$D(\nu, z, \eta) \equiv \int_0^\infty dt t^{\nu-1} e^{2i(z-\eta)t} = [-2i(z-\eta)]^{-\nu} \Gamma(\nu) \quad (3.29)$$

for $\mathrm{Re}(\nu) > 0$ and $0 < \operatorname{Arg} z < \pi$. By the functional calculus[27] Eq. (3.28) can therefore be rewritten

$$L(\nu, z) = (i/2)^\nu \Gamma(\nu) J^* R^\nu(z) J, \quad (3.30)$$

where $R^\nu(z)$ is the νth power of the resolvent of H. Combining Eqs. (3.23), (3.24), (3.26), and (3.30) yields Eq. (3.18) in the indicated order of integration. To obtain a different order of integration, apply the spectral representations to the factors in Eq. (3.21) in a different order. The proof then proceeds in essentially the same way as before. QED

The main point of Theorem 1 is that the time-independent theory of charged particle scattering is determined by a complex power ν of the resolvent $(z-H)^{-1}$. This is in contrast to short-range theory in which ν is strictly real. The consequences of ν having a nonzero imaginary part in charged particle theory seem not to be widely appreciated, as will be discussed in more detail in Sec. VI.

It is also worth noting that the parameter γ in Theorem 1 is always set equal to unity in short-range calculations. The desirability of using a different γ for Coulomb scattering will become apparent in Sec. IVB.

Before discussing these matters, however, a Coulomb generalization of the usual transition operator will be presented. Define for all $\Phi = \oplus_\beta \phi_\beta$ in $\mathcal{H}'$ a "Coulomb identity" operator $I_C : \mathcal{H}' \to \mathcal{H}'$ by the equation

$$I_C \equiv \oplus_\beta \delta_\beta \phi_\beta, \quad (3.31)$$

where δ_β is zero if channel β has two or more clusters with nonzero charge and is one otherwise. If all of the channels have only neutral clusters, as is the case in short-range scattering theory, then I_C is the identity operator. Coulomb transition operators are then provided by the following theorem.

Theorem 2: Let Assumption (D) be true. Then the operator $S - I_C$ has on $\mathcal{H}'$ the representation

$$S - I_C = \operatorname*{w-lim}_{\epsilon \to 0^+} (-2\pi i)[\epsilon^{\gamma-1}/\Gamma(\gamma)] e^{i\alpha A} \int_\lambda dE_\lambda' \int_\mu \int_\sigma dF_\sigma \int_\tau \delta_\epsilon(\lambda - \mu) \times T(\nu, [\lambda + \mu + i\epsilon]/2) dF_\tau dE_\mu' e^{i\alpha A}, \quad (3.32)$$

where

$$\delta_\epsilon(x) \equiv (\epsilon/\pi)(x^2 + \epsilon^2)^{-1} \quad (3.33)$$

for all real x,

$$T(\nu, z) \equiv (\tfrac{1}{2}i)^{\nu-1} \Gamma(\nu) [(z - H') J^* R^\nu(z) J (z - H') - (z - H')^{2-\nu}] \quad (3.34)$$

for all complex z with nonzero imaginary part, $\nu \equiv \gamma + i\alpha(\sigma + \tau)$, $R(z) \equiv (z - H)^{-1}$, and $\Gamma(\cdot)$ is the Gamma function. The limit (3.32) is independent of γ, $\gamma > 0$. The integral in Eq. (3.32) is a repeated spectral integral which may be evaluated in any order of integration.

Proof: It is easily seen by an integration by parts that

$$\operatorname*{w-lim}_{t \to \infty} \exp[2\alpha i H_D'(t)] = I_C \quad (3.35)$$

(cf. Ref. 12, p. 29). Therefore, the operator $(S - I_C)$ has the representation

$$S - I_C = \operatorname*{w-lim}_{t \to \infty} e^{iH't} (C_t - C_t') e^{iH't}, \quad (3.36)$$

where C_t is defined by Eq. (3.20) and

$$C_t' \equiv e^{i\alpha H_D'(t)} e^{-2iH't} e^{i\alpha H_D'(t)}. \quad (3.37)$$

Proceeding as in Theorem 1 one obtains

$$S - I_C = \operatorname*{w-lim}_{\epsilon \to 0^+} e^{i\alpha A} \int_\lambda dE_\lambda' X(\epsilon, \lambda) e^{i\alpha A}, \quad (3.38)$$

$$X(\epsilon, \lambda) \equiv [\epsilon^\gamma/\Gamma(\gamma)] \int_\mu \int_\sigma dF_\sigma \int_\tau \{L(\nu, [\lambda + \mu + i\epsilon]/2)$$

$$-L_0(\nu, [\lambda + \mu + i\epsilon]/2)\} dF_\tau dE'_\mu. \quad (3.39)$$

The operator $L(\nu, z)$ is defined by Eqs. (3.27) and (3.30), and the operator $L_0(\nu, z)$ is similarly defined by

$$L_0(\nu, z) \equiv \int_0^\infty dt t^{\nu-1} e^{2izt} e^{-2itH't} = (i/2)^\nu \Gamma(\nu) R_0^\nu(z), \quad (3.40)$$

where $R_0(z) \equiv (z - H')^{-1}$. Comparing the operator $T(\nu, z)$ defined in Eq. (3.34), one notes that

$$L(\nu, z) - L_0(\nu, z) = (i/2) R_0(z) T(\nu, z) R_0(z). \quad (3.41)$$

The proof now proceeds in the same manner as the proof of Theorem 4 of Ref. 9. Consider the operator

$$Y(\epsilon, \lambda) \equiv [-2\epsilon^\gamma/\Gamma(\gamma)] \int_0^\infty dt e^{(i\lambda-\epsilon)t} (\lambda - H')(C_t - C_t^\dagger) R_0(\lambda - i\epsilon) e^{iH't} \quad (3.42)$$

and show that

$$S - I_C = \text{w-}\lim_{\epsilon\to 0^+} e^{i\alpha A} \int_\lambda dE'_\lambda \tilde{X}(\epsilon, \lambda) e^{i\alpha A}, \quad (3.43)$$

where $\tilde{X}(\epsilon, \lambda) \equiv X(\epsilon, \lambda) + Y(\epsilon, \lambda)$. The operator $\tilde{X}$ can be written in the form

$$\tilde{X}(\epsilon, \lambda) = (-2\pi i)[\epsilon^{\gamma-1}/\Gamma(\gamma)] \int_\mu \int_\sigma dF_\sigma \int_\tau \delta_\epsilon(\lambda - \mu) \times T(\nu, [\lambda + \mu + i\epsilon]/2) dF_\tau dE'_\mu \quad (3.44)$$

[cf. Eqs. (3.38) through (3.45) of Ref. 9]. In order to duplicate these steps in the present case, one needs to know that the operators $H' R_0(z) T(\nu, z) R_0(z)$ and $T(\nu, z)$ satisfy the conditions of Lemma 3. This may be proved as follows. Consider the operator

$$D(\nu, z) \equiv \int_0^\infty dt t^{\nu-1} e^{2izt} e^{-2itHt} = (i/2)^\nu \Gamma(\nu) R^\nu(z) \quad (3.45)$$

for Re $\nu > 0$ and Im $z > 0$ [cf. Eqs. (3.27) through (3.30) above]. Since

$$\|D(\nu, z)\| \le \int_0^\infty dt t^{\text{Re}\,\nu-1} e^{-2t\,\text{Im}\,z} = \Gamma(\text{Re}\,\nu)(2\text{Im}\,z)^{-\text{Re}\,\nu}, \quad (3.46)$$

$D(\nu, z)$ is a bounded operator for Re$\nu > 0$ and Im$z > 0$. Now consider the operator

$$(z - H')L(\nu, z)(z - H') = (z - H')J^* D(\nu, z) J(z - H'),$$
$$= \{(z - H')J^* R(z)\} D(\nu, z) \{(z - H) \times J R_0(z)\}(z - H')^2. \quad (3.47)$$

The operators in braces in Eq. (3.47) are bounded for Im$z > 0$ by Lemma 1 and Proposition 1 of Ref. 9. Hence, the operator $(z - H')L(\nu, z)(z - H')$ satisfies inequality (3.10) with $m = 2$. Similarly, the operator $(z - H') \times L_0(\nu, z)(z - H')$ satisfies inequality (3.10) with $m = 2$. Therefore, for Re$\nu > 0$ and Im$z > 0$, inequality (3.10) is satisfied by $T(\nu, z)$ for $m = 2$ and by $H' R_0(z) T(\nu, z) R_0(z)$ for $m = 1$. The steps leading to Eqs. (3.43) and (3.44) may now be carried out by using Lemma 3 of this paper in place of Lemma 5 of Ref. 9. QED

Remarks: Some remarks regarding Theorems 1 and 2 are in order.

(1) Theorems 1 and 2 make use of a general Abel limit which contains a parameter $\gamma > 0$ rather than the usual Abel limit ($\gamma = 1$). The reason for this generalization is that Theorem 3, below, requires $0 < \gamma < 1$. The fact that a general Abel limit may be used in place of the usual one is no doubt well known, but apparently has not previously been exploited because no one had reason to do so.

(2) In two-body theory the operator F may be considered as a function of H'.[28] This is not true in many-body theory. Thus the operators H' and F must be given equal status, as is done in Theorems 1 and 2.

(3) Note that the resolvent operator appearing in Theorems 1 and 2 is raised to a complex power ν. The presence of this complex power serves to eliminate certain mathematical divergences which arise when Coulomb potentials are present (see also the remarks in Secs. I and VI).

(4) Theorems 1 and 2 reduce to the usual short-range results (cf. Theorems 3 and 4 of Ref. 9) if $\gamma = 1$ and if all channels have only neutral clusters. In this case $\nu = 1$ and $F = A = 0$, so that $K = I_C = I$. It is clear from Eq. (3.34) that $T(1, z)$ is just the usual short-range transition operator.

(5) It is to be emphasized (cf. Sec. IV of Ref. 9) that the spectral integrals are to be performed before taking the limit $\epsilon \to 0^+$.

(6) The function $\delta_\epsilon(\lambda - \mu)$, which is supposed in the limit $\epsilon \to 0^+$ to enforce energy conservation, has been introduced in Theorem 2 in analogy with the short-range case. As will be seen in Sec. V, this may not be the most natural way to exhibit energy conservation for charged particle problems.

(7) Since δ_β in Eq. (3.31) vanishes if channel β has at least two charged fragments, Theorem 2 gives in this case a formula for the (channel) operators $S_{\gamma\beta}$ rather than $S_{\gamma\beta} - I_{\gamma\beta}$. This is not unreasonable, since I. Herbst[29] has recently shown in the two-particle case that the Coulomb scattering operator is more singular than a delta function. That is, S in the momentum space representation is more singular as a distribution than I itself. Thus there is no apparent reason why the identity operator should be subtracted from the scattering operator for channels with charged clusters.

IV. THE OPERATOR *L(ν,z)*

A. Bilateral Laplace transforms

The principal mathematical tool that will be used in the study of the operator $L(\nu, z)$ is the bilateral Laplace transform of Hilbert space-valued functions. The essential elements of the theory of such transforms are reviewed in this subsection.

To define the bilateral Laplace transform, suppose that $\tilde{f}: \mathbf{R} \to \mathcal{H}$ is a strongly measurable mapping from the real line $\mathbf{R}$ into a Hilbert space $\mathcal{H}$. Then the Bochner integral

$$f(s) \equiv \int_{\mathbf{R}} dt e^{-st} \tilde{f}(t), \quad (4.1)$$

when it exists, is called the bilateral Laplace transform of $\tilde{f}$.

Two useful properties of these transforms are the following:

(1) If the integral $f(s)$ converges at two points s_1 and

s_2, Re $s_1 <$ Re s_2, then it converges and is holomorphic in the strip Re $s_1 <$ Re $s <$ Re s_2.

(2) If the two mappings $\tilde{f}_1$ and $\tilde{f}_2$ are such that $f_1(s) = f_2(s)$ in some common domain (strip) of convergence, then $f_1(t) = f_2(t)$ for almost all t. The proof of these properties for $\mathcal{H}$-valued functions follows from a change of notation in the well-known proof for complex-valued functions.[30]

It is also useful to have an inversion theorem.

Lemma 4: Assume the following.

(i) The spectral family E_λ of a self-adjoint operator $H = \int \lambda dE_\lambda$ is defined on a separable Hilbert space $\mathcal{H}$.

(ii) A complex-valued function $f(s, \lambda)$ is defined on $\mathcal{S} \times \Lambda$, where $\mathcal{S} \equiv \{s \in \mathbf{C} \mid s = \sigma + i\tau,\ a < \sigma < b\}$ (here $\mathbf{C}$ denotes the complex numbers), and Λ is an interval, finite or infinite, of the real line $\mathbf{R}$. The function $f(s, \lambda)$ is, for fixed $\lambda \in \Lambda$, a holomorphic function of s in the strip $\mathcal{S}$ and such that

$$\lim_{|\tau| \to \infty} f(\sigma + i\tau, \lambda) = 0 \tag{4.2}$$

uniformly in every closed subinterval of $(a < \sigma < b)$.

(iii) There is a real-valued function $h(s)$ such that $|f(s, \lambda)| \le h(s)$ for all $s \in \mathcal{S}$ and $\lambda \in \Lambda$ and such that for fixed $\sigma \in (a, b)$ the function $h(\sigma + i\tau)$ is Lebesgue integrable on $(-\infty < \tau < \infty)$.

(iv) The integral $f(s, H)\phi \equiv \int_\Lambda f(s, \lambda) dE_\lambda \phi$ exists for all $s \in \mathcal{S}$ and all $\phi \in \mathcal{H}$.

(v) The integral $\tilde{f}(x, H)\phi \equiv \int_\Lambda \tilde{f}(x, \lambda) dE_\lambda \phi$ exists for all $x \in \mathbf{R}$ and all $\phi \in \mathcal{H}$, where

$$\tilde{f}(x, \lambda) \equiv \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} ds e^{xs} f(s, \lambda) \quad (a < \sigma < b) \tag{4.3}$$

is the inverse bilateral Laplace transform of f.

Then for all $\phi \in \mathcal{H}$

$$f(s, H)\phi = \int_{-\infty}^{\infty} dx e^{-sx} \tilde{f}(x, H)\phi, \tag{4.4}$$

for $a < \sigma < b$, and

$$\tilde{f}(x, H)\phi = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} ds e^{xs} f(s, H)\phi, \tag{4.5}$$

for $a < \sigma < b$ and $x \in \mathbf{R}$. The integrals in Eqs. (4.4) and (4.5) are to be understood as Bochner integrals.

Proof: The integral in Eq. (4.3) converges by hypothesis (iii), and it is independent of σ by Cauchy's integral theorem and hypothesis (ii). Equation (4.5) then follows from the definition of $\tilde{f}(x, H)\phi$ and Lemma 2. To prove Eq. (4.4), choose, for a given $\sigma \in (a, b)$, a' and b' so that $a < a' < \sigma < b' < b$. Let $\hat{h}(\sigma) \equiv (2\pi)^{-1} \int_{-\infty}^{\infty} h(\sigma + i\tau) d\tau$. Then

$$|e^{-sx} \tilde{f}(x, \lambda)| \le \begin{cases} \hat{h}(a') e^{-x(\sigma - a')} & \text{for } x \ge 0, \\ \hat{h}(b') e^{x(b' - \sigma)} & \text{for } x < 0, \end{cases} \tag{4.6}$$

for all $\lambda \in \Lambda$, and the right-hand side of inequality (4.6) is Lebesgue integrable on $(-\infty < x < \infty)$. Therefore, Eq. (4.4) follows from Lemma 2 and from Theorem 19 of Ref. 30. QED

Finally, a convolution theorem is useful.

Lemma 5: Assume that the functions f_k and the self-adjoint operators $H_k = \int \lambda dE_\lambda^{(k)}$ satisfy the assumptions of Lemma 4 on the separable Hilbert spaces $\mathcal{H}_k$, $k = 1, 2$, respectively. Let $\tilde{f}_k(x, H_k)$ be the inverse bilateral Laplace transforms of $f_k(s, H_k)$, $k = 1, 2$. Suppose that B is a transformation from $\mathcal{H}_2$ into $\mathcal{H}_1$ for which the products $f_1(s_1, H_1) B f_2(s_2, H_2)$ $(a < \sigma_k \equiv \text{Re } s_k < b,\ k = 1, 2)$, and $\tilde{f}_1(x, H_1) B \tilde{f}_2(x, H_2)$ $(x \in \mathbf{R})$, are well-defined on $\mathcal{H}_2$, and for which $\tilde{f}_1(x, H_1) B$ is bounded. Then

$$\tilde{f}_1(x, H_1) B \tilde{f}_2(x, H_2)\phi = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} ds e^{xs} F(s) \tag{4.7}$$

$(a + \sigma_2 < \sigma \equiv \text{Re } s < b + \sigma_2,\ x \in \mathbf{R})$, where almost everywhere

$$F(s) \equiv \frac{1}{2\pi i} \int_{\sigma_2 - i\infty}^{\sigma_2 + i\infty} ds_2 f_1(s - s_2, H_1) B f_2(s_2, H_2)\phi \qquad (a < \sigma_2 < b). \tag{4.8}$$

The integrals in Eqs. (4.7) and (4.8) are to be understood as Bochner integrals.

Proof: Choose $\sigma_k \equiv \text{Re } s_k \in (a, b)$, $k = 1, 2$. Since $\tilde{f}_1(x, H_1) B$ is bounded, it may be moved inside a Bochner integral. Hence, for $\phi \in \mathcal{H}_2$

$$\begin{aligned} \tilde{f}_1(x, H_1) B \tilde{f}_2(x, H_2)\phi &= \frac{1}{2\pi i} \int_{\sigma_2 - i\infty}^{\sigma_2 + i\infty} ds_2 e^{xs_2} \tilde{f}_1(x, H_1) B f_2(s_2, H_2)\phi \\ &= \frac{1}{(2\pi i)^2} \int_{\sigma_2 - i\infty}^{\sigma_2 + i\infty} ds_2 \int_{\sigma_1 - i\infty}^{\sigma_1 + i\infty} ds_1 e^{x(s_1 + s_2)} \\ &\quad \times f_1(s_1, H_1) B f_2(s_2, H_2)\phi \\ &= \frac{1}{(2\pi i)^2} \int_{\sigma_2 - i\infty}^{\sigma_2 + i\infty} ds_2 \int_{\sigma - i\infty}^{\sigma + i\infty} ds e^{xs} \\ &\quad \times f_1(s - s_2, H_1) B f_2(s_2, H_2)\phi \\ &\quad (a + \sigma_2 < \sigma \equiv \text{Re } s < b + \sigma_2). \end{aligned} \tag{4.9}$$

The order of integration in the last integral may be interchanged by Theorem 3.7.13 of Ref. 26. The result is given by Eqs. (4.7) and (4.8). QED

B. The generalized resolvent equation

The starting point for most investigations in the time-independent scattering theory for short-range forces is the resolvent equation, or some further development thereof (such as the Faddeev–Yakubovskiǐ equations). Such an equation for $L(\nu, z)$, $0 < \text{Re } \nu < 1$, is developed in this subsection.

It is more convenient to write

$$L(\nu, z) = i[2\Gamma(1 - \nu)]^{-1} J^* M(\nu, z) J, \tag{4.10}$$

where

$$\begin{aligned} M(\nu, z) &\equiv (i/2)^{\nu - 1} \Gamma(1 - \nu) \Gamma(\nu) (z - H)^{-\nu}, \\ &= (i/2)^{\nu - 1} (\pi / \sin \pi\nu) (z - H)^{-\nu}. \end{aligned} \tag{4.11}$$

The theory is then developed in terms of the operator M.

The fact that $R(z) \equiv (z - H)^{-1}$ is raised to a complex power in Eq. (4.11) is a considerable inconvenience. For this reason a representation of $M(\nu, z)$ as a linear function of R is presented.

Theorem 3: For fixed nonzero z, $0<\arg z<\pi$, and for ν in the strip $0<\operatorname{Re}\nu<1$, the operator $M(\nu, z)$ has on $\mathcal{H}$ the representation

$$M(\nu, z)=\int_{-\infty}^{\infty} dt e^{t(1-\nu)}(z+\tfrac{1}{2}ie^t-H)^{-1} \qquad (4.12a)$$

$$=\int_0^{\infty} dy y^{-\nu}(z+\tfrac{1}{2}iy-H)^{-1}. \qquad (4.12b)$$

Proof: Define $\tilde{f}(t,\lambda)\equiv e^t(z-\lambda+\frac{1}{2}ie^t)^{-1}$ for fixed nonzero z, $0<\arg z<\pi$, and all real (t,λ). The bilateral Laplace transform $f(\nu,\lambda)$ of $\tilde{f}$ is given by $f(\nu,\lambda)=(i/2)^{\nu-1}\times(\pi/\sin\pi\nu)(z-\lambda)^{-\nu}$, provided that $0<\operatorname{Re}\nu<1$. [This follows from Eq. (6.2(3)), p. 308, of Ref. 31 with the variable changes $s\to\nu=1-s$, $x\to t=\ln x$.] The function $f(\nu,\lambda)$ satisfies the requirements of Lemma 4, yielding Eq. (4.12a). A change of variables $t\to y=e^t$ yields Eq. (4.12b). QED

Remark: The fact that $\sin\pi\nu$ has zeros at the integers means, in particular, that the representation of Eq. (4.12) is not useful if $\operatorname{Re}\nu=1$. For this reason it is extremely useful to have the flexibility allowed by Theorem 1 in assigning the value of the parameter γ.

Resolvent-like equations for $M(\nu, z)$ and for

$$\tilde{M}(t,z)\equiv e^t(z+\tfrac{1}{2}ie^t-H)^{-1} \qquad (4.13)$$

can now be derived in a straightforward way. For each channel β let a self-adjoint extension H_B of the channel Hamiltonian H_β be defined. This extension must have the same domain as the full Hamiltonian H and must satisfy the equation $H_\beta P_\beta=P_\beta H_B$ on that domain. (Examples of such extensions are provided by the so-called cluster Hamiltonians.[9,12]). Operators M_B and $\tilde{M}_B$ are defined in the same way as M and $\tilde{M}$, respectively, but with H replaced by H_B.

Theorem 4: For $0<\operatorname{Re}\nu<1$ and $0<\arg z<\pi$, the operator $M(\nu,z)$ is the unique solution of

$$M(\nu,z)=M_B(\nu,z)+\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\tau M_B(\nu-\tau+1,z)(H-H_B)M(\tau,z), \qquad (4.14)$$

where $0<\operatorname{Re}\nu<c<1$. For all real t and all z with nonzero imaginary part the operator $\tilde{M}(t,z)$ is the unique solution of

$$\tilde{M}(t,z)=\tilde{M}_B(t,z)+e^{-t}\tilde{M}_B(t,z)(H-H_B)\tilde{M}(t,z). \qquad (4.15)$$

Proof: This theorem is proved in essentially the same way as Theorem 5 below. QED

This theorem provides the Coulomb analog of the resolvent equations that form the basis of the time-independent theory of scattering with short-range interactions.

It is interesting that Theorem 4 can be rewritten in a slightly more general way that does not refer to extensions of the channel Hamiltonians. To do this define the operators M' and $\tilde{M}'$ in the same way as M and $\tilde{M}$, respectively, but with H replaced by H'. Let V^* denote the adjoint of $V=HJ-JH'$.

Theorem 5: For $0<\operatorname{Re}\nu<1$ and $0<\arg z<\pi$, the operator $M(\nu,z)$ is the unique solution of

$$J^*M(\nu,z)=M'(\nu,z)J^*+\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\tau M'(\nu-\tau+1,z)V^*M(\tau,z), \qquad (4.16)$$

where $0<\operatorname{Re}\nu<c<1$. For all real t and all z with nonzero imaginary part the operator $\tilde{M}(t,z)$ is the unique solution of

$$J^*\tilde{M}(t,z)=\tilde{M}'(t,z)J^*+e^{-t}\tilde{M}'(t,z)V^*\tilde{M}(t,z). \qquad (4.17)$$

Proof: The proof follows the standard treatment of the usual resolvent equation. The operator $\tilde{M}$ is a solution of Eq. (4.17) since

$$\begin{aligned}\tilde{M}'J^*+e^{-t}\tilde{M}'V^*\tilde{M}&=\tilde{M}'J^*+(z+\tfrac{1}{2}ie^t-H')^{-1}V^*\tilde{M}\\&=(z+\tfrac{1}{2}ie^t-H')^{-1}\{J^*(z+\tfrac{1}{2}ie^t-H)\\&\quad+J^*H-H'J^*\}\tilde{M},\\&=(z+\tfrac{1}{2}ie^t-H')^{-1}(z+\tfrac{1}{2}ie^t-H')J^*\tilde{M},\\&=J^*\tilde{M}.\end{aligned} \qquad (4.18)$$

To prove that the solution of Eq. (4.17) is unique, consider solutions $\tilde{N}$ of the homogeneous equation

$$J^*\tilde{N}=(z+\tfrac{1}{2}ie^t-H')^{-1}V^*\tilde{N}. \qquad (4.19)$$

Equation (4.19) implies that $J^*\tilde{N}$ maps $\mathcal{H}$ into $\mathcal{D}_{H'}$, the domain of H', and hence that

$$\begin{aligned}0&=(z+\tfrac{1}{2}ie^t-H')J^*\tilde{N}-V^*\tilde{N}\\&=J^*(z+\tfrac{1}{2}ie^t-H)\tilde{N}.\end{aligned} \qquad (4.20)$$

Recall that P_0, where $\beta=0$ is the "free" channel, is the identity on $\mathcal{H}$. It then follows from the equation

$$J^*\psi=\oplus_\beta P_\beta\psi, \qquad (4.21)$$

valid for all $\psi\in\mathcal{H}$, that J^* is nonsingular (although J is singular). Equation (4.20) thus implies

$$(z+\tfrac{1}{2}ie^t-H)\tilde{N}=0. \qquad (4.22)$$

The self-adjointness of H and the fact that $\operatorname{Im} z\neq 0$ now imply that $\tilde{N}=0$ and hence that the solution of Eq. (4.17) is unique.

To obtain Eq. (4.16) take the bilateral Laplace transform of Eq. (4.17), using Lemma 5 to deal with the second term on the right side. Existence and uniqueness of the solution of Eq. (4.16) follow from that of Eq. (4.17) and the uniqueness and continuity properties of the bilateral Laplace transform. QED

Direct comparison of Theorems 4 and 5 is facilitated by writing the equations of Theorem 5 channel by channel. Equation (4.17) is, for example, equivalent to requiring for all channels β that

$$P_\beta\tilde{M}=\tilde{M}_\beta P_\beta+e^{-t}\tilde{M}_\beta(P_\beta H-H_\beta P_\beta)\tilde{M}, \qquad (4.23)$$

where $\tilde{M}_\beta$ is defined in the (now) obvious way. It is clear that not only does Eq. (4.23) not refer to extensions of the channel Hamiltonians but also requires equality only on $P_B H = H_B$. This subtle distinction between the equations of the two theorems is, of course, of no consequence when the extensions H_B are known, but may be important for the construction of more general theories.

Comparison of Eq. (4.16) with the resolvent equation

$$J^*(z-H)^{-1} = (z-H')^{-1}J^* + (z-H')^{-1}V^*(z-H)^{-1} \quad (4.24)$$

is also of interest. For this purpose one notes that $M(\nu, z)$ is, for z fixed, meromorphic in the right half ν plane with poles at the positive integers. In particular, the residue at $\nu = 1$ is $(H-z)^{-1}$. The Cauchy residue theorem (Ref. 26, p. 97) can therefore be applied to move the contour of integration in Eq. (4.16) to the right of the pole of the integrand at $\tau = 1$. The resulting equation is

$$J^*M(\nu, z) = M'(\nu, z)J^* + M'(\nu, z)V^*(z-H)^{-1} + \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\tau M'(\nu-\tau+1, z)V^*M(\tau, z), \quad (4.25)$$

where $0 < \text{Re}\,\nu < 1 < c < \text{Re}\,\nu + 1$. Upon substitution of Eq. (4.11) into Eq. (4.25) one obtains an equation for $(z-H)^{-\nu}$ that is valid in some open domain containing $0 < \text{Re}\,\nu \le 1$:

$$J^*(z-H)^{-\nu} = (z-H')^{-\nu}J^* + (z-H')^{-\nu}V^*(z-H)^{-1} + (\tfrac{1}{2}i)^{1-\nu}\frac{\sin \pi\nu}{\pi}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\tau M'(\nu-\tau+1, z) \times V^*M(\tau, z). \quad (4.26)$$

The strong limit as $\nu \to 1$ of the last term on the right side of Eq. (4.26) is zero, leaving one with Eq. (4.24). Thus, Eq. (4.16) can be properly said to generalize the usual resolvent equation, Eq. (4.24).

The equivalent equations (4.16) and (4.17), or alternatively Eqs. (4.14) and (4.15), are the Coulomb analogs of the resolvent equations of short-range theories. They suffer the standard ills of multichannel resolvent equations, but these can, with one exception, be overcome with a development of a Faddeev–Yakubovskiĭ type.[7-8] Such equations will not be written here, since further work should be done to ascertain the most natural way to define the transition operator T (cf. remarks following Theorem 2 and also Sec. V). Once this has been done and the analogs of the Faddeev–Yakubovskiĭ equations written down, there remains the problem of compactness of the kernels of these equations. How this is to be circumvented remains, of course, an important matter for further research.

V. THE TWO-BODY AMPLITUDE

The formulas of the preceding sections can be used to compute the two-body Coulomb scattering amplitude in a mathematically rigorous way. The calculation is done in the center of mass momentum coordinate system and recovers the well-known[32] amplitude

$$S(\mathbf{k}_f, \mathbf{k}_i) = \delta\left(\frac{|\mathbf{k}_f|^2}{2\mu} - \frac{|\mathbf{k}_i|^2}{2\mu}\right) f(\mathbf{k}_f, \mathbf{k}_i). \quad (5.1)$$

The function f is defined by

$$f(\mathbf{k}_f, \mathbf{k}_i) = -\frac{i\alpha z_1 z_2}{\pi|\mathbf{k}_f - \mathbf{k}_i|^2}\left(\frac{2k}{|\mathbf{k}_f - \mathbf{k}_i|}\right)^{2i\alpha\eta(k)} \frac{\Gamma(1+i\alpha\eta(k))}{\Gamma(1-i\alpha\eta(k))}, \quad (5.2)$$

where $k = |\mathbf{k}_f| = |\mathbf{k}_i|$ and

$$\eta(k) = \mu z_1 z_2 k^{-1}, \quad (5.3)$$

μ being the reduced mass of the system. This result is obtained in a straightforward, although lengthy, manner that is not plagued with the divergences encountered in many previous calculations.[17-19]

In the two-body calculation the motion of the center of mass is suppressed so that the operators H_0, F, and A are defined in terms of relative coordinates. The explicit representations are

$$(H_0 f)(\mathbf{x}) \equiv (2\pi)^{-3/2}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}}(|\mathbf{k}|^2/2\mu)\tilde{f}(\mathbf{k}), \quad (5.4)$$

$$(Ff)(\mathbf{x}) \equiv (2\pi)^{-3/2}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}}\eta(k)\tilde{f}(\mathbf{k}), \quad (5.5)$$

where $\eta(k)$ is defined in Eq. (5.3); and

$$(Af)(\mathbf{x}) \equiv (2\pi)^{-3/2}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}}\eta(k) ln(2|\mathbf{k}|^2/\mu)\tilde{f}(\mathbf{k}). \quad (5.6)$$

In Eqs. (5.4)–(5.6) the function $\tilde{f}$ is the Fourier transform of f. The spectral measures E'_λ and F_σ corresponding to H_0 and F, respectively, have therefore the representations

$$(E'_\lambda f)(\mathbf{x}) = (2\pi)^{-3/2}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}}\theta(\lambda - [|\mathbf{k}|^2/2\mu])\tilde{f}(\mathbf{k}) \quad (5.7)$$

and

$$(F_\sigma f)(\mathbf{x}) = (2\pi)^{-3/2}\int d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}}\theta(\lambda - \eta(k))\tilde{f}(\mathbf{k}), \quad (5.8)$$

where θ is the usual Heaviside function. Finally, the operator J is in the two-body case just the identity.

Now let ψ and ϕ be Schwartz test functions such that their Fourier transforms $\tilde{\psi}$ and $\tilde{\phi}$ have nonintersecting compact support. It is further assumed that the origin $\mathbf{k} = 0$ does not lie in the support of either $\tilde{\psi}$ or $\tilde{\phi}$. Then it follows from the previous paragraph and from Theorems 1 and 3 that the equation

$$(\psi, S\phi) = \lim_{\epsilon \to 0^+}\int d\mathbf{k}_f\, d\mathbf{k}_i\, \tilde{\psi}^*(\mathbf{k}_f)\tilde{\phi}(\mathbf{k}_i)S_\epsilon(\mathbf{k}_f, \mathbf{k}_i) \quad (5.9)$$

holds, where S_ϵ has the form

$$S_\epsilon(\mathbf{k}_f, \mathbf{k}_i) = \frac{i\epsilon^\gamma (4T_f)^{i\alpha\eta_f}(4T_i)^{i\alpha\eta_i}}{2\Gamma(\gamma)\Gamma(1-\nu)} \times \int_0^\infty dy\, y^{-\nu} G([T_f + T_i + i\epsilon + iy]/2;\, \mathbf{k}_f, \mathbf{k}_i). \quad (5.10)$$

In Eq. (5.10) the parameter γ can be arbitrarily chosen from the open unit interval (0, 1). The parameter ν is given by

$$\nu = \gamma + i\alpha(\eta_f + \eta_i), \quad (5.11)$$

where $\eta_f = \eta(|\mathbf{k}_f|)$ and $\eta_i = \eta(|\mathbf{k}_i|)$. The parameters T_f and T_i are the final and initial kinetic energies, $T_f = (|\mathbf{k}_f|^2/2\mu)$ and $T_i = (|\mathbf{k}_i|^2/2\mu)$, respectively. The function G in Eq. (5.10) is the usual Coulomb Green Function, for which the representation (2′) of Schwinger[17] is adopted:[33]

$$G(\zeta; \mathbf{k}_f, \mathbf{k}_i) = (\zeta - T_f)^{-1}\delta(\mathbf{k}_f - \mathbf{k}_i) + G_1(\zeta; \mathbf{k}_f, \mathbf{k}_i), \quad (5.12)$$

where ζ is a complex number and

$$G_1 = -(\alpha\mu z_1 z_2 \zeta/\pi^2)\int_0^1 d\rho\rho^{i\omega}(1-\rho^2)[2\rho\zeta|\mathbf{k}_f - \mathbf{k}_i|^2 - \mu(\zeta - T_f)(\zeta - T_i)(1-\rho)^2]^{-2}, \qquad (5.13)$$

$$\omega = \alpha z_1 z_2 (2\zeta/\mu)^{-1/2}. \qquad (5.14)$$

The problem now at hand is to compute the limit of Eq. (5.9) explicitly.

The contribution to $(\psi, S\phi)$ corresponding to the first term on the right side of Eq. (5.12) is easily calculated to be

$$\lim_{\epsilon\to 0^+}\int d\mathbf{k}\,\tilde{\psi}^*(\mathbf{k})\tilde{\phi}(\mathbf{k})\Gamma(\gamma + 2i\alpha\eta(k))[\Gamma(\gamma)]^{-1}\exp[-2i\alpha\eta(k)\ln\epsilon]. \qquad (5.15)$$

It is straightforward to prove with a change of variables $|\mathbf{k}| \to \eta(k)$ and an application of the Riemann–Lebesgue lemma that the expression (5.15) is zero.

Equation (5.9) is therefore true with S_ϵ replaced by

$$S_\epsilon^{(1)}(\mathbf{k}_f, \mathbf{k}_i) = \frac{i\epsilon^\gamma (4T_f)^{i\eta_f}(4T_i)^{i\eta_i}}{2\Gamma(\gamma)\Gamma(1-\nu)}\int_0^\infty dy y^{-\nu} \times G_1([T_f + T_i + i\epsilon + iy]/2; \mathbf{k}_f, \mathbf{k}_i). \qquad (5.16)$$

A change of variables $\rho \to \sigma \equiv 2\rho^{1/2}(1-\rho)^{-1}$ in Eq. (5.13) and subsequent substitution of the result into Eq. (5.16) yields

$$S_\epsilon^{(1)} = -\frac{2i\epsilon^\gamma \alpha\mu z_1 z_2 (4T_f)^{i\alpha\eta_f}(4T_i)^{i\alpha\eta_i}}{\pi^2\Gamma(\gamma)\Gamma(1-\nu)}\int_0^\infty dy\int_0^\infty d\sigma P D^{-2}, \qquad (5.17)$$

where

$$P = \sigma y^{-\nu}(T_f + T_i + i\epsilon + iy)\left(\frac{\sigma}{1 + (1+\sigma^2)^{1/2}}\right)^{2i\omega_0}, \qquad (5.18)$$

$$D = \sigma^2|\mathbf{k}_f - \mathbf{k}_i|^2(T_f + T_i + i\epsilon + iy) + \mu[(T_f - T_i)^2 + (\epsilon + y)^2]. \qquad (5.19)$$

Here ν is defined by Eq. (5.11) and ω_0 is obtained by substituting $\zeta = (T_f + T_i + i\epsilon + iy)/2$ into Eq. (5.14).

As long as $\epsilon > 0$ the integrations over the variables $\mathbf{k}_f$, $\mathbf{k}_i$, y, and σ can be performed in any order. The proof of this relies on the estimates

$$|P| \le \sigma y^{-\gamma}|T_f + T_i + i\epsilon + iy| \qquad (5.20)$$

and

$$|D|^2 \ge \epsilon^4\mu^2 + y^4\mu^2 + \sigma^4|\mathbf{k}_f - \mathbf{k}_i|^4(T_f + T_i)^2. \qquad (5.21)$$

These inequalities follow from straightforward algebra and the observations that $\mathrm{Im}\,\omega_0 > 0$ and that both Re D and Im D are sums of strictly positive terms. It follows from Eqs. (5.20)–(5.21), the assumed properties of $\tilde{\psi}$ and $\tilde{\phi}$, and Tonelli's theorem that the multiple integration in Eqs. (5.9) and (5.17) is absolutely convergent and hence, by Fubini's theorem, can be evaluated with any order of integration.

Further, if $T_f \ne T_i$ the first term on the right side of Eq. (5.21) can be dropped. This permits the application of the Lebesgue dominated convergence theorem to prove that $S_\epsilon^{(1)}$ vanishes in the limit $\epsilon \to 0$ uniformly on compact subsets of the complement of the set $T_f = T_i$. One concludes, not surprisingly, that energy is roughly conserved and that only the region $T_f \approx T_i$ contributes to the integral in Eq. (5.9).

Assume, therefore, that $|T_f - T_i| \le \delta_0$, for some arbitrarily small but nonzero δ_0, for all $\mathbf{k}_f$ and $\mathbf{k}_i$ in the (compact) supports of $\tilde{\psi}$ and $\tilde{\phi}$, respectively. Let Q_ϵ denote the integral in Eq. (5.9) with S_ϵ replaced by the $S_\epsilon^{(1)}$ given in Eq. (5.17). Then, in terms of the variables $X \equiv (T_f, \mathbf{k}_f/|\mathbf{k}_f|, \mathbf{k}_i/|\mathbf{k}_i|)$ and $\delta \equiv T_f - T_i$ the integral Q_ϵ takes the form

$$Q_\epsilon = \epsilon^\gamma \int dX\int_0^\infty dy\int_0^\infty d\sigma\int_{-\delta_0}^{\delta_0} d\delta\, RPD^{-2}, \qquad (5.22)$$

where

$$R = R(X, \delta) = -\frac{4i\alpha\mu^4 z_1 z_2 (4T_f)^{i\alpha\eta_f}(4T_i)^{i\alpha\eta_i}}{\pi^2\Gamma(\gamma)\Gamma(1-\nu)} \times T_f^{1/2}(T_f - \delta)^{1/2}\tilde{\psi}^*\tilde{\phi}. \qquad (5.23)$$

The problem now is reduced to showing how the energy conservation delta function emerges from the integration with respect to δ.

For this purpose various estimates of the δ-dependence of the integrand are needed. Application of the mean value theorem of the differential calculus yields

$$R(X, \delta) = R(X, 0) + \delta R_\delta(X, \bar{\delta}), \qquad (5.24)$$

where $R_\delta = (\partial R/\partial\delta)$ and $0 < \bar{\delta} < \delta$. Because of the assumed properties of $\tilde{\psi}$ and $\tilde{\phi}$, the function R_δ has compact support and is bounded in that support. A similar expansion can be made for P,

$$P(X, \delta, y, \sigma) = P(X, 0, y, \sigma) + \delta P_\delta(X, \bar{\delta}, y, \sigma), \qquad (5.25)$$

with $P_\delta = (\partial P/\partial\delta)$ and $0 < \bar{\delta} < \delta$. A bound for P_δ is easily constructed from the equation

$$P^{-1}P_\delta = \frac{\partial}{\partial\delta}\ln P = -\frac{\partial\nu}{\partial\delta}\ln y - (2T_f - \delta + i\epsilon + iy)^{-1} + 2i\frac{\partial\omega_0}{\partial\delta}\ln\left(\frac{\sigma}{1 + (1+\sigma^2)^{1/2}}\right). \qquad (5.26)$$

The functions $(\partial\nu/\partial\delta)$, $(2T_f - \delta + i\epsilon + iy)^{-1}$, and $(\partial\omega_0/\partial\delta)$ are all bounded in the support of $\tilde{\psi}^*\tilde{\phi}$. One needs also the straightforward estimates

$$\left|\ln\left(\frac{\sigma}{1 + (1+\sigma^2)^{1/2}}\right)\right| \le \ln 3 + |\ln\sigma| \quad (0 < \epsilon < \infty), \qquad (5.27)$$

and

$$|2T_f - \delta + i\epsilon + iy| \le (\mathrm{const})(1+y) \quad (0 < \epsilon < 1), \qquad (5.28)$$

valid on the compact support of $\tilde{\psi}^*\tilde{\phi}$. These facts, together with Eq. (5.20), yield the estimate

$$|P_\delta| \le (\mathrm{const})\sigma y^{-\gamma}(1+y)[1 + |\ln y| + |\ln\sigma|]. \qquad (5.29)$$

The denominator function D must be estimated with more care. Let Δ denote

$$\Delta(X, \delta) \equiv |\mathbf{k}_f - \mathbf{k}_i|^2, \qquad (5.30)$$

and let D_0 be given by

$$D_0 \equiv \sigma^2\Delta(X, 0)(2T_f + i\epsilon + iy) + \mu[\delta^2 + (\epsilon + y)^2]. \qquad (5.31)$$

Then

$$D_0D^{-1}-1=$$

$$\sigma^2D^{-1}\{[\Delta(X,0)-\Delta(X,\delta)](2T_f+i\epsilon+iy)+\delta\Delta(X,\delta)\}. \quad (5.32)$$

Since Re D is a sum of positive terms, the estimate

$$|D|\geq\sigma^2|\Delta(X,\delta)|\,|2T_f-\delta_0+i\epsilon+iy| \quad (5.33)$$

holds. From Eqs. (5.32) and (5.33) it follows that

$$|D_0D^{-1}-1|\leq(\text{const})|\delta| \quad (5.34)$$

for (X,δ) in the support of $\tilde{\psi}^*\tilde{\phi}$ and for $y,\sigma>0$.

Let R_0 and P_0 denote $R(X,0)$ and $P(X,0,y,\sigma)$, respectively, and write the identity

$$RPD^{-2}-R_0P_0D_0^{-2}=D_0^{-2}\{D_0^2D^{-2}[(R-R_0)P+R_0(P-P_0)]+R_0P_0(D_0D^{-1}+1)(D_0D^{-1}-1)\}. \quad (5.35)$$

The boundedness of D_0D^{-1} and R_0 and the Eqs. (5.20), (5.24), (5.25), (5.28), (5.29), and (5.34) imply the inequality

$$|RPD^{-2}-R_0P_0D_0^{-2}|\leq(\text{const})|D_0|^{-2}|\delta|\sigma y^{-\gamma}(1+y)\times[1+|\ln y|+|\ln\sigma|], \quad (5.36)$$

valid for $y,\sigma>0$ and (X,δ) in the support of $\tilde{\psi}^*\tilde{\phi}$. Now substitute the estimate

$$|D_0|\geq\text{Re}\,D_0\geq(\text{const})(\sigma^2+y^2+\delta^2) \quad (5.37)$$

into the right side of Eq. (5.36) and integrate with respect to δ. The result is obviously integrable with respect to (X,σ,y) for all X in the support of $\tilde{\psi}^*\tilde{\phi}$ and all $y,\sigma>0$. By Tonelli's theorem the right side, and hence also the left side, of Eq. (5.36) is absolutely integrable for all ϵ, $0\leq\epsilon\leq1$. Furthermore, by Fubini's theorem, the integrations can be done in any order. It then follows that in the limit as $\epsilon\to0$ the integrand in Eq. (5.22) can be replaced by $R(X,0)P(X,0,y,\sigma)D_0^{-2}$.

The problem now is to calculate the integral

$$Q_\epsilon^{(0)}\equiv\epsilon^\gamma\int dX\int_0^\infty dy\int_0^\infty d\sigma\int_{-\delta_0}^{\delta_0}d\delta\,R(X,0)P(X,0,y,\sigma)D_0^{-2} \quad (5.38)$$

$$=\epsilon^\gamma\int dX\int_0^\infty dy\int_0^\infty d\sigma R(X,0)P(X,0,y,\sigma)\mu^{-2}\times\left[\frac{\delta_0}{D_1(\delta_0^2+D_1)}+\frac{D_1^{-3/2}}{(2i)}\ln\left(\frac{\sqrt{D_1}+i\delta_0}{\sqrt{D_1}-i\delta_0}\right)\right], \quad (5.39)$$

where

$$D_1=(\epsilon+y)^2+\mu^{-1}\sigma^2\Delta(X,0)(2T_f+i\epsilon+iy). \quad (5.40)$$

The principal sheet of the logarithm is assumed cut along the negative real axis. Using the bound

$$|D_1|\geq y^2+\frac{2T_f}{\mu}\Delta(X,0)\sigma^2, \quad (5.41)$$

one easily proves that the first term on the right side of Eq. (5.39) is absolutely integrable, with the estimate being independent of ϵ. Application of the Lebesgue dominated convergence theorem then shows that it does not contribute to the limit. It only remains to estimate the second term. Since Re $D_1>0$ for $\epsilon>0$ the log term in Eq. (5.39) is well defined and bounded. Since also

$$|D_1|^2\geq(\epsilon+y)^4+(\epsilon+y)^2\sigma^4\mu^{-2}\Delta^2(X,0), \quad (5.42)$$

one finds with the aid of Eqs. (5.20) and (5.28) that

$$|PD_1^{-3/2}|\leq(\text{const})\sigma y^{-\gamma}(1+y)(\epsilon+y)^{-3/2}[(\epsilon+y)^2+\sigma^4]^{-3/4}. \quad (5.43)$$

This inequality, the boundedness of $R(X,0)$ and the log term, and Tonelli's theorem imply that the second term of the integral of Eq. (5.39) is absolutely integrable with respect to all variables for all $\epsilon>0$. Make now the change of variables $\sigma\to\rho\equiv\epsilon^{-1}\sigma$, $y\to x\equiv\epsilon^{-1}y$. Then the second term on the right side of Eq. (5.39) becomes

$$\mu^{-2}\epsilon^\gamma\int dX\int_0^\infty dx\int_0^\infty d\rho R(X,0)\epsilon^{-\nu}x^{-\nu}\rho(2T_f+i\epsilon(1+x))\times\left(\frac{\epsilon\rho}{1+(1+\epsilon^2\rho^2)^{1/2}}\right)^{2i\omega_0}\frac{D_2^{-3/2}}{2i}\ln\left(\frac{\epsilon\sqrt{D_2}+i\delta_0}{\epsilon\sqrt{D_2}-i\delta_0}\right), \quad (5.44)$$

where

$$D_2=(1+x)^2+\mu^{-1}\rho^2\Delta(X,0)(2T_f+i\epsilon(1+x)). \quad (5.45)$$

The term in (5.44) proportional to $i\epsilon(1+x)$,

$$\mu^{-2}\tfrac{1}{2}\int dX\int_0^\infty dx\int_0^\infty d\rho\,R(X,0)\,\epsilon^{1+\gamma-\nu}x^{-\nu}\rho(1+x)\times\frac{\epsilon\rho}{1+(1+\epsilon^2\rho^2)^{1/2}}{}^{2i\omega_0}\,D_2^{-3/2}\ln\left(\frac{\epsilon\sqrt{D_2}+i\delta_0}{\epsilon\sqrt{D_2}-i\delta_0}\right), \quad (5.46)$$

also does not contribute in the limit $\epsilon\to0$. To see this, write the integral as

$$\int dX\int_0^\infty dx\,R(X,0)f_\epsilon(X,x), \quad (5.47)$$

where

$$f_\epsilon(X,x)=\epsilon^{1+\gamma-\nu}\mu^{-2}x^{-\nu}\frac{(1+x)}{2}\int_0^\infty d\rho\,\rho\left(\frac{\epsilon\rho}{1+(1+\epsilon^2\rho^2)^{1/2}}\right)^{2i\omega_0}\times D_2^{-3/2}\ln\left(\frac{\epsilon\sqrt{D_2}+i\delta_0}{\epsilon\sqrt{D_2}-i\delta_0}\right). \quad (5.48)$$

The integrand of Eq. (5.48) can be bounded by using the fact that the log term is bounded (even for $\epsilon=0$) and also the estimate

$$|D_2|\geq\text{Re}D_2\geq(\text{const})[(1+x)^2+\rho^2], \quad (5.49)$$

valid for X in the support of $R(X,0)$. Thus

$$|f_\epsilon|\leq(\text{const})\,\epsilon x^{-\gamma}(1+x)\int_0^\infty d\rho\,\rho[(1+x)^2+\rho^2]^{-3/2}\leq(\text{const})\,\epsilon x^{-\gamma}. \quad (5.50)$$

Thus, $f_\epsilon(X,x)\to0$ pointwise as $\epsilon\to0$. Since f_ϵ is absolutely integrable for $\epsilon>0$ [cf. remark following Eq. (5.43)] and approaches zero pointwise, the Lebesgue dominated convergence theorem would imply that the integral of Eq. (5.46) vanishes if some integrable bound for f_ϵ could be found that is independent of ϵ. This is provided by the inequality

$$|D_2|^2\geq(\text{const})[(1+x)^4+\epsilon^2\rho^4(1+x)^2], \quad (5.51)$$

valid for X in the support of $R(X,0)$, which leads to

$$|f_\epsilon|\leq(\text{const})\,\epsilon x^{-\gamma}(1+x)\int_0^\infty d\rho\,\rho[(1+x)^4+\epsilon^2\rho^4(1+x)^2]^{-3/4}\leq(\text{const})x^{-\gamma}(1+x)^{-1}. \quad (5.52)$$

The Lebesgue dominated convergence theorem thus applies, proving that the limit as $\epsilon\to0$ of the integral of Eq. (5.46) is zero.

Finally, consider the remaining term in (5.44),

$$\mu^{-2}\frac{\epsilon^{\gamma}}{i}\int dX\int_0^{\infty}dx\int_0^{\infty}d\rho$$
$$\times R(X,0)\epsilon^{-\nu}x^{-\nu}\rho T_f\left(\frac{\epsilon\rho}{1+(1+\epsilon^2\rho^2)^{1/2}}\right)^{2i\omega_0}$$
$$\times D_2^{-3/2}\ln\left(\frac{\epsilon\sqrt{D_2}+i\delta_0}{\epsilon\sqrt{D_2}-i\delta_0}\right). \qquad (5.53)$$

It is easy, using Eq. (5.49), to see that the Lebesgue dominated convergence theorem holds so that the limit as $\epsilon\to 0$ can be taken through the integrals in (5.53). In that limit, ω_0 approaches $\alpha\eta_f=\alpha\eta_i=(\nu-\gamma)/2$ and the log term approaches $i\pi$. The limit is

$$(\psi,S\phi)=\int dX\int_0^{\infty}dx\int_0^{\infty}d\rho\,\mu^{-2}\pi T_f R(X,0)x^{-\nu}\rho(\tfrac{1}{2}\rho)^{\nu-\gamma}$$
$$\times[(1+x)^2+2T_f\,\mu^{-1}\Delta(X,0)\rho^2]^{-3/2}, \qquad (5.54)$$

where now it is understood that $|\mathbf{k}_i|=|\mathbf{k}_f|$. This integral can actually be done. By making the change of variables $\rho\to\tilde{\rho}\equiv(1+x)[2T_f\mu^{-1}\Delta(X,0)]^{-1/2}\rho$ in Eq. (5.54) one obtains

$$(\psi,S\phi)=\int dXR(X,0)\mu^{-2}\pi T_f 2^{\gamma-\nu}\left(\frac{\mu}{2T_f\Delta(X,0)}\right)^{1+(\nu-\gamma)/2}$$
$$\times\int_0^{\infty}dx\,x^{-\nu}(1+x)^{-1+\nu-\gamma}\int_0^{\infty}d\tilde{\rho}\tilde{\rho}^{1+\nu-\gamma}(1+\tilde{\rho}^2)^{3/2} \qquad (5.55)$$

$$=\int dX\,R(X,0)\frac{\pi 2^{\gamma-\nu}}{2\Delta(X,0)\mu^2}\left(\frac{\mu}{2T_f\Delta(X,0)}\right)^{(\nu-\gamma)/2}$$
$$\times\left\{\frac{\Gamma(1-\nu)\Gamma(\gamma)}{\Gamma(1+\gamma-\nu)}\right\}\left\{\frac{\Gamma[1+(\nu-\gamma)/2]\Gamma[\frac{1}{2}-(\nu-\gamma)/2]}{2\Gamma(\frac{3}{2})}\right\}. \qquad (5.56)$$

Now recall the classical doubling formula [cf. Eq. (1.2(15)), page 5, of Ref. 34] for the gamma function,

$$\Gamma(2z)=\pi^{-1/2}2^{2z-1}\Gamma(z)\Gamma(z+\tfrac{1}{2}), \qquad (5.57)$$

and recall that $\Gamma(\frac{3}{2})=2^{-1}\pi^{1/2}$. Setting $z=(1+\gamma-\nu)/2$ in Eq. (5.57) and substituting the result into Eq. (5.56) yields

$$(\psi,S\phi)=\int dX\,R(X,0)\frac{\pi}{2\Delta(X,0)}\left(\frac{\mu}{2T_f\Delta(X,0)}\right)^{(\nu-\gamma)/2}$$
$$\times\frac{\Gamma(1-\nu)\Gamma(\gamma)\Gamma[1+(\nu-\gamma)/2]}{\mu^2\Gamma[1-(\nu-\gamma)/2]}. \qquad (5.58)$$

Substituting the definition of R into Eq. (5.58) and writing the result in terms of the original momentum variables yields the result

$$(\psi,S\phi)=\int d\mathbf{k}_f d\mathbf{k}_i\tilde{\psi}^*(\mathbf{k}_f)\tilde{\phi}(\mathbf{k}_i)\delta(T_f-T_i)f(\mathbf{k}_f,\mathbf{k}_i), \qquad (5.59)$$

which was to be proved.

Remarks: (1) The wave functions ϕ and ψ have been chosen to be of a type that are dense in the space of square integrable functions. Since S is bounded, extension of the left side of Eq. (5.59) to arbitrary square integrable functions is immediate. Extension of the right side would also be immediate were it not for the strong singularity of the function $f(\mathbf{k}_f,\mathbf{k}_i)$ when $\mathbf{k}_f=\mathbf{k}_i$. An extensive discussion of this problem has been given by *I*. Herbst.[29]

(2) In Theorem 2 an approximation $\delta_\epsilon(T_f-T_i)$ to the energy conservation delta function was introduced. This was done in analogy to short-range formulas. It is noteworthy that the function δ_ϵ does not appear in a natural way in the two-body calculation. Energy conservation is enforced in a far more subtle way by the function D_0 in Eq. (5.38). This leads one to suspect that exhibiting energy conservation via the function δ_ϵ may not be useful. One should look for alternative, more natural, ways of achieving that goal.

VI. DISCUSSION

In the foregoing sections the foundations of a time-independent multichannel scattering theory for nonrelativistic charged particle systems have been examined. An important feature of the theory is that the scattering operator is specified, not by the resolvent operator, but by a complex power of the resolvent operator. As a first step in development of the theory a generalized resolvent equation was developed to encompass these complex powers. This equation was shown to have a unique solution and to reduce to the usual resolvent equation in the absence of Coulomb potentials. Finally, the two-body problem was treated in the context of this formulation of scattering theory.

The objections to the present theory that were outlined in Sec. I are apparently circumvented by the theory of this paper.

For example, the channel operator F_β is multiplicative in the momentum space representation with the form [cf. Eq. (71) of Ref. 11]

$$F_\beta g(\mathbf{k}_1,\ldots,\mathbf{k}_n)\equiv f_\beta(\mathbf{k}_1,\ldots,\mathbf{k}_n)g(\mathbf{k}_1,\ldots,\mathbf{k}_n), \qquad (6.1)$$

where

$$f_\beta(\mathbf{k}_1,\ldots,\mathbf{k}_n)=\sum_{1\le r<s\le n}z_r z_s|(\mathbf{k}_r/m_r)-(\mathbf{k}_s/m_s)|^{-1}. \qquad (6.2)$$

Here it is assumed that there are n clusters in channel β with charge numbers z_r, masses m_r, and momenta $\mathbf{k}_r$. In this representation the differentials $dF_{\beta,\tau}$ are to be replaced by $\delta(\tau-f_\beta(\mathbf{k}_1,\ldots,\mathbf{k}_n))d\tau$, where $\delta(\cdot)$ is the Dirac delta function. The imaginary part of the complex power ν in Theorems 1 and 2 therefore consists of terms of the form αf_β, where α is the fine structure constant. As this is what is expected on the basis of relativistic theories,[13–15] the objection raised in this regard in Sec. I is apparently overcome.

In addition, none of the previously encountered divergences appeared in the two-body calculation of Sec. V. This can be directly attributed to the incorporation of complex powers of the resolvent into the theory. We conclude that previous difficulties[5,17–20] with the two-body problem are the result of studying the wrong operator!

The next step in the development of the theory is to write down equations of the Faddeev–Yakubovskiĭ type. The problem here is how to exhibit energy conservation, a matter of some subtlety as was pointed out in Sec. V. Research on this topic is in progress and will be the subject of a forthcoming paper.

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The maximal solvable subgroups of the $SU(p,q)$ groups and all subgroups of $SU(2,1)$*

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A general method is proposed for obtaining all conjugacy classes of maximal solvable subalgebras of an arbitrary semisimple Lie algebra over a zero characteristic field F. The method is applied to explicitly construct all $q+1$ maximal solvable subalgebras S_κ of the algebra of $SU(p,q)$ for $p \geq q > 0$ (over the field of real numbers). The dimension of S_κ for $0 \leq \kappa \leq q$ is $(2\kappa+1) \times (p+q-\kappa)-1$ and it contains $p+q-\kappa-1$ compact elements. The low-dimensional pseudounitary groups with $0 \leq p+q \leq 4$, $0 \leq q \leq p$ are considered in detail and different realizations of the maximal solvable subalgebras are presented. Finally, all subalgebras of the physically interesting algebra $SU(2,1)$ are found (not only the maximal solvable ones). The invariants of the subalgebras are found in all cases when they exist.

I. INTRODUCTION

In many applications of group theory and group representation theory in physics it is important to know all the subgroups of a given group, in particular to classify all possible chains of subgroups into equivalence classes with respect to inner automorphisms of the group itself.

There are several reasons for the interest in this problem. Thus, a typical situation is when a physical system has a certain symmetry, described by a group (e.g., a Lie group) G, then a further interaction is introduced, e.g., an external field, decreasing the symmetry to $G_0 \subset G$. A list of subgroups of G will thus provide a classification of possible breakings of the initial symmetry.

A further reason for the importance of subgroup chains is their connection to group representation theory and in particular to the choice of bases for representations of Lie groups. Thus a basis for the representations of a given Lie group G may be obtained by considering a complete set of commuting operators, containing all the Casimir operators of the group, some further operators from the algebra or enveloping algebra of G (and possibly some further operators like reflections, etc). The basis functions will be the common eigenfunctions of such a set of commuting operators and nonequivalent sets of operators lead to nonequivalent bases. In particular, if all the continuous operators in the set are chosen to be Casimir operators of G or its subgroups, then we obtain the most commonly used "subgroup type" bases. In the opposite case we obtain "nonsubgroup type" bases which are also of considerable physical interest,[1] but will not be discussed in this paper.

The wavefunctions (or state vectors) of quantum theory can very often be identified with basis vectors of the representations of a certain group, e.g., the Poincaré group[2] (inhomogeneous Lorentz group), the Galilei group,[3] the group $SU(3)$ (e.g., when considering internal symmetries of elementary particles[4] or the motion of nucleons in the average field of a nucleus[5]) or some other group. Different complete sets of commuting operators, determining the basis, correspond to the observability of different physical quantities (to the appearance of different quantum numbers, e.g., linear momentum versus angular momentum) and thus to different physical situations. Consider for example the group $SU(3)$. In elementary particle physics the important chain of subgroups is $SU(3) \supset S[U(2) \times U(1)] \supset U(1) \times U(1)$, where the $SU(2)$ subgroup is associated with isotopic spin. In nuclear physics, on the other hand, the important chain is $SU(3) \supset O(3) \supset O(2)$, where the group $O(3)$ is imbedded irreducibly into $SU(3)$ and corresponds to the angular momentum of the particles involved.

A very important application of group representation theory in physics is due to the fact that it is possible to expand physical quantities, e.g., scattering amplitudes in terms of the basis functions of representations of a given group. Thus, the group $O(3)$ provides the standard formulas of partial wave analysis, the group $O(2,1)$ underlies Regge pole theory,[6] etc. The homogeneous Lorentz group $O(3,1)$ has been used to provide two-variable expansions of relativistic scattering amplitudes,[7,8] the Galilei group to provide the same for nonrelativistic amplitudes.[9] The different subgroup reductions, corresponding to different bases, lead to expansions in terms of different special functions, each of which may be particularly appropriate in a definite physical situation. Thus, the reduction $O(3,1) \supset O(3) \supset O(2)$ leads to expansions that simplify specifically for low energy scattering; those corresponding to the reduction $O(3,1) \supset O(2,1) \supset O(2)$ simplify to the contrary for the limit of very high energies.[7]

The subgroup structure of the groups $O(3,1)$,[8,10] $E(3)$,[9] and their subgroups has been completely clarified. Some work has also been done on the subgroups of the Poincaré group[11] and $SU(2,1)$.[12] Dynkin[13] has solved the problem of finding all the semisimple subgroups of an arbitrary complex semisimple Lie group (see also Ref. 14). The case of real semisimple Lie algebras has also been treated.[15]

For physical applications one would like to know all subalgebras, not only the semisimple ones and particularly those with invariants; thus we attack the problem from the opposite end, namely find all the maximal solvable subalgebras of the algebra of $SU(p,q)$. The method is however directly applicable to the case of maximal solvable subalgabras of an arbitrary semisimple Lie algebra.

Let us finally mention that the $SU(p,q)$ groups and their algebras are of interest in physics for a multitude of reasons. Thus, $SU(1,1)$, being isomorphic to the three-dimensional Lorentz group $O(2,1)$, underlies Regge pole theory[6] and also figures in various models in elementary particle physics[16] and also in atomic physics.[17] The group $SU(2,1)$ can be used to provide crossing symmetric expansions of scattering amplitudes.[18] The group $SU(3,1)$ has been studied in various connections in elementary particle theory[19] and the group $SU(2,2)$ is of course of special importance, being locally isomorphic to the conformal group of space–time (for reviews see, e.g., Ref. 20). Higher groups, in particular $SU(6,6)$ have been studied[21] in attempts to combine intrinsic symmetries [like $SU(3)$] with the Lorentz group.

A complete classification of all subgroups of $SU(p,q)$ is thus of considerable interest. One-parameter subgroups (and the corresponding subalgebras) have already been classified.[22] The classification of maximal solvable subalgebras, given in this article, should together with the work on one-parameter subgroups and on semisimple subgroups considerably simplify the task of finding all subalgebras. In this article we do indeed list all subalgebras of $SU(2,1)$.

II. MAXIMAL SOLVABLE SUBGROUPS OF SEMISIMPLE GROUPS

A. Discussion of the problem of finding all classes of subgroups of a given Lie group

We consider the problem of classifying all chains of subgroups

$$G=G_0\supset G_1\supset G_2\supset\cdots\supset G_n=1 \tag{1}$$

(the G_i for $i=1,\ldots,n$ are continuous subgroups of the Lie group G) under the continuous automorphism group of G.

In terms of the Lie algebra $L=L(G)$ of the infinitesimal operators of G, the problem is to classify the chains

$$L=L_0\supset L_1\supset L_2\supset\cdots\supset L_n=0 \tag{2}$$

of properly descending subalgebras of L over the real number field R under the automorphism group $\mathrm{Aut}(L)$ of L over R.

In the final analysis one wants to represent the classes of conjugacy of the R-subalgebras of L under $\mathrm{Aut}(L)$ by a list of representatives.

In more general terms one wants to establish a list $\mathcal{L}(L,F)$ of the classes of conjugacy of a finite-dimensional Lie algebra L over a zero characteristic field F under the group of automorphisms $\mathrm{Aut}_F(L)$ of L over F.

By Levi's theorem[23] for every F-subalgebra S of L there exists a decomposition

$$S=R(S)\dotplus X \tag{3}$$

of S into the direct sum of the maximal solvable ideal $R(S)$ of S and a semisimple subalgebra X of S.

Moreover, assuming F to be the real number field, any two Levi decompositions (3) are conjugate under the group of automorphisms $\mathrm{Inn}(S,L)$ of L that is generated by the automorphisms

$$\exp[\mathrm{ad}_L(x)]:L\to L$$

$$\exp[\mathrm{ad}_L(x)]u=\sum_{j=0}^{\infty}\frac{\mathrm{ad}_L(x)^j}{j!}u\quad (x\in S,\ u\in L)$$

of L over R with the adjoint representation

$$\mathrm{ad}:L\to L$$

over R refined by Lie multiplication

$$\mathrm{ad}_L(x)u=[x,u]\quad (x\in L,\ u\in L).$$

According to Whitehead's proof, which later on was greatly simplified by various authors,[24] the task of performing a Levi decomposition (3) can be carried out by solving certain systems of inhomogeneous linear equations over F. In particular, for any given semisimple F-subalgebra Y of L, one can find a solution X containing Y.

In view of these facts our task can be broken up into the following four tasks.

(i) To represent the conjugacy classes of solvable subalgebras S_0 of L under $\mathrm{Aut}_F(L)$.

(ii) To determine the normalizer subalgebra

$$\mathrm{Nor}_L(S_0)=\{x\mid x\in L \text{ and } [x,S_0]\subseteq S_0\}$$

for any solvable F-subalgebra S_0 in L and to determine its maximal solvable ideal (radical) $R\,\mathrm{Nor}_L(S_0)$.

(iii) To perform a Levi decomposition of $\mathrm{Nor}_L(S_0)$:

$$\mathrm{Nor}_L(S_0)=R(\mathrm{Nor}_L(S_0))\dotplus Y.$$

(iv) To represent the conjugacy classes of the semisimple subalgebras of Y under the normal subgroup $\mathrm{Inn}(Y,Y)=\mathrm{Inn}(Y)$ (inner automorphism group) of the automorphism group of Y over R.

The task of determining the normalizer subalgebra $\mathrm{Nor}_L(S)$ of a subalgebra S reduces after extending an F basis $b_1,\ldots,b_\sigma$ of S to an F basis $b_1,\ldots,b_\tau$ of L to the task of finding a solution basis $\zeta_{\sigma+1,i},\ldots,\zeta_{\tau,i}$ $(1\leqslant i\leqslant\rho)$ of the system of linear homogeneous equations

$$\left[\left(\sum_{k=\sigma+1}^{\tau}\zeta_{k,i}b_k\right),b_j\right]\equiv 0 \pmod S,\quad i\leqslant j\leqslant\sigma,$$

inasmuch as the $\sigma+\rho$ elements $b_1,\ldots,b_\sigma$ and $\sum_{k=\sigma+1}^{\tau}\zeta_{k,i}b_k$ $(1\leqslant i\leqslant\rho)$ form an F basis of $\mathrm{Nor}_L(S)$.

The task of determining the Killing radical $KR(S)$ of the F-subalgebra S with F-basis $b_1,\ldots,b_\sigma$ and multiplication rule

$$[b_i,b_j]=\sum_{k=1}^{\sigma}Y_{ij}^{k}b_k\quad (Y_{ij}^k\in F)$$

reduces to the task of finding a solution basis $\eta_{1k},\ldots,\eta_{\sigma k}$ $(1\leqslant k\leqslant\rho')$ of the system of linear homogeneous equations

$$\sum_{i=1}^{\sigma}\sum_{j=1}^{\sigma}Y_{\alpha\beta}^{i}Y_{ij}\eta_j=0\quad (1\leqslant\alpha<\beta\leqslant\sigma)$$

with Killing constants

$$Y_{ij}=\sum_{\alpha=1}^{\sigma}\sum_{\beta=1}^{\sigma}Y_{\alpha i}^{\beta}Y_{\beta j}^{\alpha},$$

inasmuch as the elements $\sum_{i=1}^{\sigma}\eta_{ik}b_i$ $(1\leqslant k\leqslant\rho')$ form an F basis of $R(S)$. Similarly deal with centralizer, radical.

Regarding task (iv), we view it as an extension of the task of the ordinary representation theory of classical Lie algebra, which is simply the task of representing the classes of conjugacy under $\mathrm{Inn}DF^{f\times f}$ of the F-homomorphisms of a semisimple Lie algebra X of finite dimension over F in the simple matrix algebra $DF^{f\times f}$ formed by all matrices of degree f over F with vanishing trace. Progress has been made for $F=\mathbb{C}$. For the field of real numbers, we are still far away from a complete solution of task (iv), though we believe we know the methods to achieve it.

Task (i) of representing the conjugacy classes of solvable subalgabras can be reduced to the following steps.

(i.a) To represent the classes of conjugacy of the maximal solvable subalgebras of L under $\mathrm{Aut}_F(L)$.

(i.b) To represent the classes of solvable subalgebras S_0 of a maximal solvable subalgebra S of L under $\mathrm{Aut}_F(S,L)$, the stabilizer of S in $\mathrm{Aut}_F(L)$. Reduce to:

(i.b.a.) To represent the conjugacy classes of the F-subalgebras S_{00} of the radical $R(L)$ under $\mathrm{Aut}(R(L),L)$.

(i.b.b) To determine for a given F-subalgebra S_{00} of $R(L)$ the normalizer $\mathrm{Nor}_L(S_{00})$ and a representative set of the classes of conjugacy under $\mathrm{Aut}_F(\mathrm{Nor}_L(S_{00}),L)$ of those solvable subalgebras S_0 of $\mathrm{Nor}_L(S_{00})$ that intersect $R(L)$ in S_{00}.

In regard to (i.a) we remark that every maximal solvable F-subalgebra S of L contains the radical $R(L)$ of L and that for any Levi decomposition $L=R(L)\dotplus X$ of L there exists the decomposition $S=R(L)\dotplus(S\cap X)$ and vice versa ($S\cap X$ is a maximal solvable F-subalgebra of X).

Finally the following task remains:

(i.a.a) To form a representative set $MS(L)$ of the conjugacy classes under $\mathrm{Aut}_F(L)$ of the maximal solvable subalgebras of a finite-dimensional semisimple Lie algebra L over a field F of characteristic zero.

In view of the fact that L is the direct sum of its minimal ideals

$$L=\sum_{i=1}^{r}L_i,$$

where $L_1,\ldots,L_r$ are simple non-Abelian finite-dimensional Lie algebras over F and that a solvable F-subalgebra S of L is maximal solvable precisely if $S\cap L_i$ is a maximal solvable Lie subalgebra of L_i for $i=1,\ldots,r$ and $S=\sum_{i=1}^{r}S\cap L_i$, it follows that we need to solve task (i.a.a) only for simple non-Abelian Lie algebras of finite dimension over F.

Since for any solvable F-subalgebra S of L also the F-subalgebra of L generated by S and by the scalar ring

$$\mathcal{S}(L)=\{\sigma\,|\,\sigma\in\mathrm{End}(L)\ \&\ \forall x\ [x\in L\Rightarrow\sigma\,\mathrm{ad}_L(x)=\mathrm{ad}_L(x)\sigma]\}$$

is solvable, it suffices to deal only with the case in which L is centrally simple and finite dimensional over F. Hence

$$\mathcal{S}(L)=\{\lambda 1_L\,|\,\lambda\in F\}.$$

In this paper we develop a general method for solving the task (i.a.a) and apply it to the special case of the special pseudounitary Lie groups $SU(p,q)$. Note that $\mathcal{S}(L)$ is Abelian if L is semisimple.

B. General theorems on maximal solvable subgroups

We shall derive a theorem, stated precisely in the end of this section, giving a criterion for a subalgebra S of L to be maximal solvable. The theorem is stated in terms of a certain decreasing chain of linear subspaces, called a flag (defined below).

By Lie's theorem, for any finite-dimensional Lie algebra L over a zero characteristic field F and for any solvable F-subalgebra of L, the elements X of S for which the adjoint linear transformation $\mathrm{ad}_L(x)$ is nilpotent form a nilpotent ideal $N(S,L)$ of S with an Abelian factor algebra.

For any field extension E of F we obtain the extended Lie algebra

$$L\underset{F}{\otimes}E=EL=L_E$$

of L over E such that

$$N(S_E,L_E)=N(S,L)_E.$$

This is because of the linearity of the definition of $N(S,L)$.

The Killing ideal KR of L is defined as the radical of the Killing bilinear form on L. Since the Killing bilinear form on L stays invariant under field extension, the same is true for the Killing radical:

$$KR(L_E)=KR(L)_E.$$

For any ideal X of L also the radical ideal $R(X)$ of X is an ideal of L (*N.B.*: only for characteristic zero!).

Because of linearity the normalizer concept is invariant under field extension, in other words for any F-subalgebra S of L we have

$$\mathrm{Nor}_{L_E}(S_E)=(\mathrm{Nor}_L(S))_E.$$

The centralizer of S in L is the ideal

$$Z_L(S)=\{x\,|\,x\in L\ \&\ [x,S]=0\}$$

of $\mathrm{Nor}_L(S)$. Again we have the invariance

$$Z_{L_E}(S_E)=(Z_L(S))_E.$$

The intersection, sum and product of ideals are also invariant under extension, in particular the center of S defined as $z(S)=Z_L(S)\cap S$ and the derived algebra $DS=[S,S]$, also $R(L)/KR(L)=z(L/KR(L))$ and $R(L)$.

A solvable F-subalgebra S of L is said to be of *maximal type* if

$$S\supseteq R(\mathrm{Nor}_L(N(S,L))).$$

This concept is invariant under field extension. For any solvable subalgebra S of L we have

$$[S,R(\mathrm{Nor}_L(N(S,L)))]\subseteq R(\mathrm{Nor}_L(N(S,L))),$$

and hence $S+R(\mathrm{Nor}_L(N(S,L)))$ is solvable. An invariant embedding of S into another solvable F-algebra is obtained in this way, such that the new solvable subalgebra coincides with S precisely if S is of maximal type.

For any solvable F-subalgebra S of L the factor algebra $\mathrm{Nor}_L(N(S,L))$ over its radical is semisimple so that there is a Levi decomposition

$$\mathrm{Nor}_L(N(S,L)) = R(\mathrm{Nor}_L(N(S,L))) \dot{+} X,$$

where X is a semisimple F-subalgebra X of $\mathrm{Nor}_L(N(S,L))$.

Supposing now that S is of maximal type, then we have

$$N(S,L) \subseteq R(\mathrm{Nor}_L(N(S,L))) \subseteq S \subseteq \mathrm{Nor}_L(N(S,L))$$

so that it follows that

$$N(R(\mathrm{Nor}_L(N(S,L))),L) = N(S,L),$$
$$S = R(\mathrm{Nor}_L(N(S,L))) \dot{+} S \cap X, \tag{4}$$

$S \cap X$ is Abelian, and $N(S\cap X, L) = 0$.

Note that the nilpotency of $\mathrm{ad}_X(x)$ for some element x of the semisimple Lie algebra X implies the nilpotency of $\Delta(x)$ for any representation Δ of X in a ring of matrices over F (or an extension of F). Conversely, if for some faithful matrix representation Δ of X over F or an extension of F the matrix $\Delta(x)$ is nilpotent, then $\mathrm{ad}_X(x)$ is nilpotent, also ad_L is nilpotent.

Hence in particular

$$N(S\cap X, L) = N(S \cap X, X) = 0. \tag{5}$$

If S is a maximal solvable subalgebra of L, then $S\cap X$ is a maximal solvable subalgebra of X. Because of (5) we find that $S \cap X$ is a Cartan subalgebra.

An element x of a semisimple Lie algebra X of finite dimension over F is said to be compact if it is contained in a Cartan subalgebra of L that is a maximal solvable subalgebra. A Cartan subalgebra H of L consists only of compact elements precisely if H is a maximal solvable subalgebra of L. This is due to the existence of elements of H which belong only to one Cartan subalgebra (regular elements).

The Cartan subalgebra H of a finite-dimensional semisimple Lie algebra over the real number field is compact precisely if all roots are purely imaginary on H. Indeed, if for some element x of H one of the roots would not be purely imaginary, then among the roots of H there is one, say α, for which the real part of $x\alpha$ would be maximal and positive. If α is real on H, then the sum of the root space of α and of H is a solvable subalgebra of X larger than H, which is a contradiction. Hence α is not real on H which means that the complex conjugate α^* of α is a root distinct from α and that there is a two-dimensional linear subspace M of X, intersecting H in zero and invariant under H with roots α and α^*. In view of the maximal property of H we find that $[M,M]=0$ so that again $M+H$ is a solvable subalgebra of X larger than M, which is a contradiction.

Our concept of compactness finds its justification by the remark that a Cartan subalgebra H of X is compact precisely if the set of linear transformations $\exp \mathrm{ad}(x)$ $(x\in H)$ is compact in the standard topologization of $\mathrm{End}_{\mathcal{R}} X$.

We note that an element of a finite-dimensional semisimple Lie algebra X over the complex number field is compact precisely if X vanishes. Hence a solvable subalgebra S of a Lie algebra L over the complex number field (or any algebraically closed field of zero characteristic) is maximal solvable precisely if it coincides with the radical of $\mathrm{Nor}_L(N(S,L))$.

Without proof we mention that all maximal solvable subalgebras of L are conjugate under $\mathrm{Inn}(L)$ and also that any two compact Cartan subalgebras of a semisimple Lie algebra L of finite dimension over $\mathcal{R}$ are conjugate under $\mathrm{Inn}(L)$.

We continue the study of a solvable subalgebra S of maximal type of finite-dimensional semisimple Lie algebra L over a zero characteristic field F, using some faithful representation space M of L of finite dimension over F or over some extension of F (e.g., for the adjoint representation we have $M=L$). Again we note that the application of an element of L to M is nilpotent if and only if its adjoint representation is nilpotent.

Using this remark, we associate with S a properly decreasing set of linear subspaces $M_0 = M$, $M_{i+1} = N(S,L)M_i$,

$$M = M_0 \supset M_1 \supset \cdots \supset M_r = 0,$$

called a flag.

The flag normalizer in L is defined as

$$\overline{\mathrm{Nor}}_L = \mathrm{Nor}_L(M_0, \ldots, M_r) = \{x \mid x\in L \,\&\, xM_i \subseteq M_i \quad (0 \le i \le r)\}.$$

The flag centralizer in L is defined as

$$\overline{Z}_L = Z_L(M_0,\ldots,M_r) = \{y \mid y \in L \,\&\, yM_i \subseteq M_{i+1} \quad (0 \le i < r)\}.$$

Both subsets are subalgebras of L such that $\overline{Z}_L = N(\overline{Z}_L, L)$ is an ideal of $\overline{\mathrm{Nor}}_L$.

Moreover, for the particular flag associated with S we find that $N(S,L)\subseteq \overline{Z}_L$, $S \subseteq \overline{\mathrm{Nor}}_L$, and $\overline{Z}_L \cap \mathrm{Nor}_L(N(S,L))$ is an ideal of $\mathrm{Nor}_L(N(S,L))$, contained in the radical of $\mathrm{Nor}_L(N(S,L))$. Since S is of maximal type, it follows that $\overline{Z}_L \cap \mathrm{Nor}_L(N(S,L))$

$$N(S,L) \subseteq \overline{Z}_L \cap \mathrm{Nor}_L(N(S,L)) \subseteq N(S,L),$$

$$\overline{Z}_L \cap \mathrm{Nor}_L(N(S,L)) = N(S,L).$$

However, the normalizer of a proper subalgebra of any nilpotent Lie algebra is always larger than the proper subalgebra itself.

Hence

$$N(S,L) = Z_L(M_0, M_1, \ldots, M_r) = \overline{Z}_L. \tag{6}$$

The flag factors M_{i-1}/M_i define representations Δ_i of $\mathrm{Nor}_L(M_0,\ldots,M_r) = \overline{\mathrm{Nor}}_L$ over F (or an extension of F) by setting

$$\Delta_i(x)(u/M_i) = xu/M_i$$

for u of M_{i-1} and x of $\overline{\mathrm{Nor}}_L$ $(i=1,2,\ldots,r)$. The representation Δ_i maps the radical of $\overline{\mathrm{Nor}}_L$ onto the radical of $\Delta_i(\overline{\mathrm{Nor}}_L)$ as is well known from the representation theory of Lie algebras of zero characteristic.

Hence

$$\overline{Z}_L \subseteq R(\overline{\mathrm{Nor}}_L)$$

$$= \{x \mid x \in \overline{\mathrm{Nor}}_L \,\&\, \Delta_i(x) \in R(\Delta_i(\overline{\mathrm{Nor}}_L)), \quad (1 \le i \le r)\}.$$

Asuming now that S is a maximal solvable subalgebra of L it follows that S contains $R(\overline{\mathrm{Nor}_L})$ as an ideal. Moreover, from the general representation theory for zero characteristic fields we know that

$$[\overline{\mathrm{Nor}_L},\ R(\overline{\mathrm{Nor}_L})]\subseteq N(\overline{\mathrm{Nor}_L},\ L).$$

Since $R(\overline{\mathrm{Nor}_L})$ is contained in S, it follows that $[\overline{\mathrm{Nor}_L},\ R(\overline{\mathrm{Nor}_L})]$ belongs to S and hence

$$[\overline{\mathrm{Nor}_L},\ R(\overline{\mathrm{Nor}_L})]\subseteq N(S,L)=\overline{Z}_L,$$

$$\Delta_i([\overline{\mathrm{Nor}_L},\ R(\overline{\mathrm{Nor}_L})])=[\Delta_i(\overline{\mathrm{Nor}_L}),\ R(\Delta_i(\overline{\mathrm{Nor}_L}))]=0$$

$$(1\leqslant i\leqslant r).$$

It follows that the Lie algebras $\Delta_i(\overline{\mathrm{Nor}_L})$ are the direct sum of the center and the derived algebra.

Hence the center z of $\Delta_i(\overline{\mathrm{Nor}_L})$ satisfies

$$z(\Delta_i(\overline{\mathrm{Nor}_L}))=R(\Delta_i(\overline{\mathrm{Nor}_L})). \tag{7}$$

Using the Levi decomposition

$$\overline{\mathrm{Nor}_L}=R(\overline{\mathrm{Nor}_L})\dot{+}Y, \tag{8}$$

we find that

$$S=R(\overline{\mathrm{Nor}_L})\dot{+}S\cap Y, \tag{9}$$

where $S\cap Y$ is a compact Cartan subalgebra of Y.

Conversely, let us assume that for the solvable subalgebra S of L we have (6)–(9), where $S\cap Y$ is a compact Cartan subalgebra of the semisimple subalgebra Y of L. For any solvable subalgebra S_1 of L properly containing S we either have

$$N(S,L)\subset N(S_1,L),\quad N(S,L)\subset \mathrm{Nor}_{N(S_1,L)}(N(S,L)),$$

$$\mathrm{Nor}_{N(S_1,L)}(N(S,L))\subseteq \overline{Z}_L,$$

which is a contradiction, or

$$N(S,L)=N(S_1,L),\quad S\subset S_1,\quad S_1\subseteq\overline{\mathrm{Nor}_L}.$$

However, according to (6)–(9), S is already a maximal solvable subalgebra of $\overline{\mathrm{Nor}_L}$ and we again have a contradiction.

It follows that S is a maximal solvable subalgebra of L. We have thus established the following theorem.

Theorem: A solvable subalgebra S of a semisimple Lie algebra L of finite dimension over a zero characteristic field F is maximal solvable precisely if for a given faithful representation space M of finite dimension over F (or an extension of F) the conditions (6)–(9) are satisfied by the flag associated with M under S and its centralizer and normalizer under L [note that $S\cap Y$ is a compact Cartan subalgebra of the semisimple Lie algebra Y as is mentioned after Eq. (9)].

The proof of the above theorem also yields the following result.

Corollary: Every nonzero solvable subalgebra S of a semisimple Lie algebra L of finite dimension over the field F of characteristic zero determines a maximal solvable subalgebra S^* of L containing S as follows. If $S\subset S+R(\mathrm{Nor}_L N(S,L))$, then set $S^*=(S+\mathrm{Nor}_L N(S,L))^*$. If $R(\mathrm{Nor}_L(N(S,L)))\subseteq S$, then let S_1 be a maximal solvable subalgebra of $\mathrm{Nor}_L(S)\cap \mathrm{Nor}_L(N(S,L))$ containing S and set $S^*=S_1^*$.

C. Application to the $SU(p,q)$ Lie groups

Let us now pursue the case when $F=R$ is the field of real numbers and

$$L=LSU(p,q)$$
$$=\{x\,|\,x\in C^{(p+q)\times(p+q)}\ \&\ x^+(I_p\oplus -I_q)+(I_p\oplus -I_q)x=0_{p+q},$$
$$p\geqslant q\geqslant 0\},$$

(where I_p is the unit matrix of dimension p and x^+ is the matrix Hermitian conjugate to x).

In this case the complexification of L is the simple algebra $LSL(p+q,C)=DC^{(p+q)\times(p+q)}$ of dimension $(p+q)^2-1$ over the field of complex numbers C.

The maximal solvable subalgebras of L_C over C are known to be conjugate under $\mathrm{Inn}(SL(n,C))$ to the rings of matrices $LST(p+q,C)$ formed by the upper triangular matrices of degree $p+q$ and zero trace over C [Borel subalgebras of $LSL(p+q,C)$].

We want to determine the maximal solvable R-subalgebras of $L=LSU(p,q)$ under $\mathrm{Inn}(L)$. We use the faithful representation space $M=C^{(p+q)\times 1}$ of L over the extension C of R that is formed by the $(p+q)$-columns over C.

After a suitable Hermitian equivalence transformation of $I_p\oplus -I_q$ to an Hermitian symmetric nonsingular matrix D, the R-algebra $N(S,L)$ is contained in the upper triangular nilpotent algebra

$$DLT(p+q,C)$$
$$=\{y\,|\,y=(y_{ik})\in C^{(p+q)\times(p+q)}\ \&\ y_{ik}=0 \text{ if } i\geqslant k\}$$

so that we have

$$N(S,L)\subseteq N(f_1,\ldots,f_s;C)$$
$$=\{Y=(Y_{ik})\ \&\ Y_{ik}\in C^{f_i\times f_k}\ \&\ Y_{ik}=0_{f_i\times f_k}$$
$$\text{if } i\geqslant k,\ i,k=1,2,\ldots,s;$$
$$s,f_1,\ldots,f_s \text{ are natural numbers satisfying}$$
$$f_1+f_2+\cdots+f_s=p+q\},$$

such that the linear subspaces

$$M_i=\dot{\sum} C\, c^{(p+q)\times 1}_{f_1+\cdots+f_{i-1}+j},\quad 1\leqslant j\leqslant p+q-(f_1+\cdots+f_{i-1})$$

(note that $c_k^{n\times 1}$ denotes the kth unit column) of the $(p+q)$-column space $C^{(p+q)\times 1}$ over C are characterized by the property that

$$M_{i+1}=N(S,L)M_i\quad (0\leqslant i<s).$$

Hence

$$M_0=C^{(p+q)\times 1}\supset M_1\supset\cdots\supset M_s=0,$$

$$\mathrm{Nor}_L(N(S,L))M_i\subset M_i,$$

$$\mathrm{Nor}_L(N(S,L))\cap N(R(\mathrm{Nor}_L(N(S,L))),L).$$

Because of the nilpotency of $N(f_1,\ldots,f_s;C)$ and the maximal property of S it follows that

$$CN(S,L)=N(R(\mathrm{Nor}_{CL}(CS,CL)),CL)=N(f_1,\ldots,f_s;C),$$

$$X=\dot{\sum_{f_j>1}} X_j,$$

where X_j is a simple R-algebra for which

$CX_j = \{(x_{ik}) \mid x_{ik} = 0_{f_i \times f_k}$ if $i \neq j$ or $k \neq j$ and
x_{ik} = element of $DLC^{f_j \times f_j}$ if $i = k = j\}$,
$D = (D_{ik}), \quad D_{ik} \in C^{f_i \times f_k}$.

Since

$$x^+ D + Dx = 0$$

for x of X_j, it follows that $D_{ik} = 0$ if $i \neq k$ and either $f_i > 1$ or $f_k > 1$.

Furthermore, because of the nonsingularity of D it follows that the matrices D_{jj} are nonsingular if $f_j > 1$. Also, D_{jj} is Hermitian symmetric.

The matrix

$$D_0 = (D_{ik} \mid f_i = 1 \,\&\, f_k = 1)$$

is also nonsingular, Hermitian symmetric and subject to the condition

$$x_0^+ D_0 + D_0 x_0 = 0$$

for $x_0 = (x_{ik} \mid f_i = f_k = 1 \,\&\, x = (x_{\alpha\beta}) \in N(S, L))$.

Since the complexification of the R-Lie-algebra formed by all matrices x_0 is the full upper triangular nilalgebra of the corresponding degree, it follows that after a suitable transformation of S by an upper triangular matrix we shall have

$$D_0 = \begin{bmatrix} & & & & & 1 \\ & & & & 1 & \\ & & & \cdot & & \\ & & \cdot & & & \\ & \cdot & & & & \\ & 1 & & & & \\ 1 & & & & & \end{bmatrix}.$$

In view of the fact that the complexification of $N(S, L)$ is $N(f_1, \ldots, f_s; C)$ and that $x^+ D + Dx = 0$ for all x of $N(S, L)$, it follows that

(a) There are no two distinct indices j with $f_j > 1$.

(b) If $f_j > 1$, then the number of f_i's with $i < j$ is equal to the number of f_i's with $i > j$.

Since it is our aim to establish a list of representatives of certain classes of subalgebras of $LSU(p, q)$ conjugate under transformations by elements of $SU(p, q)$ it is permissible to transform the Lie algebra $LSU(p, q)$ itself by some nonsingular matrix.

Thus, in order to obtain all nonconjugate [under $SU(p, q)$] maximal solvable subalgebras of the Lie algebra $LSU(p, q)$ with $p \geq q \geq 0$ it is convenient to utilize the $q+1$ distinct realizations of this algebra that are formed by the matrices X of degree $p+q$ over C satisfying

$$X^+ D_\kappa + D_\kappa X = 0, \quad \kappa = 0, 1, \ldots, q, \tag{10}$$

where

$$D_0 = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}, \quad D_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & I_{p-1} & 0 & 0 \\ 0 & 0 & -I_{q-1} & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix},$$

$$D_\kappa = \begin{bmatrix} 0 & 0 & 0 & H_\kappa \\ 0 & I_{p-\kappa} & 0 & 0 \\ 0 & 0 & -I_{q-\kappa} & 0 \\ H_\kappa & 0 & 0 & 0 \end{bmatrix} \tag{11}$$

and where I_s is the identity matrix of degree s and H_r is the r-dimensional matrix of the type

$$H_r = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 1 & 0 \\ \cdot & \cdot & \cdots & \cdot & \cdot \\ 1 & 0 & \cdots & 0 & 0 \end{bmatrix}$$

(note that the zeros in D_κ are in general square or rectangular matrices with all elements equal to zero).

We then require that the matrices X satisfying (10) leave the flag of the $p+q$ subspaces $\sum_{h=1}^{j} Cc_h^{(p+q)\times 1}$ $(1 \leq j \leq p+q)$, i.e.,

$$C^{(p+q)\times 1} \supset \sum_{h=1}^{p+q-1} Cc_h^{(p+q)\times 1} \supset \cdots \supset Cc_1^{(p+q)\times 1} \supset 0, \tag{12}$$

invariant.

In this manner we obtain the following $q+1$ distinct maximal solvable subalgebras S_κ of the Lie algebra $LSU(p, q)$ [and any other maximal solvable subalgebra is conjugate to precisely one of these under $SU(p, q)$]:

1. S_0 is compact, has the R-dimension $p+q-1$ and consists of the $(p+q)$-dimensional diagonal matrices

$$S_0 = \begin{pmatrix} i\lambda_1 & & & & \\ & i\lambda_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & i\lambda_{p+q} \end{pmatrix}, \quad \lambda_j = \text{real},$$

$$\lambda_1 + \lambda_2 + \cdots + \lambda_{p+q} = 0, \tag{13}$$

and D_κ is D_0.

We have

$$\dim S_0 = p+q-1, \quad N_0 = p+q-1 \tag{14}$$

(where N_κ is the number of compact elements in S_κ).

2. S_q in the case when $p = q$ or $p = q+1$ is of special interest since its complexification coincides with a Borel subalgebra of $LSL(p+q, C)$. In this case we have $D_q = H_q$.

For $p=q$ we have

$$S_q=\begin{pmatrix} r_1+is_1, & \alpha_{12} & ,\alpha_{13} & & & & \alpha_{1\,2q-1}, & ia_1 \\ 0 & ,r_2+is_2, & \alpha_{23}, & & & & ia_2, & -\alpha^*_{1\ 2q-1} \\ & & \ddots & & & \cdot^{\cdot^{\cdot}} & & \\ & & & r_q+is_q, & ia_q & & & \\ & & & 0 & ,-r_q+is_q & & & \\ & & & & & \ddots & & \\ 0 & & & & & -r_3+is_3, & -\alpha^*_{23} & ,-\alpha^*_{13} \\ & & & & & 0 & ,-r_2+is_2, & -\alpha^*_{12} \\ & & & & & 0 & ,\quad 0 & ,-r_1+is_1 \end{pmatrix} \qquad (15a)$$

with $s_1+s_2+\cdots+s_2=0$.

For $p=q+1$ we have

$$S_q=\begin{pmatrix} r_1+is_1, & \alpha_{12} & ,\alpha_{13} & & & & & \alpha_{1\,2q}, & ia_1 \\ 0 & ,r_2+is_2, & \alpha_{23} & & & & & ia_2 & ,-\alpha^*_{1\,2q} \\ & & \ddots & & & & \cdot^{\cdot^{\cdot}} & & \\ & & & r_q+is_q, & \alpha_{q,q+1}, & ia_q & & & \\ & & & 0 & ,ia_{q+1} & ,-\alpha^*_{q,q+1} & & & \\ & & & 0 & ,\ 0 & ,-r_q+is_q & & & \\ & & & & & & \ddots & & \\ 0 & & & & & & -r_3+is_3, & -\alpha^*_{23} & ,-\alpha^*_{13} \\ & & & & & & 0 & ,-r_2+is_2, & -\alpha^*_{12} \\ & & & & & & 0 & ,\quad 0 & ,-r_1+is_1 \end{pmatrix} \qquad (15b)$$

with $2(s_1+s_2+\cdots+s_q)+a_{q+1}=0$ (here and below Latin letters correspond to real numbers and Greek ones to complex numbers).

The dimensions of the maximal solvable algebra and its compact (and Abelian) subalgebra in this case are

$$\dim S_q=\tfrac{1}{2}(p+q)(p+q+1)-1,\quad N_q=p-1. \qquad (16)$$

3. S_κ for $0<\kappa\leq q$ in the case when the complex extension of S_κ is not a Borel subalgebra of $SL(p+q,C)$ and S_κ not compact. The matrix D_κ has the general form, given in (11). In this case we have

$$S_\kappa=\begin{pmatrix} S_{11} & S_{12} & S_{13} \\ 0 & S_{22} & S_{23} \\ 0 & 0 & S_{33} \end{pmatrix} \qquad (17)$$

with

$$S_{11}=\begin{pmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1\kappa} \\ 0 & \alpha_{22} & \cdots & \alpha_{2\kappa} \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & \alpha_{\kappa\kappa} \end{pmatrix},$$

$$S_{22}=\begin{pmatrix} ia_{\kappa+1} & & 0 \\ & \ddots & \\ 0 & & ia_{p+q-\kappa} \end{pmatrix},$$

$$S_{12}=\begin{pmatrix} \alpha_{1\,\kappa+1}, & \ldots, & \alpha_{1\,p+q-\kappa} \\ \alpha_{\kappa\,\kappa+1}, & \ldots, & \alpha_{\kappa\,p+q-\kappa} \end{pmatrix}$$

$$S_{13}=\begin{pmatrix} \alpha_{1\,p+q-\kappa+1}, & \ldots, & \alpha_{1\,p+q-1} & ,ib_1 \\ \alpha_{2\,p+q-\kappa+1}, & \ldots, & ib_2 & ,-\alpha^*_{1\,p+q-1} \\ \cdots & \cdots & \cdots & \cdots \\ ib_\kappa, & \ldots\ldots, & -\alpha^*_{2\,p+q-\kappa+1}, & -\alpha^*_{1\,p+q-\kappa+1} \end{pmatrix}$$

$$S_{23}=-D_\kappa^{-1}S_{12}^+H_\kappa,\quad D_\kappa=\begin{pmatrix} I_{p-\kappa} & 0 \\ 0 & -I_{q-\kappa} \end{pmatrix}$$

$$S_{33}=-H_\kappa^{-1}S_{11}^+H_\kappa, \quad (S_{13}^+H_\kappa+H_\kappa S_{13}=0)$$

with $2\,\mathrm{Im}(\alpha_{11}+\alpha_{22}+\cdots+\alpha_{\kappa\kappa})+a_{\kappa+1}+\cdots+a_{p+q-\kappa}=0$.

The dimensions of S_κ and their maximal compact subalgebras are

$$\dim S_\kappa=(2\kappa+1)(p+q-\kappa)-1, \quad N_\kappa=p+q-\kappa-1. \tag{18}$$

In the following section we shall consider specific examples in detail.

III. MAXIMAL SOLVABLE SUBGROUPS OF LOW DIMENSIONAL PSEUDOUNITARY GROUPS

Let us now specify the results of the previous section for the cases of greatest physical interest, when $p\geq q\geq 1$, $p+q\leq 4$. We shall make use of the results summarized in Eqs. (10)–(18).

A. The group $SU(1,1)$

We have two possible realizations, corresponding to

$$D_0=\begin{pmatrix}1&0\\0&-1\end{pmatrix} \quad\text{and}\quad D_1=\begin{pmatrix}0&1\\1&0\end{pmatrix}.$$

It is easy to see that Eq. (10) implies

$$X_0=\begin{pmatrix}ia&\alpha\\\alpha^*&-ia\end{pmatrix} \text{ and } X_1=\begin{pmatrix}c&ib\\id&-c\end{pmatrix},$$

respectively, where Latin letters correspond to real numbers and Greek letters to complex ones. The unitary matrix Z transforming one realization into the other

$$ZX_1Z^{-1}=X_0 \tag{19}$$

can be chosen to be

$$Z=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\-1&1\end{pmatrix}.$$

The flag determining the two different maximal solvable subalgebras consists of the subspaces

$$\begin{pmatrix}1\\0\end{pmatrix} \text{ and } \left\{\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix}\right\}.$$

Indeed the condition

$$X_\kappa\begin{pmatrix}1\\0\end{pmatrix}=\omega\begin{pmatrix}1\\0\end{pmatrix}, \quad \kappa=0,\ 1,$$

implies $\beta=0$ or $d=0$, respectively (ω is an arbitrary complex number). Thus, we obtain two maximal solvable subalgebras

$$S_0=\begin{pmatrix}ia&0\\0&-ia\end{pmatrix}, \quad S_1=\begin{pmatrix}c&ib\\0&-c\end{pmatrix}.$$

Clearly the subgroup generated by the one-parameter subalgebra S_0 is the group of rotations $O(2)$. The two parameter subalgebra S_1 generates the group of translations and dilatations of a straight line. The algebra S_0 contains (consists of) one compact element, the algebra S_1 contains none.

The usual physical notations correspond to the invariant form determined by D_0. The generators are denoted

$$K_1=\tfrac{1}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}, \quad K_2=\tfrac{1}{2}\begin{pmatrix}0&i\\-i&0\end{pmatrix}, \quad L_3=\tfrac{1}{2}\begin{pmatrix}i&0\\0&-i\end{pmatrix}. \tag{20}$$

The subalgebra S_0 then corresponds to L_3, S_1 to $\{K_1,\ L_3+K_2\}$.

B. The group $SU(2,1)$

Again we have only two possible realizations of the invariant form, corresponding to

$$D_0=\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix} \text{ and } D_1=\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix},$$

so that the general element of the algebra can be written as

$$X_0=\begin{pmatrix}ia&\alpha&\beta\\-\alpha^*&ib&\gamma\\\beta^*&\gamma^*&-i(a+b)\end{pmatrix} \text{ or } X_1=\begin{pmatrix}b-\frac{1}{2}ic&\delta&id\\\epsilon&ic&-\delta^*\\ie&-\epsilon^*&-b-\frac{1}{2}ic\end{pmatrix}, \tag{21}$$

respectively. The operator Z transforming X_1 into X_0 as in (19) can be chosen in the form

$$Z=\begin{pmatrix}1/\sqrt{2}&0&1/\sqrt{2}\\0&1&0\\-1/\sqrt{2}&0&1/\sqrt{2}\end{pmatrix}. \tag{22}$$

Introduce the three vectors

$$e_1=\begin{pmatrix}1\\0\\0\end{pmatrix}, \quad e_2=\begin{pmatrix}0\\1\\0\end{pmatrix}, \quad e_3=\begin{pmatrix}0\\0\\1\end{pmatrix}. \tag{23}$$

We impose the condition $X_\kappa e_1=\omega e_1$ (the second flag condition $X_\kappa e_2=\omega_1e_1+\omega_2e_2$ is satisfied automatically) and find the maximal solvable subalgebras:

$$S_0=\begin{pmatrix}ia&0&0\\0&ib&0\\0&0&-i(a+b)\end{pmatrix} \text{ and } \tilde{S}_1=\begin{pmatrix}b-\frac{1}{2}ic&\delta&id\\0&ic&-\delta^*\\0&0&-b-\frac{1}{2}ic\end{pmatrix}. \tag{24}$$

The algebra S_0 contains two independent compact elements, $\tilde{S}_1$ has dimension five but contains only one compact element obtained by putting $b=d=\delta=0$. The five-dimensional solvable algebra could of course also have been obtained using the other realization of $SU(2,1)$. The invariance of the vector space determined by the vector e_1 must then be replaced by the invariance of the space $Ze_1=(1/\sqrt{2})(e_1-e_3)$. The maximal solvable subalgebra S_1 is then obtained in the form

$$S_1=Z\tilde{S}_1Z^{-1}=\begin{pmatrix}ia&\alpha&c+i(a+b/2)\\-\alpha^*&ib&-\alpha^*\\c-i(a+b/2)&-\alpha&-i(a+b)\end{pmatrix}. \tag{24'}$$

C. The group $SU(3,1)$

The two possible realizations of the algebra of $SU(3,1)$ are given by the invariant forms corresponding to

$$D_0=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix} \text{ and } D_1=\begin{pmatrix}0&0&0&1\\0&1&0&0\\0&0&1&0\\1&0&0&0\end{pmatrix}.$$

The general element of the algebra can be written as

$$X_0=\begin{pmatrix} ia^* & \alpha & \beta & \gamma \\ -\alpha^* & ib & \delta & \epsilon \\ -\beta^* & -\delta^* & ic & \zeta \\ \gamma^* & \epsilon^* & \zeta^* & -i(a+b+c) \end{pmatrix}$$

or

$$X_1=\begin{pmatrix} d-i(e+f)/2 & \mu & \nu & ig \\ \rho & ie & \sigma & -\mu^* \\ \tau & -\sigma^* & if & -\nu^* \\ ih & -\rho^* & -\tau^* & -d-i(e+f)/2 \end{pmatrix}$$

and the matrix, transforming one form into the other, is

$$Z=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}.$$

We introduce the vectors

$$e_1=\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad e_2=\begin{pmatrix}0\\1\\0\\0\end{pmatrix},\quad e_3=\begin{pmatrix}0\\0\\1\\0\end{pmatrix},\quad e_4=\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

and impose the flag conditions

$$X_\kappa e_1=\omega e_1,\quad X_\kappa e_2=\omega_1 e_1+\omega_2 e_2$$

($X_\kappa e_3=\omega_1 e_1+\omega_2 e_2+\omega_3 e_3$ follows automatically).

We obtain two maximal solvable algebras:

$$S_0=\begin{pmatrix} ia & 0 & 0 & 0 \\ 0 & ib & 0 & 0 \\ 0 & 0 & ic & 0 \\ 0 & 0 & 0 & -i(a+b+c) \end{pmatrix},$$

$$S_1=\begin{pmatrix} d-i(e+f)/2 & \mu & \nu & ig \\ 0 & ie & 0 & -\mu^* \\ 0 & 0 & if & -\nu^* \\ 0 & 0 & 0 & -d-i(e+f)/2 \end{pmatrix}. \tag{25}$$

The dimension and number of compact elements in these cases is:

$$\dim S_0=3,\quad N_0=3,$$

and

$$\dim S_1=8,\quad N_1=2.$$

D. The group $SU(2,2)$

For the group $SU(2,2)$ we have three distinct possible realizations, corresponding to

$$D_0=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},\quad D_1=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

and

$$D_2=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

Using (10), we find that a general element of the $SU(2,2)$ algebra is

$$X_0=\begin{pmatrix} ia & \beta & \gamma & \delta \\ -\beta^* & ib & \epsilon & \zeta \\ \gamma^* & \epsilon^* & ic & \eta \\ \delta^* & \zeta^* & -\eta^* & -i(a+b+c) \end{pmatrix},$$

$$X_1=\begin{pmatrix} e-\frac{1}{2}i(b+c) & \beta & \gamma & ia \\ \delta & ib & \epsilon & -\beta^* \\ \zeta & \epsilon^* & ic & \gamma^* \\ id & -\delta^* & \zeta^* & -e-\frac{1}{2}i(b+c) \end{pmatrix},$$

and

$$X_2=\begin{pmatrix} p+iq & \beta & \gamma & ia \\ \delta & r-iq & ib & -\gamma^* \\ \epsilon & ic & -r-iq & -\beta^* \\ id & -\epsilon^* & -\delta^* & -p+iq \end{pmatrix}, \tag{26}$$

respectively. The connection between these realizations is

$$ZX_2Z^{-1}=X_0 \quad\text{and}\quad \tilde{Z}X_1\tilde{Z}^{-1}=X_0$$

with

$$Z=\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \text{ and } \tilde{Z}=\begin{pmatrix} 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \end{pmatrix}.$$

Imposing the usual flag conditions

$$X_\kappa\begin{pmatrix}1\\0\\0\\0\end{pmatrix}=\omega\begin{pmatrix}1\\0\\0\\0\end{pmatrix},\quad X_\kappa\begin{pmatrix}0\\1\\0\\0\end{pmatrix}=\begin{pmatrix}\omega_1\\\omega_2\\\omega\\0\end{pmatrix},$$

$$X_\kappa\begin{pmatrix}0\\0\\1\\0\end{pmatrix}=\begin{pmatrix}\omega_1\\\omega_2\\\omega_3\\0\end{pmatrix},$$

we find that the three maximal solvable subalgebras are

$$S_0=\begin{pmatrix} ia & 0 & 0 & 0 \\ 0 & ib & 0 & 0 \\ 0 & 0 & ic & 0 \\ 0 & 0 & 0 & -i(a+b+c) \end{pmatrix},$$

$$S_1=\begin{pmatrix} e-\frac{1}{2}i(b+c) & \beta & \gamma & ia \\ 0 & ib & 0 & -\beta^* \\ 0 & 0 & ic & \gamma^* \\ 0 & 0 & 0 & -e-\frac{1}{2}i(b+c) \end{pmatrix},$$

and

$$S_2=\begin{pmatrix} p+iq & \beta & \gamma & ia \\ 0 & r-iq & ib & -\gamma^* \\ 0 & 0 & -r-iq & -\beta^* \\ 0 & 0 & 0 & -p+iq \end{pmatrix}. \quad (27)$$

The dimensions of interest are

$$\dim S_0=3,\quad \dim S_1=8,\quad \dim S_2=9,$$
$$N_0=3,\qquad N_1=2,\qquad N_2=1.$$

Finally let us note that we could have obtained all three maximal solvable subalgebras using one realization, e.g., the one usually considered in physics, namely X_0. The flag conditions would, however, have to be applied to three different flags, namely

$$F_0=\left\{\begin{pmatrix} x\\0\\0\\0\end{pmatrix};\begin{pmatrix} x\\y\\0\\0\end{pmatrix};\begin{pmatrix} x\\y\\z\\0\end{pmatrix}\right\},$$

$$F_1=\tilde{Z}F_0=\left\{\begin{pmatrix} x\\0\\0\\-x\end{pmatrix};\begin{pmatrix} x\\y\\0\\-x\end{pmatrix};\begin{pmatrix} x\\y\\z\\-x\end{pmatrix}\right\},$$

and

$$F_2=ZF_0=\left\{\begin{pmatrix} x\\0\\0\\-x\end{pmatrix};\begin{pmatrix} x\\y\\-y\\-x\end{pmatrix};\begin{pmatrix} x\\y+z\\-y+z\\-x\end{pmatrix}\right\}.$$

The general element of the corresponding maximal solvable algebra is respectively.

$$S_0=S_0,\ \tilde{S}_1=\begin{pmatrix} ia & \beta & \gamma & d+i[a+(b+c)/2] \\ -\beta^* & ib & 0 & -\beta^* \\ \gamma^* & 0 & ic & \gamma^* \\ d-i[a+(b+c)/2] & -\beta & -\gamma & -i(a+b+c) \end{pmatrix}$$

and

$$\tilde{S}_2=\begin{pmatrix} ia & \beta & \gamma & d+\tfrac{1}{2}i(2a+b+c) \\ -\beta^* & ib & e+\tfrac{1}{2}i(b-c) & -\beta^* \\ \gamma^* & e-\tfrac{1}{2}i(b-c) & ic & \gamma^* \\ d-\tfrac{1}{2}i(2a+b+c) & -\beta & -\gamma & -i(a+b+c) \end{pmatrix}.$$

IV. COMPLETE CLASSIFICATION OF ALL CONTINUOUS SUBGROUPS OF $SU(2,1)$

A. Discussion of the methods

The problem of classifying the general chains of subgroups (1) of a given Lie group G was discussed in Sec. II A. We have already found all maximal solvable subgroups of $SU(p,q)$ in Sec. II C and made the results more explicit for $SU(1,1)$, $SU(2,1)$, $SU(3,1)$, and $SU(2,2)$ in Sec. III.

It should be pointed out that it sometimes happens that the continuous group generated by a linear Lie algebra L over the real number field is not closed in the standard topology. In that case its closure is a linear continuous group with a Lie algebra $\bar{L}$ containing L as a proper ideal with an Abelian factors algebra. Such cases will be pointed out below.

To continue further, we must examine the Lie algebra L of G, and

(1) find all classes of solvable subalgebras (contained in the already found maximal ones),

(2) find all classes of semisimple algebras,

(3) find all classes of subalgebras having a nontrivial Levi decomposition (i.e., both a nontrivial semisimple and solvable subalgebra).

For low-dimensional Lie groups we find it advantageous to approach the problem from two ends.

1. We first classify all one-dimensional subalgebras L_1 and write down a representative A of each class explicitly. [For the algebra $LSU(p,q)$ this has been performed.[21]] We then turn to two-dimensional subalgebras $L_2=\{A,B\}$ and consider separately the case when the derived algebra L_2' has dimension $\dim L_2'=0$ or 1. We then let one of the generators, say A, run through all classes of one-dimensional algebras, always writing it in a specific simple form, leaving B as a general element of L and requiring that A and B satisfy the appropriate commutation relations. This allows us to specify B and thus to obtain all classes of two-dimensional subalgebras and specific representatives of each class.

Three-dimensional subalgebras $L_3=\{A,B,C\}$ can then be studied, using our classification of one- and two-dimensional subalgebras. Indeed, the derived algebra L_3' can have dimension 3, 2, 1, or 0. If $\dim L_3'=3$, then L_3 is semisimple and easy to find; if $\dim L_3'=2$, then we can let L_3' run through all two-dimensional subalgebras that we have already classified and search only for a third element, forming the subalgebra L_3. If $\dim L_3'=1$, we can similarly make use of our classification of one-dimensional subalgebras. If $\dim L_3'=0$, then L_3 is Abelian and easy to find. Thus we proceed from k-dimensional subalgebras to $(k+1)$-dimensional ones, always making use of the already existing classification of lower dimensional subalgebras.

2. The second approach is opposite in spirit to the first one, in that we start from the highest dimensional subalgebras and proceed to the lower ones. We proceed by searching for all elements of L that satisfy certain additional conditions (making sure that these conditions are group properties). Thus we may require that a certain flag is invariant, that a certain vector subspace is invariant, that a certain vector space is annihilated, that a real vector remains real or is given a specific phase, etc. Imposing successively stronger and stronger conditions, we obtain lower dimensional subalgebras.

As an illustration we consider subalgebras of $SU(1,1)$ when both procedures are essentially trivial and then proceed to $SU(2,1)$ (this last algebra has been treated previously,[12] using less general techniques and some subalgebras were unfortunately omitted, in particular the maximal solvable subalgebra S_1).

B. Subgroups of $SU(1, 1)$

Let us first start from the one-dimensional subalgebras. We denote the generators of Lorentz transformations (boosts), along space axis 1 and 2, K_1 and K_2 and the generator of rotations L_3 [we use the local isomorphism between $SU(1,1)$ and $O(2,1)$]. The relations are

$$[K_1, K_2] = -L_3, \quad [K_2, L_3] = K_1, \quad [L_3, K_1] = K_2$$

and the generators can be represented as in (20).

It has been shown earlier[22] that there are three distinct classes of one-dimensional subalgebras, represented, e.g., by

$$L_3, \ K_2, \text{ and } L_3 - K_1. \tag{28}$$

The two-dimensional subalgebras $\{A, B\}$

$$[A, B] = 0 \text{ or } [A, B] = A. \tag{29}$$

Putting A equal to L_3 or K_2, we find that no operator B can be found in the algebra to satisfy either of Eqs. (29). However, putting

$$A = L_3 - K_1 = \tfrac{1}{2}\begin{pmatrix} i & i \\ -i & -i \end{pmatrix}, \quad B = \begin{pmatrix} ia & \alpha \\ \alpha^* & -ia \end{pmatrix},$$

we find that for $a = 0$, $\alpha = \frac{1}{2}$ we have a two-dimensional subalgebra

$$\{L_3 - K_1, K_2\} \text{ satisfying } [L_3 - K_1, K_2] = L_3 - K_1$$

of the type $[A, B] = A$. It has been shown[8] that an algebra of this type has no invariants [no nonconstant polynomial $P(A, B)$ exists, commuting with both A and B].

The alternative procedure, starting from the highest dimensional algebras and imposing successive restrictions, is equally simple in this case. Indeed, the one-parameter subalgebra L_3 is obtained by requiring that a general element X_0 of the algebra leaves the vector space $\binom{1}{0}$ invariant. The two-parameter maximal solvable subalgebra $\{L_3 - K_1, K_2\}$ is obtained by requiring that, e.g., the vector $\binom{1}{-1}$ is invariant. If we add the condition that X_0 annihilates the vector $\binom{1}{-1}$ we obtain the subalgebra $L_3 - K_1$ and if we require that X leaves $\binom{1}{1}$ invariant, in addition to $\binom{1}{-1}$, we obtain the subalgebra K_2.

The results are summarized in Table I.

C. Subgroups of $SU(2,1)$

We shall obtain the subalgebras of dimension $\dim L \geq 3$ by imposing restrictions on general elements of $SU(2,1)$. Those with $\dim L = 2$ will be obtained starting from the one-dimensional ones, classified earlier.[22] We find it convenient to use the three-dimensional defining representation of $SU(2,1)$ in the form X_0 of Eq. (21). With apologies to mathematicians, who use different notations and to physicists, who use still different ones, we introduce a basis of the algebra in the form

$$A = \begin{pmatrix} i & 0 & 0 \\ 0 & -2i & 0 \\ 0 & 0 & i \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & i & 0 \\ i & 0 & i \\ 0 & -i & 0 \end{pmatrix},$$

$$D = \begin{pmatrix} i & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & -i \end{pmatrix}, \quad E = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad F = \begin{pmatrix} i & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -i \end{pmatrix},$$

$$G = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad H = \begin{pmatrix} 0 & i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{30}$$

so that a general element is

$$X = \begin{pmatrix} i(a+d+f) & b+g+i(c+h) & e+id \\ -b-g+i(c+h) & -2ia & -b+ic \\ e-id & -b-ic & i(a-d-f) \end{pmatrix}. \tag{31}$$

We make use of the vectors e_1, e_2, and e_3 introduced in Eq. (23) [note that e_1 and e_2 can be transformed into each other by an $SU(2,1)$ transformation, whereas e_3 cannot be thus transformed].

Let us first obtain all maximal subalgebras. The requirement that the space $e_1 - e_3$ be invariant, i.e., $X(e_1 - e_3) = \alpha(e_1 - e_3)$ with α complex, leads to the conditions $f = g = h = 0$ and we obtain the maximal solvable subalgebra S_1 of Eq. (24′)

$$\{A, B, C, D, E\} = S_1, \tag{32}$$

satisfying the commutation relations

$$[A,B] = 3C, \quad [A,C] = -3B, \quad [A,D] = 0, \quad [A,E] = 0,$$
$$[B,C] = 2D, \quad [B,D] = 0, \quad [B,E] = B, \tag{33}$$
$$[C,D] = 0, \quad [C,E] = C, \quad [D,E] = 2D.$$

TABLE I. Subalgebras of $LSU(1, 1)$.

Class	No. of elements	Generators	Algebra	Invariants of algebra	Group
1	1	L_3		L_3	$O(2)$ (a rotation)
2	1	K_2		K_2	$O(1,1)$ (a pure Lorentz transformation)
3	1	$L_3 - K_1$		$L_3 - K_1$	$E(1)$ (a translation)
4	2	$A = L_3 - K_1$, $B = K_2$	$[A, B] = A$	—	Translations and dilatations of a straight line

The requirement $Xe_2=\alpha e_2$ similarly leads to the algebra

$$\{A,D,E,F\}\sim LS[U(1)\times U(1,1)], \tag{34}$$

satisfying

$$[A,D]=[A,E]=[A,F]=0,$$
$$[F-D,E]=-2F,\quad [E,F]=2(F-D),\quad [F,F-D]=2E. \tag{35}$$

The condition $Xe_3=\alpha e_3$ leads to the subalgebra

$$\{A,F,G,H\}\sim LS[U(2)\times U(1)] \tag{36}$$

with the commutation relations

$$[Y,T]=[Y,G]=[Y,H]=0,$$
$$[T,G]=2H,\quad [G,H]=2T,\quad [H,T]=2G, \tag{37}$$

where $T=\frac{1}{2}(A+F)$ and $Y=\frac{1}{2}(-A+3F)$.

If we require that the operator X leaves a real vector real, i.e., $Xf=f'$, where $f=x_ie_i$ and $f'=x_i'e_i$ with x_i, x_i' real, then we obtain the algebra

$$\{B,E,G\}\sim LO(2,1), \tag{38}$$

satisfying

$$[X,E]=-G,\quad [E,G]=X,\quad [G,X]=E \tag{39}$$

with $X=-B+G$.

This completes the list of all maximal subalgebras of $LSU(2,1)$—a five-dimensional solvable algebra (32), two four-dimensional ones (34) and (36), and one three-dimensional simple algebra (38).

Let us now find all four- and three-dimensional subalgebras of the above maximal subalgebras. We start from the maximal solvable subalgebra S_1, so that the element X already satisfies $S(e_1-e_3)=\alpha(e_1-e_3)$. Let us add additional requirements. If we require $|\alpha|^2=1$, e.g., $X(e_1-e_3)=ie^{i\phi}(e_1-e_3)$, we obtain the restriction $a^2+e^2=1$, i.e., we obtain a one-parameter class of four-dimensional algebras

$$\{B,C,D,R=\cos\phi A+\sin\phi E;\ 0\leqslant\phi<\pi\}, \tag{40}$$

satisfying

$$[B,C]=2D,\quad [B,D]=0,\quad [C,D]=0, \tag{41}$$
$$[B,R]=3\cos\phi C+\sin\phi B,\quad [C,R]=3\cos\phi B+\sin\phi C,$$
$$[D,R]=2\sin\phi D.$$

Demanding that X annihilates the space (e_1-e_3), i.e., $X(e_1-e_3)=0$, we obtain the three-parameter nilpotent algebra

$$\{B,C,D\}, \tag{42}$$

satisfying

$$[B,C]=2D,\quad [B,D]=0,\quad [C,D]=0. \tag{43}$$

Let us now require that, in addition to conserving the e_1-e_3 space, X should act in a definite manner on the vector e_2.

Thus, the requirement $Xe_2=\alpha e_2$, α complex, implies $b=c=0$, i.e., gives the algebra

$$\{A,D,E\}, \tag{44}$$

satisfying

$$[A,D]=0,\quad [A,E]=0,\quad [D,E]=2D. \tag{45}$$

The condition that X projects the space e_2 onto e_1-e_3, i.e., $Xe_2=\alpha(e_1-e_3)$, α complex, again leads to the algebra (40) (with $\phi=\pi/2$); however, the condition $|\alpha|^2=1$, e.g., $Xe_2=e^{i\phi}(e_1-e_3)$ yields a new algebra, generated by D, E, and $Y=\cos\phi B+\sin\phi C$, $0\leqslant\phi<\pi$. This algebra can be simplified by an $SU(2,1)$ transformation so that $UDU^{-1}=D$, $UEU^{-1}=E$, $UYU^{-1}=B$. Indeed, it is sufficient to put

$$U=\begin{pmatrix}\exp[-i(\phi+\pi)/3 & 0 & 0\\ 0 & \exp[i2(\phi+\pi)/3 & 0\\ 0 & 0 & \exp[-i(\phi+\pi)/3\end{pmatrix}.$$

Thus we obtain the subalgebra

$$\{B,D,E\}, \tag{46}$$

satisfying

$$[B,D]=0,\quad [B,E]=B,\quad [D,E]=2D. \tag{47}$$

Further restrictions on elements of the maximal solvable algebra S_1 lead to two- and one-dimensional subalgebras, which we shall consider below. The semisimple subalgebras (34) and (36) do, however, contain further three-dimensional subalgebras.

Indeed, an element $X\in LS[U(1)\times U(1,1)]$ of (34) by necessity satisfies $Xe_2=-2iae_2$. If we add the requirement $Xe_2=0$, i.e., $a=0$, we obtain the subalgebra

$$\{D,E,F\}\sim LSU(1,1). \tag{48}$$

If we impose $X(e_1-e_2)=\alpha(e_1-e_3)$, in addition to $Xe_2=2iae_2$, we obtain the intersection of S_1 with $LS[U(1)\times U(1,1)]$, which is again the algebra $\{A,D,E\}$ of (44). Further restrictions lead to lower dimensional subalgebras.

An element $X\in LS[U(2)\times U(1)]$ of (36) satisfies $Xe_3=i(a-f)e_3$. The condition $Xe_3=0$, i.e., $a=f$ gives the algebra

$$\{A+F,\ G,H\}\sim LSU(2). \tag{49}$$

Thus, we have so far found that $SU(2,1)$ has one five-dimensional solvable subalgebra, one continuous family of solvable four-dimensional ones, two further four-dimensional subalgebras, and six three-dimensional subalgebras.

Let us now simply list the classes of one-dimensional subalgebras found previously.[12,22] Changing the notations of Ref. 22 slightly, we can list the following classes of one-dimensional subalgebras:

A continuous family of compact algebras

$$\cos\phi A+\sin\phi F,\quad 0\leqslant\phi<\pi, \tag{50}$$

all corresponding to $U(1)$ groups.

A continuous family of noncompact algebras

$$\cos\phi A+\sin\phi E,\quad 0<\phi<\pi, \tag{51}$$

corresponding to $O(1,1)$ groups.

Four individual mutually nonequivalent noncompact algebras represented by

$B,\ D,\ A+D,$ and $A-D.$ (52)–(55)

Finally, let us obtain all classes of two-dimensional subalgebras of $LSU(2,1)$. The basis elements of the algebra $\{X, Y\}$ can be chosen to satisfy either $[X, Y]=0$ or $[X, Y]=X$. We can always choose X in one of the standard forms (50)–(55), leave Y general and find all Y satisfying one of the above commutation relations. In this manner we obtain a number of two-dimensional algebras, some of which can be further simplified by an $SU(2,1)$ transformation, leaving X invariant and simplifying Y. We drop all details and simply list the four Abelian and two solvable nonabelian algebras obtained.

Taking X in the form (50), we obtain one algebra for any $0 \leq \phi < \pi$, namely,

$$\{A,F\} \text{ with } [A,F]=0 \tag{56}$$

and two nonequivalent algebras for $\phi=0$ only:

$$\{A,E\} \text{ with } [A,E]=0 \tag{57}$$

and

$$\{A,D\} \text{ with } [A,D]=0. \tag{58}$$

The choice of X in the form (51) yields no new two-dimensional subalgebra, $X=B$ yields two new subalgebras, namely

$$\{B,D\} \text{ with } [B,D]=0 \tag{59}$$

and

$$\{B,E\} \text{ with } [B,E]=-B. \tag{60}$$

The choice $X=D$ yields one continuous class of algebras, namely,

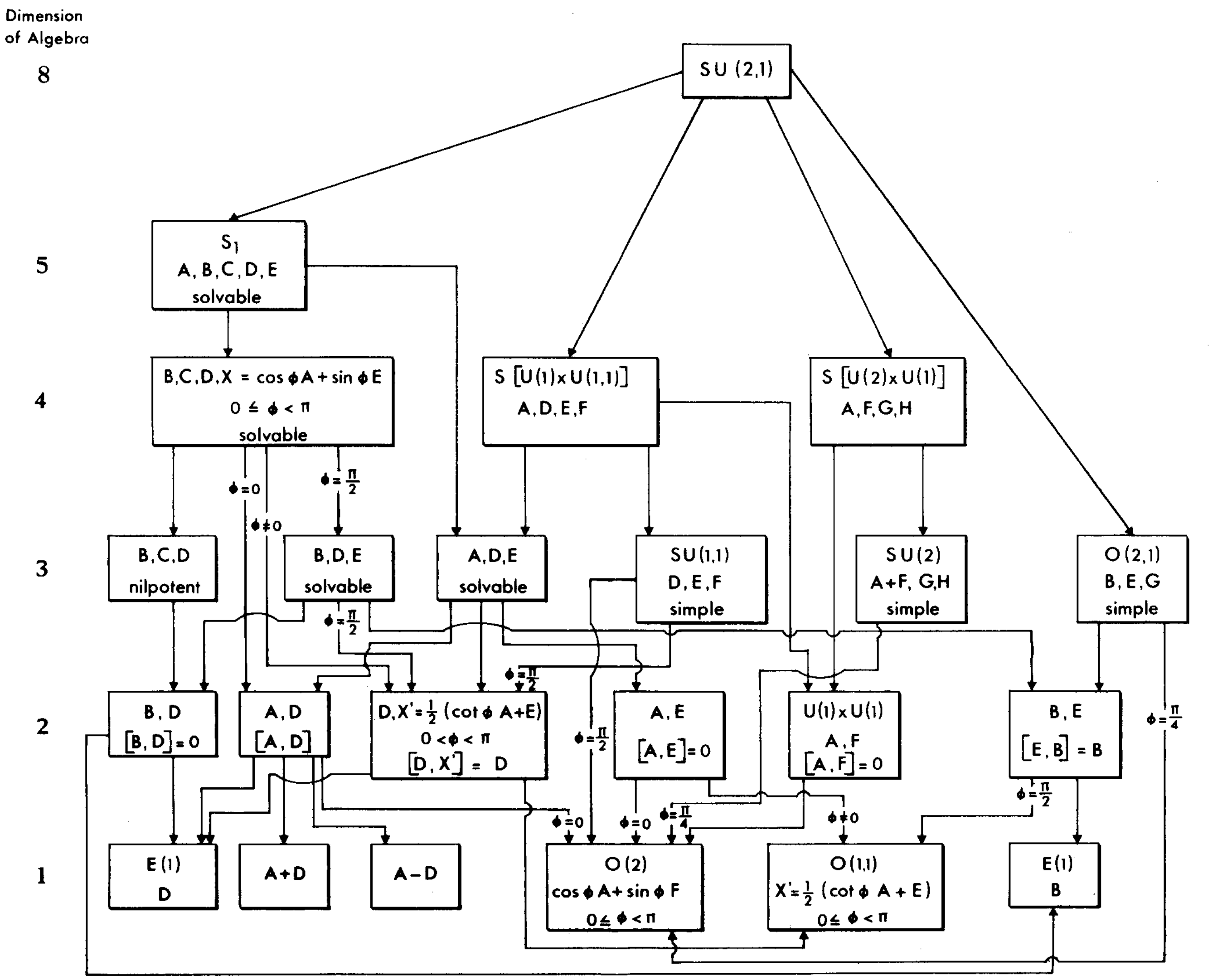
$$\{D,\tfrac{1}{2}[\cot(\phi A+E)]\} \text{ with } [D,\tfrac{1}{2}[\cot(\phi A+E)]]=D,\quad 0<\phi<\pi. \tag{61}$$

Finally, the choices $X=A+D$ or $X=A-D$ yield no new subalgebras.

Thus, we have obtained a complete classification of all subalgebras of the algebra of $SU(2,1)$, each of them corresponding to a Lie subgroup of $SU(2,1)$ itself. The results of this section are summarized in Table II, showing all the subalgebras and all mutual inclusions amongst them. All subgroup chains of the type (1) for $SU(2,1)$ can be directly read off from this diagram.

Let us remark here that the connected *closed* sub-

TABLE II. Continuous subgroup structure of $SU(2, 1)$.



group structure of $SU(2,1)$ is identical with the one given on Table II, except that the subalgebra $O(2)$ in the last row generates a nonclosed group whenever $\tan\phi$ is irrational. Its closure in this case is obviously the two-parameter compact group $U(1)\times U(1)$ generated by A and F.

D. Invariants of the subalgebras of $SU(2,1)$

We are mainly interested in subalgebras that have invariants (Casimir operators), i.e., subalgebras, the enveloping algebras of which have nontrivial centers. Let us find the invariants of all the subalgebras of $LSU(2,1)$

One-dimensional subalgebras

A one-dimensional algebra $\{X\}$ always has an invariant, namely X itself.

In order to find the invariants of the two- and higher-dimensional algebras, we shall make use of the adjoint representation of the corresponding algebra and consider functions $f(x_1, x_2, \ldots, x_n)$, when n is the dimension of the algebra. We construct the generators of the algebra as differential operators and require that they all annihilate the function $f(x_1, \ldots, x_n)$ [so that $f(x_1, \ldots, x_n)$ is invariant under the transformations of the adjoint representation of the group]. Each such invariant that can be expressed as a homogeneous polynomial in $x_1, \ldots, x_n$ corresponds to an invariant of the algebra.

Two-dimensional subalgebras

(a) If $\{X, Y\}$ is Abelian, then both X and Y are obviously invariants. Thus both generators of the following algebras are invariants of the algebras:

$$\{B,D\},\quad \{A,D\},\quad \{A,E\},\quad \{A,F\}.$$

(b) If $[X, Y]=X$, then we write the generators as

$$X=x\frac{\partial}{\partial y},\quad Y=-x\frac{\partial}{\partial x}$$

and let X and Y act on the space of functions $f(x,y)$. The conditions

$$Xf(x,y)=0 \quad\text{and}\quad Yf(x,y)=0$$

clearly imply $f(x,y)=\text{const}$, so that the algebra $\{X, Y\}$ has no invariant (this agrees with a general theorem on the absence of invariants for certain solvable Lie algebras, proven earlier[8]).

Three-dimensional subalgebras

The invariants of the simple three-dimensional subalgebras of $LSU(2,1)$ are obvious, namely,

$$LSU(2)\sim\{A+F,\ G,H\},\quad I_a=\tfrac{1}{4}(A+F)^2+G^2+H^2, \tag{62}$$

$$LSU(1,1)\sim\{D,E,F\}\qquad I_b=(D-F)^2+E^2-F^2, \tag{63}$$

$$LO(2,1)\sim\{B,E,G\},\qquad I_c=(B-G)^2+E^2-G^2. \tag{64}$$

Now let us consider the solvable subalgebras.

Consider algebra (42), put

$$B=2d\frac{\partial}{2c},\quad C=-2d\frac{\partial}{\partial b},\quad D=0 \tag{65}$$

and operate on the functions $f(b,c,d)$. The condition $Bf=Cf=Df=0$ implies

$$f(b,c,b)=f(d).$$

Thus we find that only a function of d is an invariant, hence the only operators that commute with B, C, and D are polynomials in D and we find that the only independent invariant is the obvious one:

$$\{B,C,D\},\quad \text{Invariant}=D. \tag{66}$$

The algebra (44) can be represented by

$$A=0,\quad D=2d\frac{\partial}{\partial e},\quad E=-2d\frac{\partial}{\partial d}.$$

The requirement $Af=DF=EF=0$ implies $f(a,d,e)=f(\text{a})$ and hence we again have only one independent invariant

$$\{A,D,E\},\quad \text{Invariant: } A. \tag{67}$$

Finally, the algebra (46) is represented by

$$B=b\frac{\partial}{\partial e},\quad D=2d\frac{\partial}{\partial e},\quad E=-b\frac{\partial}{\partial b}-2d\frac{\partial}{\partial d}.$$

This time $Bf(b,d,e)=0$ implies $f(b,d,e)=f(b,d)$, $Df=0$ is automatically satisfied, and

$$Ef(b,d)=-b\frac{\partial f}{\partial b}-2d\frac{\partial f}{\partial d}=0$$

implies

$$\frac{\partial f}{\partial b}\Big/\frac{\partial f}{\partial d}=-\frac{d(d)}{db}=-\frac{2d}{b}\quad\text{so that } d=\text{const } b^2.$$

Hence the invariants are arbitrary functions of one variable $f(d/b^2)$. Since no function of d/b^2 can be written as a polynomial in b, d, and e the algebra $\{B,D,E\}$ has no invariant (D/B^2 is not an operator in the enveloping algebra).

Four-dimensional subalgebras

The invariants of the algebras (34) and (36) are again obvious, namely

$$LS[U(2)\times U(1)]\sim\{A,F,G,H\},\qquad I_a=\tfrac{1}{4}(A+F)^2+G^2+H^2,\quad \tilde{I}_a=-A+3F, \tag{68}$$

$$LS[U(1)\times U(1,1)]\sim\{A,D,E,F\},\quad I_b=(D-F)^2+E^2-F^2,\quad \tilde{I}_b=A. \tag{69}$$

Consider now the solvable subalgebra (40). The generators can be represented as

$$B=2d\frac{\partial}{\partial c}+(-3\cos\phi\, c+\sin\phi\, b)\frac{\partial}{\partial r},$$

$$C=-2d\frac{\partial}{\partial b}+(3\cos\phi\, b+\sin\phi\, c)\frac{\partial}{\partial r},$$

$$D=2\sin\phi\, d\frac{\partial}{\partial r},$$

$$R=(3\cos\phi\, c-\sin\phi\, b)\frac{\partial}{\partial b}-(3\cos\phi\, b+\sin\phi\, c)\frac{\partial}{\partial c}-2\sin\phi\, d\frac{\partial}{\partial d}.$$

The requirement $Df(b,c,d,r)=0$ implies $f=f(b,c,d)$ or $\phi=0$. For $\phi\neq 0$ the condition $Bf=0$ then gives $f=f(b,d)$ and $Cf=0$ implies $f=f(d)$. Finally $Rf=0$ implies that $\{B,C,D,R\}$ for $\phi\neq 0$ has no invariant.

Consider now the special case of (40) for $\phi=0$ when the algebra is represented as

$$B=2d\frac{\partial}{\partial c}-3c\frac{\partial}{\partial a},\quad C=-2d\frac{\partial}{\partial b}+3b\frac{\partial}{\partial a},\quad D=0,$$

$$A=3c\frac{\partial}{\partial b}-3b\frac{\partial}{\partial c}.$$

We have $Df(a,b,c,d)=0$, hence D is an invariant.

The condition

$$\tfrac{1}{3}Af=c\frac{\partial f}{\partial b}-b\frac{\partial f}{\partial c}=0$$

implies

$$f(a,b,c,d)=f(a,b^2+c^2,d).$$

Further, $Bf=0$ and $Cf=0$ lead to the same condition

$$4d\frac{\partial f}{\partial x}-3\frac{\partial f}{\partial a}=0,\quad x=b^2+c^2.$$

This equation can be immediately solved and we find that f is an arbitrary function of two variables $f(d,3(b^2+c^2)+4ad)$. An arbitrary polynomial in the operators D and $3(B^2+C^2)+4AD$ will hence commute with A, B, C, and D, and we find that the algebra for $\phi=0$ has two independent invariants:

$$\{A,B,C,D\},\quad I_1=D,\quad I_2=3(B^2+C^2)+4AD. \tag{70}$$

Let us note that the algebra $\{A,B,C,D\}$ is of some interest in physics since after complexification it can be identified with the "harmonic oscillator algebra,"[25] i.e., the algebra of a boson creation a^+ and annihilation operator a, the number-of-particles operator a^+a, and the identity operator I. Indeed, we have

$$[a^+,a]=-I,\quad [N,a^+]=a^+,\quad [N,a]=-a,$$

$$[a^+,I]=[a,I]=[N,I]=0,$$

so that we can identify

$$I=4iD,\quad a=B-iC,\quad a^+=B+iC,\quad N=iA/3.$$

Five-dimensional subalgebra

Let us finally show that the maximal solvable algebra S_1 itself has no invariant. Indeed, the commutation relations (3.3) are satisfied by the operators

$$A=3c\frac{\partial}{\partial b}-3b\frac{\partial}{\partial c},\qquad D=2d\frac{\partial}{\partial e},$$

$$B=c\frac{\partial}{\partial a}+2d\frac{\partial}{\partial c}+b\frac{\partial}{\partial e},\quad E=-b\frac{\partial}{\partial b}-c\frac{\partial}{\partial c}-2d\frac{\partial}{\partial d},$$

$$C=3b\frac{\partial}{\partial a}-2d\frac{\partial}{\partial b}+c\frac{\partial}{\partial e}.$$

The condition $Df(a,b,c,d,e)=0$ implies $f=f(a,b,c,d)$; $Af=0$ gives

$$c\frac{\partial f}{\partial b}-b\frac{\partial f}{\partial c}=0,$$

i.e., $f=f(a,b^2+c^2,d)$. Condition $Ef=0$ gives

$$x\frac{\partial f}{\partial x}+d\frac{\partial f}{\partial d}=0,\quad x=b^2+c^2,$$

implying that $f=f(a,(b^2+c^2)/d)$. Finally $Bf=0$ and $Cf=0$ give the equation

$$-3\frac{\partial f}{\partial a}+4\frac{\partial f}{\partial y}=0,\quad y=\frac{b^2+c^2}{d}.$$

Solving this equation, we find that in order to be invariant under the regular representation f must depend on one variable only, namely

$$f=f\left(\frac{3(b^2+c^2)+4ad}{4d}\right).$$

Since $[3(B^2+C^2)+4AD]/4D$ is not an operator in the enveloping algebra, we find that S_1 has no invariant.

Some results of this section are summarized in Table III, where we list all nonconjugate chains of subgroups of $SU(2,1)$, including only groups the algebras of which satisfy the conditions:

TABLE III. Chains of $SU(2,1)$ subgroups with invariants providing state labels.

1. $SU(2,1)$	$S[U(2)\times U(1)]$ $\{A,F,G,H\}$ $I_1=\frac{1}{4}A+F)^2+G^2+H^2$ $I_2=-(A+3F)/2$	$S[U(1)\times U(1)]$ $\{-(A+3F)/2,A+F\}$ $I_3=A+F$
2a. $SU(2,1)$	$S[U(1)\times U(1,1)]$ $\{A,D,E,F\}$ $I_1=(D-F)^2+E^2-F^2$ $I_2=A$	$S[U(1)\times U(1)]$ $\{A,F\}$ I_3-F
b.		$S[U(1)\times O(1,1)]$ $\{A,E\}$ $I_3=E$
c.		$S[U(1)\times E(1)]$ $\{A,D\}$ $I_3=D$
3a. $SU(2,1)$	$O(2,1)$ $\{B,E,G\}$ $I_1=(B_1-G)^2+E^2-G^2$	$O(2)$ $\{G\}$ $I_2=G$
b.		$O(1,1)$ $\{E\}$ $I_2=E$
c.		$E(2)$ $\{B\}$ $I_2=B$
4a. $SU(2,1)$	Harm. oscillator group $\{A,B,C,D\}$ $I_1=D$ $I_2=3(B^2+C^2)+4AD$	$E(1)$ $\{B\}$ $I_3=B$
b.		$\{A,D\}$ $I_3=A$

(a) They have at least one invariant.

(b) That invariant is not simultaneously an invariant of a larger algebra in the same chains of subalgebras. We also list the corresponding invariants.

Several comments are in order here.

(i) Besides the seven obvious chains of subgroups 1, 2a–c, 3a–c, leading through a maximal semisimple subgroup, we obtain two less obvious ones 4a, b, leading through the solvable group generated by $\{A,B,C,D\}$.

(ii) Each of the subgroup chains, except those involving $O(2,1)$, provides a complete set of commuting operators. Thus, the common eigenfunctions of each of these sets will provide a nondegenerate system of basis functions for the representations of $SU(2,1)$. If we wish to use the $O(2,1)$ chain, then one operator is missing and states labeled by the same eigenvalues of the invariants I_1 and I_2 (in Table III) may occur more than once in a given representation of $SU(2,1)$. It follows that we have a "missing label problem," which can, however, be resolved, e.g., by constructing a further operator, commuting with the invariants I_1 and I_2, but not related to any subgroup. The analogous missing label problem for the $SU(3)\supset O(3)\supset O(2)$ reduction has been resolved in this manner.[26]

V. CONCLUSIONS

The main content of this paper is a theorem, formulated and proven in Sec. II B, which provides a method for determining all maximal solvable subalgebras of any semisimple Lie algebra over a zero characteristic field F. The method was then applied in Sec. II C to explicitly construct all $q+1$ maximal solvable subalgebras of $LSU(p,q)$. In Sec. III we have presented very explicitly the maximal solvable subalgebras of $LSU(p,q)$ for $4\geqslant p+q\geqslant 0$, $p\geqslant q\geqslant 0$. Finally, in Sec. IV we have classified all subalgebras of $LSU(2,1)$, constructed the invariants for all subalgebras that have invariants and proved that the other subalgebras have no invariants.

A continuation of this study classifying all continuous subgroups of the conformal group $SU(2,2)$ will be published separately.

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Generating functionals determining representations of a nonrelativistic local current algebra in the N/V limit*†

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Representations will be given for the nonrelativistic local current algebra consisting of $\rho(\mathbf{x})$, the particle number density, and $\mathbf{J}(\mathbf{x})$, the flux density of particles. These representations correspond to the N/V limit of (i) a free Bose gas, (ii) Bose gas in an external potential, (iii) free Fermi gas, and (iv) Bose gas (in one dimension) with a two-body interaction potential $V(x)=2/x^2$. In each case the generating functional $L(f)$, the ground state expectation value of $\exp[i\rho(f)]$, determining the representation will be given. It will also be shown the generating functional satisfies a functional equation of the form $[\nabla - i\nabla f(\mathbf{x})](1/i)[\delta/\delta f(\mathbf{x})]L(f) = \mathbf{A}(\mathbf{x}, (1/i)(\delta/\delta f))L(f)$ and that the Hamiltonian written in terms of ρ and J has the form $H=(1/8)\int d\mathbf{x}\tilde{\mathbf{K}}(\mathbf{x})^\dagger [1/\rho(\mathbf{x})]\tilde{\mathbf{K}}(\mathbf{x})$ with $\tilde{\mathbf{K}}(\mathbf{x}) = \nabla\rho(\mathbf{x}) + 2i\mathbf{J}(\mathbf{x}) - \mathbf{A}(\mathbf{x},\rho)$.

1. INTRODUCTION

Several physicists[1–5] have suggested formulating field theory in terms of local currents instead of the canonical field operators. As an aid in understanding this approach we will study in this paper the nonrelativistic local current algebra consisting of $\rho(\mathbf{x})$, the particle number density, and $\mathbf{J}(\mathbf{x})$, the flux density of particles. [Only the smeared fields, $\rho(f)=\int\rho(\mathbf{x})f(\mathbf{x})\,d\mathbf{x}$ and $J(\mathbf{g})=\int \mathbf{J}(\mathbf{x})\cdot\mathbf{g}(\mathbf{x})\,d\mathbf{x}$, where $f(\mathbf{x})$ and $\mathbf{g}(\mathbf{x})$ are test functions, are to be considered as operators.] Representations of this algebra can be determined from the generating functional $L(f,\mathbf{g})$, the ground state expectation value of $\exp[i\rho(f)]\exp[iJ(\mathbf{g})]$.[6,7] We will study representations corresponding to the N/V limit. These representations are obtained by considering the representation corresponding to an interacting system of N particles in a box of volume V, then taking the limit (of the generating functional which defines the representation) as $N\to\infty$ and $V\to\infty$ in such a way that $N/V\to\bar{\rho}$, the average particle density.

In the previous paper[6] it was shown that $L(f,\mathbf{g})$ can be expressed in terms of correlation functions and that the Hamiltonian (considered as a Hermitian form) can be expressed in terms of $\rho(\mathbf{x})$ and $\mathbf{J}(\mathbf{x})$. In this paper we will provide several illustrations of these results. All of the examples considered are systems for which the N-particle ground state wavefunction is known. Our procedure will consist of calculating all the correlation functions for the N-particle systems and then using these to determine $L(f,\mathbf{g})$ in the N/V limit. For many purposes it is sufficient to know $L(f)=L(f,0)$. For each example, $L(f)$ is shown to satisfy a functional equation of the form

$$[\nabla - i\nabla f(\mathbf{x})]\frac{1}{i}\frac{\delta}{\delta f(\mathbf{x})}L(f) = \mathbf{A}\left(\mathbf{x}, \frac{1}{i}\frac{\delta}{\delta f}\right)L(f).$$

This leads to the following expression for the Hamiltonian in terms of $\rho(\mathbf{x})$ and $\mathbf{J}(\mathbf{x})$: $H=\frac{1}{8}\int d\mathbf{x}\,\tilde{\mathbf{K}}(\mathbf{x})^\dagger[1/\rho(\mathbf{x})]\tilde{\mathbf{K}}(\mathbf{x})$, where $\tilde{\mathbf{K}}(\mathbf{x}) = \nabla\rho(\mathbf{x}) + 2i\mathbf{J}(\mathbf{x}) - \mathbf{A}(\mathbf{x},\rho)$.

Hopefully, after becoming familiar with this approach we will be able to write the Hamiltonian in terms of $\rho(\mathbf{x})$ and $\mathbf{J}(\mathbf{x})$ for any interacting system of particles. This leads directly to a functional equation for $L(f)$. By solving this equation we could determine representations in the N/V limit for cases when it is not possible to find the N-particle ground state wavefunction.

In Sec. 2 the ρ, J algebra will be defined. The N-particle representations will be reviewed along with the results on the N/V limit from the previous paper.

In the subsequent sections, $L(f)$, the functional equation for $L(f)$, and an expression for the Hamiltonian in terms of $\rho(\mathbf{x})$ and $\mathbf{J}(\mathbf{x})$ will be derived for each of the following examples:

(i) free Bose gas (Sec. 3),

(ii) Bose gas in an external potential (Sec. 4),

(iii) free Fermi gas (Sec. 5),

(iv) Bose gas (in one dimension) with a two-body interaction potential $V(x)=2/x^2$ (Sec. 6).

The last example is the most interesting since a representation of the ρ, J algebra corresponding to an interacting system is given.

2. SUMMARY OF RESULTS ON REPRESENTATIONS OF THE ρ, J ALGEBRA

The ρ, J algebra is defined by the following commutation relations among the smeared fields:

$$\begin{aligned}&[\rho(f_1),\rho(f_2)]=0,\\&[\rho(f),J(\mathbf{g})]=i\rho(\mathbf{g}\cdot\nabla f),\\&[J(\mathbf{g}_1),J(\mathbf{g}_2)]=iJ(\mathbf{g}_2\cdot\nabla\mathbf{g}_1-\mathbf{g}_1\cdot\nabla\mathbf{g}_2).\end{aligned} \tag{2.1}$$

In computing the N/V limit representation we will use the correspondence between N-particle representations and quantum mechanics. An N-particle representation[7] is defined on the Hilbert space:

$$\mathcal{H}=\begin{cases}L^2_+(R^N) = \text{symmetric functions for bosons}\\ L^2_-(R^N) = \text{antisymmetric functions for (spinless) fermions.}\end{cases}$$

In either case

$$\begin{aligned}\rho(f)&=\sum_{m=1}^N f(\mathbf{x}_m),\\ J(\mathbf{g})&=-\tfrac{1}{2}i\sum_{m=1}^N[2\mathbf{g}(\mathbf{x}_m)\cdot\nabla_m+(\nabla\cdot\mathbf{g})(\mathbf{x}_m)].\end{aligned}\tag{2.2}$$

It will be useful to introduce the quantity, $K(\mathbf{g})=-\rho(\nabla\cdot\mathbf{g})+2iJ(\mathbf{g})$. In the N-particle representation.

$$K(\mathbf{g}) = 2\sum_{m=1}^{N} \mathbf{g}(\mathbf{x}_m)\cdot\nabla_m \quad \text{or} \quad \mathbf{K}(\mathbf{x}) = 2\sum_{m=1}^{N}\delta(\mathbf{x}-\mathbf{x}_m)\,\nabla_m. \tag{2.3}$$

Once the N-particle ground state wavefunction, $\Omega_N(\mathbf{x}_1\cdots\mathbf{x}_N)$, is given, the generating functionals are determined by

$$L_N(f) = (\Omega_N, \exp[i\rho(f)]\,\Omega_N) = \int d\mathbf{x}_1\cdots\int d\mathbf{x}_N\,\Omega_N^*(\mathbf{x}_1\cdots\mathbf{x}_N) \times \exp[if(\mathbf{x}_1)]\cdots\exp[if(\mathbf{x}_N)]\,\Omega_N(\mathbf{x}_1\cdots\mathbf{x}_N) \tag{2.4a}$$

and

$$L_N(f,\mathbf{g}) = (\Omega_N, \exp[i\rho(f)]\exp[iJ(\mathbf{g})]\Omega_N) = \int d\mathbf{x}_1\cdots\int d\mathbf{x}_N\,\Omega_N^*(\mathbf{x}_1\cdots\mathbf{x}_N) \times\prod_{m=1}^{N}\{\exp[if(\mathbf{x}_m)]\exp[ij(\mathbf{x}_m,\mathbf{g})]\}\,\Omega_N(\mathbf{x}_1\cdots\mathbf{x}_N), \tag{2.4b}$$

where $j(\mathbf{x},\mathbf{g}) = -\frac{1}{2}i[2\mathbf{g}(\mathbf{x})\cdot\nabla + (\nabla\cdot\mathbf{g})(\mathbf{x})]$.

Remark: In Ref. 7 it was shown that $\exp[itj(\mathbf{x},\mathbf{g})]\psi(\mathbf{x}) = \psi(\varphi_t^{\mathbf{g}}(\mathbf{x}))\{\det[\partial_m\varphi_t^{\mathbf{g}}(\mathbf{x})_n]\}^{1/2}$, where $\varphi_t^{\mathbf{g}}(\mathbf{x})$ is the flow corresponding to the vector field $\mathbf{g}$ defined by, $(\partial/\partial t)\varphi_t^{\mathbf{g}}(\mathbf{x}) = \mathbf{g}\circ\varphi_t^{\mathbf{g}}(\mathbf{x})$ and $\varphi_0^{\mathbf{g}}(\mathbf{x}) = \mathbf{x}$.

In order to take the N/V limit, it will be convenient to express the generating functional in terms of correlation functions. The nth correlation function for an N-particle representation is defined by

$$R_n^{(N)}(\mathbf{y}_1\cdots\mathbf{y}_n;\mathbf{x}_1\cdots\mathbf{x}_n) = [N!/(N-n)!]\int d\mathbf{z}_{n+1}\cdots\int d\mathbf{z}_N \times\Omega_N^*(\mathbf{y}_1\cdots\mathbf{y}_n,\mathbf{z}_{n+1}\cdots\mathbf{z}_N)\,\Omega_N(\mathbf{x}_1\cdots\mathbf{x}_n,\mathbf{z}_{n+1}\cdots\mathbf{z}_N) \tag{2.5a}$$

Let

$$R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n) = R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n;\mathbf{x}_1\cdots\mathbf{x}_n). \tag{2.5b}$$

In the preceding paper[6] it was shown that

$$L_N(f) = \sum_{n=0}^{N}\frac{1}{n!}\int_V d\mathbf{x}_1\cdots\int_V d\mathbf{x}_n\,F(\mathbf{x}_1)\cdots F(\mathbf{x}_n)R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n), \tag{2.6a}$$

where $F(\mathbf{x}) = \exp[if(\mathbf{x})] - 1$, and

$$L_N(f,\mathbf{g}) = \sum_{n=0}^{N}\frac{1}{n!}\int_V d\mathbf{x}_1\int_V d\mathbf{y}_1\cdots\int_V d\mathbf{x}_n\int_V d\mathbf{y}_n \times\prod_{m=1}^{n}\delta(\mathbf{x}_m-\mathbf{y}_m)\{\exp[if(\mathbf{x}_m)]\exp[ij(\mathbf{x}_m,\mathbf{g})]-1\} \times R_n^{(N)}(\mathbf{y}_1\cdots\mathbf{y}_n;\mathbf{x}_1\cdots\mathbf{x}_n). \tag{2.6b}$$

Furthermore, if $R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n)\to R_n(\mathbf{x}_1\cdots\mathbf{x}_n)$ in the N/V limit and $|R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n)|\le c^n n^{n/2}$, where $c=$ const, then in the N/V limit

$$L_N(f)\to L(f) = \sum_{n=0}^{\infty}(1/n!)\int_{-\infty}^{\infty}d\mathbf{x}_1\cdots\int_{-\infty}^{\infty}d\mathbf{x}_n\,F(\mathbf{x}_1)\cdots F(\mathbf{x}_n)R_n(\mathbf{x}_1\cdots\mathbf{x}_n). \tag{2.7}$$

In addition to determining representations in the N/V limit we will be interested in expressing the Hamiltonian in terms of ρ and J. We will use the following results from the preceding paper[6]:

There is an operator of the form

$$\tilde{\mathbf{K}}(\mathbf{x}) = \mathbf{K}(\mathbf{x}) - \mathbf{A}(\mathbf{x},\rho) \tag{2.8}$$

such that $\tilde{\mathbf{K}}(\mathbf{x})$ annihilates the ground state Ω; i.e., $\tilde{\mathbf{K}}(\mathbf{x})\Omega = 0$. The Hamiltonian (for time reversal invariant systems of spinless particles) can be written as

$$H = \frac{1}{8}\int d\mathbf{x}\,\tilde{K}(\mathbf{x})^\dagger\frac{1}{\rho(\mathbf{x})}\tilde{\mathbf{K}}(\mathbf{x}). \tag{2.9}$$

Furthermore, the generating functional satisfies the functional equation

$$[\nabla - i\nabla f(\mathbf{x})]\frac{1}{i}\frac{\delta}{\delta f(\mathbf{x})}L(f) = \mathbf{A}\left(\mathbf{x},\frac{1}{i}\frac{\delta}{\delta f}\right)L(f). \tag{2.10}$$

After determining $L(f)$ in the N/V limit, we will find an $\mathbf{A}(\mathbf{x},\rho)$ such that Eq. (2.10) is satisfied. This implies $(\Omega, \exp[i\rho(f)]\tilde{\mathbf{K}}(\mathbf{x})\Omega) = 0$, where $\tilde{\mathbf{K}}(\mathbf{x}) = \mathbf{K}(\mathbf{x}) - \mathbf{A}(\mathbf{x},\rho)$. For physical reasons (explained in the previous paper), Span$\{\exp[i\rho(f)]\Omega\}$ is dense in a representation corresponding to a system of spinless particles. It therefore follows that $\tilde{\mathbf{K}}(\mathbf{x})\Omega = 0$. Then the results of the previous paper allow us to conclude H is given by Eq. (2.9).

Finally, we will show that the various N/V limit representations we determine are unitarily inequivalent. This is a consequence of translational invariance and the cluster decomposition property. A representation satisfies translational invariance and the cluster decomposition property if

$$\lim_{\lambda\to\infty} L(f + h_{\lambda\mathbf{a}}) = L(f)L(h), \quad \text{where } h_{\lambda\mathbf{a}}(\mathbf{x}) = h(\mathbf{x}-\lambda\mathbf{a}). \tag{2.11}$$

In the previous paper it was shown that two representations satisfying translational invariance and the cluster decomposition property are unitarily equivalent iff their generating functionals are equal.

3. FIRST EXAMPLE: THE INFINITE FREE BOSE GAS

The free Bose gas is the first example we will consider since it is the simplest case in which to illustrate the procedure we will be using. The representation corresponding to the free Bose gas was first given by Goldin and Sharp[8] and treated in great detail in Ref. 9. There it was shown that: (i) $L(f) = \exp[\bar{\rho}\int(\exp[if(\mathbf{x})] - 1)\,d\mathbf{x}]$, (ii) $(\nabla - i\nabla f)(1/i)[\delta/\delta f(\mathbf{x})]L(f) = 0$, and (iii) $H = \frac{1}{8}\int d\mathbf{x}\,\mathbf{K}(\mathbf{x})^\dagger[1/\rho(\mathbf{x})]\mathbf{K}(\mathbf{x})$. The Hamiltonian was originally motivated by formal manipulations when ρ and J are written in terms of the canonical fields.[1] The $1/\rho(\mathbf{x})$ term appearing in the Hamiltonian has been given a rigorous meaning in Refs. 8 and 9. In addition to giving an alternative derivation for $L(f)$, we will show the Hamiltonian follows from the N/V limit of the Hamiltonian for N free bosons in a box of volume V.

We begin by calculating the correlation functions for N free bosons in a box of volume V. The Hamiltonian for N particles is given by

$$H_N = -\frac{1}{2}\sum_{n=1}^{N}\nabla_n^2. \tag{3.1}$$

The ground state wavefunction is $\Omega_N(\mathbf{x}_1 \cdots \mathbf{x}_N) = V^{-N/2}$. The correlation functions can easily be computed from Eq. (2.5b). The result is $R_n^{(N)}(\mathbf{x}_1 \cdots \mathbf{x}_n) = N!/(N-n)!\, V^{-n}$. In the N/V limit, $R_n^{(N)} \to R_n = \bar{\rho}^n$. Equation (2.7) then gives the generating functional in the N/V limit,

$$L(f) = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\mathbf{x}_1 \cdots \int d\mathbf{x}_n F(\mathbf{x}_1) \cdots F(\mathbf{x}_n)\bar{\rho}^n,$$

$$\text{where } F(\mathbf{x}) = \exp[if(\mathbf{x})] - 1,$$

$$= \exp[\bar{\rho} \int d\mathbf{x}(\exp[if(\mathbf{x})] - 1)]. \tag{3.2}$$

Remark: $\bar{\rho}$ is the average density. It may also be thought of as the ground state expectation value of $\rho(\mathbf{x})$; $\bar{\rho} = (\Omega \rho(\mathbf{x}) \Omega)$. This expectation value is a constant for an infinite volume by translational invariance.

Since for N particles we have the ground state expressed as a wavefunction, it is easy to find the operator $\tilde{\mathbf{K}}(\mathbf{x})$ needed to obtain the Hamiltonian in terms of ρ and J. Using Eq. (2.3b), we find $\mathbf{K}(\mathbf{x})\Omega_N = 0$. Thus the Hamiltonian given by Eq. (2.9) becomes

$$H_N = \frac{1}{8} \int_V d\mathbf{x}\, \mathbf{K}^\dagger(\mathbf{x}) \frac{1}{\rho(\mathbf{x})} \mathbf{K}(\mathbf{x}). \tag{3.3}$$

This suggests in the N/V limit the Hamiltonian is given by

$$H = \frac{1}{8} \int_{-\infty}^{\infty} d\mathbf{x}\, \mathbf{K}^\dagger(\mathbf{x}) \frac{1}{\rho(\mathbf{x})} \mathbf{K}(\mathbf{x}). \tag{3.4}$$

To verify this, we must show $\mathbf{K}(\mathbf{x})\Omega = 0$ (in the N/V limit). As explained in Sec. 2, it is sufficient to prove Eq. (2.10) is satisfied. In this case Eq. (2.10) reduces to

$$(\nabla - i\nabla f) \frac{1}{i} \frac{\delta}{\delta f(\mathbf{x})} L(f) = 0. \tag{3.5}$$

By using $L(f)$ given in Eq. (3.2) it is easy to check that Eq. (3.5) is true. Thus we can conclude the Hamiltonian for a free Bose gas in the N/V limit is given by Eq. (3.4).

By similar means $L(f, \mathbf{g})$ can be calculated. The result is

$$L(f, \mathbf{g}) = \exp(\bar{\rho} \int d\mathbf{x}\{\exp[if(\mathbf{x})][\det \partial_m \varphi^{\mathbf{g}}(\mathbf{x})_n]^{1/2} - 1\}), \tag{3.6}$$

where $\varphi^{\mathbf{g}}$ is the flow corresponding to the vector field $\mathbf{g}$.

Furthermore, it can shown $L(f)$ satisfies translational invariance and the cluster decomposition property [Eq. (2.11)]. As a result, representations of the free Bose gas corresponding to different densities are unitarily inequivalent.

Finally, we mention some additional properties that can be proved for the free Bose gas representations (with given average density $\bar{\rho}$):

(i) The exponentiated currents, $\exp[i\rho(f)]$ and $\exp[iJ(\mathrm{g})]$, are irreducible.[9]

(ii) The translation operators are in the closure of the exponentiated current algebra.[6]

(iii) Span$\{\exp[i\rho(f)\Omega\}$ is dense.[9]

Other representations can be obtained by taking the direct sum of representations with different densities.

4. SECOND EXAMPLE: INFINITE BOSE GAS IN AN EXTERNAL POTENTIAL

The generating functional for a Bose Gas in an external potential $u(x)$ can be calculated in a similar manner to that of a free Bose gas. The Hamiltonian for N particles in a box of volume V is given by

$$H_N = \sum_{r=1}^{N} [-\tfrac{1}{2}\nabla_r^2 + u_N(\mathbf{x}_r) - E_g], \tag{4.1}$$

where E_g = the ground state energy per particle. Let $w_N(\mathbf{x})$ = the single-particle ground state wavefunction defined by

$$[-\tfrac{1}{2}\nabla^2 + u_N(\mathbf{x})]w_N(\mathbf{x}) = E_g w_N(\mathbf{x}) \tag{4.2}$$

with normalization $\int_V d\mathbf{x}\, w_N(\mathbf{x})^2/V = 1$. The ground state wavefunction for the N-particle system is then

$$\Omega_N = \prod_{r=1}^{N} V^{-1/2} w_N(\mathbf{x}_r) \tag{4.3}$$

Remark: (1) The Hamiltonian has been defined such that $H_N \Omega_N = 0$. (2) There are several subtle details in connection with the N/V limit which we will not discuss since we are mainly interested in the form of the representation and the Hamiltonian. However, it is well to be aware of these points. First, there is the boundary conditions at the edge of the box. Normally the wavefunction is required either to be periodic or to vanish at the edges. The boundary conditions are needed to fully specify the Hamiltonian for the system of interest. Different choices of boundary conditions may give different results in the N/V limit. Second, there is the question of how to restrict the potential to the box. The potential $u_N(\mathbf{x})$ may be chosen in any convenient manner as long as in the N/V limit we describe a system of particles in the potential $u(\mathbf{x})$. For example, we might truncate the potential, $u_N(\mathbf{x}) = u(\mathbf{x})$ for $\mathbf{x}$ in the box; or we could make the potential periodic, $u_N(\mathbf{x}) = \sum_{n=-\infty}^{\infty} u(\mathbf{x} + \mathbf{n}L)$, where L = the length of the box. Finally, the N/V limit does not exist, for perfectly good physical reasons, for every potential. For example, a harmonic oscillator potential $u(x) = kx^2$ for large x is sufficiently large and repulsive to cause particles to clump together around the origin in the N/V limit. (i.e., in the N/V limit an infinite number of particles would be found in a finite region around the origin.)

The correlation functions can be computed from Eqs. (2.3b) and (4.3). The result is

$$R_n^{(N)}(\mathbf{x}_1 \cdots \mathbf{x}_n) = \frac{N!}{(N-n)!} V^{-n} \prod_{r=1}^{n} w_N(\mathbf{x}_r)^2. \tag{4.4}$$

In order to obtain $L(f)$ in the N/V limit, we will suppose that $w_N(\mathbf{x}) \to w(\mathbf{x})$ in the N/V limit. Then

$$R_n^{(N)}(\mathbf{x}_1 \cdots \mathbf{x}_n) \to R_n = \bar{\rho}^n \prod_{r=1}^{n} w(\mathbf{x}_r)^2. \tag{4.5}$$

If we further suppose that the $w_N(\mathbf{x})$ are bounded, then the generating functional in the N/V limit is given by Eq. (2.9) which becomes

$$L(f) = \sum_{n=0}^{\infty} \frac{1}{n!} \int d\mathbf{x}_1 \cdots \int d\mathbf{x}_n F(\mathbf{x}_1) \cdots F(\mathbf{x}_n)$$

$$\times\bar{\rho}^n w(\mathbf{x}_1)^2\cdots w(\mathbf{x}_n)^2$$
$$=\exp\{\int d\mathbf{x}\,\bar{\rho}w(\mathbf{x})^2(\exp[if(\mathbf{x})]-1)\}. \quad (4.6)$$

Let $\rho_0(\mathbf{x})=$ the ground state expectation value of $\rho(\mathbf{x})$. Then,

$$\rho_0(\mathbf{x})=(\Omega,\rho(\mathbf{x})\Omega)=\frac{1}{i}\frac{\delta}{\delta f(\mathbf{x})}L(f)\bigg|_{f=0}=\bar{\rho}w(\mathbf{x})^2. \quad (4.7)$$

Now $L(f)$ can be written as

$$L(f)=\exp\{\int d\mathbf{x}\,\rho_0(\mathbf{x})(\exp[if(\mathbf{x})]-1)\}. \quad (4.8)$$

Thus $L(f)$ for a noninteracting Bose gas in an external potential has the same form as $L(f)$ for a free Bose gas. They are both determined by $(\Omega,\rho(\mathbf{x})\Omega)$. Since a free Bose gas is translational invariant, in the N/V limit $(\Omega,\rho(\mathbf{x})\Omega)=\bar{\rho}$, a constant. An external potential breaks this symmetry. It is the only nontranslational invariant system we will consider in this paper. (However, it does satisfy the cluster decomposition property).

By similar means $L(f,\mathbf{g})$ can be calculated. The result is

$$L(f,\mathbf{g})=\exp[\bar{\rho}\int d\mathbf{x}\,w(\mathbf{x})(\exp[if(\mathbf{x})]$$
$$\times\exp[\mathbf{g}(\mathbf{x})\cdot\nabla+(\nabla\cdot\mathbf{g})(\mathbf{x})/2]-1)w(\mathbf{x})\}. \quad (4.9)$$

To obtain the Hamiltonian, we must again determine the appropriate form for the operator $\tilde{\mathbf{K}}(\mathbf{x})$. Using Eqs. (2.3) and (4.3), we find

$$\mathbf{K}(\mathbf{x})\Omega_N=\left(\sum_{r=1}^{N}2\delta(\mathbf{x}-\mathbf{x}_r)\nabla_r\right)\left(\prod_{r=1}^{N}V^{-1/2}w_N(\mathbf{x}_r)\right)$$
$$=\left(\sum_{r=1}^{N}2\delta(\mathbf{x}-\mathbf{x}_r)\frac{\nabla w_N}{w_N}(\mathbf{x}_r)\right)\left(\prod_{r=1}^{N}V^{-1/2}w_N(\mathbf{x}_r)\right)$$
$$=2\rho(\mathbf{x})\frac{\nabla w_N}{w_N}(\mathbf{x})\Omega_N. \quad (4.10)$$

Thus,

$$\tilde{\mathbf{K}}_N(\mathbf{x})=\mathbf{K}(\mathbf{x})-2\rho(\mathbf{x})\frac{\nabla w_N}{w_N}(\mathbf{x})$$

and

$$H_N=\frac{1}{8}\int_V d\mathbf{x}\,\tilde{\mathbf{K}}_N(\mathbf{x})^\dagger\frac{1}{\rho(\mathbf{x})}\tilde{\mathbf{K}}_N(\mathbf{x}).$$

In the N/V limit we would expect

$$\tilde{\mathbf{K}}(x)=\mathbf{K}(\mathbf{x})-2\rho(\mathbf{x})\frac{\nabla w}{w}(\mathbf{x})$$
$$=\mathbf{K}(\mathbf{x})-\rho(\mathbf{x})\nabla\ln\rho_0(\mathbf{x}). \quad (4.11)$$

This expression can be verified by checking that Eq. (2.10), which in this case becomes

$$(\nabla-i\nabla f)\frac{1}{i}\frac{\delta}{\delta f(\mathbf{x})}L(f)=(\nabla\ln\rho_0)(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta f(\mathbf{x})}L(f), \quad (4.12)$$

is satisfied. By using Eq. (4.8) for $L(f)$, Eq. (4.12) can easily be proved true. Therefore, the Hamiltonian for a Bose gas in an external potential is given in the N/V limit by

$$H=\frac{1}{8}\int_{-\infty}^{\infty}d\mathbf{x}\,\tilde{\mathbf{K}}(\mathbf{x})^\dagger\frac{1}{\rho(\mathbf{x})}\tilde{\mathbf{K}}(\mathbf{x}), \quad (4.13)$$

where $\tilde{\mathbf{K}}(\mathbf{x})$ is given by Eq. (4.11). We can gain further understanding of this form of the Hamiltonian through the following formal manipulations. From Eq. (4.11) and (4.13),

$$H=\frac{1}{8}\int d\mathbf{x}[\mathbf{K}(\mathbf{x})-\rho(\mathbf{x})\nabla\ln\rho_0(\mathbf{x})]^\dagger\frac{1}{\rho(\mathbf{x})}[\mathbf{K}(\mathbf{x})-\rho(\mathbf{x})\nabla\ln\rho_0(\mathbf{x})]$$
$$=\frac{1}{8}\int d\mathbf{x}\,\mathbf{K}(\mathbf{x})^\dagger\frac{1}{\rho_0(\mathbf{x})}\mathbf{K}(\mathbf{x})$$
$$-\frac{1}{8}\int d\mathbf{x}\,\nabla\ln\rho_0(\mathbf{x})[\mathbf{K}(\mathbf{x})^\dagger+\mathbf{K}(\mathbf{x})]$$
$$+\frac{1}{8}\int d\mathbf{x}\,\rho(\mathbf{x})\nabla\ln\rho_0(\mathbf{x})\cdot\nabla\ln\rho_0(\mathbf{x}).$$

Since $\mathbf{K}(\mathbf{x})^\dagger+\mathbf{K}(\mathbf{x})=2\nabla\rho(\mathbf{x})$,

$$H=\frac{1}{8}\int d\mathbf{x}\,\mathbf{K}(\mathbf{x})^\dagger\frac{1}{\rho(\mathbf{x})}\mathbf{K}(\mathbf{x})$$
$$+\int d\mathbf{x}\,\rho(\mathbf{x})[\tfrac{1}{4}\nabla^2\ln\rho_0(\mathbf{x})+\tfrac{1}{8}\nabla\ln\rho_0\cdot\nabla\ln\rho_0]$$

Using $\rho_0(\mathbf{x})=\bar{\rho}w^2(\mathbf{x})$, we have

$$\tfrac{1}{4}\nabla^2\ln\rho_0(\mathbf{x})+\tfrac{1}{8}\nabla\ln\rho_0\cdot\nabla\ln\rho_0=\tfrac{1}{2}(\nabla^2w/w)(\mathbf{x}).$$

If in the N/V limit Eq. (4.2) remains true,

$$\tfrac{1}{2}(\nabla^2w/w)(\mathbf{x})=u(\mathbf{x})-E_g.$$

Therefore,

$$H=\frac{1}{8}\int d\mathbf{x}\,\mathbf{K}(\mathbf{x})^\dagger\frac{1}{\rho(\mathbf{x})}\mathbf{K}(\mathbf{x})+\int d\mathbf{x}\,\rho(\mathbf{x})(u(\mathbf{x})-E_g).$$

From Sec. 3 we may identify $\frac{1}{8}\int d\mathbf{x}\,\mathbf{K}(\mathbf{x})^\dagger[1/\rho(\mathbf{x})]\mathbf{K}(\mathbf{x})$ with the kinetic energy for bosons. The term $\int d\mathbf{x}\,\rho(\mathbf{x})[u(\mathbf{x})-E_g]$ corresponds to the potential energy. Thus H has the expected form.

The following (one-dimensional) example will illustrate some of these results:

Let

$$w(x)=\begin{cases}1-[(1/4\pi)+(1/\pi^2)\cos(\pi x)] & \text{for } |x|\le\frac{1}{2},\\ 1-(1/2\pi)[1+(1/2\pi)\sin(2\pi x)-x] & \text{for } \frac{1}{2}<|x|\le 1,\\ 1 & \text{for } 1<|x|.\end{cases}$$

Then

$$w''(x)=\begin{cases}\cos(\pi x) & \text{for } |x|\le\frac{1}{2},\\ \sin(2\pi x) & \text{for } \frac{1}{2}<|x|\le 1,\\ 0 & \text{for } 1<|x|.\end{cases}$$

Now, let $u(x)=\frac{1}{2}w''(x)/w(x)$. Then $[-\frac{1}{2}(d^2/dx^2)+u(x)]w(x)=0$. (See Fig. 1).

The ground state, for this potential, can be solved in any box (with $L>2$) if periodic boundary conditions are imposed. For N particles in a box of length L, let $u_N(x)=u(x)$ for $-\frac{1}{2}L<x<\frac{1}{2}L$. The single-particle ground state is $w_N(x)=w(x)$ for $-\frac{1}{2}L<x<\frac{1}{2}L$. Clearly in the N/V limit $w_N(x)\to w(x)$. Thus, for a Bose gas in the external potential $u(x)$ in the N/V limit $L(f)=\exp\{\bar{\rho}\int dx\,w(x)^2(\exp[if(x)]-1)\}$.

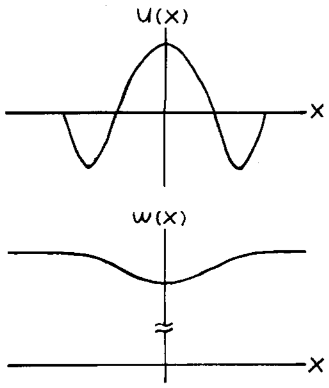

FIG. 1. The external potential $u(x)$ vs x, and the single particle wavefunction $\omega(x)$ vs x.

5. THIRD EXAMPLE: THE INFINITE FREE FERMI GAS

In this section we will compute the generating functional for a free Fermi gas. The N-particle Hamiltonian is

$$H_N = -\tfrac{1}{2}\sum_{n=1}^{N} \nabla_n^2. \tag{5.1}$$

In a cubic box with edges of length L the ground state is

$$\Omega_N = (V^{-N}/N!)^{1/2}\det_{N\times N}[\exp(i\mathbf{k}_n\cdot\mathbf{x}_m)], \tag{5.2}$$

where $\mathbf{k}_n = 2\pi/L(n_1, n_2, n_3)$ and n_1, n_2, n_3 are integers such that $|\mathbf{k}_n| \le k_f$, the Fermi momentum. The Fermi momentum is determined from the average density in the usual way. The number of particles is $N = \sum_{|\mathbf{k}|<k_f} 1$. In the limit this becomes

$$N \to \int d^3k\, V/(2\pi)^3 = V(4\pi/3)(k_f/2\pi)^3.$$

Therefore, the Fermi momentum is related to the average density by

$$\bar\rho = (4/3)\pi(k_f/2\pi)^3. \tag{5.3}$$

Remark: By picking the number of particles N such that the ground state contains all the single-particle states with $|\mathbf{k}| \le k_f$, the ground state is unique. Also, N is odd since for every occupied state $\mathbf{k}$, the state $-\mathbf{k}$ is also occupied except that $\mathbf{k}=0$ and -0 are the same. As a result $i^{(N-1)/2}\Omega_N$ is real and hence time reversal invariant.

The correlation functions can be calculated using the following theorem[10]:

Theorem 1: If $\Omega_N = (N!)^{-1/2}\det_{N\times N} f_n(\mathbf{x}_m)$ and $\int d\mathbf{x} f_n(\mathbf{x})^* f_m(\mathbf{x}) = \delta_{n,m}$, then

$$R_n(\mathbf{x}_1\cdots\mathbf{x}_n) = N!/(N-n)!\int d\mathbf{x}_{n+1}\cdots\int d\mathbf{x}_N|\Omega_N|^2 = \det_{n\times n}[K_N(\mathbf{x}_r, \mathbf{x}_s)]$$

where

$$K_N(\mathbf{y}, \mathbf{x}) = \sum_{m=1}^{N} f_m(\mathbf{y})^* f_m(\mathbf{x})$$

For the free Fermi ground state, $f_n(\mathbf{x}) = V^{-1/2}\times\exp(i\mathbf{k}_n\cdot\mathbf{x})$. Therefore, the correlation functions are given by

$$R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n) = \det_{n\times n}[G_N(\mathbf{x}_r - \mathbf{x}_s)], \tag{5.4}$$

where

$$G_N(\mathbf{x}) = V^{-1}\sum_{|\mathbf{k}_n|<k_f} \exp(i\mathbf{k}_n\cdot\mathbf{x}). \tag{5.5}$$

In the N/V limit

$$G_N(\mathbf{x}) \to G(\mathbf{x}) = (2\pi)^{-3}\int_{|\mathbf{k}|<k_f} d^3k \exp(i\mathbf{k}\cdot\mathbf{x}) = 3\bar\rho(\sin z - z\cos z)/z^3|_{z=k_f|\mathbf{x}|} \tag{5.6}$$

and $R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n) \to R_n(\mathbf{x}_1\cdots\mathbf{x}_n) = \det_{n\times n} G(\mathbf{x}_r - \mathbf{x}_s)$.

In order to obtain $L(f)$ in the N/V limit from Eq. (2.7), we must show $R_n^{(N)}$ is bounded. To do this, we need to introduce a few theorems on matrices.

Let L be a linear vector space with an inner product $(\cdot,\cdot)$ and let $w_1, w_2\cdots w_n \in L$. The quantity

$$V(w_1, w_2\cdots w_n) = [\det_{n\times n}(w_r, w_s)]^{1/2}$$

can be interpreted as the volume of a hyperparallelepiped formed from the vectors $w_1, w_2\cdots w_n$.[11]

Let

$h_1 = (w_1, w_1)^{1/2}$,

$h_r =$ the magnitude of the component of vector w_r orthogonal to the subspace spanned by the vectors $w_1, w_2, \ldots, w_{r-1}$.

Then it can be shown that[11]

$$V(w_1, w_2\cdots w_n) = h_1 h_2\cdots h_n$$

By using this relation the following result can easily be proved:

Theorem 2: $V(w_1\cdots w_n) \le V(w_1\cdots w_r)V(w_{r+1}\cdots w_n)$

Corollary 1: $V(w_1\cdots w_n) \le V(w_1)V(w_2)\cdots V(w_n)$

In Sec. 6 we will need the following corollary:

Corollary 2 (*Hadamard's Theorem*): If A is an $N\times N$ matrix, then

$$|\det A|^2 \le \prod_{j=1}^{N}\left(\sum_{k=1}^{N}|A_{jk}|^2\right).$$

Proof: Apply Corollary 1 to the matrix $A^\dagger A$.

Corollary 3: If A is an $N\times N$ matrix and $|A_{jk}| < c$ for $1\le j, k\le N$, then $|\det A| < c^N N^{N/2}$.

We can now show the correlation functions are bounded. Let the vector space L be $\{(a_1, a_2\cdots a_N); a_j \in \mathbb{C}\}$ with inner produce $(A, B) = V^{-1}\sum_{j=1}^{N} a_j^* b_j$, and let X_r be the vector with components $(X_r)_j = \exp(i\mathbf{k}_j\cdot\mathbf{x}_r)$. Then

$$G_N(\mathbf{x}_r - \mathbf{x}_s) = (X_r, X_s) \quad\text{and}\quad R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n) = \det_{n\times n}(X_r, X_s).$$

By Theorem 2,

$$R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n) \le R_r^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_r)R_{n-r}^{(N)}(\mathbf{x}_{r+1}\cdots\mathbf{x}_n).$$

Furthermore, by Corollary 1,

$$R_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n) \le R_1^{(N)}(\mathbf{x}_1)\cdots R_1^{(N)}(\mathbf{x}_n) = \bar\rho^n.$$

We can now obtain the generating functional for a free Fermi gas in the N/V limit from Eq. (2.7). The result is

$$L(f) = \sum_{n=0}^{\infty}\frac{1}{n!}\int d\mathbf{x}_1\cdots\int d\mathbf{x}_n F(\mathbf{x}_1)\cdots F(\mathbf{x}_n) \det_{n\times n} G(\mathbf{x}_r - \mathbf{x}_s), \tag{5.7}$$

where $F(\mathbf{x})=\exp[if(\mathbf{x})-1]$ and $G(\mathbf{x})$ is given by Eq. (5.6).

An alternative expression for $L(f)$ can also be derived. For this purpose we will use the identity

$$\int d\mathbf{x}_1\cdots\int d\mathbf{x}_N(\det_{N\times N}[h_r(\mathbf{x}_s)])^*(\det_{N\times N}[g_r(\mathbf{x}_s)])$$
$$=N!\,\det_{N\times N}[\int d\mathbf{x}h_r(\mathbf{x})^*g_s(\mathbf{x})]. \tag{5.8}$$

Now, using Eqs. (2.5) and (5.2), we obtain, for the N-particle generating functional,

$$L_N(f)=(1/N!)\int_V(d\mathbf{x}_N/V)\cdots\int_V(d\mathbf{x}_N/V)$$
$$\times\det_{N\times N}[\exp(i\mathbf{k}_n\cdot\mathbf{x}_m)]\exp[if(\mathbf{x}_1)]\cdots\exp[if(\mathbf{x}_N)]$$
$$\times\det_{N\times N}[\exp(i\mathbf{k}_n\cdot\mathbf{x}_m]$$
$$=\det_{N\times N}\{\int(d\mathbf{x}/V)\exp[if(\mathbf{x})]\exp[i(\mathbf{k}_n-\mathbf{k}_m)\cdot\mathbf{x}]\} \tag{5.9}$$
$$=\det_{N\times N}\{\delta_{m,n}+\int_V(d\mathbf{x}/V)(\exp[if(\mathbf{x})]-1)$$
$$\times\exp[i(\mathbf{k}_n-\mathbf{k}_m)\cdot\mathbf{x}]\}.$$

By using the expansion

$$\det(\delta_{m,n}+A_{m,n})=\exp\{\mathrm{Tr}[\ln(\delta_{m,n}+A_{m,n})]\}$$
$$=\exp\left(\sum_{n=1}^{\infty}\frac{(-)^{(n-1)}}{n}\mathrm{Tr}\,A^n\right), \tag{5.10}$$

Eq. (5.9) becomes

$$L_N(f)=\exp\left(\sum_{n=1}^{\infty}\frac{(-)^{n-1}}{n!}\int_V d\mathbf{x}_1\cdots\int_V d\mathbf{x}_n\right.$$
$$\left.\times F(\mathbf{x}_1)\cdots F(\mathbf{x}_n)T_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n)\right), \tag{5.11}$$

where

$$T_n^{(N)}(\mathbf{x}_1\cdots\mathbf{x}_n)$$
$$=(n-1)!\,(1/V)\sum_{\mathbf{k}_1}\cdots(1/V)\sum_{\mathbf{k}_n}(\exp[i(\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{x}_1]$$
$$\times\exp[i(\mathbf{k}_2-\mathbf{k}_3)\cdot\mathbf{x}_2]\cdots\exp[i(\mathbf{k}_n-\mathbf{k}_1)\cdot\mathbf{x}_n])$$
$$=(n-1)!\,G_N(\mathbf{x}_1-\mathbf{x}_2)G_N(\mathbf{x}_2-\mathbf{x}_3)\cdots G_N(\mathbf{x}_n-\mathbf{x}_1). \tag{5.12}$$

In the N/V limit

$$L_N(f)\to L(f)$$
$$=\exp\left(\sum_{n=1}^{\infty}\frac{(-)^{n-1}}{n!}\int d\mathbf{x}_1\cdots\int d\mathbf{x}_nF(\mathbf{x}_1)\cdots F(\mathbf{x}_n)T_n(\mathbf{x}_1\cdots\mathbf{x}_n)\right), \tag{5.13}$$

where

$$T_n(\mathbf{x}_1\cdots\mathbf{x}_n)=(n-1)!\;G(\mathbf{x}_1-\mathbf{x}_2)\,G(\mathbf{x}_2-\mathbf{x}_3)\cdots G(\mathbf{x}_n-\mathbf{x}_1). \tag{5.14}$$

Furthermore, $(1/n!)\sum_{\mathrm{perm}}T_n(\mathbf{x}_{\tau_1}\cdots\mathbf{x}_{\tau_n})$ are the cluster functions of the correlation functions $R_n(\mathbf{x}_1\cdots\mathbf{x}_n)$. The expansion for $L(f)$ given in Eq. (5.13) was discussed in the previous paper.[6]

With a little more work $L(f,\mathbf{g})$ can be calculated explicitly by similar means. The result is

$$L(f,\mathbf{g})=\sum_{n=0}^{\infty}\frac{1}{n!}\int d\mathbf{x}_1\int d\mathbf{y}_1\cdots\int d\mathbf{x}_n\int d\mathbf{y}_n$$
$$\prod_{r=1}^{n}[\delta(\mathbf{x}_r-\mathbf{y}_r)\{\exp[if(\mathbf{x}_r)]\exp[ij(\mathbf{x}_r,\mathbf{g})]-1\}]$$
$$\times R_n(\mathbf{y}_1\cdots\mathbf{y}_n;\,\mathbf{x}_1\cdots\mathbf{x}_n), \tag{5.15}$$

where

$$R_n(\mathbf{y}_1\cdots\mathbf{y}_n;\,\mathbf{x}_1\cdots\mathbf{x}_n)=\det_{n\times n}[G(\mathbf{x}_r-\mathbf{y}_s)] \tag{5.16}$$

and

$$j(\mathbf{x},\mathbf{g})=-\tfrac{1}{2}i[2\mathbf{g}(\mathbf{x})\cdot\nabla+(\nabla\cdot\mathbf{g})(\mathbf{x})].$$

Alternatively,

$$L(f,\mathbf{g})=\exp\sum_{n=1}^{\infty}\frac{(-)^{n-1}}{n!}\int d\mathbf{x}_1\int d\mathbf{y}_1\cdots\int d\mathbf{x}_n\int d\mathbf{y}_n$$
$$\times\prod_{r=1}^{n}[\delta(\mathbf{x}_r-\mathbf{y}_r)\{\exp[if(\mathbf{x}_r)]\exp[ij(\mathbf{x}_r,\mathbf{g})]-1\}]$$
$$\times T_n(\mathbf{y}_1\cdots\mathbf{y}_n;\,\mathbf{x}_1\cdots\mathbf{x}_n), \tag{5.17}$$

where

$$T_n(\mathbf{y}_1\cdots\mathbf{y}_n;\,\mathbf{x}_1\cdots\mathbf{x}_n)$$
$$=(n-1)!\,G(\mathbf{x}_1-\mathbf{y}_2)G(\mathbf{x}_2-\mathbf{y}_3)\cdots G(\mathbf{x}_n-\mathbf{y}_1). \tag{5.18}$$

Remark: Clearly $R_n(\mathbf{x}_1\cdots\mathbf{x}_n;\,\mathbf{x}_1\cdots\mathbf{x}_n)=R_n(\mathbf{x}_1\cdots\mathbf{x}_n)$. Furthermore, it can be shown that $|R_n(\mathbf{y}_1\cdots\mathbf{y}_n;\,\mathbf{x}_1\cdots\mathbf{x}_n)|^2\le R_n(\mathbf{y}_1\cdots\mathbf{y}_n)R_n(\mathbf{x}_1\cdots\mathbf{x}_n)$.

In three dimensions neither the functional equation for $L(f)$ nor an expression for the Hamiltonian in terms of ρ and J are known at present. However, for a one-dimensional free Fermi gas both of them will be given in the next section.

Remarks: (1) For a Fermi gas in an external potential the correlation functions have the same form as those for a free Fermi gas. Only the function $G(\mathbf{x})$ occurring in Eqs. (5.16) and (5.18) need be changed.

(2) It can be shown that $L(f)$ for a free Fermi gas satisfies the cluster decomposition property [Eq. (2.11)]. As a result, representations with different average densities are unitarily inequivalent. Also, the free Bose and free Fermi representations are unitarily inequivalent since their generating functionals are unequal and satisfy translational invariance and the cluster decomposition property.

(3) For both the free Bose gas and the free Fermi gas there is nothing in the Hamiltonian to set a scale of distance. Consequently, a scale transformation can only effect the average density. It can be shown for both cases that $R_{n,\bar\rho}(\mathbf{x})=(\bar\rho/\rho_0)^nR_{n,\bar\rho_0}((\bar\rho/\rho_0)^{1/3}\mathbf{x})$. As a result,

$$L_{\bar\rho}(f)=L_{\rho_0}(f_{\bar\rho/\rho})\quad\text{where }f_{\bar\rho/\rho_0}(\mathbf{x})=f((\bar\rho/\rho_0)^{1/3}\mathbf{x}). \tag{5.19}$$

(4) The cluster decomposition property expressed in terms of the correlation functions is trivial for a free

Bose gas since

$$R_{n+m}=\bar{\rho}^{n+m}=\bar{\rho}^{n}\bar{\rho}^{m}=R_nR_m.$$

For the free Fermi Gas it can be shown that

$$R_{n+m}(\mathbf{x}_1\cdots\mathbf{x}_n,\ \mathbf{y}_1+\mathbf{a},\cdots,\ \mathbf{y}_m+\mathbf{a})$$

$$=\det_{(n+m)\times(n+m)}\begin{pmatrix}G(\mathbf{x}_r-\mathbf{x}_s) & O(1/a^2)\\ O(1/a^2) & G(\mathbf{y}_p-\mathbf{y}_q)\end{pmatrix}$$

$$\to\det_{n\times n}G(\mathbf{x}_r-\mathbf{x}_s)\det_{m\times m}G(\mathbf{y}_p-\mathbf{y}_q)\quad\text{as }|\mathbf{a}|\to\infty$$

$$=R_n(\mathbf{x}_1\cdots\mathbf{x}_n)\,R_m(\mathbf{y}_1\cdots\mathbf{y}_m).$$

6. FOURTH EXAMPLE: INTERACTION OF THE FORM $\lambda(\lambda-1)/x^2$ IN ONE DIMENSION

In this section we will calculate the generating functional and find an expression for the Hamiltonian in terms of ρ and J for a one-dimensional Bose gas interacting via a two-body potential $U(x)=2/x^2$. We first consider a system consisting of N particles on a ring of length L. We can associate a periodic potential with the potential g/x^2 by writing

$$U(x)=g\sum_{n=-\infty}^{\infty}(x+nL)^{-2}=\frac{g\pi^2}{L^2}\left[\sin\left(\frac{\pi x}{L}\right)\right]^{-2}. \qquad (6.1)$$

Sutherland[12] has found the exact N particle ground state for this potential. We will first write his results in terms of currents and then proceed to the N/V limit.

Consider the N-particle wave function

$$\Psi_N=\prod_{j<k=1}^{N}|\psi(x_j-x_k)|^{\lambda}. \qquad (6.2)$$

Suppose $\psi(x)=\pm\psi(-x)$. Let $\varphi(x)=(d/dx)\ln\psi=\psi'/\psi(x)$. Then $\varphi(x)=-\varphi(-x)$ and $\varphi(0)=0$ (if ψ is well behaved). By direct computation it can be shown that

$$-\tfrac{1}{2}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2}\Psi_N=\Big(-\tfrac{1}{2}\lambda\sum_{j\neq k}[\varphi'(x_j-x_k)+\lambda\varphi(x_j-x_k)^2]$$

$$+\tfrac{1}{2}\lambda^2\sum_{j\neq k\neq m}\varphi(x_j-x_k)\varphi(x_k-x_m)\Big)\Psi_N. \qquad (6.3)$$

If there is a function $\alpha(x)$ such that

$$\varphi(x_1-x_2)\varphi(x_2-x_3)+\varphi(x_2-x_3)\varphi(x_3-x_1)+\varphi(x_3-x_1)\varphi(x_1-x_2)$$

$$=\alpha(x_1-x_2)+\alpha(x_2-x_3)+\alpha(x_3-x_1), \qquad (6.4)$$

then

$$\Big(-\tfrac{1}{2}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2}+\tfrac{1}{2}\sum_{j\neq k}U(x_j-x_k)\Big)\Psi_N=0, \qquad (6.5)$$

where

$$U(x)=\lambda\varphi'(x)+\lambda^2\varphi(x)^2-\lambda^2(N-2)\alpha(x). \qquad (6.6)$$

Remark: We have started with a special form for a wavefunction Ψ and constructed a potential such that Ψ is an eigenvalue of Schrodinger's equation. This procedure (due to Sutherland[12]) only works when functions Ψ and α can be found such that Eq. (6.4) is satisfied.

It is easy to show that $K(x)\Psi_N=2\lambda\rho(x)\int dy\,\varphi(x-y)\rho(y)\Psi_N$. Let

$$\tilde{K}(x)=K(x)-2\lambda\rho(x)\int dy\,\varphi(x-y)\rho(y). \qquad (6.7)$$

If Ψ is the ground state, then the Hamiltonian, given by Eq. (2.9), can be written as

$$H_N=\tfrac{1}{8}\int_{-L/2}^{L/2}\tilde{K}(x)^\dagger\frac{1}{\rho(x)}\tilde{K}(x). \qquad (6.8)$$

We will check that this Hamiltonian formally agrees with what is expected for a system of particles interacting via the two body potential $U(x)$. Substituting Eq. (6.7) into Eq. (6.8), we obtain

$$H=\tfrac{1}{8}\int dx\,K(x)^\dagger\frac{1}{\rho(x)}K(x)$$

$$+\tfrac{1}{2}\lambda^2\int dx\int dy\int dz\,\rho(x)\rho(y)\rho(z)\varphi(x-y)\varphi(x-z)$$

$$=\tfrac{1}{4}\lambda\int dx\int dy\,\varphi(x-y)[K(x)^\dagger\rho(y)+\rho(y)K(x)]. \qquad (6.9)$$

We can identify $\tfrac{1}{8}\int dx\,K(x)^\dagger[1/\rho(x)]K(x)$ with the kinetic energy (for bosons). From the commutation relations [Eq. (2.1)] we find

$$K(x)^\dagger\rho(y)+\rho(y)K(x)=2\frac{d}{dx}\rho(x)\rho(y)+2\frac{d}{dy}[\delta(x-y)\rho(y)]$$

and from Eq. (2.2)

$$-\int dx\int dy\,\varphi(x-y)[K(x)^\dagger\rho(y)+\rho(y)K(x)]$$

$$=\int dx\int dy\,\rho(x)(\rho(y)-\delta(x-y))\varphi'(x-y)$$

$$=\sum_{j\neq k}\varphi'(x_j-x_k).$$

Furthermore,

$$\int dx\int dy\int dz\,\rho(x)\rho(y)\rho(z)\varphi(x-y)\varphi(x-z)$$

$$=\sum_{j,k,m}\varphi(x_j-x_k)\varphi(x_j-x_m)$$

$$=-\sum_{j\neq k\neq m}\varphi(x_k-x_j)\varphi(x_j-x_m)+\sum_{j\neq k}\varphi(x_j-x_k)^2.$$

Therefore, Eq. (6.9) becomes

$$H=-\tfrac{1}{2}\sum_j\frac{\partial}{\partial x_j^2}+\tfrac{1}{2}\lambda\sum_{j\neq k}[\varphi'(x_j-x_k)+\varphi(x_j-x_k)^2]$$

$$-\tfrac{1}{2}\lambda^2\sum_{j\neq k\neq m}\varphi(x_j-x_k)\varphi(x_k-x_m)$$

$$=-\tfrac{1}{2}\sum_j\frac{\partial^2}{\partial x_j^2}+\tfrac{1}{2}\sum_{j\neq k}U(x_j-x_k)$$

$$=\tfrac{1}{8}\int dx\,K(x)^\dagger\frac{1}{\rho(x)}K(x)$$

$$+\tfrac{1}{2}\int dx\int dy\,\rho(x)[\rho(y)-\delta(x-y)]U(x-y). \qquad (6.10)$$

This is the expected form of the Hamiltonian.

It can also be verified that the generating functional,

$$L_N(f)=\int_{-L/2}^{L/2}dx_1\cdots\int_{-L/2}^{L/2}dx_N|\Psi_N|^2\exp[if(x_1)]\cdots\times\exp[if(x_N)]$$

satisfies the functional equation

$$\left(\frac{d}{dx}-if'(x)\right)\frac{1}{i}\frac{\delta}{\delta f(x)}L_N(f)=2\lambda\int_{-L/2}^{L/2}dy\,\varphi(x-y)\frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)}L_N(f). \tag{6.11}$$

We will now consider the case (Sutherland[12]) in which

$$\psi(x)=\sin(\pi x/L),\quad \varphi(x)=(\pi/L)\cot(\pi x/L),\quad\text{and}\quad g=\lambda(\lambda-1).$$

Then the normalized wavefunction,

$$\Psi_N=\{(\lambda!)^N/[(\lambda N)!L^N]\}^{1/2}\prod_{j>k}|2\sin[\pi(x_j-x_k)/L]|^\lambda \tag{6.12}$$

with $\int_{-L/2}^{L/2}dx_1\cdots\int_{-L/2}^{L/2}dx_N|\Psi_N|^2=1$,

satisfies the Schrödinger equation

$$H\Psi_N=(\lambda^2\pi^2N/6)\cdot(N^2-1)/L^2\Psi_N \tag{6.13}$$

with

$$H=-\tfrac{1}{2}\sum_j\frac{\partial^2}{\partial x_j^2}+\tfrac{1}{2}g\sum_{j\neq k}\frac{\pi^2}{L^2}\left[\sin\left(\frac{\pi(x_j-x_k)}{L}\right)\right]^{-2} \tag{6.14}$$

It also turns out Ψ is the Bose ground state for this Hamiltonian.[12]

A Fermi wavefunction for this Hamiltonian can also be constructed. Let $R=$ the region for which $x_1<x_2<\cdots<x_n$. Let P be the permutation such that $(x_{p_1}, x_{p_2},\ldots,x_{p_n})\in R$. Define $\Psi_F=(-)^P\Psi$. To see that Ψ_F is the Fermi ground state notice: (i) Ψ_F is antisymmetric, (ii) Ψ_F satisfies the Schrödinger equation in the region R, (iii) for $\lambda>1$, if $x_k=x_m$ for any $k\neq m$, then $\Psi=\Psi_F=0$ and $(d/dx)\Psi=(d/dx)\Psi_F=0$. Therefore, Ψ_F and $(d/dx)\Psi_F$ are continuous at the boundary of the region R. Finally, if N is odd, then Ψ_F is periodic; i.e., $\Psi_F(-\tfrac{1}{2}L, x_2,\ldots,x_N)=\Psi_F(x_2,\ldots,x_N,\tfrac{1}{2}L)$.

Since $L_N(f)$ depends only on $|\Psi|^2$, for this interaction it is the same for both bosons and fermions. Also,

$$L_N(f,g)=\int_{-L/2}^{L/2}dx_1\cdots\int_{-L/2}^{L/2}dx_N\times\Psi_N(x_1\cdots x_N)\exp[if(x_1)]\cdots\exp[if(x_N)]J(x_1)^{1/2}\cdots\times J(x_N)^{1/2}\Psi_N(\xi(x_1),\ldots,\xi(x_N))],$$

where ξ is the flow corresponding to the vector field g, and $J(x)=[(d/dx)\xi](x)$. Since $\Psi_F(x_1\cdots x_N)=(-)^P\Psi$ and $\Psi_F(\xi(x_1),\ldots,\xi(x_N))=(-)^{P'}\Psi$, and the flow ξ is a one-to-one continuous map on a ring, $(-)^P=(-)^{P'}$. As a result $L(f,g)$ is the same for both bosons and fermions. Therefore, for this particular one-dimensional example the boson and fermion representations of the ρ,J algebra are unitarily equivalent. This result depends crucially on the nature of flows in one dimension; i.e., there are no flows that can interchange two points. In three dimensions we expect the bose and fermi generating functionals $L(f,g)$ to give rise to inequivalent representations of the ρ,J algebra.

As the coupling constant is changed continuously the ground state wavefunction changes continuously. When $\lambda\to1$, the coupling constant $g=\lambda(\lambda-1)\to0$. Since the potential is infinite when two particles are at the same point, the ground state wavefunction must vanish for those points. Thus we might expect the Fermi ground state (Ψ_F) to go to the free Fermi ground state as $\lambda\to1$, while the Bose ground state (Ψ) changes abruptly in character when $\lambda\to1$. This result is in fact true. When $\lambda=1$, $(d/dx_j)\Psi|_{x_j=x_k}$ is no longer continuous. Therefore, Ψ no longer satisfies Schrödinger's equation (6.13). However, it can be shown[12] that

$$\Psi_F=(N!L^N)^{-1/2}\prod_{j>k}[2\sin(\pi(x_j-x_k)/L)]=(N!L^N)^{-1/2}\det_{N\times N}[\exp(ik_mx_n)]$$

where $k_m=2\pi m/L$ and $m=-\tfrac{1}{2}(N-1), -\tfrac{1}{2}(N-3),\ldots,\tfrac{1}{2}(N-1)$

= the free Fermi ground state (in one dimension) for N particles.

Since for this interaction $L(f)$ is the same for both bosons and fermions as $\lambda\to1$, $L(f)\to$ the generating function for a free Fermi gas (in one dimension).

A. The case λ = 1: The free Fermi gas in one dimension

We will now examine the N/V limit for a free Fermi gas in one dimension. From Eqs. (6.7), (6.8), and 6.11 we have for N free Fermions on a ring of length L

$$\tilde{K}_N(x)=K(x)-2\int_{-L/2}^{L/2}dy\frac{\pi}{L}\cot\left(\frac{\pi(x-y)}{L}\right)\rho(x)\rho(y), \tag{6.15}$$

$$H_N=\tfrac{1}{8}\int_{-L/2}^{L/2}dx\,\tilde{K}_N(x)^\dagger\frac{1}{\rho(x)}\tilde{K}_N(x), \tag{6.16}$$

$$\left(\frac{d}{dx}-if'(x)\right)\frac{1}{i}\frac{\delta}{\delta f(x)}L_N(f)=2\int_{-L/2}^{L/2}dy\frac{\pi}{L}\cot\left(\frac{\pi(x-y)}{L}\right)\times\frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)}L_N(f). \tag{6.17}$$

If we could interchange the N/V limit with the integrals in Eq. (6.15), we would obtain

$$\tilde{K}(x)=K(x)-2\int_{-\infty}^{\infty}dy\frac{1}{(x-y)}\rho(x)\rho(y), \tag{6.18}$$

$$H=\tfrac{1}{8}\int_{-\infty}^{\infty}dx\,\tilde{K}(x)^\dagger\frac{1}{\rho(x)}\tilde{K}(x), \tag{6.19}$$

$$\left(\frac{d}{dx}-if'(x)\right)\frac{1}{i}\frac{\delta}{\delta f(x)}L(f)$$

$$=2\int_{-\infty}^{\infty} dy \frac{1}{(x-y)} \frac{1}{i} \frac{\delta}{\delta f(x)} \frac{1}{i} \frac{\delta}{\delta f(y)} L(f). \qquad (6.20)$$

In Sec. 5 we calculated $L(f)$ in the N/V limit for a free Fermi gas in three dimensions. By a similar calculation, $L(f)$ in the N/V limit for a free Fermi gas in one dimension is given by Eq. (5.7) with

$$G(x)=\int_{-k_f}^{k_f} \frac{dk}{2\pi} \exp(ikx)=\frac{1}{\pi x} \sin k_f x, \quad \text{where } \bar{\rho}=\frac{k_f}{\pi}.$$

Since we know $L(f)$ in the N/V limit, we can verify that Eq. (6.19) gives the correct Hamiltonian by checking that Eq. (6.20) for $L(f)$ is satisfied.

Remark: The singular nature of the term $1/(x-y)$ appearing in Eqs. (6.18) and (6.20) makes it necessary to consider the integrals as the principle value, $P\int dy[1/(x-y)]\cdot=\lim_{\epsilon\to 0}(\int_{\epsilon}^{\infty}+\int_{-\infty}^{-\epsilon})dy[1/(x-y)]\cdot$, or as the limit of a sequence $\lim_{\epsilon\to 0}\int_{-\infty}^{\infty} dy(x-y)/[\epsilon^2+(x-y)^2]$. In addition we will need to take advantage of the antisymmetry. Therefore, we will use, $\int_{-\infty}^{\infty} dy/(x-y)\cdot = \lim_{L\to\infty} P\int_{-L}^{L} dy/(x-y)\cdot$ and as a result $\int_{-\infty}^{\infty} dy/(x-y)\cdot \text{const}=0$. Alternatively the right-hand side of Eq. (6.20) may be written as

$$[\text{rhs Eq. (6.20)}]=2P\int_{-\infty}^{\infty} \frac{dy}{(x-y)} \frac{1}{i} \frac{\delta}{\delta f(x)} \times\left(\frac{1}{i} \frac{\delta}{\delta f(y)}-\bar{\rho}\right)L(f).$$

Recall that

$$L(f)=\sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1\cdots \int dx_n (\exp[if(x_1)]-1)\cdots (\exp[if(x_n)]-1)R_n.$$

Therefore,

$$\left(\frac{d}{dx_1}-if'(x_1)\right)\frac{1}{i}\frac{\delta}{\delta f(x_1)}L(f) =\sum_{n=2}^{\infty} \frac{1}{(n-1)!} \exp[if(x_1)]\int dx_2\cdots\int dx_n \times(\exp[if(x_2)]-1)\cdots (\exp[if(x_n)]-1)\frac{d}{dx_1}R_n$$

and

$$\frac{1}{i}\frac{\delta}{\delta f(x_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2)}L(f) =\sum_{n=2}^{\infty} \frac{1}{(n-2)!} \exp[if(x_1)]\exp[if(x_2)]\int dx_3\cdots\int dx_n \times[(\exp[if(x_3)]-1)\cdots (\exp[if(x_n)]-1)R_n] +\delta(x_1-x_2)\frac{1}{i}\frac{\delta}{\delta f(x_1)}L(f).$$

Due to the principle value the $\delta(x_1-x_2)$ term will vanish when integrated. Therefore,

$$P\int \frac{dx_2}{x_1-x_2}\frac{1}{i}\frac{\delta}{\delta f(x_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2)}L(f)$$

$$=\sum_{n=2}^{\infty}\frac{\exp[if(x_1)]}{(n-2)!}P\int dx_2\frac{\exp[if(x_2)]}{x_1-x_2}\int dx_3\cdots\int dx_n \times(\exp[if(x_3)]-1)\cdots(\exp[if(x_n)]-1)R_n$$

$$=\sum_{n=2}^{\infty}\frac{\exp[if(x_1)]}{(n-1)!}\int dx_2\cdots\int dx_n(\exp[if(x_2)]-1)\cdots(\exp[if(x_n)]-1) \times\left(\sum_{j=2}^{n}\frac{R_n}{x_1-x_j}+P\int dx_{n+1}\frac{R_{n+1}}{x_1-x_{n+1}}\right)$$

Remark: In the case we are considering $R_{n+1}/(x_1-x_{n+1})$ is a continuous function. Therefore the principle value is not needed and interchanging the order of integration is valid.

Equation (6.20) can now be written as

$$\sum_{n=2}^{\infty}\frac{\exp[if(x_1)]}{(n-1)!}\int dx_2\cdots\int dx_n(\exp[if(x_2)]-1)\cdots(\exp[if(x_n)]-1) \times\left(\frac{1}{2}\frac{d}{dx_1}R_n-\sum_{j=2}^{n}\frac{R_n}{x_1-x_j}-\int dx_{n+1}\frac{R_{n+1}}{x_1-x_{n+1}}\right)=0.$$

Therefore, to show that $L(f)$ satisfies Eq. (6.20), it is sufficient to show that

$$\frac{1}{2}\frac{d}{dx_1}R_n=\sum_{j=2}^{n}\frac{R_n}{x_1-x_j}+\int dx_{n+1}\frac{R_{n+1}}{x_1-x_{n+1}}. \qquad (6.21$$

Recall that

$$R_n=\det_{n\times n}[G(x_r-x_s)] =\int_{-k_f}^{k_f}\frac{dk_1}{2\pi}\cdots\int_{-k_f}^{k_f}\frac{dk_n}{2\pi}\det_{n\times n}\{\exp[i(k_r-k_s)x_r]\}.$$

Let the matrix

$$A_{n-1}\begin{pmatrix}1\cdots \hat{r}'\cdots n\\ 1\cdots \hat{s}'\cdots n\end{pmatrix}=A_{rs},$$

where $A_{rs}=\exp[k_r-k_s)x_r]$ and $r=1,2,\ldots,n$ with r' deleted and $s=1,2,\ldots,n$ with s' deleted. By expanding the determinant by minors twice, first by the $(n+1)$ column and then by the $(n+1)$ row, we obtain

$$\det A_{n+1}\begin{pmatrix}1\cdots n+1\\ 1\cdots n+1\end{pmatrix} =\det A_n\begin{pmatrix}1\cdots n\\ 1\cdots n\end{pmatrix}-\sum_{r,s=1}^{n}(-)^{r+s}\exp[i(k_r-k_{n+1})x_r] \times\exp[i(k_{n+1}-k_s)x_{n+1}]\det A_{n-1}\begin{pmatrix}1\cdots \hat{r}\cdots n\\ 1\cdots \hat{s}\cdots n\end{pmatrix}.$$

As a result we have

$$P\int_{-\infty}^{\infty}\frac{dx_{n+1}}{x_1-x_{n+1}}R_{n+1} =\int\frac{dk_1}{2\pi}\cdots\int\frac{dk_n}{2\pi}\sum_{r,s=1}^{n}-(-)^{r+s}\det A_{n-1}\begin{pmatrix}1\cdots \hat{r}\cdots n\\ 1\cdots \hat{s}\cdots n\end{pmatrix}$$

$$\times \int \frac{dk_{n+1}}{2\pi} \exp[i(k_r - k_{n+1})x_r]\, P\int_{-\infty}^{\infty} \frac{dx_{n+1}}{x_1 - x_{n+1}}$$

$$\times \exp[i(k_{n+1} - k_s)x_{n+1}],$$

$$P\int_{-\infty}^{\infty} \frac{dx_{n+1}}{x_1 - x_{n+1}} \exp[i(k_{n+1} - k_s)x_{n+1}$$

$$= \exp[i(k_{n+1} - k_s)x_1(-i)\int_{-\infty}^{\infty} \frac{dy}{y} \sin(k_{n+1} - k_s)y$$

$$= -i\pi\, \mathrm{sgn}(k_{n+1} - k_s) \exp[i(k_{n+1} - k_s)x_1]$$

and

$$\int_{-k_f}^{k_f} \frac{dk_{n+1}}{2\pi} \exp[i(k_r - k_{n+1})x_r](-i\pi)\, \mathrm{sgn}(k_{n+1} - k_s)$$

$$\times \exp[i(k_{n+1} - k_s)x_1] = \frac{\exp[i(k_r - k_s)x_r}{x_1 - x_r}$$

$$- \exp(ik_r x_r)\exp(-ik_s x_1)\frac{\cos[k_f(x_1 - x_r)]}{x_1 - x_r}.$$

Therefore,

$$P\int \frac{dx_{n+1}}{x_1 - x_{n+1}} R_{n+1}$$

$$= \int \frac{dk_1}{2\pi} \cdots \int \frac{dk_n}{2\pi} \sum_{r,s=1}^{n} -(-)^{r+s}\Bigg(\frac{\exp[i(k_r - k_s)x_r]}{x_1 - x_r}$$

$$- \exp(ik_r x_r)\exp(-ik_s x_1)\frac{\cos[k_f(x_1 - x_r)]}{x_1 - x_r}\Bigg)$$

$$\times \det A_{n-1}\begin{pmatrix} 1 \cdots \hat{r} \cdots n \\ 1 \cdots \hat{s} \cdots n \end{pmatrix}. \qquad (6.22)$$

When $r \neq 1$, the first term equals $\sum_{r=2}^{n}[-1/(x_1 - x_r)]\det A_n$, while the second term vanishes since

$$\sum_{s=1}^{n}(-)^s \exp(-ik_s x_1)\det A_{n-1}\begin{pmatrix} 1 \cdots \hat{r} \cdots n \\ 1 \cdots \hat{s} \cdots n \end{pmatrix}$$

is equal to a determinant with the 1st and rth rows proportional. For $r = 1$ the two terms added together give

$$\sum_{s=1}^{n}(-)^s ik_s \exp[i(k_1 - k_s)x_1 \det A_{n-1}\begin{pmatrix} 2 & \cdots & n \\ 1 \cdots & \hat{s} \cdots & n \end{pmatrix}.$$

Next consider

$$\frac{d}{dx}R_n = \frac{d}{dx_1}\det G(x_r - x_s)$$

$$= \det\begin{pmatrix} 0 & G'(x_1 - x_2) & \cdots & G'(x_1 - x_n) \\ G(x_2 - x_1) & G(x_2 - x_2) & \cdots & G(x_2 - x_n) \\ & \cdot \quad \cdot \quad \cdot & & \\ G(x_n - x_1) & G(x_n - x_2) & \cdots & G(x_n - x_n) \end{pmatrix}$$

$$- \det\begin{pmatrix} 0 & G(x_1 - x_2) & \cdots & G(x_1 - x_n) \\ G'(x_2 - x_1) & G(x_2 - x_2) & \cdots & G(x_2 - x_n) \\ & \cdot \quad \cdot \quad \cdot & & \\ G'(x_n - x_1) & G(x_n - x_2) & \cdots & G(x_n - x_n) \end{pmatrix}.$$

Since $G(x) = G(-x)$, $G'(x) = -G'(-x)$, and $\det A = \det A^T$, we have

$$\frac{d}{dx_1}R_n = -2\det\begin{pmatrix} G'(x_1 - x_1)G(x_1 - x_2) \cdots G(x_1 - x_n) \\ \cdot \quad \cdot \quad \cdot \\ G'(x_n - x_1)G(x_n - x_2) \cdots G(x_n - x_n) \end{pmatrix}$$

$$= \int \frac{dk_1}{2\pi} \cdots \int \frac{dk_n}{2\pi} \sum_{s=1}^{n}(-)^{s+1}(-2ik_s)\exp[i(k_1 - k_s)x_1]$$

$$\times \det A_{n-1}\begin{pmatrix} 2 & \cdots & n \\ 1 \cdots & \hat{s} \cdots & n \end{pmatrix}.$$

Substituting these results into Eq. (6.22), we obtain Eq. (6.21). Therefore, we can conclude the Hamiltonian in the N/V limit for a free Fermi gas in one dimension is given by Eq. (6.19).

B. The case $\lambda = 2$: Interacting potential $2/x^2$ in one dimension

We will now derive the generating functional and Hamiltonian for the interacting case when $\lambda = 2$, $[U(x) = 2/x^2]$. We begin by computing the N-particle correlation functions. Substituting equation 6.12 into equation 2.5, we obtain

$$R_n^{(N)}(x_1 \cdots x_n) = \frac{N!}{(N-n)!}\frac{1}{L^n}\frac{2^N}{(2N)!}\int_{-L/2}^{L/2}\frac{dx_{n+1}}{L} \cdots \int_{-L/2}^{L/2}\frac{dx_N}{L}$$

$$\times \prod_{j>k}\left[2\sin\left(\frac{\pi(x_j - x_k)}{L}\right)\right]^4. \qquad (6.23)$$

The square of the ground state for the interaction we are considering is the same as the joint probability density function for the eigenvalues of a unitary self-dual random matrix.[13] Consequently, we will find some results from random matrices very useful in explicitly calculating the correlation functions. In particular, it can be shown[13] that

$$\prod_{j>k}\{2\sin[\pi(x_j - x_k)/L]\}^4$$

$$= \det_{2N\times 2N}[\exp(i2\pi p x_j/L),\ p\exp(i2\pi x_j/L)], \qquad (6.24)$$

where $j = 1, 2, \ldots, N$ and $p = -(N - \frac{1}{2}), -(N - \frac{3}{2}), \ldots, (N - \frac{1}{2})$. We are using the notation

$$\det_{2N\times 2N}[\varphi_k(x_j), \psi_k(x_j)]$$

$$= \det\begin{pmatrix} \varphi_1(x_1)\psi_1(x_1)\varphi_1(x_2)\psi_1(x_2) \cdots \varphi_1(x_N)\psi_1(x_N) \\ \varphi_2(x_1)\psi_2(x_1)\varphi_2(x_2)\psi_2(x_2) \cdots \varphi_2(x_N)\psi_2(x_N) \\ \varphi_{2N}(x_1)\psi_{2N}(x_1)\varphi_{2N}(x_2)\psi_{2N}(x_2) \cdots \varphi_{2N}(x_N)\psi_{2N}(x_N) \end{pmatrix}.$$

We will also use the result[14] that

$$\int dx_1 \cdots \int dx_N \det_{2N\times 2N}[\varphi_k(x_j), \psi_k(x_j)]$$

$$= N!\,\{\det_{2N\times 2N}\int dx[\psi_p(x)\varphi_q(x) - \varphi_p(x)\psi_q(x)]\}^{1/2}. \qquad (6.25)$$

Finally, we will need to use Laplace's theorem[15] to the effect that

$$\det_{n\times n} A = \sum_{\{j\}} (-)^s \det A\begin{pmatrix} i_1 \cdots i_s \\ j_1 \cdots j_s \end{pmatrix} \det A\begin{pmatrix} i_{s+1} \cdots i_n \\ j_{s+1} \cdots j_n \end{pmatrix}, \qquad (6.26)$$

where $i_1 < i_2 < \cdots < i_s, i_{s+1} < i_{s+2} < \cdots < i_n, \sigma = i_1 + i_2 \cdots + i_s + j_1 + j_2 + \cdots j_s$ and $\sum_{\{j\}}$ = sum over all permutations such that $j_1 < j_2 < \cdots < j_s$ and $j_{s+1} < j_{s+2} < \cdots < j_n$.

Substituting Eqs. (6.24) and (6.26) into Eq. (6.23), we obtain

$$R_n^{(N)}(x_1 \cdots x_n) = \frac{N!}{(N-n)!} \frac{1}{L^n} \frac{2^N}{(2N)!} \sum_{\{p,q\}} \det_{2n\times 2n} [\exp(i2\pi p x_j/L), p\exp(i2\pi p x_j/L)] \times (-)^\sigma \int \frac{dx_{n+1}}{L} \cdots \int \frac{dx_N}{L} \det_{2(N-n)\times 2(N-n)} [\exp(i2\pi q x_{j'}/L), \; q\exp(i2\pi q x_{j'}/L)], \qquad (6.27)$$

where $j = 1, 2, \ldots, n$, $j' = n+1, \ldots, N$ and $\{p, q\} = \{(-N - \frac{1}{2}), \ldots, (N - \frac{1}{2})\}$.

Next, by Eq. (6.25) we have

$$\int \frac{dx_{n+1}}{L} \cdots \int \frac{dx_N}{L} \det_{2(N-n)\times 2(N-n)} [\exp(i2\pi q x_{j'}/L), q\exp(i2\pi q x_{j'}/L)]$$
$$= (N-n)! \left(\det_{2(N-n)\times 2(N-n)} \int_{-L/2}^{L/2} \frac{dx}{L} (q - q') \times \exp[i2\pi(q' + q)x/L]\right)^{1/2}$$
$$= (N-n)! \{\det[(q - q')\delta q', -q]\}^{1/2}$$
$$= \begin{cases} (N-n)! \prod_{q>0} 2q & \text{if for every } q \text{ there is a } -q, \\ 0 & \text{otherwise.} \end{cases}$$

Therefore in Eq. (6.27) we can write

$$\sum_{\{p\}} = \sum_{\{-p_1, p_1, p_2, -p_2 \cdots -p_n, p_n\}} = \frac{1}{n!} \sum_{p_n = 1/2}^{N-1/2} \cdots \sum_{p_n = 1/2}^{N-1/2}$$

and $(-)^\sigma = +1$. Equation (6.27) becomes

$$R_n^{(N)}(x_1 \cdots x_n) = N! \; L^{-n} \frac{2^N}{(2N)!} \frac{1}{n!} \sum_{p_1 = 1/2}^{N-1/2} \sum_{p_n = 1/2}^{N-1/2} \frac{\prod_{q=1/2}^{N-1/2}(2q)}{\prod_{j=1}^{n}(2p_j)} \det_{2n\times 2n}[\exp(i2\pi p x_j/L, \; p\exp(i2\pi p x_j/L)],$$

where $p = -p_1, p_1, \ldots, -p_n, p_n$ and $j = 1, 2, \ldots, n$.

Since $[N! \, 2^N/(2N)!] \prod_{q=1/2}^{N-1/2}(2q) = 1$, by applying Eq. (6.25) with the indices x and p interchanged and with $\int dx$ replaced by $(1/L)\sum_{p=1/2}^{N-1/2}(1/2p)$, we obtain

$$R_n^{(N)}(x_1 \cdots x_n) = (\det_{2n\times 2n} A_{jk}^{(N)})^{1/2}, \qquad (6.28)$$

where the $2n \times 2n$ matrix A_{jk} is defined as follows:

$$A_{2j,2k}^{(N)} = \frac{1}{L} \sum_{p=1/2}^{N-1/2} \frac{1}{2p/L} \times \det\begin{pmatrix} -(p/L)\exp(-i2\pi p x_j/L) & -(p/L)\exp(-i2\pi p x_k/L) \\ (p/L)\exp(i2\pi p x_j/L) & (p/L)\exp(i2\pi p x_k/L) \end{pmatrix}$$
$$= \frac{1}{L} \sum_{p=1/2}^{N-1/2} i\left(\frac{p}{L}\right) \sin\frac{2\pi p}{L}(x_j - x_k), \qquad (6.29a)$$

$$A_{2j,2k-1}^{(N)} = -A_{2k-1,2j}^{(N)} = \frac{1}{L} \sum_{p=1/2}^{N-1/2} \frac{1}{2p/L} \times \det\begin{pmatrix} -(p/L)\exp(-i2\pi p x_j/L) & \exp(-i2\pi p x_k/L) \\ (p/L)\exp(i2\pi p x_j/L) & \exp(i2\pi p x_k/L) \end{pmatrix}$$
$$= \frac{1}{L} \sum_{p=1/2}^{N-1/2} -\cos\frac{2\pi p}{L}(x_j - x_k), \qquad (6.29b)$$

$$A_{2j-1,2k-1}^{N} = \frac{1}{L} \sum_{p=1/2}^{N-1/2} \frac{1}{2p/L} \times \det\begin{pmatrix} \exp(-i2\pi p_j/L) & \exp(-i2\pi p x_k/L) \\ \exp(i2\pi p_j/L) & \exp(i2\pi p x_k/L) \end{pmatrix}$$
$$= \frac{1}{L} \sum_{p=1/2}^{N-1/2} (-i) \frac{1}{p/L} \sin\frac{2\pi p}{L}(x_j - x_k). \qquad (6.29c)$$

In order to take the N/V limit of $L(f)$, we need to show that $R_n^{(N)} = (\det A^{(N)})^{1/2}$ is bounded. We can find a bound for $\det A$ by using Corollary 3 (Hadamard's theorem).

A few preliminary steps are needed before we can apply the corollary to find a bound on $R_n^{(N)}$. Let

$$G_N(x) = \frac{1}{2L} \sum_{p=-(N-1/2)}^{N-1/2} \exp(i2\pi p x/L) = \tfrac{1}{2} L^{-1} \frac{\sin(2\pi N x/L)}{\sin(\pi x/L)}.$$

Then from Eq. (6.29) we have

$$A_{2j,2k}^{(N)} = (-i/2\pi) G_N'(x_j - x_k),$$
$$A_{2j,2k-1}^{(N)} = -A_{2k-1,2j}^{(N)} = -G_N(x_j - x_k),$$
$$A_{2j-1,2k-1}^{(N)} = -i2\pi \int_0^{x_j - x_k} dx \, G_N(x).$$

We can bound each matrix element of A as follows:

$$|G_N(x)| \leq \frac{1}{2L} \sum_{p=-N+1/2}^{N-1/2} |\exp(i2px/L)| \leq \frac{2N}{2L} = \bar{\rho},$$

$$|G_N'(x)| \leq \frac{1}{2L} \sum_{p=-N+1/2}^{N-1/2} \left|\frac{2\pi p}{L} \exp(i2\pi x/L)\right|.$$

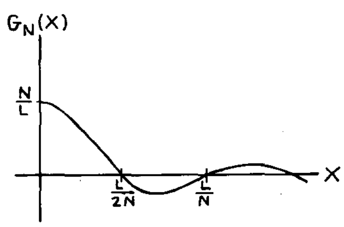

FIG. 2. The function $G_N(x)$ vs x.

Since $(p/L)<\bar{\rho}$, $|G_N'(x)|\le 2\pi\bar{\rho}^2$. Furthermore, since $G_N(x)$ is an oscillating function of decreasing amplitude (for $-\frac{1}{2}L\le x\le\frac{1}{2}L$, see Fig. 2),

$$\max_{|x|<L/2}\left|\int_0^x dx\, G_N(x)\right|$$

$$=\int_0^{L/2N} dx\, G_N(x)\le\frac{L}{2N}\max|G_N(x)|=\tfrac{1}{2}.$$

Therefore, $|A_{jk}|\le c=\max(\bar{\rho},\bar{\rho}^2,\pi)$. Finally, by the corollary to Hadamard's theorem:

$$R_n^{(N)}=(\det A)^{1/2}\le(\sqrt{2}c)^n n^{n/2}.$$

Therefore, $L(f)$ in the N/V limit is given by Eq. (2.7) which becomes

$$L_N(f)\to L(f)$$

$$=\sum_{n=0}^{\infty}\frac{1}{n!}\int dx_1\cdots\int dx_n F(x_1)\cdots F(x_n)R_n(x_1\cdots x_n), \tag{6.30}$$

where

$$F(x)=\exp[if(x)]-1 \text{ and } R_n^{(N)}\to R_n=\bar{\rho}^n(\det{}_{2n\times 2n}A)^{1/2}, \tag{6.31}$$

$A_{2j,2k}=-G'(\delta_{jk})$, $A_{2j,2k-1}=-A_{2k-1,2j}=-G(\delta_{jk})$, $A_{2j-1,2k-1}=\int_0^{\delta_{jk}}dx\, G(x)$, $\delta_{jk}=2\pi\bar{\rho}(x_j-x_k)$, and $G(x)=(\sin x)/x$.

For example: $R_1(x)=\bar{\rho}$ and $R_2(x_1,x_2)=\bar{\rho}^2[1+G'(\delta)\int_0^\delta dx\, G(x)-G(\delta)^2]$, where $\delta=2\pi\bar{\rho}(x_1-x_2)$.

Remark: Under the scale transformation $x\to\alpha x$, $H\to(1/\alpha^2)H$. Therefore, $L(f)$ for representations with different average densities are related as in Eq. (5.19).

The Hamiltonian may be determined by the same method we used for the $\lambda=1$ case. Formally taking the N/V limit of the N-particle Hamiltonians suggests the following:

$$\tilde{K}(x)=K(x)-4\int_{-\infty}^{\infty}\frac{dy}{x-y}\rho(x)\rho(y), \tag{6.32}$$

$$H=\tfrac{1}{8}\int_{-\infty}^{\infty}dx\,\tilde{K}(x)^\dagger\frac{1}{\rho(x)}\tilde{K}(x), \tag{6.33}$$

and

$$\left(\frac{d}{dx}-f'(x)\right)\frac{1}{i}\frac{\delta}{\delta f(x)}L(f)$$

$$=4P\int_{-\infty}^{\infty}\frac{dy}{x-y}\frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)}L(f). \tag{6.34}$$

By checking that the functional equation (6.34) for $L(f)$ is satisfied, we can verify the form of the Hamiltonian. Proceeding as we did in going from Eq. (6.20) to (6.21), we find that Eq. (6.34) is satisfied if the correlation functions satisfy the equation

$$\frac{1}{4}\frac{d}{dx}R_n=\sum_{j\neq 1}R_n/(x_1-x_j)+P\int_{-\infty}^{\infty}dx_{n+1}R_{n+1}/(x_1-x_{n+1}). \tag{6.35}$$

A sketch of the proof of this equation is given in the Appendix. We may therefore conclude the Hamiltonian is given by Eqs. (6.32) and (6.33).

The generating functional $L(f,g)$ can also be calculated for this interaction. To do this, we need to compute

$$R_n^{(N)}(y_1\cdots y_n;x_1\cdots x_n)$$

$$=\frac{N!}{(N-n)!}\int_{-L/2}^{L/2}dz_1\cdots\int_{-L/2}^{L/2}dz_{N-n}\Psi_N(y_1\cdots y_n,\ z_1\cdots z_{N-n})$$

$$\times\Psi_N(x_1\cdots x_n,\ z_1\cdots z_{N-n}).$$

By the same method used to obtain Eq. (6.24) it can be shown that

$$\Psi^{(N)}(y_1\cdots y_n,\ z_1\cdots z_{N-n})\Psi^{(N)}(x_1\cdots x_n,\ z_1\cdots Z_{N-n})$$

$$=\frac{2^N}{(2N)!}\frac{1}{L^N}(i)^{2n^2-n}$$

$$\times\frac{\prod_{j>k}\{2\sin[(\pi/L)(x_j-x_k)]\cdot 2\sin[(\pi/L)(y_j-y_k)]\}}{\prod_{j,k}2\sin[(\pi/L)(y_j-x_k)]}$$

$$\times\det{}_{2N\times 2N}[\exp(ip\eta_j),\ \exp(ip\xi_k),\ \exp(ip\theta_m),\ p\exp(ip\theta_m)]$$

where

$$\eta_j=2\pi x_j/L,\quad j=1,2,\ldots,n,$$

$$\xi_k=2\pi y_k/L,\quad k=1,2,\ldots,n,$$

$$\theta_m=2\pi z_m/L,\quad m=1,2,\ldots,(N-n),$$

and

$$p=-(N-\tfrac{1}{2}),\ -(N-\tfrac{3}{2}),\ldots,(N-\tfrac{1}{2})$$

Then by calculations similar to those used to compute $R_n^{(N)}$ [Eqs. (6.23)–(6.29)], we obtain

$$R_n^{(N)}(y_1\cdots y_n;\ x_1\cdots x_n)$$

$$=\left[\left(\frac{\prod_{j>k}\{2\sin[\pi(x_j-x_k)/L]2\sin[\pi(y_j-y_k)/L]\}}{L^n\prod_{j,k}[2\sin\pi(y_j-y_k)/L]}\right)^2\det{}_{2n\times 2n}A_{jk}^{(N)}\right]^{1/2} \tag{6.36}$$

where

$$A_{jk}^{(N)}=L^{-1}\sum_{p=1/2}^{N-1/2}\left(\frac{p}{L}\right)^{-1}\sin 2\pi\frac{p}{L}(z_j-z_k),$$

and $z_{2j-1}=x_j$ and $z_{2j}=y_j$.

In the N/V limit

$$R_n^{(N)}(;)\to R_n(;)$$

$$=\left(\frac{\prod_{j>k}(x_j-x_k)^2(y_j-y_k)^2}{(2\pi)^{2n}\prod_{j,k}(y_j-x_k)^2}\det{}_{2n\times 2n}\mathrm{Si}(2\pi\bar{\rho}(z_j-z_k))\right)^{1/2}, \tag{6.37}$$

where $\mathrm{Si}(x)=\int_0^x dx\,(\sin x)/x$, and

$$L(f,g)=\sum_{n=0}^{\infty}\frac{1}{n!}\int dx_1\int dy_1\cdots\int dx_n\int dy_n$$

$$\times \prod_{m=1}^{n} \delta(x_m - y_m)\{\exp[if(x_m)]\exp[ij(x_m,g)] - 1\}$$

$$R_n(y_1\cdots y_n;\, x_1\cdots x_n), \tag{6.38}$$

where

$$j(x,g) = -\tfrac{1}{2}i[2g(x)\partial_x + g'(x)].$$

Remarks: (1) It can be checked that

$$\lim_{y_1\to x_1}\cdots \lim_{y_n\to x_n} R_n(y_1\cdots y_n;\, x_1\cdots x_n) = R_n(x_1\cdots x_n).$$

(2) The correlation functions $R_n^{(N)}(y;x)$ given by Eq. (6.36) have been calculated for the Bose ground state. The Fermi ground state would give different correlation functions since $R_n^{(N)}(y;x)$ is determined by the integral $\int dz\, \Psi_N(y,z)\Psi_N(x,z)$ and for bosons $\Psi_N(y,z)\Psi(x,z)$ is positive while for fermions it has the same magnitude but varies in sign. [The correlation functions $R_n^{(N)}(x) = R_n^{(N)}(x;x)$ are the same for both systems.] However, we have previously mentioned that the generating functional $L_N(f,g)$ is the same for bosons and fermions. Therefore, for this N-particle system the generating functional $L_N(f,g)$ is not determined by a unique set of correlation functions $R_n^{(N)}(y;x)$. Thus $R_n^{(N)}(y;x)$ contains more information than is needed to determine a representation of the ρ, J current algebra. This result may be due to the one-dimensional nature of the system and not be true in three dimensions. The correlation functions $R_n^{(N)}(y;x)$ for the Fermi ground state have not been calculated. Nor is it known if the correlation functions $R_n(y;x)$ in the N/V limit for bosons and fermions are different.

(3) For the two body potential $\lambda(\lambda-1)/x^2$, we have calculated $L(f,g)$ in the N/V limit for the cases when $\lambda=1$ and 2. The N/V limit might be expected to exist for other cases when $\lambda>1$ [i.e., $\lambda(\lambda-1)>0$] and that

$$\left(\frac{d}{dx} - if'(x)\right)\frac{1}{i}\,\frac{\delta}{\delta f(x)}L(f)$$

$$= 2\lambda P\int_{-\infty}^{\infty} \frac{dy}{x-y}\,\frac{1}{i}\,\frac{\delta}{\delta f(x)}\,\frac{1}{i}\,\frac{\delta}{\delta f(y)}L(f), \tag{6.39}$$

$$\tilde{K}(x) = K(x) - 2\lambda\rho(x)\int \frac{dy}{x-y}\,\rho(y), \tag{6.40}$$

$$H = \tfrac{1}{8}\int dx\, \tilde{K}(x)^{\dagger}\,\frac{1}{\rho(x)}\,\tilde{K}(x). \tag{6.41}$$

On physical grounds we can expect $L(f)$ to satisfy the cluster decomposition property. Since for different λ the operator $\tilde{K}(x)$ is different, we may conclude by a theorem in Ref. 6 that the representations corresponding to different λ are all unitarily inequivalent. By considering the ground state energy we can give a possible physical reason for this. From Eq. (6.13) the ground state energy per particle for a system of N particles is $E/N = \lambda^2\pi^2\rho^2/6$. As expected, the ground state energy in the N/V limit is infinite. However, for different coupling constants the difference in the ground state energies is infinite since the energy per particle is different. As a consequence of the unitary inequivalence of the representations, if we tried to relate the ground states for different coupling constants by a perturbation series in λ, the series would diverge. However, it is possible that series in λ for matrix elements would converge. (For example, the ground state energy per particle given above.)

(4) After calculating the correlation functions $R_n(x_1\cdots x_n)$ for the case $\lambda = 2(u(x) = 2/x^2)$, the author discovered that Dyson[16] had previously calculated them using a different method. In his case they were the correlations for the eigenvalues of random matrices from the symplectic ensemble.

7. CONCLUSION

It is hoped the examples presented here are helpful in gaining further insight into expressing field theory in terms of the local currents. They also may be useful in testing new approximation schemes.

Other work has been done in connection with this approach. Girard[17] has studied the thermodynamics of the free Bose gas and the free Fermi gas using currents. Goldin and Sharp[18] have shown how to calculate the time dependent n-point functions, $(\Omega, \rho(x_1,t_1)\cdots\rho(x_n,t_n)\Omega)$, where $\rho(x,t) = \exp(itH)\rho(x)\exp(-itH)$, for the free Bose gas. In Ref. 9 it was shown that for the free Bose gas the functional equation (3.8) subject to the appropriate boundary conditions uniquely determines $L(f)$.

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APPENDIX

We have used the result that the correlation functions for a system of particles interacting via the two-body potential $U(x) = 2/x^2$ satisfies Eq. (6.36), namely

$$\frac{1}{4}\frac{d}{dx_1}R_n = \sum_{j\neq 1}\frac{R_n}{(x_1-x_j)} + P\int_{-\infty}^{\infty} dx_{n+1}\frac{R_{n+1}}{(x_1-x_{n+1})}. \tag{A1}$$

In this section we sketch the calculation needed to verify the equation.

To facilitate the computation we introduce the following notation:

Let

$$\det\begin{pmatrix} x_1 & x_1\cdots & x_n & x_n \\ -k_1 & k_1\cdots & -k_n & k_n \end{pmatrix} = \det B,$$

where B is the $2n\times 2n$ matrix

$$B = \begin{pmatrix} b(k_1,x_1) & \cdots & b(k_1,x_n) \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ b(k_n,x_1) & \cdots & b(k_n,x_n) \end{pmatrix},$$

and b is the 2×2 matrix

$$b(k,x) = \begin{pmatrix} \exp(-i2\pi kx) & -k\exp(-i2\pi kx) \\ \exp(i2\pi kx) & k\exp(i2\pi kx) \end{pmatrix}$$

and

$$[a,b]\det\begin{pmatrix}\hat{x}_m\, x_m\\ \bar{k}_p\end{pmatrix} = -a\det\begin{pmatrix}\hat{x}_m\, x_m\\ -\hat{k}_p\, k_p\end{pmatrix} + b\det\begin{pmatrix}\hat{x}_m\, x_m\\ -k_p\, \hat{k}_p\end{pmatrix},$$

where ˆ means that the row (column) is deleted.

The expansion of the determinant by minors is then

$$\det\begin{pmatrix}x_1\, x_1 \cdots x_n x_n\\ -k_1\, k_1 \cdots -k_n k_n\end{pmatrix}$$

$$=\sum_{p=1}^{n} -[\exp(-i2\pi k_p x_m),\ \exp(i2\pi k_p x_m)]\det\begin{pmatrix}\hat{x}_m\, x_m\\ \bar{k}_p\end{pmatrix}$$

$$=\sum_{p=1}^{n}[-k_p\exp(-i2\pi k_p x_m),\ k_p\exp(i2\pi k_p x_m)]\det\begin{pmatrix}x_m\,\hat{x}_m\\ \bar{k}_p\end{pmatrix}.$$

It is convenient to use R_n in the form given by Eq. (6.28),

$$R_n=\frac{1}{n!}\int_{-\bar{p}}^{\bar{p}}\frac{dk_1}{4k_1}\cdots\int_{-\bar{p}}^{\bar{p}}\frac{dk_n}{4k_n}\det\begin{pmatrix}x_1\, x_1 \cdots x_n x_n\\ -k_1\, k_1\cdots -k_n k_n\end{pmatrix}. \qquad \text{(A2)}$$

To compute $P\int[dx_{n+1}/(x_1-x_{n+1})]R_{n+1}$ expand the determinant in Eq. (A2)by the last two columns using Laplace's theorem [Eq. (6.26)]. We get terms of the form

$$(k_m\pm k_p)\exp[ix_{n+1}(k_m\mp k_p)]\det\begin{pmatrix}x_1\, x_1 & \cdots & \hat{x}_{n+1}\,\hat{x}_{n+1}\\ -k_1\, k_1 & \hat{k}_m\,\hat{k}_p & -k_{n+1}\, k_{n+1}\end{pmatrix}.$$

Expand the determinants for those terms proportional to $k_m(k_p)$ by minors about the $-k_m(-k_p)$ row and interchange the variables $k_{n+1}\rightarrow k_m(k_p)$. Taking into account the terms that vanish when integrated, we are left with

$$P\int\frac{dx_{n+1}}{x_1-x_{n+1}}R_{n+1}$$

$$=\frac{1}{(n+1)!}\int\frac{dk_1}{4k_1}\cdots\int\frac{dk_n}{4k_n}\int_{-\bar{p}}^{\bar{p}}\frac{dk_{n+1}}{4k_{n+1}}P\int\frac{dx_{n+1}}{x_1-x_{n+1}}\sum_{m=1}^{n}\sum_{p=1}^{n}2(n+1)k_{n+1}\exp(i2\pi k_{n+1}x_m)$$

$$\times\Big[\{\exp[-i2\pi x_{n+1}(k_{n+1}+k_p)],\ k_p\rightarrow -k_p\}\det\begin{pmatrix}\hat{x}_m\, x_m & \hat{x}_{n+1}\,\hat{x}_{n+1}\\ \bar{k}_p & -\hat{k}_{n+1}\,\hat{k}_{n+1}\end{pmatrix} - k_{n+1}\{\exp[-i2\pi x_{n+1}(k_{n+1}+k_p)],\ k_p\rightarrow -k_p\}$$

$$\times\det\begin{pmatrix}x_m\,\hat{x}_m & \hat{x}_{n+1}\,\hat{x}_{n+1}\\ \bar{k}_p & -\hat{k}_{n+1}\,\hat{k}_{n+1}\end{pmatrix}\Big]=\frac{1}{n!}\int\frac{dk_1}{4k_1}\cdots\int\frac{dx_n}{4k_n}$$

$$\times\sum_{m=1}^{n}\sum_{p=1}^{n}\Big[[a_m(k_p),a_m(-k_p)]\det\begin{pmatrix}\hat{x}_m\, x_m\cdots & \hat{x}_{n+1}\,\hat{x}_{n+1}\\ \bar{k}_p & -\hat{k}_{n+1}\,\hat{k}_{n+1}\end{pmatrix}+[b_m(k_p),\ b_m(-k_p)]\det\begin{pmatrix}x_m\,\hat{x}_m & \hat{x}_{n+1}\,\hat{x}_{n+1}\\ \bar{k}_p & \hat{k}_{n+1}\,\hat{k}_{n+1}\end{pmatrix}\Big],$$

where

$$a_m(k_p)=\begin{cases}\tfrac{1}{2}(-2\pi k_p)\exp(-i2\pi k_p x_1) & \text{for } m=1,\\ -\tfrac{1}{2}(x_1-x_m)^{-1}\exp(-i2\pi k_p x_m)+\tfrac{1}{2}(x_1-x_m)^{-1}\cos\bar{p}(x_1-x_m)\exp(-i2\pi k_p x_1) & \text{for } m\neq 1,\end{cases}$$

and

$$b_m(k_p)=\begin{cases}\tfrac{1}{4}(-2\pi i k_p)(-k_p\exp(-i2\pi k_p x_1)-\tfrac{1}{2}i\bar{p}^2\exp(-i2\pi k_p x_1) & \text{for } m=1,\\ \Big(-\frac{1}{2}\frac{1}{(x_1-x_m)}[-k_p\exp(-i2\pi k_p x_m)]+\frac{i\bar{p}\sin(x_m-x_1)}{2(x_1-x_m)}\exp(-i2\pi x_1 k_p) & \\ +\frac{1}{4i\pi(x_1-x_m)^2}\cos 2\pi\bar{p}(x_1-x_m)[\exp(-i2\pi x_1 k_p)-\exp(-i2\pi x_m k_p)]\Big) & \text{for } m\neq 1.\end{cases}$$

Upon summing over p and reconstructing the determinants we obtain Eq. (A1).

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