The infinitely renormalized field in the scalar field model

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The system consisting of a relativistic scalar boson field interacting with a single spinless nucleon with kinetic energy taken to be independent of momentum is studied in d space dimensions. The interaction Hamiltonian is taken to be $H_I(f)=\int_R{}^d\phi_f(x)\psi^*(x)\psi(x)\,dx$, where f is a momentum cutoff. The physical Hilbert space $\mathcal{K}$ corresponding to the case $f\equiv 1$ in d space dimensions is discussed. The time smoothed nucleon annihilation operator is constructed as a closable operator on $\mathcal{K}$. First order estimates are established for $\psi(h)$ in terms of the local (in momentum space) number operators on $\mathcal{K}$ for the case $d=3$. It is shown that the union of the ranges of the adjoints $\psi^*(h)$ is dense in $\mathcal{K}$. The one particle Hamiltonian is related to the nucleon creation operator on $\mathcal{K}$.

INTRODUCTION

The objective of this paper is to study the phenomenon of infinite field strength renormalization in a simple model. We investigate the infinitely renormalized nucleon field operator in the scalar field model. We restrict our attention to the action of this operator on the one nucleon physical Hilbert space, where the phenomenon of principle interest already occurs; the range of the operator restricted to this subspace is contained in the zero nucleon space.

Much has been written dealing with the mathematical aspects of this model.[1–8] The work closest to this paper is Ref. 2. In that paper the physical Hilbert space is constructed via the Wightman functions for the case of three space dimensions. We obtain more information than is obtained in Ref. 2 in that we get estimates for the time-smoothed nucleon field operator in terms of the local number operator (in momentum space) for three space dimensions. We also construct the nucleon field operator for d space dimensions, where $d>3$. For this case we must use more regular test functions for time smoothing than those in $\mathcal{S}(\mathbb{R}^1)$, and we do not obtain estimates on the operator.

An interesting question is to determine whether the infinitely renormalized nucleon operator is unbounded. For Fermion fields, equal-time anticommutation relations imply boundedness of the spatially smoothed field operators. In this model, however, there are no sharp-time nucleon field operators (after cutoffs are removed); there are only time-smoothed field operators. Hence there are no equal-time anticommutation relations, and so the boundedness is in question. In fact, the indications are that the field operators are unbounded. We feel that our techniques are a step in settling this question.

The scalar field model may be described as follows. Consider a system of spinless nucleons interacting with a boson field. We will consider a Hamiltonian for which the kinetic energy is independent of the nucleon momentum. This is customarily interpreted as meaning that the nucleon mass is "very large" relative to the nucleon momentum.

The total Hamiltonian of the system in the presence of a momentum cutoff f is $H_f=H_0+H_I(f)$, where

$$H_0=M\int_{\mathbb{R}^d}\psi(x)^*\psi(x)\,dx+\int_{\mathbb{R}^d}a(k)^*\mu(k)a(k)\,dK,$$

$$H_I(f)=(1/\sqrt{2})(2\pi)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d}[f(k)/\mu^{1/2}(k)]$$

$$\times[\exp(ik\cdot x)a(k)^*+\exp(-ik\cdot x)a(k)]\psi(x)^*\psi(x)\,dx\,dk,$$

$$\mu(k)=(k^2+m^2)^{1/2},\quad m,\ M>0$$

and $\psi(x)$ and $a(k)$ are the annihilation operators for the nucleons and bosons respectively. M is the nucleon mass and m is the boson mass. H_f is an operator on $\mathcal{F}_{\text{nucleons}}\otimes\mathcal{F}_{\text{mesons}}$ which commutes with the nucleon number operator, so that H_f leaves the number of nucleons invariant. Hence, in studying H_f we can consider a subspace in which a fixed number of nucleons are present. H_f also commutes with the nucleon position operator. This means we can reduce H_f with respect to position; that is, we can consider the nucleons as being located at fixed points in $\mathbb{R}^d$. To treat nuclear annihilation and creation operators, we need to consider states with different numbers of nucleons, but it turns out that for our purposes it suffices to restrict attention to the subspace with zero and one nucleon, and the one nucleon may be assumed located at the origin. The Hamiltonian H_f restricted to the no nucleon states is

$$H_f=\int_{\mathbb{R}^d}a(k)^*\mu(k)a(k)\,dk$$

while for the one nucleon states under consideration it is

$$H_f=M+\int_{\mathbb{R}^d}a(k)^*\mu(k)a(k)\,dk+(1/\sqrt{2})(2\pi)^{-d}$$

$$\times\int_{\mathbb{R}^d}[f(k)/\mu^{1/2}(k)][a(k)^*+a(k)]\,dk.$$

These are operators on $\mathcal{F}_{\text{mesons}}$; we will henceforth denote this space simply by $\mathcal{F}$. To remove the cutoff, we choose a sequence $\{f_n\}$ of smooth functions with compact support that converges in a suitable sense to the function $\mu(k)^{-1/2}$. Write $H_n=H_{f_n}$. For each n, we renormalize the nucleon mass so that the lower bound of H_n is zero. If $d\geqslant 2$, the renormalized mass M_n will go to infinity as $n\to\infty$. Thus for $d\geqslant 2$ the model exhibits infinite mass renormalization.

Let Λ_n denote the ground state for H_n. This is a unit eigenvector corresponding to eigenvalue zero. If $d=2$, then Λ_n converges strongly in $\mathcal{F}$ and H_n converges in the generalized strong sense to a positive operator on $\mathcal{F}$. If $d > 2$, then Λ_n converges weakly to zero. In this case, it is necessary to construct another space $\mathcal{K}$, the physical Hilbert space, with the property that the sequence $\{\Lambda_n\}$ "converges" in a certain sense to a nontrivial vector in $\mathcal{K}$. Then the Hamiltonian may be constructed on $\mathcal{K}$ as a "limit" of the sequence H_n.

Briefly, the procedure for constructing $\mathcal{K}$ is to define a sequence of linear functionals $\{\omega_n\}$ by $\omega_n(A) = (A\Lambda_n, \Lambda_n)$ for $A \in \mathcal{A} =$ the algebra generated by

$$\{\exp(i \int_{\mathbb{R}^d} [\overline{g(k)a}(k) + g(k)a(k)^*] dk) \,|\, g \in L^2(\mathbb{R}^d) \text{ and has compact support}\}.$$

Then ω_n converges to a linear functional ω on $\mathcal{A}$. We let $\mathcal{K}$ be the space obtained from $(\mathcal{A}, \omega)$ via the Gel'fand–Naimark–Segal construction. Thus setting $\ker\omega = \{A \in \mathcal{A} \,|\, \omega(A^*A) = 0\}$, $\mathcal{K}$ is the Hilbert space completion of $\mathcal{A}/\ker\omega$ in the inner product $([A],[B]) = \omega(B^*A)$, where $[A] = A + \ker\omega$. H can be defined on $\mathcal{K}$ in a standard way.

In this paper we consider the nucleon annihilation operator restricted to those states in which there is one nucleon at the origin and any number of mesons. It maps those states into ones with no nucleons and any number of mesons. Since the Hilbert space of states of one nucleon at the origin is one-dimensional, this restriction of the nucleon annihilation operator can be regarded as a mapping of meson states; it will be constructed as a mapping of $\mathcal{K}$ into $\mathcal{F}$. In the following, when the nucleon annihilation operator is referred to it denotes this restriction. The construction of the nucleon annihilation operator begins with the time smoothed annihilation nucleon operator on $\mathcal{F}$ given by

$$\psi_n(h) = \int dt\, h(t) \exp(itH_0) \exp(-itH_n) \quad \text{for } h \in \mathcal{S}(\mathbb{R}^1).$$

This sequence of operators converges weakly to zero on $\mathcal{F}$. To remedy this, we multiply ψ_n by a suitable sequence $\{c_n\}$ of constants tending to infinity. This procedure is called infinite field strength renormalization. We show that the sequence $\{\psi_n(h)A\Omega_n\}$ converges strongly in $\mathcal{F}$ for A in $\mathcal{B}$, where $\mathcal{B}$ is a subset of $\mathcal{A}$ such that $\{[A] \,|\, A \in \mathcal{B}\}$ is a dense subset of $\mathcal{K}$. The limit we call $\psi(h)[A]$. $\psi(h)$ is called the annihilation operator without cutoffs; we show that it is a closable operator from $\mathcal{K}$ to $\mathcal{F}$. We also show that the union of the ranges of $\psi^*(h)$ over $h \in \mathcal{S}(\mathbb{R}^1)$ is dense in $\mathcal{K}$. Finally, we establish the relationship between the Hamiltonian without cutoffs and the annihilation operator without cutoffs

$$\exp(itH)\psi^*(h) = \psi^*(h_t) \exp(itH_0),$$

where h_t is the translate of h by t. In this equation each side is an operator from $\mathcal{F}$ to $\mathcal{K}$.

I. PRELIMINARIES

A. Fock space

Before we can discuss the physics of a spinless nucleon interacting with a boson field, we need to define the space which is used to represent the nucleon and bosons and the operators which describe the interaction of these particles.

First we define the state space for the bosons. Let $\mathcal{H}$ be a complex Hilbert space. Let $\mathcal{H}^0 = \mathbb{C}$, $\mathcal{H}^j = \mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H}$ (j factors), and $\mathcal{L} = \sum_{j=0}^{\infty} \oplus \mathcal{H}^j$. $\mathcal{L}$ is called the Fock space over $\mathcal{H}$. For every permutation $\sigma \in S_n$, the symmetric group of degree n, there exists a unique unitary operator $U(\sigma)$ defined by the equation

$$U(\sigma)(x_1 \otimes x_2 \otimes \cdots \otimes x_n) = x_{\sigma^{-1}(1)} \otimes x_{\sigma^{-1}(2)} \otimes \cdots \otimes x_{\sigma^{-1}(n)}$$

for $x_1, \ldots, x_n \in \mathcal{H}$. A tensor $u \in \mathcal{H}^n$ is called symmetric if $U(\sigma)u = u$ for all $\sigma \in S_n$. Define

$$P_S^{(n)} = \begin{cases} I, & n = 0, \\ (1/n!) \sum_{\sigma \in S_n} U(\sigma), & n > 0. \end{cases}$$

Then $P_S^{(n)}: \mathcal{H}^{(n)} \xrightarrow{\text{onto}} \mathcal{F}^n$, the space of all symmetric n tensors; moreover, $P_S^{(n)}$ is an orthogonal projection. Put $\mathcal{F} = \sum_{n=0}^{\infty} \mathcal{F}^n$ and $P_S = \sum_{n=0}^{\infty} P_S^{(n)}$. Then P_S is the orthogonal projection of $\mathcal{L}$ onto $\mathcal{F}$. $\mathcal{F}$ is called the symmetric Fock space over $\mathcal{H}$. The state space used to describe the bosons is the Fock space $\mathcal{F}$ over $\mathcal{H} = L^2(\mathbb{R}^d)$. The subspace $\mathcal{F}^n$ is the state space for a system of n bosons. Since $\mathcal{F}$ is the direct sum of $\{\mathcal{F}_n \,|\, n = 0, 1, 2, \cdots\}$ we can regard an element $\psi = \sum_{n=0}^{\infty} \psi_n$, $\psi_n \in \mathcal{F}^n$, of $\mathcal{F}$ as a state that contains n bosons with probability $\|\psi_n\|^2 / \|\psi\|^2$. We can now define an operator which creates bosons, i.e., takes a pure state $\psi_n \in \mathcal{F}^n$ with n bosons to a state in $\mathcal{F}^{n+1}$. Let $\mathcal{V}$ denote the subspace of algebraic symmetric tensors over $\mathcal{H}$. Then $\mathcal{V}$ is dense in $\mathcal{F}$. For $x \in \mathcal{H}$ and $u \in \mathcal{V} \cap \mathcal{F}^n$, define $C_x u = \sqrt{n+1} P_S(x \otimes u)$. C_x extends linearly to $\mathcal{V}$. Then C_x: $\mathcal{V} \to \mathcal{V}$ and $\mathcal{V} \cap \mathcal{F}^n \to \mathcal{V} \cap \mathcal{F}^{n+1}$. C_x is a closable operator.[1] We denote its closure by C_x also, and we denote its adjoint by A_x. C_x and A_x are called respectively the creation and annihilation operators for the state x. Let R_x be the closure of $(1/\sqrt{2})(A_x + C_x)$. R_x is called the boson field operator. We will use R_x later on to express the potential of the interaction between a nucleon and a system of bosons. R_x is related to the usual field operators, ϕ and π, as follows. If $\mathcal{H} = L^2(\mathbb{R}^d)$, then

$$R_{(\hat{h}/\mu^{1/2} + i\hat{g}\mu^{1/2})} = \int_{\mathbb{R}^d} [\phi(x,0)h(x) + \pi(x,0)g(x)] dx$$

for h and g real-valued functions in $C_{\text{com}}^{\infty}(\mathbb{R}^d)$. We now state several results concerning the operators A_x, C_x, and R_x which will be useful later on.

Theorem I.1: R_x is self-adjoint.

Theorem I.2: For any x and y in $\mathcal{H}$, $\exp(iR_x)$ leaves invariant $\mathcal{D}(R_y)$ and $\exp(iR_x)R_y - R_y \exp(iR_x) = \operatorname{Im}(x,y) \times \exp(iR_x)$ on $\mathcal{D}(R_y)$.

Theorem I.3: (Weyl relations) For any x and y in $\mathcal{H}$, $\exp(iR_{x+y}) = \exp(iR_y) \exp[-i \operatorname{Im}(x,y)/2]$.

Theorem I.4: If u is in $\mathcal{V}$, then $\exp(iR_x)u = \exp(-\|x\|^2/4) \exp(iC_x) \exp(iA_x)u$.

Theorem I.5: The map $x \to \exp(iR_x)$ is strongly continuous on $\mathcal{H}$.

Let Λ be the zero rank tensor $1 \in \mathbb{C}$. Λ is called the vacuum state in $\mathcal{F}$.

Theorem I.6: Let K_1 be a closed subspace of $\mathcal{H}$. Let $K_2 = K_1^{\perp}$. Let $\mathcal{F}(K)$ denote the symmetric Fock space over K. There is a unique unitary transformation L from $\mathcal{F}(K_1) \otimes \mathcal{F}(K_2)$ onto $\mathcal{F}(\mathcal{H})$ such that

$$L(\exp(iR_x^{(1)})\Lambda_1)\otimes(\exp(iR_y^{(2)})\Lambda_2)=\exp(iR_{x+y})\Lambda$$

for all $x\in K_1$ and $y\in K_2$. Here Λ_j is the vacuum state in $\mathcal{F}(K_j)$ and $R_x^{(j)}$ acts in $\mathcal{F}(K_j)$. L satisfies

$$L(\exp(iR_x^{(1)})\otimes I)L^{-1}=\exp(iR_x),\quad x\in K_1,$$

and

$$L(I\otimes\exp(iR_y^{(2)}))L^{-1}=\exp(iR_y),\quad y\in K_2.$$

Theorem I.7: The linear span of $\{\exp(iR_x)\Lambda\mid x\in\mathcal{H}\}$ is dense in $\mathcal{F}$.

These theorems may be found or easily deduced from results in Ref. 1.

As we mentioned above, the boson field operator is used to express the potential energy. We need to define another operator representing kinetic energy.

Definition I.8: Let U be a unitary operator on $\mathcal{H}$. Define $\Gamma(U)$: $\mathcal{F}\rightarrow\mathcal{F}$ by $\Gamma(U)=I\oplus U\oplus(U\oplus U)\oplus(U\oplus U\oplus U)\oplus\cdots$.

$\Gamma(U)$ is clearly a unitary operator. If A is a self-adjoint operator on $\mathcal{H}$, then, for all $t\in\mathbb{R}$, $\exp(itA)$ is a unitary operator on $\mathcal{H}$ which gives rise to the unitary operator $\Gamma(\exp(itA))$ on $\mathcal{F}$.

Theorem I.9: $\Gamma(\exp(itA))$ is a strongly continuous one-parameter group in t.

Proof: Strong continuity on $\mathcal{V}$ is clear, and this implies strong continuity on the whole space.

Hence, by Stone's theorem, $\Gamma(\exp(itA))$ has a unique infinitesimal generator $d\Gamma(A)$, a self-adjoint operator on $\mathcal{F}$ such that $\Gamma(\exp(itA))=\exp(it\,d\Gamma(A))$.

Definition I.10: $N=d\Gamma(I)$. N is called the number operator.

Theorem I.11: For all $x\in\mathcal{H}$, $R_x(N+I)^{-1/2}$ is a bounded operator.

If A is the kinetic energy operator for a single boson, then $d\Gamma(A)$ represents the kinetic energy of the system of bosons. We shall need the following results concerning $\Gamma(U)$, $d\Gamma(A)$, and R_x:

Theorem I.12: If $x\in\mathcal{H}$ and U is a unitary operator on $\mathcal{H}$, then

$$\Gamma(U)R_x\Gamma(U)^{-1}=R_{Ux}.$$

Proof: See Ref. 1.

Theorem I.13: Let A be a self-adjoint operator on $\mathcal{H}$, and let $x\in\mathcal{D}_A$. If $\psi\in\mathcal{D}(d\Gamma(A)\cap\mathcal{D}(N^{1/2}))$, then $\psi\in\mathcal{D}$ $\in\mathcal{D}_{d\Gamma(A)\exp(iR_x)}$ and

$$d\Gamma(A)\exp(iR_x)\psi=\exp(iR_x)\{d\Gamma(A)\psi+\tfrac{1}{2}(Ax,x)\psi+R_{iAx}\psi\}.$$

For a proof, see Ref. 9.

B. Operators with cutoffs

1. The one nucleon Hamiltonian

We are now in a position to define an operator that represents the boson kinetic energy.

Definition I.14: Let m be a positive constant. Let μ be the function on $\mathbb{R}^d$ defined by $\mu(k)=(m^2+|k|^2)^{1/2}$ for all $k\in\mathbb{R}^d$ and let $\mathcal{M}_\mu$ be the operator of multiplication by μ on $\mathbb{R}^d$. Finally, let $H_0=d\Gamma(\mathcal{M}_\mu)$. H_0 is called the free Hamiltonian.

H_0 is the operator on $\mathcal{F}$ which represents the boson kinetic energy. m is equal to the mass of a single boson. H_0 also represents the total Hamiltonian for a system of bosons, since, for a system of bosons, there is no interaction and hence no potential energy term in the Hamiltonian. Let us now define the Hamiltonian for the system of bosons interacting with a nucleon. The Hilbert space for the nucleon is $L^2(\mathbb{R}^d)$, and hence the Hilbert space for the nucleon and bosons is $L^2(\mathbb{R}^d)\otimes\mathcal{F}$. Note that this space can be identified in a natural way with the space $L^2(\mathbb{R}^d;\mathcal{F})$. We make use of this identification in the following definition.

Definition I.15: Let $w\in L^2(\mathbb{R}^d)$. For all $x\in\mathbb{R}^d$, define the function $w_x\in L^2(\mathbb{R}^d)$ by $w_x(k)=w(k)\exp(ik\circ x)$ for all $k\in\mathbb{R}^d$. Let $u\in L^2(\mathbb{R}^d;\mathcal{F})$ be such that $u(x)\in\mathcal{D}_{(N+I)}{}^{1/2}$ for all $x\in\mathbb{R}^d$. It is clear that the set of such u is dense in $L^2(\mathbb{R}^d;\mathcal{F})$. Define V_wu by $V_w(u)(x)=R_{w_x}u(x)$ for all $x\in\mathbb{R}^d$.

Let f_n be a sequence of nonnegative C^∞ functions on $\mathbb{R}^d$ with compact support such that

(1) $f_n(-x)=f_n(x)$ for all $x\in\mathbb{R}^d$ and for all n,

(2) f_n is a monotonically increasing sequence, and

(3) $f_n(x)=1$ for $|x|\leqslant n$ and $f_n(x)=0$ for $|x|>n+1$.

Let $w_n=(2\pi)^{-d}f_n/\mu^{1/2}$, where $\mu(k)=(m^2+k^2)^{1/2}$ for all $k\in\mathbb{R}^d$ and m is a positive constant. Let $V_n=V_{w_n}$. We call V_n the potential corresponding to the cutoff function f_n.

In this paper, we are studying the scalar field model. The principal simplifying assumption in this model is that the nucleon has infinite mass. This implies that the nucleon does not recoil, and hence the nucleon kinetic energy is zero. Therefore, the Hamiltonian consists of the sum of the boson kinetic energy H_0 and the potential energy V_n. However, the inf of the spectrum of H_0+V_n is $-\frac{1}{2}(w_n,\mu^{-1}w_n)$. It is convenient to add a constant term to the Hamiltonian so as to make the inf of the spectrum 0. This is justifiable, since the potential may be altered by a constant without changing the physics. So we set $H_n=H_0+V_n+\frac{1}{2}(w_n,\mu^{-1}w_n)$. (Note that here we are writing H_0 instead of $I\otimes H_0$. We shall continue this convention.) H_n is the one nucleon Hamiltonian corresponding to the cutoff f_n. It is the same as the Hamiltonian described in Ref. 10 except that we are considering only one nucleon where Schweber is considering a whole field of nucleons, and we are representing the nucleon with configuration space rather than momentum space. (We are representing the bosons, however, with momentum space, as Schweber does.)

Now if $u\in L^2(\mathbb{R}^d;\mathcal{F})$ and is in the domain of H_n, then

$$(H_nu)(x)=H_0u(x)+R_{(w_n)_x}u(x)+\tfrac{1}{2}(w_n,\mu^{-1}w_n)u(x).$$

Hence, setting $H_n(x)=H_0+R_{(w_n)_x}+\frac{1}{2}(w_n,\mu^{-1}w_n)$, we have $H_n=\int_{\mathbb{R}^d}H_n(x)\,dx$. $H_n(x)$ is an operator on $\mathcal{F}$ called the reduced H_n at x.

2. The nucleon annihilation operator

In analogy with the boson creation operator, we can define the nucleon creation operator.

Definition I. 16: Let $h \in L^2(\mathbb{R}^d)$ and $u \in \mathcal{J}$. We define the creation operator $\psi^*(h)$ applied to u by $\psi^*(h)u = h \otimes u$. Thus $\psi^*(h)\colon \mathcal{J} \to L^2(\mathbb{R}^d) \otimes \mathcal{J}$.

Now let us calculate the adjoint, which we denote by $\psi(h)$. Let $h_1 \in L^2(\mathbb{R}^d)$ and u and $v \in \mathcal{J}$. Then

$$\begin{aligned}(\psi(h)h_1 \otimes u, v) &= (h_1 \otimes u, \psi^*(h)v)\\ &= (h_1 \otimes u, h \otimes v)\\ &= (h_1, h)(u, v)\\ &= ((h_1, h)u, v).\end{aligned}$$

Hence $\psi(h)h_1 \otimes u = (h, h_1)u$. What we are interested in is the pointwise annihilation operator.

Definition I. 17: Let $x \in \mathbb{R}^d$. The annihilation operator at x, $\psi(x)$, is a map from $L^2(\mathbb{R}^d) \otimes \mathcal{J} \to \mathcal{J}$ defined by $\psi(x)h \otimes u = h(x)u$ for $h \in C^\infty(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ and $u \in \mathcal{J}$.

Note that, formally, $\psi(x)$ is a special case of $\psi(h)$ resulting from letting h equal the δ-function at x. Also, we we have the relationship $\psi(h) = \int_{\mathbb{R}^d} h(x)\psi(x)\,dx$, so that we can study the annihilation operator $\psi(h)$ (also called the spatially smoothed annihilation operator) by studying the pointwise annihilation operator $\psi(x)$.

II. THE TIME SMOOTHED NUCLEON ANNIHILATION OPERATOR WITHOUT CUTOFFS IN THREE DIMENSIONS

A. The physical Hilbert space

In the preceding section, we have considered an interaction with a cutoff; now we remove the cutoff. If $d > 2$, i.e., if we are in more than two spatial dimensions, then it is necessary to move out of Fock space into another space, called the physical Hilbert space. Put $w = (2\pi)^{-d}/\mu^{1/2}$, where, as before, μ is the function $\mu(k) = (m^2 + |k|^2)^{1/2}$. Then, recalling that $H_n = H_0 + V_{w_n} + \frac{1}{2}(w_n, \mu^{-1}w_n)$, we would expect formally that the limit of the sequence $\{H_n\}$ should be given by $H = H_0 + V_w + \frac{1}{2}(w, \mu^{-1}w)$. However, this last expression does not make sense for two reasons: $w \notin L^2(\mathbb{R}^3)$ (so that V_w does not make sense) and $(w, \mu^{-1}w) = \infty$.

The first thing we do to construct the limiting Hamiltonian is to simplify the problem by looking at the reduced Hamiltonian $H_n(x)$. For each $x \in \mathbb{R}^d$, we can construct a space $\mathcal{K}_x$ and an operator $H(x)$ that is in some sense a limit of the sequence $\{H_n(x)\}$. The spaces $\mathcal{K}_x$ can all be identified in a natural way, i.e., there exists a canonical unitary operator U_x for each x such that $\mathcal{K}_x = U_x \mathcal{K}_0 U_x^{-1}$. Then we can construct the limiting Hamiltonian H acting on $L^2(\mathbb{R}^d) \otimes \mathcal{K}$ by the formula $H = \int_{\mathbb{R}^d} U_x^{-1} H(x) U_x\,dx$. Since the problem is analogous at different points x, we confine our attention to the construction of the limiting Hamiltonian for $H_n(0)$, which we will henceforth call H_n. We will also call the limiting reduced Hamiltonian H and put $\mathcal{K} = \mathcal{K}_0$.

$\mathcal{K}$ is constructed by making sense of the limit of the cutoff ground states. Recall that the inf of the spectrum of H_n is 0. There is an eigenvector Λ_n of multiplicity one for 0, and Λ_n is called the ground state for the cutoff f_n. We can find Λ_n explicitly. Put $g_n = -iw_n/\mu$. Then putting $A = \mathcal{M}_\mu$ and $x = g_n$, we have by Theorem I. 13 that $H_n = \exp(iR_{g_n})H_0\exp(-iR_{g_n})$. A straightforward calculation shows that $H_0\Lambda = 0$ and hence that $\exp(iR_{g_n})H_0 \times \exp(-iR_{g_n})[\exp(iR_{g_n})\Lambda] = 0$. Thus if $\Lambda_n = \exp(iR_{g_n})\Lambda$, then $H_n\Lambda_n = 0$. $\|\Lambda_n\| = 1$ for all n, but the sequence converges weakly to 0. Nevertheless, we shall make sense of a limiting ground state, a unit vector in another Hilbert space which is a "limit" of the sequence $\{\Lambda_n\}$.

The motivation for the method we will use for making sense of the limit comes from the fact that the Fock space is determined by the action of a certain set of operators on the ground state Λ_n; the linear span of $\{\exp(iR_x)\Lambda_n \mid x \in L^2(\mathbb{R}^d)\}$ is dense in $\mathcal{J}$. (This follows from Theorems I. 7 and I. 3.)

We will construct the limit of the sequence $\{\Lambda_n\}$ by regarding Λ_n as a linear functional on a certain space for each n. Let S be a bounded open subset of $\mathbb{R}^d$ and let $\mathcal{A}(S) =$ the von Neumann algebra on $\mathcal{J}$ generated by $\{\exp(iR_g \mid g \in L^2(\mathbb{R}^d)$ and $\operatorname{supp} g \subset S\}$. Let $\mathcal{A}$ denote the norm closure of the union of $\mathcal{A}(S)$, where S ranges over all bounded open sets in $\mathbb{R}^d$. Define the linear functional ω_n on $\mathcal{A}$ by $\omega_n(A) = (A\Lambda_n, \Lambda_n)$. Each ω_n is continuous relative to the norm topology on $\mathcal{A}$. A calculation shows that $\{\omega_n\}$ converges pointwise to a continuous linear functional ω on $\mathcal{A}$ with norm 1. Applying the Gel'fand–Naimark–Segal (GNS) construction to the pair $(\mathcal{A}, \omega)$, we obtain a Hilbert space $\mathcal{K}$ in which $\mathcal{A}/\ker\omega$ is dense. We call $\mathcal{K}$ the physical Hilbert space. We can now define the limiting Hamiltonian H on $\mathcal{K}$. We do this by defining $\exp(itH)$ and then applying Stone's Theorem. Let $A \in \mathcal{A}(S)$. Let $g = -iw/\mu$ and put $r = g\chi_S$ and $r_n = g_n - r$. Since $H_n = \exp(iR_{g_n})H_0\exp(-iR_{g_n})$, we have by the functional calculus that $\exp(itH_n) = \exp(iR_{g_n})\exp(itH_0) \times \exp(-iR_{g_n})$. Hence

$$\begin{aligned}\exp(itH_n) &= \exp(iR_{r_n+r})\exp(itH_0)\exp(-iR_{r_n+r})\\ &= \exp(iR_{r_n})\exp(iR_r)\exp\{it[d\Gamma(\mu\chi_S) + d\Gamma(\mu\chi_{S^c})]\}\\ &\quad\times\exp(-iR_{r_n})\exp(-iR_r)\\ &\quad(\text{where } S^c \text{ denotes the complement of } S)\\ &= \exp(iR_{r_n})\exp(-R_r)\exp[it\,d\Gamma(\mu\chi_S)]\\ &\quad\times\exp[it\,d\Gamma(\mu\chi_{S^c})]\exp(-iR_{r_n})\exp(-iR_r)\\ &= \exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)\exp(iR_{r_n})\\ &\quad\times\exp[it\,d\Gamma(\mu\chi_{S^c})]\exp(-iR_{r_n}).\end{aligned}$$

Therefore,

$$\begin{aligned}&\exp(itH_n)A\Lambda_n\\ &\quad= \exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)\exp(iR_{r_n})\\ &\qquad\times\exp[it\,d\Gamma(\mu\chi_{S^c})]\exp(-iR_{r_n})A\Lambda_n\\ &\quad= \exp(iR_r)[it d\Gamma(\mu\chi_{S^c})]\exp(-iR_r)A\exp(iR_{r_n})\\ &\qquad\times\exp[it\,d\Gamma(\mu\chi_{S^c})]\exp(-iR_{r_n})\exp(iR_{r+r_n})\Lambda\\ &\quad= \exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)A\exp(iR_{r_n})\\ &\qquad\times\exp[it\,d\Gamma(\chi_{S^c})]\exp(iR_r)\Lambda\\ &\quad= \exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)A\exp(iR_r)\exp(iR_{r_n})\\ &\qquad\times\exp[it\,d\Gamma(\mu\chi_{S^c})]\Lambda\end{aligned}$$

$$=\exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)A\exp(iR_r)\Lambda$$
$$=\exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)A\Lambda_n.$$

Put $U(t)[A]=[\exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)A]$. Then $U(t)$ maps $[\mathcal{A}(S)]$ onto $[\mathcal{A}(S)]$ and preserves the $\mathcal{K}$ norm. It is clear that if $A\in\mathcal{A}(S)\cap\mathcal{A}(T)$, where S and T are bounded open sets in $\mathbb{R}^3$, then $U(t)[A]$ defined in the above manner is the same whether A is regarded as an element of $\mathcal{A}(S)$ or of $\mathcal{A}(T)$. Thus we have defined $U(t)$ in a consistent manner as a map from the union $\mathcal{U}$ of $[\mathcal{A}(S)]$ over bounded open sets onto $\mathcal{U}$. Since $\mathcal{U}$ is dense in $[\mathcal{A}]$ relative to the operator norm, $\mathcal{U}$ is dense in $[\mathcal{A}]$ relative to the $\mathcal{K}$ norm. Since $[\mathcal{A}]$ is dense in $\mathcal{K}$, $\mathcal{U}$ is dense in $\mathcal{K}$. Thus $U(t)$ extends to a unitary map from $\mathcal{K}$ onto $\mathcal{K}$. It is easy to show that $U(t)$ is strongly continuous in t. Hence $U(t)$ is a strongly continuous unitary group, and by Stone's theorem, there exists a self-adjoint operator H on $\mathcal{K}$ such that $U(t)=\exp(itH)$. This H we call the one nucleon Hamiltonian without cutoffs.

B. Existence of the annihilation operator without cutoffs

We now proceed to construct the nucleon annihilation operator without cutoffs. As with the Hamiltonian, we shall construct the annihilation operator reduced at the origin, since the same procedure serves to construct the annihilation operator reduced at x for all $x\in\mathbb{R}^3$ and the full annihilation operator can be constructed from the reduced ones. For $x\in\mathbb{R}^d$, let e_x denote the pointwise evaluation functional on $L^2(\mathbb{R}^d)$, i.e., if $h\in L^2(\mathbb{R}^d)\cap C^\infty(\mathbb{R}^d)$, then $e_x h=h(x)$. Then recalling Definition I.17, we have $\psi(x)=e_x\otimes I$, where I is the identity operator on $\mathcal{J}$. Hence the annihilation operator reduced at x is simply the identity operator on $\mathcal{J}$. We see that the procedure used to define $\exp(itH)$ will not work here, for if $A\in\mathcal{A}$, the sequence $IA\Lambda_n$ is equal to $A\Lambda_n$, which converges weakly to zero. If we consider the spatially smoothed annihilation operator $\psi(h)$, we run into the same problem that is, $\psi(h)A\Lambda_n$ converges weakly to zero for $A\in\mathcal{A}$.

The way we get around this difficulty is by time smoothing. Up to now, all the operators considered have been at the fixed time $t=0$. From quantum mechanics, we know that an observable $V(t)$ evolves in time according to the formula

$$V(t)=\exp(itH)V(0)\exp(-itH),$$

where H is the Hamiltonian. In this case, the annihilation operator corresponding to the cutoff f_n and reduced at the origin is an operator from the reduced one nucleon space $\mathcal{J}$, where the Hamiltonian is H_n, to the zero nucleon space $\mathcal{J}$, where the Hamiltonian is H_0. Hence the annihilation operator at time t corresponding to the cutoff f_n and reduced at the origin is $\exp(itH_0)I\exp(-itH_n)=\exp(itH_0)\exp(-itH_n)$. We wish to time-smooth with a function h belonging to some suitable space of test functions. The result is

$$\tilde{\psi}_n(h)=\int_{\mathbb{R}^1}dt\,h(t)\exp(itH_0)\exp(-itH_n),$$

where we are using the strong integral. If $A\in\mathcal{A}(S)$ for some bounded open set S in $\mathbb{R}^3$, then it is easy to show that the sequence $\tilde{\psi}_n(h)A\Lambda_n$ converges weakly to zero. To correct this, we multiply the operators $\tilde{\psi}_n(h)$ by a suitably chosen sequence $\{c_n\}$ of constants that tend to infinity.

Put $c_n=(\Lambda_n,\Lambda)^{-1}=(\exp(iR_{g_n})\Lambda,\Lambda)^{-1}$. By Theorem I.4,

$$(\exp(iR_{g_n})\Lambda,\Lambda)$$
$$=\exp(-\|g_n\|^2/4)(\exp(iC_{g_n})\exp(iA_{g_n})\Lambda,\Lambda)$$
$$=\exp(-\|g_n\|^2/4)(\exp(-C_{g_n})\Lambda,\Lambda)$$
$$=\exp(-\|g_n\|^2/4)(\Lambda,\Lambda)$$
$$=\exp(-\|g_n\|^2/4).$$

Hence, $c_n=\exp(\|g_n\|^2/4)$. Put

$$\psi_n(h)=c_n\tilde{\psi}_n(h)=c_n\int dt\,h(t)\exp(itH_0)\exp(-itH_n).$$

We will determine what sort of test function space h should lie in, and then we will construct a "limit" of the sequence $\psi_n(h)$. Let us first find conditions on h which will insure that $\psi_n(h)\Lambda_n$ is a sequence bounded in norm:

$$\psi_n(h)\Lambda_n=c_n\int dt\,h(t)\exp(itH_0)\exp(itH_n)\Lambda_n$$
$$=c_n\int dt\,h(t)\exp(itH_0)\Lambda_n$$
$$=c_n\sqrt{2\pi}\,\check{h}(H_0)\exp(iR_{g_n})\Lambda$$
$$=2\pi\check{h}(H_0)\exp(iC_{g_n})\Lambda,$$

where

$$\check{h}(t)=(1/\sqrt{2\pi})\int h(s)\exp(its)\,ds,\quad g_n=[-i/(2\pi)^d]f_n/\mu^{3/2},$$

and f_n is as defined above in Sec. I.B.1. [We will also use the notation

$$\check{h}(t)=(1/\sqrt{2\pi})\int h(s)\exp(-its)\,ds$$

and

$$h_1*h_2(t)=(1/\sqrt{2\pi})\int h_1(t-s)h_2(s)\,ds.]$$

Suppose that the restriction of $\check{h}$ to the positive half-line is the Laplace transform of a function γ:

$$\check{h}(t)=\int_0^\infty\gamma(s)\exp(-st)\,ds=\mathcal{L}\gamma(t)\quad(t>0).$$

Then $\check{h}(H_0)=\int_0^\infty\gamma(s)\exp(-sH_0)\,ds$ and, since H_0 is a positive operator,

$$\|\check{h}(H_0)\exp(iC_{g_n})\Lambda\|_2^2\leqslant\int_0^\infty|\gamma(s)|\,\|\exp(-sH_0)\exp(iC_{g_n})\Lambda\|_2^2\,ds.$$

Now

$$\exp(-sH_0)\exp(iC_{g_n})\Lambda=\exp(iC_{\exp(-s\mu_{g_n})})\Lambda$$
$$=\exp[\|\exp(-s\mu_{g_n})\|^2/4]$$
$$\times\exp(iR_{\exp(-s\mu_{g_n})})\Lambda$$

so that

$$\|\exp(-sH_0)\exp(iC_{g_n})\Lambda\|_2^2=\exp[\|\exp(-s\mu_{g_n})\|^2/2].$$

After some further estimates, we find that

$$\lim_{n\to\infty}\|\exp(-sH_0)\exp(iC_{g_n})\Omega\|_2^2\sim 1/s^{1/2}\quad\text{as } s\to 0 \text{ for } d=3,$$

$$\lim_{n\to\infty}\|\exp(-sH_0)\exp(iC_{g_n})\Omega\|_2^2\sim\exp(\tfrac{1}{2}s^{3-d})\quad\text{as } s\to 0 \text{ for } d>3,$$

and $\lim_{n\to\infty}\|\exp(-sH_0)\exp(iC_{g_n})\Omega\|_2^2$ remains bounded as $s\to\infty$ for $d\geqslant 3$, where $K_1(s)\sim K_2(s)$ as $s\to a$ means that $\lim_{s\to a}[K_1(s)/K_2(s)]=1$. In order that the integral

$$\int_0^\infty|\gamma(s)|\exp(-sH_0)\Lambda_n\|_2^2\,ds \tag{1}$$

converge for the case $d=3$, it suffices to have $\int_0^1[|\gamma(s)|/s^{1/2}]\,ds<\infty$ and $\int_1^\infty|\gamma(s)|\,ds<\infty$. Now suppose that $h\in\mathcal{S}(R^1)$, the space of rapidly decreasing functions on R^1.

Then (a) $\gamma(s)/s$ remains bounded as $s \to 0$ and (b) $s^2\gamma(s)$ remains bounded as $s \to \infty$. (a) and (b) follow from the fact that

$$\lim_{s\to\infty} s\mathcal{L}\, f(s) = \lim_{t\to 0} f(t) \quad \text{and} \quad \lim_{s\to 0} s\mathcal{L}\, f(s) = \lim_{t\to\infty} f(t)$$

provided that f and f' are Laplace transformable and $\lim_{t\to\infty} f(t)$ exists.[11] Since $\gamma(s)/s$ remains bounded as $s \to 0$ and $s^2\gamma(s)$ remains bounded as $s \to \infty$, $\int_0^1 [|\gamma(s)|/s^{1/2}]ds < \infty$ and $\int_1^\infty |\gamma(s)|\, ds < \infty$. Thus, in the case $d=3$, it suffices to have $\hat{h} \in \mathcal{S}(R^1)$ or, equivalently, $h \in \mathcal{S}(R^1)$.

In the case $d > 3$, the condition $\hat{h} \in \mathcal{S}(R^1)$ does not insure that $\|\psi_n(h)\Lambda_n\|_2^2$ is a bounded sequence. If, for example, $\hat{h}(t) = \int_0^\infty \exp(-s^{-p})\exp(-s^t)\,ds$, where $0 < p < d-3$, then $\hat{h} \in \mathcal{S}$, and it can be shown that

$$\lim_{n\to\infty} \sup \|\psi_n(h)\Lambda_n\|_2^2 = \infty.$$

If $\hat{h} \in \mathcal{S}(R^1)$ and has compact support, then (1) converges. Hence we would use as test function space the set $\hat{\mathcal{D}}$ of all functions in $\mathcal{S}(R^1)$ whose Fourier transforms have compact support. However, $\mathcal{D}$ contains no nontrivial functions with compact support. The physical significance of this is that using $\mathcal{D}$ as test function space would not permit one to make measurements localized in time. Since this is an undesirable restriction, we need a larger space of test functions.

The problem of choosing a suitable test function space for a field theory is discussed in a paper by Jaffe.[12] The test function space should be the set of infinitely differentiable functions $\hat{h}$ whose Fourier transform h satisfies

$$\|\hat{h}\|_{n,m,A} = \sup_{P\in R} G(A|p|^2)(1+|p|^2)^n |D^m\hat{h}(p)| < \infty$$

for all integers n, m, and A, where $D^m\hat{h}$ denotes the mth derivative of $\hat{h}$ and G is an entire function satisfying

$$\int_0^\infty \frac{\ln[G(t^2)]}{1+t^2}\, dt < \infty. \tag{2}$$

The condition (2) insures that the test function space contains nontrivial functions of compact support. Note that if we take $G \equiv 1$, we obtain the space $\mathcal{S}$. As we have seen, this space is not restrictive enough to insure that the sequence $\|\psi_n(h)\Lambda_n\|_2^2$ remain bounded. Let $\mathcal{J}$ be the test function space corresponding to

$$G(z) = 2\sum_{n=0}^{\infty} \frac{z^n}{(4n)!} = \begin{cases} \cos z^{1/4} + \cosh z^{1/4}, & z \neq 0, \\ 2, & z = 0. \end{cases}$$

As $t \to \pm\infty$, $G(t^2) \sim \exp(\sqrt{|t|})$, so that $\int_0^\infty \{\ln[G(t^2)]/(1+t^2)\}\,dt < \infty$. If $\check{h} \in \mathcal{J}$, then $\check{h}(t)\exp(\sqrt{|t|})$ remains bounded as $t \to \pm\infty$. Hence there exists a constant M such that $|\check{h}(t)| \leqslant M\exp(-\sqrt{|t|})$ for all t. Then

$$\|\check{h}(H_0)\exp(iC_{g_n})\Lambda\|_2^2 \leqslant \|M\exp(-\sqrt{H_0})\exp(iC_{g_n})\Lambda\|_2^2$$
$$= M^2\exp(\|Jg_n\|_2^2/4), \quad \text{where } J(t) = \exp(-\sqrt{|t|}).$$

Hence,

$$\lim_{n\to\infty} \sup \|\psi_n(h)\Lambda_n\|_2^2 \leqslant 2\pi M^2 \exp(\|Jg\|_2^2/2)$$

since $\|Jg\|_2^2 < \infty$.

We will construct the time smoothed annihilation operator without cutoffs for the cases $d=3$ and $d>3$, using the test function spaces $\mathcal{S}$ and $\mathcal{J}$, respectively.

Let S be a bounded open set in R^d, and let F be a function in $L^2(R^d)$ with support in S. Let $g = -i/(2\pi)^d\mu^{3/2}$, $r = g_n X_S$, $r_n = g_n - r$, and $A = \exp(iR_F)$. We will show that the sequence $\psi_n(h)A\Lambda_n$ converges in $\mathcal{F}$. By the definition of $\psi_n(h)$ and the fact that

$$\exp(-itH_n) = \exp(iR_{g_n})\exp(-itH_0)\exp(-iR_{g_n}),$$

we have

$$\psi_n(h)A\Lambda_n = c_n \int dt\, h(t)\exp(itH_0)\exp(iR_{g_n})\exp(-itH_0)$$
$$\times \exp(-iR_{g_n})A\exp(iR_{g_n})\Lambda.$$

By Theorem I.12 and the functional calculus, $\exp(itH_0) \times \exp(iR_{g_n})\exp(-itH_0) = \exp(iR_{\exp(it\mu)g_n})$. Using this fact, the fact that $A \in \mathcal{A}(S)$, and Theorem I.3, we have

$$\psi_n(h)A\Lambda_n = c_n \int dt\, h(t)\exp(iR_{\exp(it\mu)g_n})\exp(-iR_{(r+r_n)})A$$
$$\times \exp(iR_{(r+r_n)})\Lambda$$
$$= c_n \int dt\, h(t)\exp(iR_{\exp(it\mu)g_n})\exp(-iR_r)\exp(-iR_{r_n})A$$
$$\times \exp(iR_{r_n})\exp(iR_r)\Lambda$$
$$= c_n \int dt\, h(t)\exp(iR_{\exp(it\mu)g_n})\exp(-iR_r)A\exp(iR_r)\Lambda.$$

By Theorem I.3,

$$\exp(-iR_r)\exp(R_F)\exp(R_r) = \exp(i\,\mathrm{Im}(F, r)\exp(iR_F)$$

and

$$\exp(iR_{\exp(it\mu)g_n})\exp(iR_F)$$
$$= \exp[\tfrac{1}{2}\mathrm{Im}(\exp(it\mu)_{g_n}, F)]\exp\{iR[\exp(it\mu)_{g_n} + F]\}.$$

Hence,

$$\psi_n(h)A\Lambda_n = c_n \int dt\, h(t)\exp[i\,\mathrm{Im}(F, r)]$$
$$\times \exp[\tfrac{1}{2}\mathrm{Im}(\exp(it\mu)_{g_n}, F)]\exp\{iR[\exp(it\mu)_{g_n} + F]\}\Lambda.$$

By Theorem I.4,

$$\exp(iR_{\exp(it\mu)g_n+F})\Lambda$$
$$= \exp[-\|\exp(it\mu)_{g_n} + F\|^2/4]\exp(iC_{\exp(it\mu)g_n+F})$$
$$\times \exp(iA_{\exp(it\mu)g_n+F})\Lambda$$
$$= \exp(-\|g_n\|^2/4)\exp(-\|F\|^2/4)$$
$$\times \exp[-\tfrac{1}{2}\mathrm{Re}(\exp(it\mu)_{g_n}, F)\exp(iC_{i\exp(it\mu)g_n+F})\Lambda.$$

Therefore, using the fact that $c_n = \exp(\|g_n\|^2/4)$, we have

$$\psi_n(h)A\Lambda_n = \int dt\, h(t)\exp(-\|F\|^2/4)\exp[i\,\mathrm{Im}(F, r)]$$
$$\times \exp[-\tfrac{1}{2}(F, \exp(it\mu)_{g_n})]\exp(iC_{\exp(it\mu)g_n+F})\Lambda.$$

By property (3) of the sequence $\{f_n\}$ and the boundedness of S, there exists an integer N such that, for $n \geqslant N$, $g_n = -[i/(2\pi)^d]/\mu^{3/2} = g$ on S so that $(F, \exp(it\mu)_{g_n}) = (F, \exp(it\mu)_{g_n}$. From now on, we will only consider $n \geqslant N$. Put

$$\eta(t) = \exp(-\|F\|^2/4)h(t)\exp[-\tfrac{1}{2}(F, \exp(it\mu)_{g_n})].$$

Then

$$\psi_n(h)A\Lambda_n = \int dt\, \eta(t) \exp(iC_{\exp(it\mu)_{g_n}+F})\Lambda. \tag{3}$$

To make sense of the limit of the sequence $\{\psi_n(h)\}$, first we note that the Fock space h can be identified in a natural way with the space $\mathbb{C} \oplus \sum_{j=1}^{\infty} \oplus L^2((\mathbb{R}^d)^j)$.[13] This space, in turn, can be identified with the space $L^2(X)$, where X is the set $\{a\} \cup \cup_{j=1}^{\infty}(\mathbb{R}^d)^j$. The measure on X is defined as the disjoint union of the measures on $\{a\}$ and $(\mathbb{R}^d)^j$, $j=1,2,\cdots$, where the measure on $\{a\}$ is the counting measure and the measure on $(\mathbb{R}^d)^j$ is Lebesgue measure. The spaces $\mathbb{C} \oplus \sum_{j=1}^{\infty} \oplus L^2((\mathbb{R}^d)^j)$ and $L^2(X)$ are identified as follows: If $\lambda \oplus \sum_{j=1}^{\infty} \varphi_j \in \mathbb{C} \oplus \sum_{j=1}^{\infty} \oplus L^2((\mathbb{R}^d)^j)$, then we identify it with the element Φ in $L^2(X)$ defined by $\Phi(a)=\lambda$, $\Phi(k_1, \ldots, k_j) = \varphi_j(k_1, \ldots, k_j)$ for all $j = 1,2,\cdots$ and for all $(k_1, \ldots, k_j) \in (\mathbb{R}^d)^j$. Similarly, we can identify $\mathcal{J}$ with the symmetric elements of $L^2(X)$, that is, those elements Φ of $L^2(X)$ with the property that

$$\Phi(k_1, \ldots, k_{j_1}, \ldots, k_{j_2}, \ldots, k_j)$$
$$= \Phi(k_1, \ldots, k_{j_2}, \ldots, k_{j_1}, \ldots, k_j)$$

for all j, $j=1,2,\cdots$, for all j_1, j_2 such that $1 \le j_1 < j_2 \le j$, and for all $(k_1, \ldots, k_j) \in (\mathbb{R}^d)^j$. Under this identification, the element $\exp(iC_{\exp(it\mu)_{g_n}})\Lambda$ in $\mathcal{J}$ is identified with the function Φ_n^t in $L^2(X)$ given by $\Phi_n^t(a)=1$,

$$\Phi_n^t(k_1, \ldots, k_j) = [\exp(it\mu)\, g_n + F]^{(j)}(k_1, \ldots, k_j)\, i^j$$
$$= \prod_{p=1}^{j} i[\exp(it\mu)\, g_n + F](k_p).$$

Define a function Φ^t on X by $\Phi^t(a)=1$. $\Phi^t(k_1, \ldots, k_j) = \prod_{p=1}^{j} i(\exp(it\mu)g + F)(k_p)$. The sequence Φ_n^t coverges pointwise on X to Φ^t for each t, but does not converge in the L^2 sense because $\Phi^t \notin L^2(X)$. (This follows from the fact that $(\exp(it\mu)g + F) \notin L^2(\mathbb{R}^d)$. Now put $\Psi_n(h) = \int_{\mathbb{R}^{\prime}} dt\, \eta(t)\Phi_n^t$ and $\Psi(h) = \int_{\mathbb{R}^{\prime}} dt\, \eta(t)\Phi^t$. Then for each n, $\Psi_n(h)$ is the element of $L^2(X)$ corresponding to $\Psi_n(h)A\Lambda_n$. We wish to show that $\Psi(h) \in L^2(X)$ and that $\Psi_n(h) \to \Psi(h)$ in the L^2 sense. To do this, it suffices by the dominated convergence theorem to show that $\Psi_n(h)$ is dominated in L^2 norm by a function in $L^2(X)$. It is clear that $|\Psi_n(h)|$ is an increasing sequence, so that $\|\Psi(h)\|_2 = \lim_{n\to\infty} \|\Psi_n(h)\|_2$ by the monotone convergence theorem and $\|\Psi_n(h)\|_2 \le \|\Psi(h)\|_2$ for all n (where we are allowing the possibility that $\|\Psi(h)A\|_2 = \infty$). If we can show that the sequence $\{\|\Psi_n(h)\|_2\}$ is bounded, it will follow that $\|\Psi(h)\|_2 < \infty$ and that $\Psi(h)$ dominates $\{\Psi_n(h)\}$ in L^2 norm. Also, the bound on the sequence $\{\|\Psi_n(h)\|_2\}$ will be a bound on $\|\Psi(h)\|_2$.

Since $\|\Psi_n(h)\|_2 = \|\psi_n(h)A\Lambda_n\|$, we have reduced the problem to showing that $\{\|\psi_n(h)A\Lambda_n\|\}$ is bounded. Actually, we will prove an even stronger result.

Definition II.1: For $u \in \mathcal{K}$, let $\|u\|_{\mathcal{K}}$ denote its norm in $\mathcal{K}$. If S is a bounded open set in R^d, let $[A]$ denote the element in $\mathcal{A}(S)$ determined by A, i.e.,

$$[A] = \{B \in \mathcal{A}(S) \mid \lim_{n\to\infty} ((A-B)^* (A-B)\Lambda_n, \Lambda_n).$$

Definition II.2: N_S denotes the closure of the unbounded operator N_S° defined on the closure of $[\mathcal{A}(S)]$ in $\mathcal{K}$ as follows. The domain of N_S° is $\{[A] \mid A \in \mathcal{A}(S)$ and $d\Gamma(X_S)A$ is a bounded operator on Fock space$\}$. N_S° is defined on this domain by the formula

$$N_S[A] = [d\Gamma(X_S)A].$$

Theorem II.3: Let S be a bounded open set in $\mathbb{R}^3$. Then there exist constants M_1, M_2, and L such that

$$\|\psi_n(h)A\Lambda_n\| \le M_1(L\|h\|_1 + \|h'\|_1)\|[A]\|_{\mathcal{K}}$$
$$+ M_2\|h\|_1\|(N_S + I)^{1/2}[A]\|_{\mathcal{K}}$$

for all $h \in \mathcal{S}$ and $[A] \in \mathcal{D}_{(N_S+I)^{1/2}}$.

From this theorem and our previous remarks, we have the following corollary:

Corollary II.4: For every bounded open set S in $\mathbb{R}^3$, $\psi(h)$ is definable on all $[A] \in \mathcal{D}_{(N_S+I)^{1/2}}$ as a strong limit in $\mathcal{J}$ of the sequence $\{\psi_n(h)A\Lambda_n\}$. Moreover, for such S, there exist constants $M_1(S)$, $M_2(S)$, and $L(S)$ such that

$$\|\psi(h)\| \le M_1(S)(L(S)\|h\|_1 + \|h'\|_1)\|[A]\|_{\mathcal{K}}$$
$$+ M_2(S)\|h\|_1\|(N_S + I)^{1/2}[A]\|_{\mathcal{K}}$$

for all $[A] \in \mathcal{D}_{(N_S+I)^{1/2}}$ and $h \in \mathcal{S}$.

Remark II.5: A straightforward calculation shows that for each $F \in L^2(\mathbb{R}^3)$ with support in S, a bounded open set in $\mathbb{R}^3$, $[\exp(iR_F)] \in \mathcal{D}_{(N_S+I)^{1/2}}$. Since $\mathcal{B} = \cup[\mathcal{A}(S)]$ is dense in $\mathcal{K}$, Corollary II.4 implies that $\psi(h)$ is densely defined on $\mathcal{K}$.

Remark II.6: Corollary II.4 asserts that for fixed $h \in \mathcal{S}$, $\psi(h)|_{\mathcal{A}(s)}$ is bounded with respect to $(N_S + I)^{1/2}$ and that for fixed $A \in \mathcal{D}_{(N_S+I)^{1/2}} \psi(h)A$ is a continuous function of h relative to the norm $(\|h\|_1 + \|h'\|_1)$.

Proof of Theorem II.3: Put $E_n = \|\psi_n(h)A\Lambda_n\|^2$. Then

$$E_n = c_n^2\Big(\int dt\, h(t) \exp(itH_0)\exp(-itH_n)A\Lambda_n,$$
$$\int ds\, h(s)\exp(isH_0)\exp(-isH_n)A\Lambda_n\Big).$$

By Fubini's theorem,

$$E_n = c_n^2 \int\int dt\, ds\, h(t)\overline{h(s)}$$
$$(\exp(itH_0)\exp(-itH_n)A\Lambda_n, \exp(isH_0)\exp(-isH_n)A\Lambda_n).$$

By Theorem I.6, we may regard $\mathcal{J}$ as $\mathcal{J}_1 \otimes \mathcal{J}_2$, where $\mathcal{J}_1$ is the Fock space over $L^2(S)$ and $\mathcal{J}_2$ is the Fock space over $L^2(S^c)$. Let Λ_1 and Λ_2 denote the vacuum states for $\mathcal{J}_1$ and $\mathcal{J}_2$. Let

$$H_0^1 = d\Gamma(\mu\chi_S), \quad H_0^2 = d\Gamma(\mu\chi_{S^c}),$$

$$H_n^1 = \exp(iR_r)H_0^1\exp(-iR_r), \quad \text{and} \quad H_n^2 = \exp(-R_{r_n})H_0^2\exp(-iR_{r_n}).$$

Then

$$\exp(itH_0)\exp(-itH_n)A\Lambda_n$$
$$= \exp[it(H_0^1 + H_0^2)]\exp[-it(H_n^1 + H_n^2)]A\exp(iR_r)\exp(iR_{r_n})\Lambda$$
$$= \exp(itH_0^1)\exp(-itH_n^1)A\exp(iR_r)\exp(itH_0^2)$$
$$\times\exp(-itH_n^2)\exp(iR_{r_n})\Lambda$$
$$= [\exp(itH_0^1)\exp(-itH_n^1)A\exp(iR_r)][\exp(itH_0^2)\exp(iR_{r_n})]\Lambda.$$

Letting $B = \exp(-iR_r)A\exp(iR_r)$, we have

$$(\exp(itH_0)\exp(-itH_n)A\Lambda_n, \exp(isH_0)\exp(-isH_n)A\Lambda_n)$$
$$= (\exp(itH_0^1)\exp(-itH_n^1)A\exp(-iR_r)\Lambda_1,$$
$$\exp(isH_0^1)\exp(-isH_n^1)A\exp(-iR_r)\ \Lambda_1)$$
$$\times(\exp(itH_0^2)\exp(iR_{r_n})\Lambda_2, \exp(isH_0^2)\exp(iR_{r_n})\Lambda_2)$$

$$= (\exp(itH_0^1)\exp(iR_r)\exp(-itH_0^1)B\Lambda_1,$$
$$\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1)$$
$$\times(\exp(itH_0^2)\exp(iR_{r_n})\Lambda_2,\ \exp(isH_0^2)\exp(iR_{r_n})\Lambda_2).$$

Let $\sigma(t,s) = (\exp(itH_0^1)\exp(iR_r)\exp(-itH_0^1)B\Lambda_1,\ \exp(isH_0^1) \times \exp(iR_r)\exp(-isH_0^1)B\Lambda_1)$. Then

$$E_n = c_n^2 \int\int dt\,ds\, h(t)\overline{h(s)}\sigma(t,s)$$
$$\times(\exp(itH_0^2)\exp(iR_{r_n})\Lambda_2,\ \exp(isH_0^2)\exp(iR_{r_n})\Lambda_2).$$

By Theorem I.4,

$$E_n = \exp(\|r\|^2/2)\int\int dt\,ds\, h(t)\overline{h(s)}\sigma(t,s)$$
$$\times(\exp(itH_0^2)\exp(iC_{r_n})\Lambda_2,\ \exp(isH_0^2)\exp(iC_{r_n})\Lambda_2).$$

Now putting $\mu_2 = \mu\chi_{S^c}$ and using Theorems I.3 and I.12, we have

$$(\exp(itH_0^2)\exp(iC_{r_n})\Lambda_2,\ \exp(isH_0^2)\exp(iC_{r_n})\Lambda_2)$$
$$= (\exp[iC_{\exp(it\mu_2)r_n}]\Lambda_2,\ \exp[iC_{\exp(is\mu_2)r_n}]\Lambda_2)$$
$$= \sum_{p=0}^{\infty}\frac{1}{p!}([\exp(it\mu_2)r_n]^{(p)},\ [\exp(is\mu_2)r_n]^{(p)})$$
$$= \sum_{p=0}^{\infty}\frac{1}{p!}(\exp(it\mu_2)r_n,\ \exp(is\mu_2)r_n)^p$$
$$= \sum_{p=0}^{\infty}\frac{1}{p!}\left(\int dk\,\exp(it\mu_2)\exp(-is\mu_2)|r_n(k)|^2\right)^p$$
$$= \sum_{p=0}^{\infty}\frac{1}{p!}\int\circ\circ\circ\int\prod_{\alpha=1}^{p} dk_\alpha |r_n(k_\alpha)|^2$$
$$\times\exp[it\mu_2(k_\alpha)]\exp[-is\mu_2(k_\alpha)].$$

Hence we have

$$E_n = \exp(\|r\|^2/2\int\int dt\,ds\,h(t)\overline{h(s)}\sum_{p=0}^{\infty}\frac{1}{p!}$$
$$\times\int\circ\circ\circ\int\prod_{\alpha=1}^{p} dk_\alpha|r_n(k_\alpha)|^2$$
$$\times\ \exp[it\mu_2(k_\alpha)]\ \ \exp[-is\mu_2(k_\alpha)]\sigma(t,s).$$

Then by Fubini's Theorem,

$$E_n = \exp(\|r\|^2/2)\sum_{p=0}^{\infty}\frac{1}{p!}\int\circ\circ\circ\int\prod_{\alpha=1}^{p}dk_\alpha|r_n(k_\alpha)|^2$$
$$\times\int\int dt\,ds\,h(t)\overline{h(s)}\exp\left(it\sum_{\alpha=1}^{p}\mu_2(k_\alpha)\right)$$
$$\times\exp\left(-is\sum_{\alpha=1}^{p}\mu_2(k_\alpha)\right)\sigma(t,s).$$

We are trying to obtain an estimate of E_n that depends on $\|[A]\|_K$, $\|N_S^{1/2}[A]\|_K$, $\|h\|_1$, and $\|h'\|_1$, but not on n. To do this, we shall need the following lemma.

Lemma II.7: If θ is a function on $\mathbb{R}_1^+$ (the nonnegative half-line) with the property that $|\theta(t)| \leqslant \min M(1/t^2, 1/e)$ for all $t \geqslant 0$, then $|\theta(t)| \leqslant M(\int_0^1 s\exp(-st)\,ds + 2\exp(-t))$ for all $t \geqslant 0$.

Proof: Let t be greater than 0. Consider $\int_0^\infty s\exp(-st)\,ds$. Integrating by parts, with $u = s$ and $dv = \exp(-st)\,ds$, we obtain $1/t^2 = \int_0^\infty s\exp(-st)\,ds = \int_0^1 s\exp(-st)\,ds + \int_1^\infty s\exp(-st)\,ds$. Integrating $\int_1^\infty s\exp(-sr)\,ds$ by parts with $u = s$ and $dv = \exp(-st)$, we obtain

$$\int_1^\infty s\exp(-st)\,ds = -(1/t)s\exp(-st)\Big|_1^\infty + (1/t)\int_1^\infty\exp(-st)ds$$
$$= (1/t)\exp(-t) + (1/t^2)\exp(-t).$$

Hence, $1/t^2 = \int_0^1 s\exp(-st)\,ds + (1/t)\exp(-t) + (1/t^2) \times \exp(-t)$. If $t \geqslant 1$, the above expression is less than or equal to $\int_0^1 ds\, s\exp(-st) + 2\exp(-t)$. If $0 \leqslant t < 1$, then $1/e < 2/e \leqslant 2\exp(-t) \leqslant \int_0^1 ds\,s\exp(-st) + 2\exp(-t)$. Now since $|\theta(t)| \leqslant \min M(1/t^2,\ 1/e)$ for all $t \geqslant 0$, $|\theta(t)| \leqslant M(\int_0^1 s\exp(-st)\,ds + 2\exp(-t))$ for all $t \geqslant 0$. ■

Now put $\theta(T) = \int\int dt\,ds\,h(t)\overline{h(s)}\exp(itT)\exp(-isT)\sigma(t,s)$. In order to apply the lemma, we will show that $|\theta(t)| \leqslant \|[A]\|_K^2\ \|h\|_1^2$ and $|\theta(T)| \leqslant (1/T^2)(\|h'\|_1\|[A]\|_K + \|C\|\ \|h\|_1 \times\|h\|_1\|(N_S+I)^{1/2}[A]\|_K)^2$. To prove the first estimate, we note that $|\theta(T)| \leqslant \int\int dt\,ds|h(t)|\ |h(s)|\ |\sigma(t,s)|$ and, by the definition of σ and the Schwarz inequality,

$$|\sigma(t,s)| \leqslant \|\exp(itH_0^1)\exp(iR_r)\exp(-itH_0^1)B\Lambda_1\|$$
$$\times\|\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1\|$$
$$= \|B\Lambda_1\|^2 = \|\exp(-iR_r)A\exp(iR_r)\Lambda_1\|^2$$
$$= \|A\exp(iR_r)\Lambda_1\|^2$$
$$= \|[A]\|^2.$$
$$\therefore\ |\theta(T)| \leqslant \int\int dt\,ds|h(t)|\ |h(s)|\ \|[A]\|_K^2$$
$$= \|[A]\|_K^2\ \ \|h\|_1^2.$$

To obtain the second estimate, we integrate by parts in s and t, obtaining

$$\theta(T) = (1/T^2)\int\int dt\,ds[h'(t)\overline{h'(s)}\sigma(t,s)$$
$$+ h'(t)\overline{h(s)}\sigma_s(t,s) + h(t)\overline{h'(s)}\sigma_t(t,s)$$
$$+ h(t)\overline{h(s)}\sigma_{t,s}(t,s)].$$

Then

$$|\theta(T)| \leqslant (1/T^2)[\int\int dt\,ds|h'(t)|\ |h'(s)|\ |\sigma(t,s)|$$
$$+ \int\int dt\,ds|h'(t)|\ |h(s)|\ |\sigma_s(t,s)|$$
$$+ \int\int dt\,ds|h(t)|\ |h'(s)|\ |\sigma_t(t,s)|$$
$$+ \int\int dt\,ds|h(t)|\ |h(s)|\ |\sigma_{t,s}(t,s)|].$$

Since $\sigma(t,s)$ is symmetric in t and s,

$$\int\int dt\,ds|h'(t)|\ |h(s)|\ |\sigma_s(t,s)|$$
$$= \int\int dt\,ds|h(t)|\ |h'(s)|\ |\sigma_t(t,s)|,$$

and the previous equation reduces to

$$|\theta(T)| \leqslant [\int\int dt\,ds|h'(t)|\ |h'(s)|\ |\sigma(t,s)|$$
$$+ 2\int\int dt\,ds|h'(t)|\ |h(s)|\ |\sigma_s(t,s)|$$
$$+ \int\int dt\,ds|h(t)|\ |h(s)|\ |\sigma_{t,s}(t,s)|].$$

Since $\sigma(t,s)| < \|[A]\|_K^2$, the first of these three double integrals is less than or equal to $\|[A]\|_K^2\ \|h'\|_1^2$.

To estimate the second integral, we first note that

$$\sigma_s(t,s) = \frac{\partial}{\partial s}(\exp(itH_0^1)\exp(iR_r)\exp(-itH_0^1)B\Lambda_1,$$
$$\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1)$$
$$= \Big(\exp(itH_0^1)\exp(iR_r)\exp(-itH_0^1)B\Lambda_1,$$

$$\frac{\partial}{\partial s}[\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1]\Big),$$

$$\frac{\partial}{\partial s}[\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1]$$

$$=iH_0^1\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1$$

$$-i\exp(isH_0^1)\exp(iR_r)H_0^1\exp(-isH_0^1)B\Lambda_1$$

$$=i\exp(isH_0^1)[H_0^1,\exp(iR_r)]\exp(-isH_0^1)B\Lambda_1.$$

Put $\mu_1=\mu\chi_s$. Then by Theorem I.13

$$\frac{\partial}{\partial s}[\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1]$$

$$=i\exp(isH_0^1)(\tfrac{1}{2}(\mu_1 r,r)+R_{i\mu_1 r})\exp(-isH_0^1)B\Lambda_1$$

$$=i\exp(isH_0^1)(\tfrac{1}{2}(\mu_1 r,r)+R_{i\mu_1 r})\exp(-isH_0^1)$$

$$\times\exp(-iR_r)A\exp(iR_r)\Lambda_1.$$

By Theorem I.12 and the functional calculus, this last expression is equal to

$$i\exp(isH_0^1)(\tfrac{1}{2}(\mu_1 r,r)+R_{i\mu_1 r})\exp(-iR_{\exp-is\mu_1 r)})$$

$$\times\exp(-isH_0^1)A\exp(iR_r)\Lambda_1.$$

Put $C=[\frac{1}{2}(\mu_1 r,r)+R_{i\mu_1 r}]\exp(-iR_{\exp-is\mu_1 r)})\ (\tilde{N}_S+I)^{-1/2}$, where $\tilde{N}_S=d\Gamma(\chi_S)$. By Theorem I.2,

$$R_{i\mu_1}\exp(-iR_{\exp(-is\mu_1 r)}$$

$$=\exp(-iR_{\exp(-is\mu_1 r)})R_{i\mu_1 r}$$

$$+\operatorname{Im}(\exp(-is\mu_1)r,\mu_1 r)\exp(-iR_{\exp(-is\mu_1 r)})$$

on $\mathcal{D}_{R_{i\mu_1 r}}$. Hence by Theorem I.11, C is a bounded operator for each s and the bound is independent of s. Then we have

$$\frac{\partial}{\partial s}[\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1]$$

$$=i\exp(isH_0^1)C(\tilde{N}_S+I)^{1/2}\exp(-isH_0^1)A\exp(iR_r)\Lambda_1$$

$$=i\exp(isH_0^1)C\exp(-isH_0^1)(\tilde{N}_S+1)^{1/2}A\exp(iR_r)\Lambda_1.$$

Therefore,

$$\Big\|\frac{\partial}{\partial s}[\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1]\Big\|$$

$$=\|i\exp(isH_0^1)C(\exp(-isH_0^1)[(\tilde{N}_S+I)^{1/2}A]\exp(iR_r)\Lambda_1\|$$

$$\leqslant\|C\|\ \|(\tilde{N}_S+I)^{1/2}A)\exp(iR_r)\Lambda_1\|$$

$$=\|C\|\ \|(N_S+I)^{1/2}[A]\|.$$

From this it follows that

$$|\sigma_s(t,s)|\leqslant\|\exp(itH_0^1)\exp(iR_r)\exp(-itH_0^1)B\Lambda_1\|$$

$$\times\Big\|\frac{\partial}{\partial s}[\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1]\Big\|$$

$$\leqslant\|[A]\|_K\ \|C\|\ \|(N_S+I)^{1/2}[A]\|_K.$$

Thus, the second integral is less than or equal to

$$2\iint dt\,ds\,|h'(t)|\ |h(s)|\ \|[A]\|_K\|C\|\ \|(N_S+I)^{1/2}[A]\|_K$$

$$=2\|C\|\ \|h\|_1\|h'\|_1\|[A]\|_K\|(N_S+I)^{1/2}[A]\|_K.$$

To estimate the third integral, we observe that

$$|\sigma_{t,s}(t,s)|=\Big|\Big(\frac{\partial}{\partial t}[\exp(itH_0^1)\exp(iR_r)\exp(-itH_0^1)B\Lambda_1],$$

$$\frac{\partial}{\partial s}[\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1]\Big)\Big|$$

$$\leqslant\Big\|\frac{\partial}{\partial t}[\exp(itH_0^1)\exp(iR_r)\exp(-itH_0^1)B\Lambda_1]\Big\|$$

$$\times\Big\|\frac{\partial}{\partial s}[\exp(isH_0^1)\exp(iR_r)\exp(-isH_0^1)B\Lambda_1]\Big\|$$

$$\leqslant\|C\|^2\|(N_S+I)^{1/2}[A]\|_K^2,$$

implying that the third integral is less than or equal to $\|C\|^2\|h\|_1^2\|(N_S+I)^{1/2}[A]\|_K^2$. Using the estimates on these integrals, we have

$$|\theta(T)|\leqslant(1/T^2)(\|h'\|_1^2\|[A]\|_K^2+2\|C\|\|h\|_1\|h'\|_1\|[A]\|_K$$

$$\times\|(N_S+I)^{1/2}[A]\|_K+\|C\|^2\|h\|_1^2\|(N_S+I)^{1/2}[A]\|_K^2)$$

$$=(1/T^2)(\|h'\|_1\|[A]\|_K+\|C\|\ \|h\|_1\|(N_S+I)^{1/2}\|[A]\|_K)^2.$$

Put $M=(\|h'\|_1\|[A]\|_K+\|C\|\ \|h\|_1\|(N_S+I)^{1/2}A\|)^2+e\|[A]\|_K^2\|h\|_1^2$. Then by our two estimates on θ, we have $|\theta(T)|\leqslant\min M(1/T^2,1/e)$. Therefore, by Lemma II.7, $|\theta(T)|\leqslant M(\int_0^1 s\exp(-sT)\,ds+2\exp(-T)$ for all $T\geqslant 0$, and, recalling the definition of θ, we get

$$\Big|\iint dt\,ds\,h(t)\overline{h(s)}\exp(itT)\exp(-isT)\sigma(t,s)\Big|$$

$$=M(\int_0^1 s\exp(-sT)\,ds+2\exp(-T)).$$

Putting $T=\sum_{\alpha=1}^{p}\mu_2(k_\alpha)$ in this last inequality, we have

$$\iint dt\,ds\,h(t)\overline{h(s)}\exp\Big(it\sum_{\alpha=1}^{p}\mu_2(k_\alpha)\Big)$$

$$\times\exp\Big(-is\sum_{\alpha=1}^{p}\mu_2(k_\alpha)\Big)\sigma(t,s)\Big|$$

$$\leqslant M\Big[\int_0^1 s\exp\Big(-s\sum_{\alpha=1}^{p}\mu_2(k_\alpha)\Big)ds+2\exp\Big(-\sum_{\alpha=1}^{p}\mu_2(k_\alpha)\Big)\Big].$$

Using this result in Eq. (1), we get

$$E_n\leqslant M\exp(\|r\|^2/2)\sum_{p=0}^{\infty}\frac{1}{p!}\int\cdots\int\prod_{\alpha=1}^{p}dk_\alpha|r_n(k_\alpha)|^2$$

$$\times\Big[\int_0^1 s\exp\Big(-s\sum_{\alpha=1}^{p}\mu_2(k_\alpha)\Big)ds+2\exp\Big(-\sum_{\alpha=1}^{p}\mu_2(k_\alpha)\Big)\Big].$$

By Fubini's theorem, this is equal to

$$M\exp(\|r\|^2/2)\Big(\int_0^1 ds\,s\sum_{p=0}^{\infty}\frac{1}{p!}\int\cdots\int\prod_{\alpha=1}^{p}dk_\alpha|r_n(k_\alpha)|^2$$

$$\times\exp[-s\mu_2(k_\alpha)]+2\sum_{p=0}^{\infty}\frac{1}{p!}\int\cdots\int\prod_{\alpha=1}^{p}dk_\alpha$$

$$\times|r_n(k_\alpha)|^2\exp[-\mu_2(k_\alpha)]\Big)$$

$$=M\exp(\|r\|^2/2)\Big(\int_0^1 ds\,\{s\exp[\|\ |r_n|^2\exp(-s\mu_2)\|_1]\}$$

$$+2\exp[\|\ |r_n|^2\exp(-\mu_2)\|_1]$$

$$\leqslant M\exp(\|r\|^2/2)\int_0^1 ds[s\exp(\|\ |g|^2\exp(-s\mu)\|_1)]$$

$$+2\exp(\|\ |g|^2\exp(-\mu)\|_1)\Big).$$

Put $K=\exp(\|r^2/2)(\int_0^1 ds\,[\exp(\|\ |g|^2\exp(-s\mu)\|_1)]+2\exp(\|\ |g|^2\exp(-\mu)\|_1)$. We claim that $K<\infty$. Since

$\| |g|^2 \exp(-\mu)\|_1$ is clearly finite, it suffices to show that $\int_0^1 ds\, [s \exp(\| \, |g|^2) \quad \exp(-s\mu\|_1)] < \infty$. Now

$$\| \, |g|^2 \exp(-s\mu)\|_1 = \frac{1}{4\pi^6} \int_{\mathbb{R}^3} \frac{1}{\mu^3(k)} \exp(-s\mu)\, dk$$

$$= \frac{1}{4\pi^6} \int_{\mathbb{R}^3} \frac{1}{(|k|^2 + m^2)^{3/2}}$$

$$\times \exp[-s(|k|^2 + m^2)^{1/2}]\, dk.$$

By the spherical symmetry of the integrand, we have

$$\| \, |g|^2 \exp(-s\mu)\|_1 = \frac{1}{\pi^5} \int_0^\infty \frac{\rho^2}{(\rho^2 + m^2)^{3/2}}$$

$$\times \exp[s(\rho^2 \; m^2)^{1/2}]\, d\rho.$$

Put

$$\beta(s) = \frac{1}{\pi^5} \int_0^1 \frac{\rho^2}{(p^2 + m^2)^{3/2}} \exp[-s(\rho^2 + m^2)^{1/2}]\, d\rho$$

and

$$\gamma(s) = \frac{1}{\pi^5} \int_1^\infty \frac{\rho^2}{(\rho^2 + m^2)^{3/2}} \exp[-s(\rho^2 + m^2)^{1/2}]\, d\rho.$$

Then

$$\int_0^1 ds\, [s \exp(\| \, |g|^2 \exp(-s\mu)\|_1)]$$

$$= \int_0^1 s \exp[\beta(s) + \gamma(s)]\, ds$$

$$= \int_0^1 (s \exp[\gamma(s)]) \exp(\beta(s))\, ds.$$

It is clear that $\beta(s)$ and hence $\exp(\beta(s))$ are bounded functions on $[0,1]$. Hence to show convergence of the integral, it suffices to show that $\int_0^1 s \exp(\gamma(s))\, ds < \infty$. But

$$\gamma(s) \leq \frac{1}{\pi^5} \int_1^\infty \frac{\rho^2}{(\rho^2)^{3/2}} \exp(-s\rho)\, d\rho$$

$$= \frac{1}{\pi^5} \int_1^\infty \frac{1}{\rho} \exp(-s\rho)\, d\rho$$

$$= \frac{1}{\pi^5} \int_s^\infty \frac{\exp(-u)}{u}\, du$$

$$\leq \frac{1}{\pi^5} \left(\int_s^1 \frac{du}{u} + \int_1^\infty \exp(-u)\, du \right)$$

$$= \frac{1}{\pi^5} \left((-\ln s) + \frac{1}{e} \right).$$

$$\therefore \int_0^1 s \exp(\gamma(s))\, ds \leq \int_0^1 s \exp\left[\frac{1}{\pi^5} \left((-\ln s) + \frac{1}{e} \right) \right] ds$$

$$= \int_0^1 s \left(\frac{1}{s} \exp(1/e) \right)^{1/\pi^5} ds$$

$$\leq (\exp(1/e))^{1/\pi^5} \int_0^1 s \circ \frac{1}{s}\, ds$$

$$= (\exp(1/e))^{1/\pi^5} < \infty.$$

Thus $\int_0^1 ds[s \exp(\| \, |g|^2 \exp(-s\mu)\|_1)] < \infty$ and hence $K < \infty$. So we have

$$E_n \leq MK = K[(\|h'\|_1 \|[A]\|_K + \|C\| \, \|h\|_1$$

$$\times \|(N_S + I)^{1/2}[A]\|_K)^2 + e\|[A]\|_K^2 \, \|h\|_1^2]$$

$$\leq K[\|h'\|_1 \|[A]\|_K + \|C\| \, \|h\|_1$$

$$\times \|(N_S + I)^{1/2}[A]\|_K + e\|[A]\|_K \, \|h\|_1]^2.$$

Recalling the definition of E_n, we have

$$\|\psi_n(h) A \Lambda_n\| \leq K^{1/2}[\|h'\|_1 \|[A]\|_K + \|C\| \, \|h\|_1$$

$$\times \|(N_S + I)^{1/2}[A]\| + e\|[A]\|_K \, \|h\|_1]$$

$$= M_1(L\|h\|_1 + \|h'\|_1)\|[A]\|_K$$

$$+ M_2 \|h\|_1 \|(N_S + I)^{1/2}[A]\|_K,$$

where $M_1 = K^{1/2}$, $M_2 = K^{1/2}\|C\|$, and $L = e/M_1$. This completes the proof of Theorem II.3.

For the case $d > 3$, we cannot prove a detailed estimate like the one in Theorem II.3; in fact, we cannot even construct $\psi(h)$ for $h \in \mathcal{S}$ in general. We will construct $\psi(h)$ for $h \in \mathcal{G}$. To do this, we will show that the sequence $\|\psi_n(h) A \Lambda_n\|_2^2$ is a bounded sequence when $A = \exp(iR_F)$ and F is a continuous function with compact support on R^d. (Note that the set of all finite linear combinations of operators $[\exp(iR_F)]$, where F is continuous and has compact support is dense in $\mathcal{K}$; hence when we have shown that $\|\psi_n(h) A \Lambda_n\|_2^2$ is bounded for such A, we will have shown $\psi(h)$ can be defined on a dense set.)
By the remarks preceding Definition II.1, we see that it suffices to show that $\|\Psi(h)\|_2 < \infty$ where, as before, $\Psi(h) = \int_{R^1} dt\, \eta(t) \Phi^t$ and $\eta(t) = \exp(-\|F\|^2/4) h(t) \exp[-\frac{1}{2}(F, \exp(it\mu)g)]$. First we need some lemmas. In the following we write Zh for $\hat{h}$ and $Z^{-1}h = \check{h}$.

Lemma II.8:

$$\|Z^{-1}(h \exp\{\tfrac{1}{2} \exp[-it\mu(k)]Ag(k)\})(s) \exp(\sqrt{|s|}\|_{\infty,s}$$

$$\leq \exp\{\tfrac{1}{2}|Ag(k)| \exp[\sqrt{\mu(k)}]\} \|Z^{-1}h(s) \exp(\sqrt{|s|}\, \|_{\infty,s},$$

where $k \in R^d$, A is a constant, and $\|f(s)\|_{\infty,s}$ denotes $\sup_{-\infty < s < \infty} |f(s)|$.

Proof:

$$Z^{-1}(h \exp\{\tfrac{1}{2} \exp[-it\mu(k)]Ag(k)\})$$

$$= Z^{-1}(h) * Z^{-1}(\exp\{\tfrac{1}{2} \exp[-it\mu(k)]Ag(k)\}).$$

Note that if δ_x denotes the Dirac delta distribution centered at x, then

$$Z\left(\sum_{j=0}^\infty \frac{[\frac{1}{2}Ag(k)]^j \delta_{j\mu(k)}}{j!} \right)(t)$$

$$= \sum_{j=0}^\infty \frac{[\frac{1}{2}Ag(k)]^j Z(\delta_{j\mu(k)})(t)}{j!}$$

$$= \sum_{j=0}^\infty \frac{[\frac{1}{2}Ag(k)]^j \exp(-itj\mu)(k)}{j!}$$

$$= \exp\{\tfrac{1}{2}Ag(k) \exp[-it\mu(k)]\}$$

in the sense of distributions. Therefore,

$$Z^{-1}(\exp\{\tfrac{1}{2} \exp[-it\mu(k)]Ag(k)\}) = \sum_{j=0}^\infty \frac{[\frac{1}{2}Ag(k)]^j \delta_{+j\mu(k)}}{j!}$$

and

$$Z^{-1}(h) * Z^{-1}(\exp\{\tfrac{1}{2} \exp[-it\mu(k)]Ag(k)\})(s)$$

$$= \sum_{j=0}^\infty \frac{[\frac{1}{2}Ag(k)]^j Z^{-1}h(-j\mu(k) + s)}{j!}.$$

From this it follows that

$$\|Z^{-1}(h) * Z^{-1}(\exp\{\tfrac{1}{2}\exp[-it\mu(k)]Ag(k)\})(s)\exp(\sqrt{|s|})_{\infty,s}$$

$$\leqslant \sum_{j=0}^{\infty} \frac{|\frac{1}{2}Ag(k)|^{j}}{j\,!} \|h[-j\mu(k)+s]\exp(\sqrt{|s|})\|_{\infty,s}$$

$$\leqslant \sum_{j=0}^{\infty} \frac{|\frac{1}{2}Ag(k)|^{j}}{j!} \|h(s)\exp(\sqrt{|s+j\mu(k)|})\|_{\infty,s}$$

$$\leqslant \sum_{j=0}^{\infty} \frac{|\frac{1}{2}Ag(k)|^{j}}{j!} \exp(\sqrt{j\mu(k)})\|h(s)\exp(\sqrt{|s|})\|_{\infty,s}$$

$$\leqslant \sum_{j=0}^{\infty} \frac{|\frac{1}{2}Ag(k)\exp(\sqrt{\mu(k)})|^{j}}{j\,!} \|h(s)\exp(\sqrt{|s|})\|_{\infty,s}$$

$$=\exp\{\tfrac{1}{2}|Ag(k)|\exp[\sqrt{\mu(k)}]\}\|h(s)\exp(\sqrt{|s|})\|_{\infty,s}.$$

Lemma II. 9: Let $k_j \in R^d$ and $D_j \in \mathbb{C}$ for $j=1,\ldots,n$. Let

$$M = \max_{j=1,\ldots,n} \tfrac{1}{2}|g(k_j)D_j\exp[\sqrt{\mu(k_j)}]|.$$

Then

$$Z^{-1}\left[h\exp\left(\frac{1}{2}\sum_{j=1}^{n}\frac{\exp[-it\mu(k_j)g(k_j)D_j]}{n}\right)\right](s)\exp(\sqrt{|s|})\|_{\infty,s}$$

$$\leqslant e^{M}\|h(s)\exp(\sqrt{|s|})\|_{\infty,s}.$$

Proof: We will use induction on n. For $n=1$, the result is true by Lemma II. 8. If the result is true for $n-1$, then

$$Z^{-1}\left[h\exp\left(\frac{1}{2}\sum_{j=1}^{n}\frac{\exp[-it\mu(k_j)]g(k_j)D_j}{n}\right)\right](s)\exp(\sqrt{|s|})\Big\|$$

$$=\Big\|Z^{-1}\left\{\left[h\exp\left(\frac{1}{2}\frac{n-1}{n}\sum_{j=1}^{n-1}\frac{\exp[-it\mu(k_j)]g(k_j)D_j}{n-1}\right)\right]\right.$$

$$\left.\times\exp\left(\frac{1}{2}\frac{1}{n}\exp[it\mu(k_n)]g(k_n)D_n\right)\right\}(s)\exp(\sqrt{|s|})\Big\|_{\infty,s}$$

$$\leqslant \exp(M/n)\Big\|Z^{-1}\left\{h\exp\left[\frac{1}{2}\sum_{j=1}^{n-1}\frac{\exp[-it\mu(k_j)]g(k_j)}{n-1}\right.\right.$$

$$\left.\left.\times\left(D_j\frac{n-1}{n}\right)\right]\right\}(s)\exp(\sqrt{|s|})\Big\|_{\infty,s} \qquad \text{(by Lemma II.8)}$$

$$\leqslant \exp(M/n)\exp[(n-1)M/n]\|\check{h}(s)\exp(\sqrt{|s|})\|_{\infty,s}$$

(by the induction hypothesis)

$$=e^{M}\|\check{h}(s)\exp(\sqrt{|s|})\|_{\infty,s}.$$

Lemma II. 10: Let F be a continuous function with compact support on R^d. Suppose the support is contained in the set $B=\{x\in R^d|\ |x_j|\leqslant L,\ j=1,\ldots,d$ (where x_j denotes the jth coordinate of x)$\}$. Let $M=\frac{1}{2}L^d \times \sup_{k\in R^d}|g(k)F(k)\exp[\sqrt{\mu(k)}]|$. Then

$$\|Z^{-1}\{h\exp[\tfrac{1}{2}(F,\exp(it\mu)g)]\}(s)\exp(\sqrt{|s|})\|_{\infty,s}$$

$$\leqslant \exp(M)\|\check{h}(s)\exp(|s|^{1/2})\|_{\infty,s}\ .$$

Proof: For each positive integer n, let P_n be the partition of B into n^d boxes of equal size. Choose one point from each box in P_n and call the set so obtained Q_n. Then by the continuity of F,

$$\lim_{n\to\infty}\tfrac{1}{2}(L^d/n^d)\sum_{k_j\in Q_n}\exp[-it\mu(k_j)]g(k_j)F(k_j)$$

$$=(F,\exp(it\mu)g)\ \text{ for each } t.$$

Hence,

$$\lim_{n\to\infty}h(t)\exp\left(\frac{1}{2}\frac{L^d}{n^d}\sum_{k_j\in Q_n}\exp[-it\mu(k_j)]g(k_j)F(k_j)\right)$$

$$=h(t)\exp[\tfrac{1}{2}(F,\exp(it\mu)g)]\ \text{ for all } t.$$

Put

$$\not f_n(t)=h(t)\exp\left(\frac{1}{2}\frac{L^d}{n^d}\sum_{k_j\in Q_n}\exp[-it\mu(k_j)]g(k_j)F(k_j)\right)$$

and

$$\not f(t)=h(t)\exp[\tfrac{1}{2}(F,\exp(it\mu)g)].$$

Then $|\not f_n(t)|\leqslant|h(t)|e^M$ and $|\not f(t)|\leqslant|h(t)|e^M$.

Since $h\in L^1(R^d)$, $\not f_n \to \not f$ dominatedly, and so $\not f_n \to \not f$ in $L^1(R^d)$. Therefore, $\not f_n \to \not f$ uniformly, and $\check{\not f}_n(s)\exp(\sqrt{|s|})\to\check{\not f}(s)\exp(\sqrt{|s|})$ pointwise. But, by Lemma II. 9,

$$\|\check{\not f}_n(s)\exp(\sqrt{|s|})\|_{\infty,s}\leqslant e^M\|\check{h}(s)\exp(\sqrt{|s|})\|_{\infty,s}$$

and so

$$\|\check{\not f}(s)\exp(\sqrt{|s|})\|_{\infty,s}\leqslant e^M\|\check{h}(s)\exp(\sqrt{|s|})\|_{\infty,s}.$$

Theorem II. 11: $\|\Psi(h)\|_2<\infty$.

Proof:

$$\Psi(h)=\sum_{p=0}^{\infty} i^p\,\frac{\sqrt{(p+1)!}}{p!}\int dt\,\eta(t)(\exp(it\mu)+F)^{(p)},$$

$$\|\Psi(h)\|_2^2$$

$$=\sum_{p=0}^{\infty}\frac{(p+1)!}{(p!)^2}\int\cdots\int\prod_{j=1}^{p}dk_j$$

$$\times\left|\int dt\,\eta(t)(\exp(it\mu)g+F)^{(p)}\right|^2$$

$$=\sum_{p=0}^{\infty}\frac{(p+1)!}{(p!)^2}\int\cdots\int\left|\int dt\,\eta(t)\sum_{T\subseteq T_p}\prod_{j\in T}\exp[it\mu(k_j)]\right.$$

$$\left.\times g(k_j)\prod_{j\in T_p-T}F(k_j)\right|^2\prod_{j=1}^{p}dk_j$$

(where $T_p=\{1,2,\ldots,p\}$)

$$=\sum_{p=0}^{\infty}\frac{(p+1)!}{(p!)^2}\int\cdots\int\left|\sum_{T\subseteq T_p}\prod_{j\in T_p-T}F(k_j)\int dt\,\eta(t)\right.$$

$$\left.\times\prod_{j\in T}\exp[it\mu(k_j)]g(k_j)\right|^2\prod_{j=1}^{p}dk_j$$

$$=2\pi\sum_{p=0}^{\infty}\frac{(p+1)!}{(p!)^2}\int\cdots\int\left|\sum_{T\subseteq T_p}\prod_{j\in T_p-T}F(k_j)\right.$$

$$\left.\times\check{\eta}\left(\sum_{j\in T}\mu(k_j)\right)\prod_{j\in T}g(k_j)\right|^2\prod_{j=1}^{p}dk_j$$

$$\leqslant 2\pi\sum_{p=0}^{\infty}\frac{2^p(p+1)!}{(p!)^2}\int\cdots\int\prod_{j=1}^{p}dk_j$$

$$\times\left[\sum_{T\subseteq T_p}\left|\prod_{j\in T_p-T}F(k_j)\check{\eta}\left(\sum_{j\in T}\mu(k_j)\right)\prod_{j\in T}g(k_j)\right|^2\right].$$

Recall that $\eta(t) = \exp(-\|F\|^2/4)h(t)\exp[-\frac{1}{2}(F, \exp(it\mu)g)]$ where $h \in \mathcal{J}$. If M is chosen as in Lemma 3 and $M' = \|h(s)\exp(\sqrt{|s|})\|_{\infty,s}$, then, putting $M'' = 2\pi\exp(-\|F\|^2/4)e^M M'$, we have

$$\|\Psi(h)\|_2^2$$

$$\leqslant M''\sum_{p=0}^{\infty}\frac{2^p(p+1)!}{(p!)^2}\int\circ\circ\circ\int\prod_{j=1}^{p}dk_j$$

$$\times\left[\sum_{T\leqslant T_p}\prod_{j\in T_p-T}\left|F(k_j)\right|\exp\left[\left(\sum_{j\in T}\mu(k_j)\right)^{1/2}\prod_{j\in T}\left|g(k_j)\right|\right]^2.$$

Using this last inequality and the fact that for $a_i \geqslant 0$, $i = 1, \ldots, n$,

$$\left(\sum_{i=1}^{n}a_i\right)^{1/2} \geqslant \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\sqrt{a_i},$$

we have

$$\|\Psi(h)\|_2^2$$

$$\leqslant M''\sum_{p=0}^{\infty}\frac{2^p(p+1)!}{(p!)^2}\int\circ\circ\circ\int\prod_{j=1}^{p}dk_j$$

$$\times\left[\sum_{T\subseteq T_p}\prod_{j\in T_p-T}|F(k_j)|\prod_{j\in T}|g(k_j)|\exp\left(-\frac{1}{\sqrt{p}}\mu(k_j)\right)\right]^2$$

$$= M''\sum_{p=0}^{\infty}\frac{2^p(p+1)!}{(p!)^2}$$

$$\times\int\circ\circ\circ\int\left[|F|\exp\left(-\frac{1}{\sqrt{p}}\mu\right)(|g|)^{(p)}\right]^2\prod_{j=1}^{p}dk_j$$

$$= M''\sum_{p=0}^{\infty}\frac{2^p(p+1)!}{(p!)^2}$$

$$\times\left\{\int\left[|F(k)| + \exp\left(-\frac{1}{\sqrt{p}}\mu(k)\right)|g(k)|\right]^2 dk\right\}^p < \infty.$$

C. Closability of the annihilation operator

We have defined $\psi(h)$ on a dense subset of $\mathcal{K}$. Although $\psi_n(h)$ is a bounded operator for all n, we cannot expect $\psi(h)$ to be bounded, for the sequence $\{c_n\}$ tends to infinity. However, we can show that $\psi(h)$ is closable. This is tantamount to showing that the adjoint, $\psi^*(h)$: $\mathcal{J} \to \mathcal{K}$, is densely defined.

Theorem II.12: $\psi^*(h)$ is densely defined.

Proof: Let $v = A\Lambda = \exp(iR_F)\Lambda \in \mathcal{J}$, where F has bounded support and is an element of $L^2(\mathbb{R}^3)$. $v \in \mathcal{D}_{\psi^*(h)}$ iff $(\psi(h)[G], v)$ is a continuous function of $[G]$ on $[\mathcal{A}]$. Note that

$$\begin{aligned}(\psi(h)[G], v) &= (\lim_{n\to\infty}\psi_n(h)G\Lambda_n, v)\\ &= \lim_{n\to\infty}(\psi_n(h)G\Lambda_n, v)\\ &= \lim_{n\to\infty}(G\Lambda_n, \psi_n^*(h)v).\end{aligned}$$

To show that $(\psi(h)[G], v)$ is a continuous function of $[G]$, we must show that there exists an M such that

$$|(\psi(h)[G], v)| \leqslant M\|G\|_K \quad \text{for all } [G] \in [\mathcal{A}].$$

Thus we must show that $|\lim_{n\to\infty}(G\Lambda_n, \psi_n^*(h)v)| \leqslant M\|G\|_K$. Now

$$\begin{aligned}\left|\lim_{n\to\infty}(G\Lambda_n, \psi_n^*(h)v)\right| &\leqslant \lim_{n\to\infty}\sup\|G\Lambda_n\|\,\|\psi_n^*(h)v\|\\ &\leqslant \lim_{n\to\infty}\sup\|G\Lambda_n\|\lim_{n\to\infty}\sup\|\psi_n^*(h)v\|.\end{aligned}$$

But $\lim_{n\to\infty}\sup\|G\Lambda_n\| = \lim_{n\to\infty}\|G\Lambda_n\| = \|G\|_{\mathcal{K}}$. We claim that there exists an M such that $\|\psi_n^*(h)v\| \leqslant M$ for all n. Then $\lim_{n\to\infty}\sup\|\psi_n^*(h)v\| \leqslant M$, so that $|\psi(h)G, v)| \leqslant M\|G\|$. Thus we have reduced the problem to showing that the sequence $\{\|\psi_n^*(h)v\|\}$ is bounded. Recalling the definition of $\psi_n(h)$ and taking adjoints, we get

$$\begin{aligned}\psi_n^*(h)v &= c_n\int dt\,h(t)\exp(itH_n)\exp(-itH_0)\exp(iR_F)\Lambda\\ &= c_n\int dt\,h(t)\exp(iR_{g_n})\exp(itH_0)\exp(-iR_{g_n})\\ &\quad\times\exp(-itH_0)\exp(iR_F)\Lambda\\ &= c_n\exp(iR_{g_n})\int dt\,h(t)\exp(-iR_{\exp(it\mu)g_n})\exp(iR_F)\Lambda\\ &= c_n\exp(iR_{g_n})\int dt\,h(t)\exp[\tfrac{1}{2}i\,\mathrm{Im}(F, \exp(it\mu)g_n)]\\ &\quad\times\exp(iR_{F-\exp(it\mu)g_n})\Lambda\\ &= c_n\exp(iR_{g_n})\int dt\,h(t)\exp[\tfrac{1}{2}i\,\mathrm{Im}(F, \exp(it\mu)g_n)]\\ &\quad\times\exp(-\|F-\exp(it\mu)g_n\|^2/4)\exp(iC_{F-\exp(it\mu)g_n})\Lambda\\ &= c_n\exp(iR_{g_n})\int dt\,h(t)\exp[\tfrac{1}{2}(F, \exp(it\mu)g_n)]\\ &\quad\times\exp(-\|F\|^2/4)\exp(-\|g_n\|^2/4)\exp(iC_{F-\exp(it\mu)g_n})\Lambda\\ &= \exp(iR_{g_n})\int dt\,h(t)\exp[\tfrac{1}{2}(F, \exp(it\mu)g_n)]\\ &\quad\times\exp(-\|F\|^2/4)\exp(iC_{F-\exp(it\mu)g_n})\Lambda.\end{aligned}$$

Choose N such that, for $n \geqslant N$, $g_n \equiv [-i/(2\pi)^3]/(1/\mu^{3/2})$ on the support of F. Suppose $n \geqslant N$. Put $g = -[i/(2\pi)^3](1/\mu^{3/2})$. Then $(F, \exp(it\mu)g_n) = (F, \exp(it\mu)g)$. Put $\eta(t) = h(t)\exp[\frac{1}{2}(F, \exp(it\mu)g)]\exp(-\|F\|^2/4)$. Then $\psi_n^*(h) = \exp(iR_{g_n})\int dt\,\eta(t)\exp(iC_{F-\exp(it\mu)g_n})\Lambda$. Since $\exp(iR_{g_n})$ is unitary,

$$\begin{aligned}\|\psi_n^*(h)v\| &= \left\|\int dt\,\eta(t)\exp(iC_{F-\exp(it\mu)g_n})\Lambda\right\|\\ &= \left\|\int dt\,\eta(t)\exp(iC_{\exp(it\mu)g_n-F})\Lambda\right\|.\end{aligned}$$

By Eq. (3), this gives

$$\|\psi_n^*(h)v\| = \|\psi_n(h)\exp(iR_{(-F)})\Lambda_n\|$$

By Theorem II.3, Remark II.5, and Theorem II.11, $\{\|\psi_n(h)\exp(iR_{(-F)})\Lambda_n\|\}$ is a bounded sequence. Hence $\{\|\psi_n^*(h)v\|\}$ is a bounded sequence and thus $v \in \mathcal{D}_{\psi^*(h)}$.

Now by Theorem I.7 and the strong continuity of $\exp(iR_x)$ (Theorem I.5), $\{\exp(iR_F)\Lambda \mid F \in L^2(\mathbb{R}^3)$ and F has bounded support$\}$ is dense in $\mathcal{J}$. Thus $\psi^*(h)$ is densely defined, and $\psi(h)$ is closable.

III. THE ONE PARTICLE HAMILTONIAN WITHOUT CUTOFFS

A. Denseness of the range of the creation operator

In Sec. IIA, we constructed the one nucleon Hamiltonian H without cutoffs by specifying that it satisfy the equation

$$\exp(itH)[A] = [\exp(iR_{g\chi_S})\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_{g\chi_S})A]$$

for $A \in \mathcal{A}(S)$. We will now give an alternate method of constructing the one nucleon Hamiltonian by using the nucleon creation operator. Although we already have a method of constructing the one nucleon Hamiltonian in this model, it is to be hoped that the alternate method can be used in other models to construct the Hamiltonian from the nucleon creation operator.

The alternate method of constructing the Hamiltonian is simply to define it as the infinitesimal generator of the unitary group $U(t)$, where $U(t)$ is given by $U(t)\psi^*(h)v = \psi^*(h_t)\exp(itH_0)v$, where $h_t(x)=h(x+t)$. In order to show that $U(t)$ is unitary, it is necessary to show that this defines $U(t)$ on a dense set. Thus, we must show that $\cup_{h\in\mathcal{S}}$ range $\psi^*(h)$ is dense in $\mathcal{K}$. First we will need some lemmas. Put $D=\cup_{h\in\mathcal{S}(\mathbb{R}^1)}\psi^*(h)D'$, where D' = the linear span of $\{\exp(iR_F)\Lambda \mid F$ has compact support and is an element of $L^2(\mathbb{R}^d)\}$.

Lemma III.1: $[\exp(iR_F)\exp(-iR_{\exp(-s\mu)g}]\in D$ for $F\in L \in L^2(\mathbb{R}^d)$ with compact support.

Proof: Put $\eta(t)=h(t)\exp[-i\,\mathrm{Im}(\exp(it\mu)g,F)] \times\exp(i\,\mathrm{Im}(g,F))$ and choose $h\in\mathcal{S}$ such that $\hat{\eta}(x) =\exp(-s|x|)$. (There is a unique h with this property, since the Fourier transform operator is a bijection from $\mathcal{S}$ onto $\mathcal{S}$.) We claim that

$$\psi^*(h)\exp(iR_F)\Lambda=[\exp(\|\exp(-s\mu)g\|^2/4)\exp(iR_F)$$
$$\times\exp(-iR_{\exp(-s\mu)g})],$$

which will establish the desired result since the left side of this equation is an element of D and the right side side is a scalar multiple of $[\exp(iR_F)\exp(-iR_{\exp(-s\mu)g})]$. Let $G\in L^2(\mathbb{R}^d)$ and have compact support. Then

$$(\psi^*(h)\exp(iR_F)\Lambda,[\exp(iR_G)])$$
$$=(\exp(iR_F)\Lambda,\psi(h)[\exp(iR_G)])$$
$$=\lim_{n\to\infty}(\exp(iR_F)\Lambda,\psi_n(h)\exp(iR_G)\Lambda_n)$$
$$=\lim_{n\to\infty}(\psi_n^*(h)\exp(iR_F)\Lambda,\exp(iR_G)\Lambda_n)$$
$$=\lim_{n\to\infty}(c_n\textstyle\int dt\,h(t)\exp(itH_n)\exp(-itH_0)\exp(iR_F)\Lambda,$$
$$\exp(iR_G)\Lambda_n)$$
$$=\lim_{n\to\infty}(c_n\textstyle\int dt\,h(t)\exp(iR_{g_n})\exp(itH_0)$$
$$\times\exp(-iR_{g_n})\exp(-itH_0)\exp(iR_F)\Lambda,\exp(iR_G)\Lambda_n).$$

Now

$$c_n\textstyle\int dt\,h(t)\exp(iR_{g_n})\exp(itH_0)\exp(-iR_{g_n})\exp(-itH_0)\exp(iR_F)\Lambda$$
$$=c_n\textstyle\int dt\,h(t)\exp(iR_{g_n})\exp(-iR_{\exp(it\mu)g_n})\exp(iR_F)\Lambda$$
$$=c_n\exp(iR_F)\textstyle\int dt\,h(t)\exp[-i\,\mathrm{Im}(\exp(it\mu)g_n,F)]$$
$$\times\exp[i\,\mathrm{Im}(g_n,F)]\exp(iR_{g_n})\exp(-iR_{\exp(it\mu)g_n})\Lambda.$$

For n sufficiently large, this is equal to

$$c_n\exp(iR_F)\textstyle\int dt\,h(t)\exp[-i\,\mathrm{Im}(\exp(it\mu)g,F)]$$
$$\times\exp[i\,\mathrm{Im}(g,F)]\exp(iR_{g_n})\exp(-iR_{\exp(it\mu)g_n})\Lambda$$
$$=\exp(iR_F)\textstyle\int dt\,\eta(t)\exp(iR_{g_n})\exp(-iC_{\exp(it\mu)g_n})\Lambda$$
$$=\exp(iR_F)\exp(iR_{g_n})\textstyle\int dt\,\eta(t)\exp(-iC_{\exp(it\mu)g_n})\Lambda.$$

Now we have

$$\int dt\,\eta(t)\exp(-iC_{\exp(it\mu)g_n})$$
$$=\int dt\,\eta(t)\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}(C_{\exp(it\mu)g_n})^p$$
$$=\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}\int dt\,\eta(t)(C_{\exp(it\mu)g_n})^p$$
$$=\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}\int dt\,\eta(t)\left(\int dk\exp[it\mu(k)]g_n(k)a^*(k)\right)^p$$
$$=\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}\int dt\,\eta(t)\int\circ\circ\circ\int\prod_{j=1}^{p}dk_j\exp[it\mu(k_j)]$$
$$\times g_n(k_j)a^*(k_j)$$
$$=\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}\int\cdots\int\prod_{j=1}^{p}dk_jg_n(k_j)a^*(k_j)\,dt$$
$$\times\eta(t)\exp\left(it\sum_{j=1}^{p}\mu(k_j)\right)$$
$$=\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}\int\circ\cdots\int\left(\prod_{j=1}^{p}dk_jg_n(k_j)a^*(k_j)\right)$$
$$\times\hat{\eta}\left(\sum_{j=1}^{p}\mu(k_j)\right)$$
$$=\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}\int\cdots\int\prod_{j=1}^{p}dk_j\,g_n(k_j)a^*(k_j)\exp[-s\mu(k_j)]$$
$$=\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}\left(\int dk\,g_n(k)\exp[-s\mu(k)]a^*(k)\right)^p$$
$$=\sum_{p=0}^{\infty}\frac{(-i)^p}{p!}(C_{\exp(-s\mu)g_n})^p=\exp(-iC_{\exp(-s\mu)g_n}).$$

Therefore,

$$c_n\textstyle\int dt\,h(t)\exp(iR_{g_n})\exp(itH_0)\exp(-iR_{g_n})$$
$$\times\exp(-itH_0)\exp(iR_F)\Lambda$$
$$=\exp(iR_F)\exp(iR_{g_n})\exp(-iC_{\exp(-s\mu)g_n})\Lambda$$
$$=\exp(\|\exp(-s\mu)g_n\|^2/4)\exp(iR_F)\exp(iR_{g_n})$$
$$\times\exp(-iR_{\exp(-s\mu)g_n})\Lambda$$
$$=\exp(\|\exp(-s\mu)g_n\|^2/4)\exp(iR_F)$$
$$\times\exp(-iR_{\exp(-s\mu)g_n})\exp(iR_{g_n})\Lambda,$$

where the last step follows from the fact that $\mathrm{Im}(\exp(-s\mu)g_n,g_n)=0$. Hence

$$(\psi^*(h)\exp(iR_F)\Lambda,[\exp(iR_G)])$$
$$=\lim_{n\to\infty}(\exp(\|\exp(-s\mu)g_n\|^2/4)$$
$$\times\exp(-iR_{\exp(-s\mu)})\Lambda_n,\quad\exp(iR_G)\Lambda_n)$$
$$=\exp(\|\exp(-s\mu)g\|^2/4)\lim_{n\to\infty}(\exp(iR_F)\exp(-iR_{\exp(-s\mu)g_n}$$
$$\times\exp(-iR_{\exp(-s\mu)g_n})\Lambda_n,\exp(iR_G)\Lambda_n)$$
$$=\exp(\|\exp(-s\mu)g\|^2/4)\lim_{n\to\infty}(\exp(-iR_{\exp(-s\mu)g_n})$$
$$\times\exp(iR_{g_n})\Lambda,\exp(-iR_F)\exp(iR_G)\exp(iR_{g_n})\Lambda)$$
$$=\exp(\|\exp(-s\mu)g\|^2/4)\lim_{n\to\infty}(\exp(iR_{g_n})$$

$$\times \exp(-iR_{\exp(-s\mu)g_n})\Lambda,\ \exp(-iR_F)\exp(iR_G)\exp(iR_{g_n})\Lambda)$$

$$= \exp(\|\exp(-s\mu)g\|^2/4)\lim_{n\to\infty}(\exp(-iR_{\exp(-s\mu)g_n})\Lambda,$$

$$\exp(-iR_r)\exp(-iR_F)\exp(iR_G)\exp(iR_r)\Lambda)$$

$$= \exp(\|\exp(-s\mu)g\|^2/4)\exp(-iR_{\exp(-s\mu)g})\Lambda,$$

$$\exp(-iR_r)\exp(-iR_F)\exp(iR_G)\exp(iR_r)\Lambda)$$

$$= \exp(\|\exp(-s\mu)g\|^2/4)\lim_{n\to\infty}(\exp(iR_{g_n})$$

$$\times \exp(-iR_{\exp(-s\mu)g})\Lambda,\ \exp(-iR_F)\exp(iR_G)\exp(iR_{g_n})\Lambda)$$

$$= \exp(\|\exp(-s\mu)g\|^2/4)$$

$$\times \lim_{n\to\infty}(\exp(iR_F)\exp(-iR_{\exp(-s\mu)g})\Lambda_n,\ \exp(iR_G)\Lambda_n)$$

$$= ([\exp(\|\exp(-s\mu)g\|^2/4)\exp(iR_F)$$

$$\times \exp(-iR_{\exp(-s\mu)g})],\ [\exp(iR_G)]).$$

Therefore, we have the desired result

$$\psi^*(h)\exp(iR_F)\Lambda = [\exp(\|\exp(-s\mu)g\|^2/4)$$

$$\times \exp(iR_F)\exp(-iR_{\exp(-s\mu)g})].$$

Lemma III.2: $\lim_{s\to\infty}[\exp(iR_F)\exp(-iR_{\exp(-s\mu)g})] = [\exp(iR_F)]$.

Proof:

$$\lim_{s\to\infty}\|[\exp(iR_F)] - [\exp(iR_F)\exp(-iR_{\exp(-s\mu)g})]\|$$

$$= \lim_{s\to\infty}\|[\exp(iR_F)(I - \exp(-iR_{\exp(-s\mu)g}))]\|$$

$$= \lim_{s\to\infty}\lim_{p\to\infty}(\exp(iR_F)(I - \exp[-iR_{\exp(-s\mu)g}]\Lambda_p, \Lambda_p))$$

$$= \lim_{s\to\infty}\lim_{p\to\infty}(\exp(iR_F)(I - \exp[-iR_{\exp(-s\mu)g}]\exp(iR_{g_p})\Lambda,$$

$$\exp(iR_{g_p})\Lambda)$$

$$= \lim_{s\to\infty}\lim_{p\to\infty}[(\tfrac{1}{2}i\,\mathrm{Im}(F,g_p)](\exp(iR_{g_p})\exp(iR_F)$$

$$\times (I - \exp[-iR_{\exp(-s\mu)g}])\Lambda,\ \exp(iR_{g_p})\Lambda)$$

$$= \lim_{s\to\infty}\exp[\tfrac{1}{2}i\,\mathrm{Im}(F,g)](\exp(iR_F))(I - \exp(-iR_{\exp(-s\mu)g})\Lambda, \Lambda)$$

$$= \lim_{s\to\infty}\exp[\tfrac{1}{2}i\,\mathrm{Im}(F,g)]((I - \exp[-iR_{\exp(-s\mu)g})\Lambda,$$

$$\exp(-iR_F)\Lambda) = 0,$$

since $\exp(-iR_{\exp(-s\mu)g}) \to \exp(-iR_0) = I$ strongly as $s \to \infty$.

Theorem III.3: The linear span of D is dense in $\mathcal{K}$.

Proof: This follows immediately from Lemmas III.1 and III.2 and the density of $\{[\exp(iR_F)] \mid F \in L^2(\mathbb{R}^d)$ with compact support$\}$ in $\mathcal{K}$.

B. The relationship between the one nucleon Hamiltonian and the nucleon creation operator

In the last section, we showed how to construct the one nucleon Hamiltonian from the nucleon creation operator and the free Hamiltonian; now we show that the Hamiltonian obtained this way is same as the one defined in Sec. II A. To do this, it suffices to show that

$$\exp(itH)\psi^*(h) = \psi^*(h_t)\exp(itH_0) \quad \text{for } h \in \mathcal{S}.$$

First we need some lemmas.

Lemma III.4: $\psi_n(h)\exp(itH_n) = \exp(itH_0)\psi_n(h_t)$ for $h \in \mathcal{S}$, where $h_t(x) = h(x+t)$.

Proof:

$$\psi_n(h)\exp(itH_n) = c_n\int ds\, h(s)\exp(isH_0)\exp(-isH_n)\exp(itH_n)$$

$$= c_n\int ds\, h(s)\exp(isH_0)\exp[-i(s-t)H_n]$$

$$= c_n\int ds\, h(s+t)\exp[i(s+t)H_0]\exp(-isH_n)$$

$$= \exp(itH_0)c_n\int ds\, h_t(s)\exp(isH_0)\exp(-isH_n)$$

$$= \exp(itH_0)\psi_n(h_t).$$

Lemma III.5: $\psi(h)\exp(itH) = \exp(itH_0)\psi(h_t)$ for $h \in \mathcal{S}$.

Proof: Put $T_1 = \psi(h)\exp(itH)$, $T_2 = \exp(itH_0)\psi(h_t)$, and $D =$ linear span in $\mathcal{K}$ of $\{[\exp(iR_F)] \mid F \in L^2(\mathbb{R}^d)$ and has compact support$\}$. We claim that D is a core for T_1 and T_2 and that T_1 and T_2 agree on D. From this it follows that $T_1 = T_2$.

From the construction of ψ, D is a core for $\psi(h_t)$ and hence for T_2. To show that D is a core for T_1, it suffices to show that $\exp(itH)$: $D \xrightarrow{\text{onto}} D$. Let $[\exp(iR_F)] \in D$. Then F has support in S, for some bounded open set S and

$$\exp(itH)[\exp(iR_F)]$$

$$= \{\exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)\exp(iR_F)\}$$

$$= [\exp[-\tfrac{1}{2}i\,\mathrm{Im}(r,F)]\exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]$$

$$\times \exp(iR_{F-r})]$$

$$= [\exp[-\tfrac{1}{2}i\,\mathrm{Im}(r,F)]\exp(iR_r)\exp(iR_{\exp(it\mu)(F-r)})]$$

$$\therefore \exp(itH)[\exp(iR_F)]$$

$$= [\exp[-\tfrac{1}{2}i\,\mathrm{Im}(r,F)\exp[\tfrac{1}{2}i\,\mathrm{Im}(r, \exp(it\mu)(F-r))$$

$$\times \exp(iR_{r+\exp(it\mu)(F-r)})]$$

and the right side of this equation clearly belongs to D. Thus $\exp(itH)$ carries D into D. If we put

$$G = \exp[-it\mu]\,(F-r) + r$$

and

$$G' = \exp[\tfrac{1}{2}i\,\mathrm{Im}(r,G)]\exp[-\tfrac{1}{2}i(r, \exp(it\mu)(G-r))]\exp(iR_G),$$

then $[G'] \in D$ and the above calculation shows that $\exp(itH)[G'] = \exp(iR_F)$. Thus $\exp(itH)$: $D \xrightarrow{\text{onto}} D$ and D is a core for T_1. Now we show that $T_1|_D = T_2|_D$.

Let $[A] \in D$. Then by the construction of ψ, $\psi_n(h_t)A\Lambda_n \to \psi(h_t)[A]$ strongly. Since $\exp(itH_0)$ is bounded, $\exp(itH_0)\psi_n(h_t)A\Lambda_n \to \exp(itH_0)\psi(h_t)[A]$. Again, by the construction of ψ,

$$\psi_n(h)\exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)A\Lambda_n$$

$$\to \psi(h)[\exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-R_r)A]$$

strongly.

Since $\exp(itH_n)A\Lambda_n = \exp(iR_r)\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)A\Lambda_n$ for sufficiently large n and $\exp(itH)[A] = \{\exp(iR_r) \times\exp[it\,d\Gamma(\mu\chi_S)]\exp(-iR_r)A\}$, it follows that $\psi_n(h) \times\exp(itH_n)A\Lambda_n \rightarrow \psi(h)\exp(itH)[A]$ strongly. By Lemma III. 4, $\psi_n(h)\exp(itH_n)A\Lambda_n = \exp(itH_0)\psi_n(h_t)A\Lambda_n$, and taking limits on both sides, it follows that $\psi(h)\exp(itH) = \exp(itH_0)\psi(h_t)$.

Theorem III. 6: $\exp(itH)\psi^*(h) = \psi^*(h_t)\exp(itH_0)$ for all $h \in \mathcal{S}$.

Proof: This is the adjoint of the equation proved in Lemma III. 5.

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[1] J. M. Cook, Trans. Am. Math. Soc. **74**, 222 (1953).

[2] M. Guenin, Proc. Int. School Phys. Course **45**, 234 (1969).

[3] M. Guenin and G. Velo, Helv. Phys. Acta **42**, 102 (1969).

[4] P. Kristensen, L. Mejlbo, and E. Thue Poulsen, Commun. Math. Phys. **1**, 175 (1965).

[5] P. Kristensen, L. Mejlbo, and E. Thue Poulson, Math. Scand. **14**, 129 (1964).

[6] P. Kristensen, L. Mejlbo, and E. Thue Poulson, Commun. Math. Phys. **6**, 29 (1967).

[7] L. Van Hove, Bull. Acad. Roy. Belg. Cl. Sci. **37**, 1055 (1951).

[8] L. Van Hove, Physica **18**, 145 (1952).

[9] L. Gross, Commun. Math. Phys. **31**, 25 (1973).

[10] S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, Evanston, 1961).

[11] W. Thomson, *Laplace Transformation* (Prentice-Hall, Englewood Cliffs, New Jersey, 1960), pp. 20, 21.

[12] A. Jaffe, Phys. Rev. **158**, 1454 (1967).

[13] M. Reed and B. Simon, *Methods of Modern Mathematical Physics. Vol. I: Functional Analysis* (Academic, New York, 1972), pp. 50–53.

SU(6) isoscalar factors for the product $405\times 56\to 56, 70$[*]

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SU(6) isoscalar factors for the product $405\times 56\to 56$, 70 are calculated. SU(3) isoscalar factors for the products $27\times 10\to 10$, 8 and $\overline{10}\times 8\to 8$ are also tabulated.

I. INTRODUCTION

The SU(6) symmetry group was first found useful for the classification of hadrons in the 1960's. It has recently been extended by Melosh[1] to apply to matrix elements of currents between hadron states. Following the ideas of Gell-Mann, the currents are postulated to belong to irreducible representations of an SU(6) of currents, while the particle states are classified by a different, constituent SU(6). These two different SU(6) symmetries are connected by a unitary transformation, the Melosh transformation. Melosh explicitly constructed this transformation for the free-quark model. The algebraic properties of currents transformed by the Melosh transformation have been extracted from this model and applied to physically relevant matrix elements. This method removed the inconsistencies which appeared in old SU(6) calculations of several axial coupling constants and the magnetic moments of the nucleons.[1] Gilman, Kugler, Meshkov and others,[2] used PCAC in addition to the algebraic properties of the Melosh transformed axial vector current to satisfactorily predict pionic emission amplitudes for the decays of mesons and baryons. Gilman, Karliner, and others,[3] also found that the application of the Melosh transformation technique to real photon emissions from baryons and mesons is consistent with experiment.

In each of the above applications, the basic technique is to use the Wigner–Eckart theorem to calculate a particular physically relevant matrix element. Thus, the matrix element of an operator between two hadron states is the product of appropriate SU(6) and angular momentum Clebsch–Gordan coefficients, times a reduced matrix element.[2] For each of the above applications, the Melosh transformed currents belong to 35 representations of SU(6). The baryons are classified in 56 and 70 representations, and the mesons form 35 representations of SU(6). The appropriate SU(6) Clebsch–Gordan coefficients for these applications have been calculated by Carter, Coyne, and Meshkov,[4] and by Cook and Murtaza.[5]

If one now wants to apply this technique to current-current matrix elements between baryon states which occur, for example, in nonleptonic weak decays, higher representations which originate from the product 35×35 must be considered. Explicitly, the product 35×35 is decomposed into the irreducible representations:

$$35\times 35\to 1+35+35'+189+280+\overline{280}+405. \tag{1.1}$$

The only representations in (1.1) which will contribute to a matrix element between baryon states belonging to the 56 and the 56 or 70 representations are 35 and 405.[6] In this paper, the Clebsch–Gordan coefficients for the product $405\times 56\to 56$, 70 are obtained so that such current–current processes may be treated in full. In Sec. II, the method of calculating the SU(6) isoscalar factors for the product $405\times 56\to 56$ and 70 with appropriate choice of phase is explained. In Sec. III, the SU(6) isoscalar factors for $405\times 56\to 56, 70$ are tabulated. SU(3) isoscalar factors for the products $27\times 10\to 10, 8$ and $\overline{10}\times 8\to 8$, which were used in the present calculation, are also given in Sec. III.

II. METHOD OF CONSTRUCTION

A given SU(6) representation may be reduced according to the subgroup SU(3)×SU(2). In terms of the spectroscopic notation A^{2S+1}, where A is the SU(3) representation label and $2S+1$ is the SU(2) spin multiplicity, the 35, 56, 70, and 405 representations have the following SU(3)×SU(2) contents:

$$\underline{35}=8^3, 8^1, 1^3, \tag{2.1}$$

$$\underline{56}=10^4, 8^2, \tag{2.2}$$

$$\underline{70}=8^4, 10^2, 8^2, 1^2, \tag{2.3}$$

$$\underline{405}=27^5, 27^3, 27^1, 10^3, \overline{10}^3, 8^5, 8^3_A, 8^3_B, 8^1, 1^5, 1^1. \tag{2.4}$$

Wavefunctions for these SU(6) representations are written using the 6 and $\bar{6}$ representations q_l and q^l, respectively defined in Table A1, Appendix A. A given wavefunction within an SU(6) multiplet may be classified according to its SU(3)×SU(2) quantum numbers,

$$|A; YII_3; S\,S_3\rangle, \tag{2.5}$$

where Y, I, I_3 are the hypercharge, I-spin, and third component of the I-spin, respectively, and S, S_3 are the spin and third component of the spin. The relative phases between wavefunctions within a given SU(3) multiplet are chosen to agree with the phase conventions of deSwart.[7] The relative phases of the wavefunctions within a given spin multiplet agree with the Condon–Shortley phase convention for SU(2).[8] The wavefunction of highest weight in successive SU(3)×SU(2) multiplets within a given SU(6) representation is determined by requiring orthogonality between states with the same additive quantum numbers, Y, I_3, and S_3, and that the traceless condition for each representation be satisfied. For example, the 405 wavefunctions must have the following form:

$$\begin{aligned}\xi^{kl}_{ij}\propto \{q_iq_j\}\{q^kq^l\}-\tfrac{1}{8}\sum_m\,[\delta^k_i\{q_mq_j\}\{q^mq^l\}+\delta^k_j\{q_iq_m\}\{q^mq^l\}\\ +\delta^l_i\{q_mq_j\}\{q^kq^m\}+\delta^l_j\{q_iq_m\}\{q^kq^m\}]\\ +\frac{1}{56}(\delta^k_i\delta^l_j+\delta^l_i\delta^k_j)\sum_{m,n}\{q_mq_n\}\{q^mq^n\},\end{aligned} \tag{2.6}$$

TABLE 3.1. SU(6) isoscalar factors for 405 ×56→ 56, 70

	$27^5\times 10^4$	$27^5\times 8^2$	$27^3\times 10^4$	$27^3\times 8^2$	$27^1\times 10^4$	$27^1\times 8^2$	$10^3\times 8^2$	$\overline{10}^3\times 10^4$	$\overline{10}^3\times 8^2$	$8^5\times 10^4$	$(8^5\times 8^2)_s$	$(8^5\times 8^2)_a$
$\underline{56}$												
10^4	$\frac{7}{15}$	$-2\sqrt{7}/15$	$\frac{7}{15}$	$-2\sqrt{7}/15\sqrt{5}$	$7\sqrt{2}/15\sqrt{5}$		$2\sqrt{14}/15\sqrt{3}$			$4\sqrt{14}/45$		$-2\sqrt{7}/45$
8^2	$\sqrt{14}/3\sqrt{5}$		$\sqrt{14}/15$	$\sqrt{7}/15$		$\sqrt{14}/30$	$\sqrt{7}/3\sqrt{15}$	$-2\sqrt{7}/3\sqrt{15}$	$\sqrt{7}/3\sqrt{15}$	$\sqrt{14}/9\sqrt{5}$		
$\underline{70}$												
8^4	$\sqrt{5}/3\sqrt{2}$	$-\sqrt{5}/6\sqrt{2}$	$\sqrt{5}/3\sqrt{2}$	$-1/6\sqrt{2}$	$\frac{1}{3}$		$\sqrt{5}/3\sqrt{6}$	0	0	$\sqrt{5}/9\sqrt{2}$	$\sqrt{5}/18\sqrt{2}$	$-5/18\sqrt{2}$
10^2	$\sqrt{7}/3\sqrt{2}$		$\sqrt{7}/3\sqrt{10}$	$2/3\sqrt{5}$		$2/3\sqrt{10}$	$2/3\sqrt{6}$			$\frac{4}{9}$		
8^2	$-\sqrt{5}/3\sqrt{2}$		$-1/3\sqrt{2}$	$\frac{-1}{6}$		$-1/6\sqrt{2}$	$-\sqrt{5}/6\sqrt{3}$	$-\sqrt{5}/3\sqrt{3}$	$\sqrt{5}/6\sqrt{3}$	$-\sqrt{5}/9\sqrt{2}$		
1^2								$-2\sqrt{5}/3\sqrt{3}$				

	$8_A^3\times 10^4$	$(8_A^3\times 8^2)_s$	$(8_A^3\times 8^2)_a$	$8_B^3\times 10^4$	$(8_B^3\times 8^2)_s$	$(8_B^3\times 8^2)_a$	$8^1\times 10^4$	$(8^1\times 8^2)_s$	$(8^1\times 8^2)_a$	$1^5\times 10^4$	$1^5\times 8^2$	$1^1\times 10^4$	$1^1\times 8^2$
$\underline{56}$													
10^4	0		$-2\sqrt{7}/15\sqrt{3}$	$-2\sqrt{7}/15\sqrt{3}$		$-2\sqrt{14}/15\sqrt{15}$	$2\sqrt{7}/45\sqrt{5}$			$\sqrt{7}/9\sqrt{5}$		$\sqrt{2}/45$	
8^2	$-2\sqrt{7}/3\sqrt{30}$	0	0	$2\sqrt{7}/15\sqrt{3}$	$-2\sqrt{7}/15\sqrt{6}$	0		$-4\sqrt{7}/45\sqrt{2}$	$-\sqrt{14}/9\sqrt{5}$				$-1/9\sqrt{2}$
$\underline{70}$													
8^4	0	$-\sqrt{5}/6\sqrt{6}$	$1/6\sqrt{6}$	$-\sqrt{5}/12\sqrt{3}$	$-1/4\sqrt{3}$	$\sqrt{5}/12\sqrt{3}$	$\frac{1}{36}$				$-\sqrt{5}/18\sqrt{2}$		
10^2	0		$-1/3\sqrt{3}$	$-2/3\sqrt{30}$		$-7/6\sqrt{30}$			$1/18\sqrt{10}$	$\sqrt{5}/9\sqrt{2}$			
8^2	$-\sqrt{5}/3\sqrt{6}$	$\sqrt{5}/6\sqrt{3}$	$-1/6\sqrt{3}$	$1/2\sqrt{3}$	$-1/12\sqrt{6}$	$\sqrt{5}/12\sqrt{6}$		$-7/36\sqrt{2}$	$-5\sqrt{5}/36\sqrt{2}$				$-\sqrt{7}/18\sqrt{2}$
1^2		$-\sqrt{2}/3\sqrt{3}$			$\sqrt{5}/6\sqrt{3}$			$-\sqrt{5}/6$					

where $\{q_iq_j\}=q_iq_j+q_jq_i$, with the traceless condition

$$\sum_i \xi_{ij}^{il}=0. \tag{2.7}$$

As seen in (2.4), $\underline{405}$ contains 8^3 twice. The state $|8_A;011;11\rangle$ is chosen to be the simplest state consistent with the required orthogonality and traceless conditions. $|8_B;011;11\rangle$ is then determined by requiring, in addition, that it be orthogonal to $|8_A;011;11\rangle$. The relative phases among different SU(3)×SU(2) multiplets within a given SU(6) representation is arbitrary. The phases of the wavefunctions within the 35, 56, and 70 representations are chosen to conform to Meshkov's revised phase conventions[9] for the table of SU(6) isoscalar factors for 35×56→56, 70. This table is given for reference in Appendix C. The highest weight wavefunctions, themselves, for each SU(3)×SU(2) multiplet in 35, 56, and 70 are listed in Appendix B. The present choice of relative phase for the SU(3)×SU(2) multiplets within 405 is also made explicit in Appendix B by listing the highest weight wavefunctions for each SU(3)×SU(2) multiplet within 405. The rest of the wavefunctions can easily be constructed by applying the generators $I_\pm$, $V_\pm$, and $S_\pm$.[7]

SU(6) Clebsch–Gordan coefficients can be written in terms of the product of an SU(6) isoscalar factor with SU(3) and SU(2) Clebsch–Gordan coefficients. For the product:

$$|R;A;YII_3;SS_3\rangle\times|R';A';Y'I'I_3';S'S_3'\rangle$$
$$\longrightarrow |R'';A'';Y''I''I_3'';S''S_3''\rangle,$$

where R, R', and R'' are SU(6) representation labels, and the others are SU(3)×SU(2) multiplet labels within each respective SU(6) representation, the Clebsch–Gordan coefficient is written:

$$\begin{pmatrix} R & R' & \Big| & R'' \\ A,S & A',S' & \Big| & A'',S'' \end{pmatrix}\begin{pmatrix} A & A' & A'' \\ YII_3 & Y'I'I_3', & Y''I''I_3'' \end{pmatrix}$$
$$\times (SS_3S'S_3', S''S_3''). \tag{2.8}$$

The first factor in (2.8) is the SU(6) isoscalar factor to be determined. The second factor is the full SU(3) Clebsch–Gordan coefficient for $A\times A'\rightarrow A''$, many of which have been tabulated by McNamee and Chilton.[10] The third factor is the usual SU(2) Clebsch–Gordan coefficient.[8] For the product 405×56→56, 70 the additional SU(3) Clebsch–Gordan coefficients for the products 27×10→10, 8 and $\overline{10}$×8→8 are needed. These coefficients can also be expressed, in terms of isoscalar factors times an SU(2) I-spin Clebsch–Gordan coefficient, as

$$\begin{pmatrix} A & A' & A'' \\ YII_3 & Y'I'I_3', & Y''I''I_3 \end{pmatrix}$$
$$=\begin{pmatrix} A & A' & \Big| & A'' \\ YI & Y'I' & \Big| & Y''I'' \end{pmatrix}(II_3I'I_3', I''I_3''). \tag{2.9}$$

The SU(3) isoscalar factors for 27×10→10, 8 and $\overline{10}$×8→8 were calculated according to the method of deSwart.[7] They are listed in Tables 3.2 and 3.3 in Sec. 3.

The SU(6) isoscalar factors are found by writing representative wavefunctions in each of the SU(3)×SU(2) multiplets of 56 and 70 in terms of the product wavefunctions of 405 and 56 and the Clebsch–Gordan coefficients given in (2.8). The unknown SU(6) isoscalar factors are determined by operating on these expressions with the SU(6) H_4 and H_5 operators defined in Appendix A. In particular, the expressions

$$H_4|10;1\tfrac{3}{2}\tfrac{3}{2};\tfrac{3}{2}\tfrac{3}{2}\rangle=3|10;\ 1\tfrac{3}{2}\tfrac{3}{2};\ \tfrac{3}{2}\tfrac{3}{2}\rangle, \tag{2.10}$$

TABLE 3.2 SU(3) isoscalar factors for $27\times 10\to 10,\ 8$

	Y_1I_1	$(0,2)$	$(0,2)$	$\left(1,\frac{3}{2}\right)$	$\left(1,\frac{3}{2}\right)$	$\left(-1,\frac{3}{2}\right)$	$\left(-1,\frac{3}{2}\right)$	$(2,1)$	$(2,1)$	$(0,1)$	$(0,1)$	$(0,1)$
	YI $\quad Y_2I_2$	$\left(1,\frac{3}{2}\right)$	$(0,1)$	$(0,1)$	$\left(-1,\frac{1}{2}\right)$	$\left(1,\frac{3}{2}\right)$	$(0,1)$	$\left(-1,\frac{1}{2}\right)$	$(-2,0)$	$1,\frac{3}{2}$	$(0,1)$	$\left(-1,\frac{1}{2}\right)$
10	$\left(1,\frac{3}{2}\right)$	$5/3\sqrt{7}$		$5\sqrt{2}/3\sqrt{21}$				$\sqrt{10}/3\sqrt{7}$		$-\sqrt{5}/3\sqrt{7}$		
	$(0,1)$		$5\sqrt{2}/9\sqrt{7}$		$4\sqrt{5}/9\sqrt{7}$	$10\sqrt{2}/9\sqrt{7}$			$\sqrt{10}/3\sqrt{7}$		$\sqrt{2}/\sqrt{21}$	
	$\left(-1,\frac{1}{2}\right)$						$2\sqrt{10}/3\sqrt{21}$					$4/3\sqrt{7}$
	$(-2,0)$											
8	$(0,1)$		$\sqrt{10}/9$		$\frac{4}{9}$	$-\sqrt{10}/9$			$\sqrt{2}/3$		$-\sqrt{10}/5\sqrt{3}$	
	$\left(1,\frac{1}{2}\right)$	$-\sqrt{5}/3$		$-2\sqrt{2}/3\sqrt{3}$				$\frac{-1}{3}$		$1/3\sqrt{5}$		
	$\left(-1,\frac{1}{2}\right)$						$\sqrt{2}/3\sqrt{3}$					$2/3\sqrt{5}$
	$(0,0)$					$-\sqrt{2}/\sqrt{3}$					$-2/\sqrt{15}$	

	Y_1I_1	$(-2,1)$	$(-2,1)$	$\left(1,\frac{1}{2}\right)$	$\left(1,\frac{1}{2}\right)$	$\left(1,\frac{1}{2}\right)$	$\left(-1,\frac{1}{2}\right)$	$\left(-1,\frac{1}{2}\right)$	$\left(-1,\frac{1}{2}\right)$	$(0,0)$	$(0,0)$	$(0,0)$	$(0,0)$
	YI $\quad Y_2I_2$	$\left(1,\frac{3}{2}\right)$	$(0,1)$	$(0,1)$	$\left(-1,\frac{1}{2}\right)$	$(-2,0)$	$\left(1,\frac{3}{2}\right)$	$(0,1)$	$\left(-1,\frac{1}{2}\right)$	$\left(1,\frac{3}{2}\right)$	$(0,1)$	$\left(-1,\frac{1}{2}\right)$	$(-2,0)$
10	$\left(1,\frac{3}{2}\right)$			$-4/3\sqrt{21}$						$1/3\sqrt{7}$			
	$(0,1)$				$2/9\sqrt{7}$		$-8/9\sqrt{7}$				$-5/9\sqrt{7}$		
	$\left(-1,\frac{1}{2}\right)$	$2\sqrt{5}/3\sqrt{7}$				$2/\sqrt{21}$		$\sqrt{2}/3\sqrt{21}$				$-1/3\sqrt{7}$	
	$(-2,0)$		$\sqrt{10}/\sqrt{21}$						$2\sqrt{2}/\sqrt{21}$				$1/\sqrt{7}$
8													
	$(0,1)$				$-7/9\sqrt{5}$		$4/9\sqrt{5}$				$4/9\sqrt{5}$		
	$\left(1,\frac{1}{2}\right)$			$\sqrt{2}/3\sqrt{15}$									
	$\left(-1,\frac{1}{2}\right)$	$\frac{-2}{3}$				$1/\sqrt{15}$		$-4\sqrt{2}/3\sqrt{15}$				$-2/3\sqrt{5}$	
	$(0,0)$				$-1/\sqrt{15}$								

$$H_5\,|8;1\tfrac{1}{2}\,\tfrac{1}{2};\tfrac{1}{2}\,\tfrac{1}{2}\rangle=|8;1\tfrac{1}{2}\,\tfrac{1}{2};\tfrac{1}{2}\,\tfrac{1}{2}\rangle, \tag{2.11}$$

$$H_4\,|8;1\tfrac{1}{2}\,\tfrac{1}{2};\tfrac{1}{2}\,\tfrac{1}{2}\rangle=(-4\sqrt{2}/3)\,|10;1\tfrac{3}{2}\,\tfrac{1}{2};\tfrac{3}{2}\,\tfrac{1}{2}\rangle + \tfrac{5}{3}\,|8;1\tfrac{1}{2}\,\tfrac{1}{2};\tfrac{1}{2}\,\tfrac{1}{2}\rangle, \tag{2.12}$$

for 56 and

$$H_4\,|8;1\tfrac{1}{2}\,\tfrac{1}{2};\tfrac{3}{2}\,\tfrac{3}{2}\rangle=|8;1\tfrac{1}{2}\,\tfrac{1}{2};\tfrac{3}{2}\,\tfrac{3}{2}\rangle, \tag{2.13}$$

$$H_4\,|10;1\tfrac{3}{2}\,\tfrac{3}{2};\tfrac{1}{2}\,\tfrac{1}{2}\rangle=|10;1\tfrac{3}{2}\,\tfrac{3}{2};\tfrac{1}{2}\,\tfrac{1}{2}\rangle, \tag{2.14}$$

$$H_5\,|8;1\tfrac{1}{2}\,\tfrac{1}{2};\tfrac{1}{2}\,\tfrac{1}{2}\rangle=|8;1\tfrac{1}{2}\,\tfrac{1}{2};\tfrac{1}{2}\,\tfrac{1}{2}\rangle, \tag{2.15}$$

$$H_4\,|1;000;\tfrac{1}{2}\,\tfrac{1}{2}\rangle=(-2/\sqrt{3})(|8;010;\tfrac{3}{2}\,\tfrac{1}{2}\rangle+|8;010;\tfrac{1}{2}\,\tfrac{1}{2}\rangle), \tag{2.16}$$

$$H_4\,|10;011;\tfrac{1}{2}\,\tfrac{1}{2}\rangle=H_4\,|8;011;\tfrac{3}{2}\,\tfrac{1}{2}\rangle=-H_4\,|8;011;\tfrac{1}{2}\,\tfrac{1}{2}\rangle, \tag{2.17}$$

for 70 are sufficient to determine all the isoscalar factors. These factors are tabulated in Table 3.1 in Sec. III. Each row of isoscalar factors is normalized separately. The leftmost isoscalar factor for the 56, 10^4 multiplet and the 70, 8^4 multiplet are chosen to be

TABLE A1. Basic representations 6 and $\tilde{6}$ with eigenvalue assignments for H_4 and H_5.

Name	$\vert YII_3;SS_3\rangle$	H_4	H_5
$q_1=p_\uparrow$	$\vert\frac{1}{3}\frac{1}{2}\frac{1}{2};\ \frac{1}{2}\frac{1}{2}\rangle$	1	1
$q_2=n_\uparrow$	$\vert\frac{1}{3}\frac{1}{2}-\frac{1}{2};\ \frac{1}{2}\frac{1}{2}\rangle$	-1	1
$q_3=\lambda_\uparrow$	$\vert-\frac{2}{3}\ 00;\ \frac{1}{2}\frac{1}{2}\rangle$	0	-2
$q_4=p_\downarrow$	$\vert\frac{1}{3}\frac{1}{2}\frac{1}{2};\ \frac{1}{2}-\frac{1}{2}\rangle$	-1	-1
$q_5=n_\downarrow$	$\vert\frac{1}{3}\frac{1}{2}-\frac{1}{2};\ \frac{1}{2}-\frac{1}{2}\rangle$	1	-1
$q_6=\lambda_\downarrow$	$\vert-\frac{2}{3}\ 00;\ \frac{1}{2}-\frac{1}{2}\rangle$	0	2
$q^1=\bar{p}_\downarrow$	$\vert-\frac{1}{3}\frac{1}{2}-\frac{1}{2};\frac{1}{2}-\frac{1}{2}\rangle$	-1	-1
$q^2=\bar{n}_\downarrow$	$-\vert-\frac{1}{3}\frac{1}{2}\frac{1}{2};\ \frac{1}{2}-\frac{1}{2}\rangle$	1	-1
$q^3=\bar{\lambda}_\downarrow$	$-\vert\frac{2}{3}\ 00;\ \frac{1}{2}-\frac{1}{2}\rangle$	0	2
$q^4=\bar{p}_\uparrow$	$-\vert-\frac{1}{3}\frac{1}{2}-\frac{1}{2};\ \frac{1}{2}\frac{1}{2}\rangle$	1	1
$q^5=\bar{n}_\uparrow$	$\vert-\frac{1}{3}\frac{1}{2}\frac{1}{2};\ \frac{1}{2}\frac{1}{2}\rangle$	-1	1
$q^6=\bar{\lambda}_\uparrow$	$\vert\frac{2}{3}\ 00;\ \frac{1}{2}\frac{1}{2}\rangle$	0	-2

TABLE 3.3 SU(3) isoscalar factors for $\overline{10}\times 8\rightarrow 8$

		Y_1I_1	$\left(-1,\frac{3}{2}\right)$	$\left(-1,\frac{3}{2}\right)$	(0.1)	(0,1)	(0,1)	(0,1)	$\left(1,\frac{1}{2}\right)$	$\left(1,\frac{1}{2}\right)$	$\left(1,\frac{1}{2}\right)$	(2,0)
	YI	Y_2I_2	(0,1)	$\left(1,\frac{1}{2}\right)$	(0,1)	$\left(1,\frac{1}{2}\right)$	$\left(-1,\frac{1}{2}\right)$	(0,0)	(0,1)	$\left(-1,\frac{1}{2}\right)$	(0,0)	$\left(-1,\frac{1}{2}\right)$
$\underline{8}$	(0,1)			$2\sqrt{2}/\sqrt{15}$	$-\sqrt{2}/\sqrt{15}$			$1/\sqrt{5}$		$-\sqrt{2}/\sqrt{15}$		
	$\left(1,\frac{1}{2}\right)$					$1/\sqrt{5}$			$-1/\sqrt{5}$		$1/\sqrt{5}$	$-\sqrt{2}/\sqrt{5}$
	$\left(-1,\frac{1}{2}\right)$		$2/\sqrt{5}$				$1/\sqrt{5}$					
	(0,0)				$\sqrt{3}/\sqrt{5}$					$\sqrt{2}/\sqrt{5}$		

positive. Expressions (2.12), (2.16), and (2.17), then determine the relative phases of the remaining rows. These expressions also provide an internal check on the normalization of each row.

III. RESULTS

Table 3.1 lists the SU(6) isoscalar factors for the product 405×56 → 56, 70. This table has been constructed to agree with the revised phase conventions for the isoscalar factors of the product 35×56 → 56, 70.[4,9] When necessary, this revised table for 35×56 → 56, 70, given in Appendix C, should be used with Table 3.1, rather than the table given in Ref. 4. Tables 3.2 and 3.3 list the SU(3) isoscalar factors for the products 27×10 → 10, 8 and $\overline{10}$×8 → 8, needed in the construction of the full SU(6) Clebsch–Gordan coefficients.

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APPENDIX A: GENERATORS AND BASIC REPRESENTATIONS OF SU(6) GROUP

The 35 generators of SU(6) can be written[11] as X^j_i, $i, j = 1, 2, \ldots, 6$, with the condition

$$\sum_{i=1}^{6} X^i_j = 0, \qquad \text{(A1)}$$

and the commutation relations

$$[X^j_i, X^l_k] = \delta^j_k X^l_i - \delta^l_i X^j_k. \qquad \text{(A2)}$$

The familiar SU(3) hypercharge, I-spin, V-spin, and U-spin operators are written in terms of these generators in the following way:

TABLE B1. Representative wavefunctions for 35, 56 and 70 representations. For 70, $\varphi_{ij,k} \equiv q_iq_jq_k + q_jq_iq_k - q_kq_jq_i - q_jq_kq_i$.

$|A;\, YII_3;\, SS_3\rangle$

$\underline{35}$

$$|8;\, 011;\, 11\rangle = q_1q^5$$
$$|8;\, 011;\, 00\rangle = -(1/\sqrt{2})[q_1q^2 + q_4q^5]$$
$$|1;\, 000;\, 11\rangle = (-1/\sqrt{3})[q_1q^4 + q_2q^5 + q_3q^6]$$

$\underline{56}$

$$|10;\, 1\tfrac{3}{2}\tfrac{3}{2};\, \tfrac{3}{2}\tfrac{3}{2}\rangle = q_1q_1q_1$$
$$|8;\, 011;\, \tfrac{1}{2}\tfrac{1}{2}\rangle = (1/3\sqrt{2})[2\ (q_6q_1q_1 + q_1q_6q_1 + q_1q_1q_6) - (q_4q_3q_1 + q_4q_1q_3 + q_3q_4q_1 + q_1q_4q_3 + q_3q_1q_4 + q_1q_3q_4)]$$

$\underline{70}$

$$|8;\, 011;\, \tfrac{3}{2}\tfrac{3}{2}\rangle = (1/\sqrt{6})\ \varphi_{11,3}$$
$$|10;\, 1\ \tfrac{3}{2}\tfrac{3}{2};\, \tfrac{1}{2}\tfrac{1}{2}\rangle = (1/\sqrt{6})\ \varphi_{11,4}$$
$$|8;\, 011;\, \tfrac{1}{2}\tfrac{1}{2}\rangle = -(1/3\sqrt{2})[\varphi_{11,6} + \varphi_{34,1} + \varphi_{43,1}]$$
$$|1;\, 000;\, \tfrac{1}{2}\tfrac{1}{2}\rangle = -(1/6\sqrt{3})[2\varphi_{26,1} + \varphi_{62,1} + \varphi_{21,6} + 2\varphi_{15,3} + \varphi_{53,1} + \varphi_{13,5} + 2\varphi_{34,2} + \varphi_{43,2} + \varphi_{32,4}]$$

TABLE B2. Representative 405 wavefunctions $\{q_iq_j\} \equiv q_iq_j + q_jq_i$

$|A;\, YII_3;\, SS_3\rangle$

$$|27;\, 022;\, 22\rangle = q_1q_1q^5q^5$$
$$|8;\, 011;\, 22\rangle = (1/\sqrt{20})[2\{q_1q_2\}q^5q^5 + 2q_1q_1\{q^4q^5\} + \{q_1q_3\}\{q^5q^6\}]$$
$$|1;\, 000;\, 22\rangle = (1/\sqrt{24})[2q_1q_1q^4q^4 + 2q_2q_2q^5q^5 + 2q_3q_3q^6q^6 + \{q_1q_2\}\{q^4q^5\} + \{q_2q_3\}\{q^5q^6\} + \{q_1q_3\}\{q^4q^6\}]$$
$$|27;\, 022;\, 11\rangle = (1/2)[\{q_1q_4\}q^5q^5 + q_1q_1\{q^2q^5\}]$$
$$|10;\, 1\frac{3}{2}\frac{3}{2};\, 11\rangle = (1/2)[q_1q_1\{q^2q^6\} - q_1q_1\{q^3q^5\}]$$
$$|\overline{10};\, -1\frac{3}{2}\frac{3}{2};\, 11\rangle = (1/2)[\{q_3q_4\}q^5q^5 - \{q_1q_6\}q^5q^5]$$

$$|8_A;\, 011;\, 11\rangle = (1/\sqrt{48})[2q_1q_1\{q^1q^5\} - 2q_1q_1\{q^2q^4\} + 2\{q_2q_4\}q^5q^5 - 2\{q_1q_5\}q^5q^5 + \{q_3q_4\}\{q^5q^6\} - \{q_1q_6\}\{q^5q^6\} - \{q_1q_3\}\{q^2q^6\} + \{q_1q_3\}\{q^3q^5\}]$$
$$|8_B;\, 011;\, 11\rangle = (1/\sqrt{480})[2q_1q_1\{q^1q^5\} - 8q_1q_1\{q^2q^4\} - 8\{q_2q_4\}q^5q^5 + 2\{q_1q_5\}q^5q^5 - 3\{q_1q_2\}\{q^2q^5\} - 3\{q_1q_4\}\{q^4q^5\} - 4\{q_3q_4\}\{q^5q^6\} + \{q_1q_6\}\{q^5q^6\} - 4\{q_1q_3\}\{q^2q^6\} + \{q_1q_3\}\{q^3q^5\}]$$
$$|27;\, 022;\, 00\rangle = (1/\sqrt{12})[2q_1q_1q^2q^2 + 2q_4q_4q^5q^5 + \{q_1q_4\}\{q^2q^5\}]$$

$$|8;\, 011;\, 00\rangle = (1/\sqrt{960})[2q_1q_1\{q^1q^2\} + 2\{q_1q_2\}q^2q^2 + 2q_4q_4\{q^4q^5\} + 2\{q_4q_5\}q^5q^5 + \{q_1q_3\}\{q^2q^3\} + \{q_1q_4\}\{q^1q^5\} + \{q_1q_4\}\{q^2q^4\} + \{q_1q_5\}\{q^2q^5\} + \{q_2q_4\}\{q^2q^5\} + \{q_4q_6\}\{q^5q^6\} - 7\{q_1q_6\}\{q^2q^6\} - 7\{q_3q_4\}\{q^3q^5\} + 8\{q_1q_6\}\{q^3q^5\} + 8\{q_3q_4\}\{q^2q^6\}]$$

$$|1;\, 000;00\rangle = (1/12\sqrt{14})[4q_1q_1q^1q^1 + 4q_2q_2q^2q^2 + 4q_3q_3q^3q^3 + 4q_4q_4q^4q^4 + 4q_5q_5q^5q^5 + 4q_6q_6q^6q^6 + 2\{q_1q_2\}\{q^1q^2\} + 2\{q_1q_3\}\{q^1q^3\} + 2\{q_1q_4\}\{q^1q^4\} - 5\{q_1q_5\}\{q^1q^5\} - 5\{q_1q_6\}\{q^1q^6\} + 2\{q_2q_3\}\{q^2q^3\} - 5\{q_2q_4\}\{q^2q^4\} + 2\{q_2q_5\}\{q^2q^5\} - 5\{q_2q_6\}\{q^2q^6\} - 5\{q_3q_4\}\{q^3q^4\} - 5\{q_3q_5\}\{q^3q^5\} + 2\{q_3q_6\}\{q^3q^6\} + 2\{q_4q_5\}\{q^4q^5\} + 2\{q_4q_6\}\{q^4q^6\} + 2\{q_5q_6\}\{q^5q^6\} + 7\{q_1q_5\}\{q^2q^4\} + 7\{q_1q_6\}\{q^3q^4\} + 7\{q_2q_4\}\{q^1q^5\} + 7\{q_2q_6\}\{q^3q^5\} + 7\{q_3q_4\}\{q^1q^6\} + 7\{q_3q_5\}\{q^2q^6\}]$$

$$Y = -(X_3^3 + X_6^6), \tag{A3}$$

$$I_+ = X_1^2 + X_4^5, \tag{A4a}$$

$$I_- = X_2^1 + X_5^4, \tag{A4b}$$

$$I_3 = \tfrac{1}{2}(X_1^1 + X_4^4 - X_2^2 - X_5^5), \tag{A4c}$$

$$V_+ = X_1^3 + X_4^6, \tag{A5a}$$

$$V_- = X_3^1 + X_6^4, \tag{A5b}$$

$$V_3 = \tfrac{1}{2}(X_1^1 + X_4^4 - X_3^3 - X_6^6), \tag{A5c}$$

$$U_+ = X_3^2 + X_6^5, \tag{A6a}$$

$$U_- = X_2^3 + X_5^6, \tag{A6b}$$

$$U_3 = \tfrac{1}{2}(X_3^3 + X_6^6 - X_2^2 - X_5^5). \tag{A6c}$$

The generators of spin are given by

$$S_+ = X_1^4 + X_2^5 + X_3^6, \tag{A7a}$$

$$S_- = X_4^1 + X_5^2 + X_6^3, \tag{A7b}$$

$$S_3 = X_1^1 + X_2^2 + X_3^3. \tag{A7c}$$

The basic 6 and $\bar{6}$ representations, expressed as q_1, q^l, $l = 1, 2, \ldots, 6$, respectively, are given in Table A1 along with their eigenvalue assignments. The commutation relations of the generators with these basic representations are:

$$[X_i^j, q_l] = \delta_l^j q_i - \tfrac{1}{6}\delta_i^j q_l, \tag{A8a}$$

$$[X_i^j, q^l] = -\delta_i^l q^j + \tfrac{1}{6}\delta_i^j q^l. \tag{A8b}$$

A complete set of commuting operators, linear in the generators X_i^j, is given by Y, I_3, S_3, H_4, and H_5 where H_4 and H_5 are chosen such that,[12]

$$H_4 = \pm 4\, I_3 S_3, \tag{A9a}$$

$$H_5 = \pm 6\, Y S_3, \tag{A9b}$$

for the basic 6 and $\bar{6}$ representations. The positive sign is used for the 6 representation and the negative sign for the $\bar{6}$ representation. In terms of the generators X_i^j, H_4 and H_5 are written:

$$H_4 = X_1^1 - X_2^2 - X_4^4 + X_5^5, \tag{A10a}$$

$$H_5 = X_1^1 + X_2^2 - 2X_3^3 - X_4^4 - X_5^5 + 2X_6^6. \tag{A10b}$$

APPENDIX B: REPRESENTATIVE WAVEFUNCTIONS OF HIGHEST WEIGHT

Table B1 lists the highest weight wavefunctions, written in terms of the basic representations q_l and q^l, $l = 1, 2, \ldots, 6$, for each of the SU(3)×SU(2) multiplets in the 35, 56, and 70 SU(6) representations, respectively. The relative phases of these wavefunctions are chosen to agree with the table of Carter, Coyne, and Meshkov[4] with revised phase conventions.[9] (See Appendix C.) Table B2 lists the highest weight wavefunctions for the 405 representation.

APPENDIX C SU(6) ISOSCALAR FACTORS FOR THE PRODUCT 35×56→56, 70 WITH REVISED PHASE CONVENTIONS[4,9]

	$8^3\times10^4$	$8^1\times10^4$	$1^3\times10^4$	$(8^3\times8^2)_s$	$(8^3\times8^2)_a$	$(8^1\times8^2)_s$	$(8^1\times8^2)_a$	$1^3\times8^2$
$\underline{56}$								
10^4	$2/3$	$-2/\sqrt{15}$	$-1/3$		$-2\sqrt{2}/3\sqrt{5}$			
8^2	$2/3$			$-\sqrt{2}/3$	$2\sqrt{2}/3\sqrt{5}$	0	$-\sqrt{2}/\sqrt{15}$	$-1/3\sqrt{5}$
$\underline{70}$								
8^4	$5/4\sqrt{3}$	$-\sqrt{5}/4$		$-\sqrt{5}/4\sqrt{3}$	$-1/4\sqrt{3}$			$1/2\sqrt{6}$
10^2	$\sqrt{2}/\sqrt{3}$		$-1/\sqrt{6}$		$-1/2\sqrt{6}$		$-1/2\sqrt{2}$	
8^2	$\sqrt{5}/2\sqrt{3}$			$\sqrt{5}/4\sqrt{6}$	$-5/4\sqrt{6}$	$-\sqrt{5}/4\sqrt{2}$	$1/4\sqrt{2}$	$1/2\sqrt{3}$
1^2				$\sqrt{3}/2$		$-1/2$		

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[1] H.J. Melosh, Phys. Rev. D **9**, 1095 (1974).

[2] F.J. Gilman, M. Kugler, and S. Meshkov, Phys. Rev. D **9**, 715 (1974); F.J. Gilman and M. Kugler, Phys. Rev. Lett. **30**, 518 (1973); A.J.G. Hey and J. Weyers, Phys. Lett. B **44**, 263 (1973); F.J. Gilman, M. Kugler, and S. Meshkov, *ibid.* **45**, 481 (1973); A.J.G. Hey, J. Rosner, and J. Weyers, Nucl. Phys. B **61**, 205 (1973).

[3] F.J. Gilman and I. Karliner, Phys. Rev. D **10**, 2194 (1974); A. Love and D.V. Nanopoulos, Phys. Lett. B **45**, 507 (1973); F.J. Gilman and I. Karliner, Phys. Lett. B **46**, 426 (1973).

[4] J.C. Carter, J.J. Coyne and S. Meshkov, Phys. Rev. Lett. **14**, 523 (1965).

[5] C.L. Cook and G. Murtaza, Nuovo Cimento **39**, 7095 (1965). Caution must be exercised in using these tables since inconsistencies appear in the phase conventions. This was also found by F. Gilman and I. Karliner (private communication).

[6] S. Pakvasa and S.P. Rosen, Phys. Rev. **147**, 1166 (1966); M. Machacek and Y. Tomozawa, "Nonleptonic Weak Decay and the Melosh Transformation" Phys. Rev. D (to be published).

[7] J.J. deSwart, Rev. Mod. Phys. **35**, 916 (1963). The phase convention is such that the matrix elements of $V_\pm$ are chosen to be real and positive. See Eqs. (7.5)—(7.8) in the above paper.

[8] V. Chaloupka, *et al.*, Phys. Lett. B **50**, No. 1 (April 1974).

[9] S. Meshkov (private communication).

[10] P. McNamee and F. Chilton, Rev. Mod. Phys. **36**, 1005 (1964).

[11] For example, M. Gourdin *Unitary Symmetries and Their Applications to High Energy Physics* (North-Holland, Amsterdam, 1967), Chap. IX.

[12] L. Schülke, Z. Phys. **183**, 424 (1965).

Clebsch–Gordan coefficients of magnetic space groups

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We have obtained sets of homogeneous linear equations in the Clebsch–Gordan coefficients for magnetic space groups in terms of the matrix elements of the irreducible representations of the little cogroup of the linear subgroup of index 2. Depending on the types of the co-representations in the triple product, 18 cases arise. These 18 cases can be divided into six categories. We have given explicit forms for one case in each category and have indicated how the other cases are to be treated. The formalism has been developed for projective co-representations so that both the vector and the spinor case can be treated.

1. INTRODUCTION

Clebsch Gordan (CG) coefficients for the crystallographic point groups[1,2] have been used in solving many physical problems, e.g., spectra of paramagnetic ions in solids,[3,4] paramagnetic spin Hamiltonian and relaxation phenomena,[5–9] and many other problems.[10,11] In obtaining the selection rules for transitions in crystals,[12–18] it is the coefficients in the Clebsch Gordan series[19] that are required.

Methods for calculating the CG coefficients for space groups have been treated by many authors,[20–22] and Birman and his co-workers have calculated[23–26] the CG coefficients for various space groups.

For magnetic groups[27] there is no simple formula, like the Wigner formula[19] for linear groups, for obtaining the CG coefficients. Recently some work has been done[28–31] in this direction and there are now different procedures for obtaining the CG coefficients of magnetic groups. Here, we give explicit expressions for the linear equations in the CG coefficients of the magnetic space groups from which the CG coefficients can be calculated. These expressions involve the matrix elements of the irreducible representations of the little cogroups belonging to the appropriate **k** vectors characterizing the co-representations of the magnetic space group.[27]

In Sec. 2 we give the matrix elements of the irreducible co-representations of magnetic space groups in terms of the irreducible representations of the little cogroup of the linear space group of index 2. Finally, in Sec. 3 we give explicit expressions for the linear equations in the CG coefficients for one case from each of the 6 categories that arise. We give the formulas in terms of projective co-representations,[32–34] so as to be also applicable to the case of spinor co-representations of the magnetic space groups.

2. IRREDUCIBLE COREPRESENTATIONS OF MAGNETIC SPACE GROUPS

The magnetic space group

$$M = G \; U \; a_0 G, \quad a_0^2 \in G, \tag{1}$$

has the linear subgroup G (which is a space group) of index 2 consisting of elements $(\mathbf{n} + \mathbf{t}(u) \,|\, u)$, where u is a proper or improper rotation, $\mathbf{n}$ is a lattice translation, and $\mathbf{t}(u)$ is the fixed nonprimitive translation, which may be zero or nonzero, associated with u. The antilinear operator a_0 is given by

$$a_0 = \theta(\mathbf{c} \,|\, \gamma), \tag{2}$$

where θ denotes the time reversal operator which commutes with all space operators. The co-representation theory of M has been given by Bradley and Davies,[27] and we summarize their results in the notation we shall use here. The little cogroup of G corresponding to a vector $\mathbf{k}$ in the first Brillouin zone is denoted by $K(\mathbf{k})$, and the left coset representatives of $\bar{K}(\mathbf{k})$ in $G/\mathcal{T}$, where $\mathcal{T}$ is the primitive translational subgroup of M and hence of G, are denoted by α_i, $i = 1, 2, \ldots, r$. The various irreducible representations, which may be projective ones if $\mathbf{k}$ is on the surface of the Brillouin zone,[35] of $\bar{K}(\mathbf{k})$ which appear in the irreducible representations of G are denoted by[36]

$$\Gamma^{\mathbf{k}\mu}_{mn}(u), \quad m, n = 1, 2, \ldots, p.$$

In order to treat spinor co-representations, we give the general form of the irreducible co-representations in terms of the projective co-representation of the magnetic space group, belonging to the factor system $\omega(\alpha, \beta)$,[32,34]

$$\begin{aligned} &D(\alpha)\, D(\beta)^{[\alpha]} = \omega(\alpha, \beta)^{[\alpha\beta]} D(\alpha\beta), \\ &\omega(\alpha, \beta)^{[\gamma]} \omega(\alpha\beta, \gamma) = \omega(\alpha, \beta\gamma)\, \omega(\beta, \gamma), \\ &|\omega(\alpha, \beta)| = 1, \end{aligned} \tag{3}$$

where for any complex number or for any matrix A,

$$A^{[\alpha]} = \begin{cases} A, & \text{if } \alpha \in G, \\ A^*, & \text{if } \alpha \in M - G. \end{cases} \tag{4}$$

For the spinor co-representation of M, the factor system $\omega(\alpha, \beta)$ is connected with $\bar{\omega}(\alpha, \beta)$, the factor system of the linear group

$$M' = G \; U \; (\mathbf{c} \,|\, \gamma) G, \tag{5}$$

corresponding to the spinor representation, in the following manner:

$$\begin{aligned} &\omega(u_1, u_2) = \bar{\omega}(u_1, u_2), \quad \omega(u_1, \theta\gamma u_2) = \bar{\omega}(u_1, \gamma u_2), \\ &\omega(\theta\gamma u_1, u_2) = \bar{\omega}(\gamma u_1, u_2), \quad \omega(\theta\gamma u_1, \theta\gamma u_2) = -\,\bar{\omega}(\gamma u_1, \gamma u_2). \end{aligned} \tag{6}$$

This automatically takes into account the fact that $\theta^2 = -1$ for half-integral spins. With this notation for $\omega(\alpha, \beta)$, $D(\theta^2 u)$ will be equal to $D(u)$ in the expressions used later.

We now give the expression for the (m,n)th element in the (i,j)th block of the irreducible co-representations of the magnetic space group for the three different types of co-representation.[27] The following notations have been used:

$$\mathbf{t}(\alpha_i)=\mathbf{a}_i, \qquad \alpha_i\mathbf{k}=\mathbf{k}_i,$$

$$\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}u\alpha_j)=0, \quad \text{if } \alpha_i^{-1}u\alpha_j \notin \bar{K}(\mathbf{k}),$$

$$\Phi_1(i,j,\mathbf{k};\mathbf{t}(u),u)=\exp\{i\mathbf{k}_i\circ[\mathbf{t}(u)+u\mathbf{a}_j-\mathbf{a}_i]\},$$

$$\Phi_2(i,j,\mathbf{k};\mathbf{t}(u),u)=\Phi_3(i,j,\mathbf{k};\mathbf{t}(u),u)$$
$$=\exp\{-i\gamma\mathbf{k}_i\circ[\mathbf{t}(u)+u\mathbf{c}-\mathbf{c}+u\gamma\mathbf{a}_j-\gamma\mathbf{a}_i]\},$$

$$\Phi_4(i,j,\mathbf{k};\mathbf{t}(u),u)=\exp\{i\mathbf{k}_i\bullet[\mathbf{t}(u)+u\mathbf{c}+u\gamma\mathbf{c}+u\gamma\mathbf{c}+u\gamma^2\mathbf{a}_j-\mathbf{a}_i]\}. \tag{7}$$

The matrix P (cf. Ref. 27) appearing in the following equations satisfies

$$\sum_{j'n'}\Gamma^{\mathbf{k}\mu}_{mn'}(\alpha_i^{-1}u\alpha_{j'})\ \Phi_1(i,j',\mathbf{k};\mathbf{t}(u),u)P_{j'n',jn}\exp(i\mathbf{k}_i\bullet\mathbf{n})$$
$$=\omega(u,\theta\gamma)^*\ \omega(\theta\gamma,\gamma^{-1}u\gamma)\sum_{j'n'}P_{im,j'n'}$$
$$\times\Gamma^{\mathbf{k}\mu}_{n'n}(\alpha_{j'}^{-1}\gamma^{-1}u\gamma\alpha_j)^*\circ\Phi_1(j',j,\mathbf{k};\mathbf{t}(\gamma^{-1}u\gamma),\ \gamma^{-1}u\gamma)^*$$
$$\times\exp(-i\mathbf{k}_{j'}\bullet\mathbf{n}), \qquad \forall u,\mathbf{n},i,m,j,n,$$

and

$$(PP^*)_{im,jn}=\pm\omega(\theta\gamma,\theta\gamma)\,\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}\gamma^2\alpha_j)$$
$$\times\exp[i\mathbf{k}_i\bullet(\mathbf{c}+\gamma\mathbf{c}+\gamma^2\mathbf{a}_j-\mathbf{a}_i)], \tag{8}$$

with the upper sign for co-representations of type (a) and the lower sign for co-representations of type (b). The criteria for Wigner's classification of the three types of co-representations (a, b, or c) for magnetic space groups have been given by Bradley and Davies.[27]

Type (a)

$$D^{\mathbf{k}\mu}_{im,jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)$$
$$=\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}u\alpha_j)\Phi_1(i,j,\mathbf{k};\mathbf{t}(u),u)\exp(i\mathbf{k}_i\circ\mathbf{n}),$$

$$D^{\mathbf{k}\mu}_{im,jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]$$
$$=\pm\sum_{j'n'}\omega(u,\theta\gamma)P_{j'n',jn}\,\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}u\alpha_{j'})$$
$$\times\Phi_1(i,j',\mathbf{k};\mathbf{t}(u),u)\exp(i\mathbf{k}_i\circ\mathbf{n}). \tag{9}$$

Type (b)

$$D^{\mathbf{k}\mu}_{im,jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)=D^{\mathbf{k}\mu}_{r+im,r+jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)$$
$$=\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}u\alpha_j)\Phi_1(i,j,\mathbf{k};\mathbf{t}(u),u)\exp(i\mathbf{k}_i\circ\mathbf{n}),$$

$$D^{\mathbf{k}\mu}_{r+im,jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]$$
$$=-D^{\mathbf{k}\mu}_{im,r+jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]$$
$$=\sum_{j'n'}\omega(u,\theta\gamma)P_{j'n',jn}\,\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}u\alpha_{j'})\Phi_1(i,j',\mathbf{k};\mathbf{t}(u),u)$$
$$\bullet\exp(i\mathbf{k}_i\circ\mathbf{n}),$$

$$D^{\mathbf{k}\mu}_{im,r+jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)=D^{\mathbf{k}\mu}_{r+im,jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)$$
$$=D^{\mathbf{k}\mu}_{im,jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]$$
$$=D^{\mathbf{k}\mu}_{r+im,r+jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]=0. \tag{10}$$

Type (c)

$$D^{\mathbf{k}\mu}_{im,jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)$$
$$=\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}u\alpha_j)\Phi_1(i,j,\mathbf{k};\mathbf{t}(u),u)\exp(i\mathbf{k}_i\circ\mathbf{n}),$$

$$D^{\mathbf{k}\mu}_{r+im,r+jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)=\omega(u,\theta\gamma)^*\,\omega(\theta\gamma,\gamma^{-1}u\gamma)$$
$$\times\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}\gamma^{-1}u\gamma\alpha_j)^*\,\Phi_2(i,j,\mathbf{k};\mathbf{t}(u),u)$$
$$\times\exp(-i\gamma\mathbf{k}_i\circ\mathbf{n}),$$

$$D^{\mathbf{k}\mu}_{r+im,jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]=\omega(\theta\gamma,\gamma^{-1}u\gamma)$$
$$\times\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}\gamma^{-1}u\gamma\alpha_j)^*$$
$$\times\Phi_3(i,j,\mathbf{k};\mathbf{t}(u),u)\exp(-i\gamma\mathbf{k}_i\circ\mathbf{n}),$$

$$D^{\mathbf{k}\mu}_{im,r+jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]=\omega(\theta u\gamma,\theta\gamma)$$
$$\times\Gamma^{\mathbf{k}\mu}_{mn}(\alpha_i^{-1}u\gamma^2\alpha_j)$$
$$\times\Phi_4(i,j,\mathbf{k};\mathbf{t}(u),u)\exp(i\mathbf{k}_i\circ\mathbf{n}),$$

$$D^{\mathbf{k}\mu}_{r+im,jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)=D^{\mathbf{k}\mu}_{im,r+jn}(\mathbf{n}+\mathbf{t}(u)\,|\,u)$$
$$=D^{\mathbf{k}\mu}_{im,jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]$$
$$=D^{\mathbf{k}\mu}_{r+im,r+jn}[(\mathbf{n}+\mathbf{t}(u)\,|\,u)(\mathbf{c}\,|\,\gamma)\theta]=0, \tag{11}$$

with $i,j=1,2,\ldots,r$, and $m,n=1,2,\ldots,p$.

The $\Gamma^{\mathbf{k}\mu}(u)$ matrices satisfy the relation

$$\Gamma^{\mathbf{k}\mu}(u_1)\Gamma^{\mathbf{k}\mu}(u_2)$$
$$=\omega(u_1,u_2)\Gamma^{\mathbf{k}\mu}(u_1u_2)\exp[i(u_1^{-1}\mathbf{k}-\mathbf{k})\circ\mathbf{t}(u_2)]. \tag{12}$$

Zak *et al.*[37] have given the irreducible characters of $\Gamma^{\mathbf{k}\mu}(u)$ for all the $\mathbf{k}$ vectors of the 230 space groups. For single dimensional representations we can substitute the characters for the representations. For multidimensional representations comparison of Zak's character tables and the expressions $\exp[i(u_1^{-1}\mathbf{k}-\mathbf{k})\circ\mathbf{t}(u_2)]$ enables one to use Hurley's tables[38] on projective representations of the 32 crystallographic point groups.

3. CLEBSCH GORDAN COEFFICIENTS OF MAGNETIC SPACE GROUPS

We denote by $|\mathbf{k}\mu ql\rangle$ the (ql)th basis belonging to the irreducible co-representation $D^{\mathbf{k}\mu}$. The CG coefficient $\langle\mathbf{k}_1\mu_1q_1l_1;\mathbf{k}_2\mu_2q_2l_2\,|\,\tau_3\mathbf{k}_3\mu_3q_3l_3\rangle$ connects the product function $|\mathbf{k}_1\mu_1q_1l_1;\mathbf{k}_2\mu_2q_2l_2\rangle$ with the (q_3l_3)th function $|\tau_3\mathbf{k}_3\mu_3q_3l_3\rangle$ belonging to the τ_3 repetition of the irreducible co-representation $D^{\mathbf{k}_3\mu_3}$, in the Kronecker inner direct product $D^{\mathbf{k}_1\mu_1}\otimes D^{\mathbf{k}_2\mu_2}$, i.e.,

$$|\tau_3\mathbf{k}_3\mu_3q_3l_3\rangle=\sum_{q_1l_1q_2l_2}\langle\mathbf{k}_1\mu_1q_1l_1;\mathbf{k}_2\mu_2q_2l_2\,|\,\tau_3\mathbf{k}_3\mu_3q_3l_3\rangle$$
$$\times|\mathbf{k}_1\mu_1q_1l_1;\mathbf{k}_2\mu_2q_2l_2\rangle, \tag{13}$$

$q_a=1,2,\ldots,r_a$, $l_a=1,2,\ldots,p_a$ for co-representations of type (a),

$q_a=1,2,\ldots,2r_a,\quad l_a=1,2,\ldots,p_a$ for co-representations of types (b) or (c).

This is a straightforward generalization of the symbols used in Ref. 31. Here q denotes the block and l is the index within each block of the magnetic space group co-representation. We have suppressed the index ω_a denoting the factor system; it is to be remembered that

$$\omega_3(\alpha,\beta)=\omega_1(\alpha,\beta)\,\omega_2(\alpha,\beta),\qquad \forall\alpha,\beta\in M. \tag{14}$$

If we put the matrices given in Sec. 2 for the co-representations characterized by the three **k** vectors $(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)$ in Eq. (27) of Ref. 31, we obtain a set of homogeneous equations in the CG coefficients of the magnetic space group. The summations in these equations will be restricted to elements $\cap_{a=1}^{3}\bar{K}_{i_aj_a}(\mathbf{k}_a)$ where

$$\bar{K}_{ij}(\mathbf{k})=\bar{K}(\alpha_i^{-1}\mathbf{k}\alpha_j).$$

Depending on the Wigner types to which the three co-representations characterized by the three **k** vectors $(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)$ in the triple product belong, the different cases can be classified in six categories, given in Table I. We now will give the sets of linear homogeneous equations in the CG coefficients for one case from each category. The bases forming the different repetitions of the same irreducible co-representation have been assumed to have the same transformation laws.

TABLE I. Categorization of the equations in the Clebsch–Gordan coefficients for the different types of co-representations characterized by the vectors $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$ in the first Brillouin zone that appear in the triple product.

Different cases	Types of co-representations characterized by the vectors			Categories of linear homogeneous equations
	$\mathbf{k}_1$	$\mathbf{k}_2$	$\mathbf{k}_3$	
1	a	a	a	I
2	a	a	b	II
3	a	a	c	
4	a	b	a	III
5	a	c	a	
6	b	b	a	IV
7	b	c	a	
8	c	c	a	
9	a	b	b	V
10	a	b	c	
11	a	c	b	
12	a	c	c	
13	b	b	b	VI
14	b	b	c	
15	b	c	b	
16	b	c	c	
17	c	c	b	
18	c	c	c	

The cases that have been given here, do not contain any co-representation of type (b). In the other cases in each category, co-representations of type (b) occur in place of one or more of the co-representations of type (c). To obtain the relations for these cases we make the following substitutions at the appropriate place in the relations from that category, given here.

(i) In the argument within $\Delta(\mathbf{k})$, $\gamma\mathbf{k}_{ai_a}$ is replaced by $-\mathbf{k}_{ai_a}$.

(ii) $\omega_a(u,\theta\gamma)^*\,\omega_a(\theta\gamma,\gamma^{-1}u\gamma)\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha_{i_a}^{-1}\gamma^{-1}u\gamma\alpha_{j_a})^*\times\Phi_2(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)$ is replaced by

$$\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha_{i_a}^{-1}u\alpha_{j_a})\,\Phi_1(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u).$$

(iii) $\omega_a(\theta\gamma,\gamma^{-1}u\gamma)\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha_{i_a}^{-1}\gamma^{-1}u\gamma\alpha_{j_a})^*\Phi_3(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)$ is replaced by

$$\omega_a(u,\theta\gamma)\sum_{j^an^a}\Gamma^{\mathbf{k}_a\mu_a}_{m_an^a}(\alpha_{i_a}^{-1}u\alpha_{j^a})\,\Phi_1(i_a,j^a,\mathbf{k}_a;\mathbf{t}(u),u)P^a_{j^an^a,j_an_a}.$$

(iv) $\omega_a(\theta u\gamma,\theta\gamma)\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha_{i_a}^{-1}u\gamma^2\alpha_{j_a})\Phi_4(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)$ is replaced by

$$\omega_a(u,\theta\gamma)\sum_{j^an^a}\Gamma^{\mathbf{k}_a\mu_a}_{m_an^a}(\alpha_{i_a}^{-1}u\alpha_{j^a})\Phi_1(i_a,j^a,\mathbf{k}_a;\mathbf{t}(u),u)P^a_{j^an^a,j_an_a}.$$

We use the following notation:

$$\begin{aligned}\Delta(\mathbf{k})=\;&1\quad\text{if }\mathbf{k}=\mathbf{0}\text{ or a reciprocal vector,}\\&0\quad\text{otherwise,}\\ d_a=\;&\text{dimension of the co-representation }D^{\mathbf{k}_a\mu_a},\\ f=\;&\text{order of the factor group }M/T.\end{aligned}\tag{15}$$

The occurrence of the ± sign in some of the following equations is due to the equivalence of the co-representation of type (a) with any of the two signs. Consistent use of either the upper or the lower sign will be valid.

Category I. Case 1.

$$\begin{aligned}&\langle\mathbf{k}_1\mu_1i_1m_1;\mathbf{k}_2,\mu_2i_2m_2\,|\,\tau_3\mathbf{k}_3\mu_3i_3m_3\rangle(f/d_3)\delta_{j_3j_3'}\,\delta_{n_3n_3'}\\
&\quad=\Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3})\\
&\qquad\times\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2j_2n_2\,|\,\tau_3\mathbf{k}_3\mu_3j_3n_3\rangle\\
&\qquad\times\sum_u\Big(\prod_{a=1,2}\Phi_1(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha_{i_a}^{-1}u\alpha_{j_a})\Big)\Phi_1(i_3,j_3',\mathbf{k}_3;\mathbf{t}(u),u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha_{i_3}^{-1}u\alpha_{j_3'})\pm\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2j_2n_2\,|\,\tau_3\mathbf{k}_3\mu_3j_3n_3\rangle^*\\
&\qquad\times\sum_u\sum_{j^1n^1,j^2n^2,j^3n^3}\Big(\prod_{a=1,2}\Phi_1(i_a,j^a,\mathbf{k}_a;\mathbf{t}(u),u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_an^a}(\alpha_{i_a}^{-1}u\alpha_{j^a})\,P^a_{j^an^a,j_an_a}\Big)\\
&\qquad\times\Phi_1(i_3,j^3,\mathbf{k}_3;\mathbf{t}(u),u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n^3}(\alpha_{i_3}^{-1}u\alpha_{j^3})^*P^{3*}_{j^3n^3,j_3n_3}\Big].\end{aligned}\tag{16}$$

The equations resulting from the omission of the second term on the right hand side of Eq. (16) will give the relations from which the CG coefficients of ordinary space groups can be obtained.

Category II. Case 3.

$$\begin{aligned}
&\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 i_2 m_2 \,|\, \tau_3 \mathbf{k}_3 \mu_3 i_3 m_3\rangle\,(f/d_3)\,\delta_{j_3 j_3'}\,\delta_{n_3 n_3'} \\
&\quad = \Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3}) \sum_{j_1n_1,\,j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3 \mathbf{k}_3\mu_3 j_3 n_3\rangle \sum_u \left(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathbf{t}(u), u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha_{i_a}^{-1} u \alpha_{j_a})\right) \\
&\qquad \times \Phi_1(i_3, j_3', \mathbf{k}_3; \mathbf{t}(u), u)^* \,\Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3'}(\alpha_{i_3}^{-1} u \alpha_{j_3'})^* \\
&\quad = \Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3}) \sum_{j_1n_1,\,j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3 \mathbf{k}_3\mu_3 r_3 + j_3' n_3'\rangle^* \sum_u \omega_3(u, \theta\gamma)\,\omega_3(\theta u\gamma, \theta\gamma)^*\,\Phi_4(i_3, j_3, \mathbf{k}_3; \mathbf{t}(u), u)^* \\
&\qquad \times \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha_{i_3}^{-1} u\gamma^2 \alpha_{j_3})^* \sum_{j^1n^1,\,j^2n^2} \left(\prod_{a=1,2} \Phi_1(i_a, j^a, \mathbf{k}_a; \mathbf{t}(u), u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_a n^a}(\alpha_{i_a}^{-1} u \alpha_{j^a}) P^a_{j^a n^a,\, j_a n_a}\right).
\end{aligned} \tag{17}$$

$$\begin{aligned}
&\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 i_2 m_2 \,|\, \tau_3 \mathbf{k}_3 \mu_3 r_3 + i_3 m_3\rangle(f/d_3)\,\delta_{j_3 j_3'}\delta_{n_3 n_3'} \\
&\quad = \Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}+\gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1,\,j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3 \mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle \sum_u \omega_3(u, \theta\gamma)\,\omega_3(\theta\gamma, \gamma^{-1}u\gamma)^* \\
&\qquad \times\left(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathbf{t}(u), u)\Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha_{i_a}^{-1} u \alpha_{j_a})\right) \Phi_2(i_3, j_3', \mathbf{k}_3; \mathbf{t}(u), u)^* \;\Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3'}(\alpha_{i_3}^{-1}\gamma^{-1}u\gamma\alpha_{j_3'}) \\
&\quad = \Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}+\gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1,\,j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3 \mathbf{k}_3\mu_3 j_3' n_3'\rangle^* \sum_u \omega_3(u, \theta\gamma) \\
&\qquad \times \omega_3(\theta\gamma, \gamma^{-1}u\gamma)^*\,\Phi_3(i_3, j_3, \mathbf{k}_3; \mathbf{t}(u), u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha_{i_3}^{-1}\gamma^{-1}u\gamma\alpha_{j_3}) \sum_{j^1n^1,\,j^2n^2} \left(\prod_{a=1,2} \Phi_1(i_a, j^a, \mathbf{k}_a; \mathbf{t}(u), u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_a n^a}(\alpha_{i_a}^{-1} u \alpha_{j^a}) P^a_{j^a n^a,\, j_a n_a}\right).
\end{aligned} \tag{18}$$

$$\begin{aligned}
&\Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3}) \sum_{j_1n_1,\,j_2n_2} \Bigg[\langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3 \mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle \sum_u \Bigg(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathbf{t}(u), u) \\
&\qquad \times \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha_{i_a}^{-1} u \alpha_{j_a})\Bigg)\,\Phi_1(i_3, j_3', \mathbf{k}_3; \mathbf{t}(u), u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3'}(\alpha_{i_3}^{-1} u \alpha_{j_3'})^* + \langle \mathbf{k}_1\mu_1 j_1 n_1;\; \mathbf{k}_2\mu_1 j_1 n_1; \,|\, \tau_3 \mathbf{k}_3\mu_3 j_3' n_3'\rangle^* \\
&\qquad \times \sum_u \omega_3(u, \theta\gamma)\,\omega_3(\theta u\gamma, \theta\gamma)^*\,\Phi_4(i_3, j_3, \mathbf{k}_3; \mathbf{t}(u), u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha_{i_3}^{-1} u\gamma^2 \alpha_{j_3})^* \\
&\qquad \times \sum_{j^1n^1,\,j^2n^2} \left(\prod_{a=1,2} \Phi_1(i_a, j^a, \mathbf{k}_a; \mathbf{t}(u), u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_a n^a}(\alpha_{i_a}^{-1} u \alpha_{j^a}) P^a_{j^a n^a,\, j_a n_a}\right)\Bigg] \\
&\quad = \Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}+\gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1,\,j_2n_2} \Bigg[\langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3 \mathbf{k}_3\mu_3 j_3 n_3\rangle \sum_u \omega_3(u, \theta\gamma)\,\omega_3(\theta\gamma, \gamma^{-1}u\gamma)^* \\
&\qquad \times \Phi_2(i_3, j_3', \mathbf{k}_3; \mathbf{t}(u), u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3'}(\alpha_{i_3}^{-1}\gamma^{-1}u\gamma\alpha_{j_3'}) \left(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathbf{t}(u), u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha_{i_a}^{-1} u \alpha_{j_a})\right) \\
&\qquad + \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3 \mathbf{k}_3\mu_3 r_3 + j_3' n_3'\rangle^* \sum_u \omega_3(u, \theta\gamma)\,\omega_3(\theta\gamma, \gamma^{-1}u\gamma)^*\,\Phi_3(i_3 j_3, \mathbf{k}_3;\; \mathbf{t}(u), u)^* \\
&\qquad \times \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha_{i_3}^{-1}\gamma^{-1}u\gamma\alpha_{j_3}) \sum_{j^1n^1,\,j^2n^2} \left(\prod_{a=1,2} \Phi_1(i_a, j^a, \mathbf{k}_a;\; \mathbf{t}(u), u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_a n^a}(\alpha_{i_a}^{-1} u \alpha_{j^a}) P^a_{j^a n^a,\, j_a n_a}\right)\Bigg] = 0.
\end{aligned} \tag{19}$$

Each case in this category will contain six such sets of equations with appropriate substitutions.

Category III. Case 5

$$\begin{aligned}
&\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 i_2 m_2 \,|\, \tau_3 \mathbf{k}_3 \mu_3 i_3 m_3\rangle\,(f/d_3)\,\delta_{j_3 j_3'}\,\delta_{n_3 n_3'} \\
&\quad = \Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3}) \sum_{j_1n_1,\,j_2n_2} \Bigg[\langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3 \mathbf{k}_3\mu_3 j_3 n_3\rangle \sum_u \left(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathbf{t}(u), u)\Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha_{i_a}^{-1} u \alpha_{j_a})\right)
\end{aligned}$$

$$\begin{aligned}
&\times\Phi_1(i_3,j_3',\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*+\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3'n_3'\rangle^*\sum_u\omega_2(u,\theta\gamma)^*\\
&\times\omega_2(\theta u\gamma,\theta\gamma)\sum_{j^1n^1,j^3n^3}\Phi_1(i_1,j^1,\mathbf{k}_1;\mathrm{t}(u),u)\Phi_4(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\,\Phi_1(i_3,j^3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_1\mu_1}_{m_1n^1}(\alpha^{-1}_{i_1}u\alpha_{j^1})\\
&\times\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}u\gamma^2\alpha_{j_2})\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n^3}(\alpha^{-1}_{i_3}u\alpha_{j^3})^*P^1_{j^1n^1,j_1n_1}P^{3*}_{j^3n^3,j_3n_3}\Big].
\end{aligned}\tag{20}$$

$$\begin{aligned}
&\langle\mathbf{k}_1\mu_1i_1m_1;\mathbf{k}_2\mu_2r_2+i_2m_2|\tau_3\mathbf{k}_3\mu_3i_3m_3\rangle\,(f/d_3)\,\delta_{j_3j_3'}\,\delta_{n_3n_3'}\\
&=\Delta(\mathbf{k}_{1i_1}-\gamma\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3})\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3n_3\rangle\sum_u\omega_2(u,\theta\gamma)^*\,\omega_2(\theta\gamma,\gamma^{-1}u\gamma)\Phi_1(i_1,j_1,\mathbf{k}_1;\mathrm{t}(u),u)\\
&\times\Phi_2(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\,\Phi_1(i_3,j_3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\alpha_{j_1})\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\\
&\times\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*+\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3'n_3'\rangle^*\sum_u\omega_2(u,\theta\gamma)^*\,\omega_2(\theta\gamma,\gamma^{-1}u\gamma)\\
&\times\sum_{j^1n^1,j^3n^3}\Phi_1(i_1,j^1,\mathbf{k}_1;\mathrm{t}(u),u)\,\Phi_3(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\Phi_1(i_3,j^3,\mathbf{k}_3;\mathrm{t}(u),u)^*\\
&\times\Gamma^{\mathbf{k}_1\mu_1}_{m_1n^1}(\alpha^{-1}_{i}u\alpha_{j^1})\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n^3}(\alpha^{-1}_{i_3}u\alpha_{j^3})^*P^1_{j^1n^1,j_1n_1}P^{3*}_{j^3n^3,j_3n_3}\Big]\;.
\end{aligned}\tag{21}$$

Each case in this category will contain 2 such sets of equations.

Category IV. Case 8

$$\begin{aligned}
&\langle\mathbf{k}_1\mu_1i_1m_1;\mathbf{k}_2\mu_2i_2m_2|\tau_3\mathbf{k}_3\mu_3i_3m_3\rangle\,(f/d_3)\,\delta_{j_3j_3'}\,\delta_{n_3n_3'}\\
&=\Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3})\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3n_3\rangle\sum_u\Big(\prod_{a=1,2}\Phi_1(i_a,j_a,\mathbf{k}_a;\mathrm{t}(u),u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}u\alpha_{j_a})\Big)\\
&\times\Phi_1(i_3,j_3',\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*\pm\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3'n_3'\rangle^*\\
&\times\sum_u\omega_3(u,\theta\gamma)^*\,\omega_3(\theta u\gamma,\theta\gamma)\sum_{j^3n^3}\Big(\prod_{a=1,2}\Phi_4(i_a,j_a,\mathbf{k}_a;\mathrm{t}(u),u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}u\gamma^2\alpha_{j_a})\Big)\\
&\times\Phi_1(i_3,j^3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n^3}(\alpha^{-1}_{i_3}u\alpha_{j^3})^*P^{3*}_{j^3n^3,j_3n_3}\Big].
\end{aligned}\tag{22}$$

$$\begin{aligned}
&\langle\mathbf{k}_1\mu_1i_1m_1;\mathbf{k}_2\mu_2r_2+i_2m_2|\tau_3\mathbf{k}_3\mu_3i_3m_3\rangle\,(f/d_3)\,\delta_{j_3j_3'}\delta_{n_3n_3'}\\
&=\Delta(\mathbf{k}_{1i_1}-\gamma\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3})\sum_{j_1n_1,j_2n_2}\Big(\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3n_3\rangle\sum_u\omega_2(u,\theta\gamma)^*\,\omega_2(\theta\gamma,\gamma^{-1}u\gamma)\,\Phi_1(i_1,j_1,\mathbf{k}_1;\mathrm{t}(u),u)\\
&\times\Phi_2(i_2,j_2,\mathbf{k}_3;\mathrm{t}(u),u)\,\Phi_1(i_3,j_3',\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\alpha_{j_1})\,\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*\\
&\pm\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3'n_3'\rangle^*\sum_u\omega_1(\theta u\gamma,\theta\gamma)\,\omega_2(\theta\gamma,\gamma^{-1}u\gamma)\,\omega_3(u,\theta\gamma)^*\\
&\times\sum_{j^3n^3}\Phi_4(i_1,j_1,\mathbf{k}_1;\mathrm{t}(u),u)\,\Phi_3(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\,\Phi_1(i_3,j^3,\mathbf{k}_3;\mathrm{t}(u),u)^*\\
&\times\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\gamma^2\alpha_{j_1})\,\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n^3}(\alpha^{-1}_{i_3}u\alpha_{j^3})^*P^{3*}_{j^3n^3,j_3n_3}\Big).
\end{aligned}\tag{23}$$

$$\begin{aligned}
&\langle\mathbf{k}_1\mu_1r_1+i_1m_1;\mathbf{k}_2\mu_2i_2m_2|\tau_3\mathbf{k}_3\mu_3i_3m_3\rangle\,(f/d_3)\,\delta_{j_3j_3'}\delta_{n_3n_3'}\\
&=\Delta(-\gamma\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3})\sum_{j_1n_1,j_2n_2}\Big(\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3n_3\rangle\sum_u\omega_1(u,\theta\gamma)^*\,\omega_1(\theta\gamma,\gamma^{-1}u\gamma)\,\Phi_2(i_1,j_1,\mathbf{k}_1;\mathrm{t}(u),u)\\
&\times\Phi_1(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\,\Phi_1(i_3,j_3',\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\,\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}u\alpha_{j_2})\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*
\end{aligned}$$

$$\pm \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 j_3' n_3'\rangle^* \sum_u \omega_1(\theta\gamma, \gamma^{-1}u\gamma)\, \omega_2(\theta u\gamma, \theta\gamma)\, \omega_3(u, \theta\gamma)^*$$

$$\times \sum_{j^3 n^3} \Phi_3(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_4(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_1(i_3, j^3, \mathbf{k}_3; \mathrm{t}(u), u)^* \Gamma^{\mathbf{k}_1\mu_1}_{m_1 n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*$$

$$\times \Gamma^{\mathbf{k}_2\mu_2}_{m_2 n_2}(\alpha^{-1}_{i_2}u\gamma^2\alpha_{j_2})\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n^3}(\alpha^{1}_{i_3}u\alpha_{j^3})^* P^{3*}_{j^3 n^3, j_3 n_3}\Big). \tag{24}$$

$$\langle \mathbf{k}_1\mu_1 r_1 + i_1 m_1; \mathbf{k}_2\mu_2 r_2 + i_2 m_2 | \tau_3 \mathbf{k}_3\mu_3 i_3 m_3\rangle\, (f/d_3)\, \delta_{j_3 j_3'}\delta_{n_3 n_3'}$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \times \sum_{j_1 n_1, j_2 n_2} \Big[\langle \mathbf{k}_1\mu_1 r_1 + j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 j_3 n_3\rangle \sum_u \omega_3(u, \theta\gamma)^*\, \omega_3(\theta\gamma, \gamma^{-1}u\gamma)$$

$$\times \Big(\prod_{a=1,2} \Phi_2(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^* \Big)\, \Phi_1(i_3, j_3', \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*$$

$$\pm \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 j_3' n_3'\rangle^* \sum_u \omega_3(u, \theta\gamma)^*\, \omega_3(\theta\gamma, \gamma^{-1}u\gamma) \Big(\prod_{a=1,2} \Phi_3(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)$$

$$\times \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^* \Big) \sum_{j^3 n^3} \Phi_1(i_3, j^3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n^3}(\alpha^{-1}_{i_3}u\alpha_{j^3})^* P^{3*}_{j^3 n^3, j_3 n_3} \Big]. \tag{25}$$

Each case in category IV will contain four such sets of equations.

Category V. Case 12

$$\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 i_2 m_2 | \tau_3 \mathbf{k}_3\mu_3 i_3 m_3\rangle\, (f/d_3)\delta_{j_3 j_3'}\delta_{n_3 n_3'}$$

$$= \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1 n_1, j_2 n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 j_3 n_3\rangle \sum_u \Big(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}u\alpha_{j_a}) \Big)$$

$$\times \Phi_1(i_3, j_3', \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*$$

$$= \pm \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1 n_1, j_2 n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 r_3 + j_3' n_3'\rangle^* \sum_u \omega_1(u, \theta\gamma)\, \omega_1(\theta u\gamma, \theta\gamma)^* \sum_{j^1 n^1} \Phi_1(i_1, j^1, \mathbf{k}_1; \mathrm{t}(u), u)$$

$$\times \Phi_4(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_4(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1 n^1}(\alpha^{-1}_{i_1}u\alpha_{j^1})\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2 n_2}(\alpha^{-1}_{i_2}u\gamma^2\alpha_{j_2})\Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^* P^{1}_{j^1 n^1, j_1 n_1}. \tag{26}$$

$$\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 r_2 + i_2 m_2 | \tau_3 \mathbf{k}_3\mu_3 i_3 m_3\rangle\ (f/d_3)\, \delta_{j_3 j_3'}\, \delta_{n_3 n_3'}$$

$$= \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1 n_1, j_2 n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 j_3 n_3\rangle \sum_u \omega_2(u, \theta\gamma)^*\, \omega_2(\theta\gamma, \gamma^{-1}u\gamma)\, \Phi_1(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)$$

$$\times\ \Phi_2\ (i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\Phi_1(i_3, j_3', \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1 n_1}(\alpha^{-1}_{i_1}u\alpha_{j_1})\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2 n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*$$

$$= \pm \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1 n_1, j_2 n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 r_3 + j_3' n_3'\rangle^* \sum_u \omega_1(u, \theta\gamma)$$

$$\times \omega_2(\theta\gamma, \gamma^{-1}u\gamma)\, \omega_3(\theta u\gamma, \theta\gamma)^* \sum_{j^1 n^1} \Phi_1(i_1, j^1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_3(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_4(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*$$

$$\times \Gamma^{\mathbf{k}_1\mu_1}_{m_1 n^1}(\alpha^{-1}_{i_1}u\alpha_{j^1})\Gamma^{\mathbf{k}_2\mu_2}_{m_2 n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^* P^{1}_{j^1 n^1, j_1 n_1}. \tag{27}$$

$$\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 i_2 m_2 | \tau_3 \mathbf{k}_3\mu_3 r_3 + i_3 m_3\rangle\ (f/d_3)\, \delta_{j_3 j_3'}\delta_{n_3 n_3'}$$

$$= \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{i_1 n_1, j_2 n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle \sum_u \omega_3(u, \theta\gamma)\, \omega_3(\theta\gamma, \gamma^{-1}u\gamma)^*$$

$$\Big(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}u\alpha_{j_a}) \Big) \Phi_2(i_3, j_3', \mathbf{k}_3; \mathrm{t}(u), u)^*\ \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3'}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3'})$$

$$= \pm \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1 n_1, j_2 n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3 \mathbf{k}_3\mu_3 j_3' n_3'\rangle^* \sum_u \omega_1(u, \theta\gamma)\, \omega_2(\theta u\gamma, \theta\gamma)\, \omega_3(\theta\gamma, \gamma^{-1}u\gamma)^*$$

$$\times \sum_{j^1n^1} \Phi_1(i_1, j^1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_4(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_3(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1n^1}(\alpha^{-1}_{i_1} u\alpha_{j^1})$$

$$\times \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2} u\gamma^2\alpha_{j_2})\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}\gamma^{-1} u\gamma\alpha_{j_3}) P^1_{j^1n^1, j_1n_1} . \tag{28}$$

$$\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 r_2 + i_2 m_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + i_3 m_3\rangle\, (f/d_3)\, \delta_{j_3j'_3}\, \delta_{n_3n'_3}$$

$$= \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle$$

$$\times \sum_u \omega_1(u, \theta\gamma)\, \omega_1(\theta\gamma, \gamma^{-1}u\gamma)^*\, \Phi_1(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_2(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_2(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^*$$

$$\times \Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1} u\alpha_{j_1})\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j'_3})$$

$$= \pm\Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{i_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j'_3 n'_3\rangle^* \sum_u \omega_1(u, \theta\gamma)\, \omega_2(\theta\gamma, \gamma^{-1}u\gamma)\, \omega_3(\theta\gamma, \gamma^{-1}u\gamma)^*$$

$$\times \sum_{j^1n^1} \Phi_1(i_1, j^1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_3(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_3(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1n^1}(\alpha^{-1}_{i_1} u\alpha_{j^1})$$

$$\times \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3}) P^1_{j^1n^1, j_1n_1} . \tag{29}$$

$$\Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \Big[\langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle$$

$$\times \sum_u \Big(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a} u\alpha_{j_a}) \Big)\, \Phi_1(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3} u\alpha_{j'_3})^*$$

$$\pm \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j'_3 n'_3\rangle^* \times \sum_u \omega_1(u, \theta\gamma)\, \omega_1(\theta u\gamma, \theta\gamma)^* \sum_{j^1n^1} \Phi_1(i_1, j^1, \mathbf{k}_1; \mathrm{t}(u), u)$$

$$\times \Phi_4(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_4(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1n^1}(\alpha^{-1}_{i_1} u\alpha_{j^1})\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2} u\nu^2\alpha_{j_2})\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3} u\gamma^2\alpha_{j_3})^*\, P^1_{j^1n^1, j_2n_2} \Big]$$

$$= \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \Big[\langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle$$

$$\times \sum_u \omega_2(u, \theta\gamma)^*\, \omega_2(\theta\gamma, \gamma^{-1}u\gamma) \Phi_1(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_2(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_1(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^*$$

$$\times \Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1} u\alpha_{j_1})\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3} u\alpha_{j'_3})^* \pm \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j'_3 n'_3\rangle^*$$

$$\times \sum_u \omega_1(u, \theta\gamma)\, \omega_2(\theta\gamma, \gamma^{-1}u\gamma)\, \omega_3(\theta u\gamma, \theta\gamma)^* \sum_{j^1n^1} \Phi_1(i_1, j^1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_3(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)$$

$$\times \Phi_4(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1n^1}(\alpha^{-1}_{i_1} u\alpha_{j^1})\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3} u\gamma^2\alpha_{j_3})^*\, P^1_{j^1n^1, j_1n_1} \Big]$$

$$= \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \Big[\langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j_3 n_3\rangle \sum_u \omega_3(u, \theta\gamma)$$

$$\times \omega_3(\theta\gamma, \gamma^{-1}u\gamma)^* \Big(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a} u\alpha_{j_a}) \Big)\, \Phi_2(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^*$$

$$\times \Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j'_3}) \pm \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 \,|\, \tau_3 k_3\mu_3 r_3 + j'_3 n'_3\rangle^* \sum_u \omega_1(u, \theta\gamma)\, \omega_2(\theta u\gamma, \theta\gamma)$$

$$\times \omega_3(\theta\gamma, \gamma^{-1}u\gamma)^* \sum_{j^1n^1} \Phi_1(i_1, j^1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_4(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_3(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1n^1}(\alpha^{-1}_{i_1} u\alpha_{j^1})$$

$$\times \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2} u\gamma^2\alpha_{j_2})\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3})\, P^1_{j^1n^1, j_1n_1} \Big]$$

$$= \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \Big[\langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j_3 n_3\rangle \sum_u \omega_1(u, \theta\gamma)\, \omega_1(\theta\gamma, \gamma^{-1}u\gamma)^*\, \Phi_1(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)$$

$$\times \Phi_2(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_2(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1} u\alpha_{j_1})\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*$$

$$\times \Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j'_3}) \pm \langle \mathbf{k}_1\mu_1 j_1n_1; \mathbf{k}_2\mu_2 j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + j'_3n'_3\rangle^* \sum_u \omega_1(u,\theta\gamma)\,\omega_1(\theta\gamma,\gamma^{-1}u\gamma)^*$$

$$\times \sum_{j^1n^1} \Phi_1(i_1,j^1,\mathbf{k}_1;\mathrm{t}(u),u)\,\Phi_3(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\,\Phi_3(i_3,j_3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_1\mu_1}_{m_1n^1}(\alpha^{-1}_{i_1}u\alpha_{j^1})$$

$$\times \Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3})P^1_{j^1n^1,j_1n_1}\Big] = 0. \tag{30}$$

Each case in category V will contain twelve such sets of equations.

Category VI. Case 18

$$\langle \mathbf{k}_1\mu_1 i_1m_1; \mathbf{k}_2\mu_2 i_2m_2 \,|\, \tau_3\mathbf{k}_3\mu_3 i_3m_3\rangle\,(f/d_3)\,\delta_{j_3j'_3}\,\delta_{n_3n'_3}$$

$$= \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1,j_2n_2} \langle \mathbf{k}_1\mu_1 j_1n_1; \mathbf{k}_2\mu_2 j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j_3n_3\rangle \sum_u \left(\prod_{a=1,2} \Phi_1(i_a,j_a,\mathbf{k}_a;\mathrm{t}(u),u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}u\alpha_{j_a})\right)$$

$$\times \Phi_1(i_3,j'_3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3}u\alpha_{j'_3})^*$$

$$= \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1,j_2n_2} \langle \mathbf{k}_1\mu_1 r_1 + j_1n_1; \mathbf{k}_2\mu_2 r_2 + j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + j'_3n'_3\rangle^*$$

$$\times \sum_u \left(\prod_{a=1,2} \Phi_4(i_a,j_a,\mathbf{k}_a;\mathrm{t}(u),u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}u\gamma^2\alpha_{j_a})\right)\Phi_4(i_3,j_3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^*. \tag{31}$$

$$\langle \mathbf{k}_1\mu_1 r_1 + i_1m_1; \mathbf{k}_2\mu_2 i_2m_2 \,|\, \tau_3\mathbf{k}_3\mu_3 i_3m_3\rangle\,(f/d_3)\,\delta_{j_3j'_3}\,\delta_{n_3n'_3}$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1,j_2n_2} \langle \mathbf{k}_1\mu_1 r_1 + j_1n_1; \mathbf{k}_2\mu_2 j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j_3n_3\rangle \sum_u \omega_1(u,\theta\gamma)^*\,\omega_1(\theta\gamma,\gamma^{-1}/u\gamma)\,\Phi_2(i_1,j_1,\mathbf{k}_1;\mathrm{t}(u),u)$$

$$\times \Phi_1(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\,\Phi_1(i_3,j'_3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\,\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}u\alpha_{j_2})\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3}u\alpha_{j'_3})^*$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1,j_2n_2} \langle \mathbf{k}_1\mu_1 j_1n_1; \mathbf{k}_2\mu_2 r_2 + j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + j'_3n'_3\rangle^* \sum_u \omega_1(\theta u\gamma,\theta\gamma)^*$$

$$\times \omega_1(\theta\gamma,\gamma^{-1}u\gamma)\,\Phi_3(i_1,j_1,\mathbf{k}_1;\mathrm{t}(u),u)\,\Phi_4(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\,\Phi_4(i_3,j_3,\mathbf{k}_3;\mathrm{t}(u),u)^*$$

$$\times \Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\,\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}u\gamma^2\alpha_{j_2})\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^*. \tag{32}$$

$$\langle \mathbf{k}_1\mu_1 i_1m_1; \mathbf{k}_2\mu_2 r_2 + i_2m_2 \,|\, \tau_3\mathbf{k}_3\mu_3 i_3m_3\rangle\,(f/d_3)\,\delta_{j_3j'_3}\,\delta_{n_3n'_3}$$

$$= \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1,j_2n_2} \langle \mathbf{k}_1\mu_1 j_1n_1; \mathbf{k}_2\mu_2 r_2 + j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j_3n_3\rangle \sum_u \omega_2(u,\theta\gamma)^*\,\omega_2(\theta\gamma,\gamma^{-1}u\gamma)\,\Phi_1(i_1,j_1,\mathbf{k}_1;\mathrm{t}(u),u)$$

$$\times \Phi_2(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)\,\Phi_1(i_3,j'_3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\alpha_{j_1})\,\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3}u\alpha_{j'_3})^*$$

$$= \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1,j_2n_2} \langle \mathbf{k}_1\mu_1 r_1 + j_1n_1; \mathbf{k}_2\mu_2 j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + j'_3n'_3\rangle^*$$

$$\times \sum_u \omega_2(\theta u\gamma,\theta\gamma)^*\,\omega_2(\theta\gamma,\gamma^{-1}u\gamma)\,\Phi_4(i_1,j_1,\mathbf{k}_1;\mathrm{t}(u),u)\,\Phi_3(i_2,j_2,\mathbf{k}_2;\mathrm{t}(u),u)$$

$$\times \Phi_4(i_3,j_3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\gamma^2\alpha_{j_1})\,\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^*. \tag{33}$$

$$\langle \mathbf{k}_1\mu_1 r_1 + i_1m_1; \mathbf{k}_2\mu_2 r_2 + i_2m_2 \,|\, \tau_3\mathbf{k}_3\mu_3 i_3m_3\rangle\,(f/d_3)\,\delta_{j_3j'_3}\,\delta_{n_3n'_3}$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1,j_2n_2} \langle \mathbf{k}_1\mu_1 r_1 + j_1n_1; \mathbf{k}_2\mu_2 r_2 + j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j_3n_3\rangle \sum_u \omega_3(u,\theta\gamma)^*\,\omega_3(\theta\gamma,\gamma^{-1}u\gamma)$$

$$\times \left(\prod_{a=1,2} \Phi_2(i_a,j_a,\mathbf{k}_a;\mathrm{t}(u),u)\,\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^*\right)\Phi_1(i_3,j'_3,\mathbf{k}_3;\mathrm{t}(u),u)^*\,\Gamma^{\mathbf{k}_3\mu_3}_{m_3n'_3}(\alpha^{-1}_{i_3}u\alpha_{j'_3})^*$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + j'_3 n'_3\rangle^* \sum_u \omega_3(\theta u\gamma, \theta\gamma)^* \omega_3(\theta\gamma, \gamma^{-1}u\gamma)$$

$$\times \left(\prod_{a=1,2} \Phi_3(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^*\right) \Phi_4(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^* . \qquad (34)$$

$$\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 i_2 m_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + i_3 m_3\rangle \ (f/d_3)\, \delta_{j_3 j'_3}\, \delta_{n_3 n'_3}$$

$$= \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle \sum_u \omega_3(u, \theta\gamma)\, \omega_3(\theta\gamma, \gamma^{-1}u\gamma)^*$$

$$\times \left(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}u\alpha_{j_a})\right) \Phi_2(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n'_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j'_3})$$

$$= \Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 r_1 + j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 j'_3 n'_3\rangle^* \sum_u \omega_3(\theta u\gamma, \theta\gamma)$$

$$\times \omega_3(\theta\gamma, \gamma^{-1}u\gamma)^* \left(\prod_{a=1,2} \Phi_4(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}u\gamma^2\alpha_{j_a})\right) \Phi_3(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3}). \qquad (35)$$

$$\langle \mathbf{k}_1\mu_1 r_1 + i_1 m_1; \mathbf{k}_2\mu_2 i_2 m_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + i_3 m_3\rangle \ (f/d_3)\, \delta_{j_3 j'_3}\, \delta_{n_3 n'_3}$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 r_1 + j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle \sum_u \omega_2(u, \theta\gamma)\, \omega_2(\theta\gamma, \gamma^{-1}u\gamma)^*\, \Phi_2(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)$$

$$\times \Phi_1(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_2(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^* \Gamma^{\mathbf{k}_1\mu_1}_{m_1 n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2 n_2}(\alpha^{-1}_{i_2}u\alpha_{j_2})\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n'_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j'_3})$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 j'_3 n'_3\rangle^* \sum_u \omega_2(\theta u\gamma, \theta\gamma)$$

$$\times \omega_2(\theta\gamma, \gamma^{-1}u\gamma)^*\, \Phi_3(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_4(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_3(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*$$

$$\times \Gamma^{\mathbf{k}_1\mu_1}_{m_1 n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2 n_2}(\alpha^{-1}_{i_2}u\gamma^2\alpha_{j_2})\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3}). \qquad (36)$$

$$\langle \mathbf{k}_1\mu_1 i_1 m_1; \mathbf{k}_2\mu_2 r_2 + i_2 m_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + i_3 m_3\rangle \ (f/d_3)\, \delta_{j_3 j'_3}\, \delta_{n_3 n'_3}$$

$$= \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle \sum_u \omega_1(u, \theta\gamma)\, \omega_1(\theta\gamma, \gamma^{-1}u\gamma)^*\, \Phi_1(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)$$

$$\times \Phi_2(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_2(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1 n_1}(\alpha^{-1}_{i_1}u\alpha_{j_1})\, \Gamma^{\mathbf{k}_2\mu_2}_{m_2 n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n'_3}(\alpha^{-1}_{i'_3}\gamma^{-1}u\gamma\alpha_{j'_3})$$

$$= \Delta(\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 r_1 + j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 j'_3 n'_3\rangle^* \sum_u \omega_1(\theta u\gamma, \theta\gamma)$$

$$\times \omega_1(\theta\gamma, \gamma^{-1}u\gamma)^*\, \Phi_4(i_1, j_1, \mathbf{k}_1; \mathrm{t}(u), u)\, \Phi_3(i_2, j_2, \mathbf{k}_2; \mathrm{t}(u), u)\, \Phi_3(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_1\mu_1}_{m_1 n_1}(\alpha^{-1}_{i_1}u\gamma^2\alpha_{j_1})$$

$$\times \Gamma^{\mathbf{k}_2\mu_2}_{m_2 n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3}). \qquad (37)$$

$$\langle \mathbf{k}_1\mu_1 r_1 + i_1 m_1; \mathbf{k}_2\mu_2 r_2 + i_2 m_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + i_3 m_3\rangle \ (f/d_3)\, \delta_{j_3 j'_3}\, \delta_{n_3 n'_3}$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 r_1 + j_1 n_1; \mathbf{k}_2\mu_2 r_2 + j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle \sum_u \left(\prod_{a=1,2} \Phi_2(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\right.$$

$$\left. \times \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^*\right) \Phi_2(i_3, j'_3, \mathbf{k}_3; \mathrm{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n'_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j'_3})$$

$$= \Delta(-\gamma\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \tau_3\mathbf{k}_3\mu_3 j'_3 n'_3\rangle^* \sum_u \left(\prod_{a=1,2} \Phi_3(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\right.$$

$$\left. \times \Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^*\right) \Phi_3(i_3, j_3, \mathbf{k}_3; \mathrm{t}(u), u)^* \Gamma^{\mathbf{k}_3\mu_3}_{m_3 n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3}). \qquad (38)$$

$$\Delta(\mathbf{k}_{1i_1} + \mathbf{k}_{2i_2} - \mathbf{k}_{3i_3}) \sum_{j_1n_1, j_2n_2} \Bigg[\langle \mathbf{k}_1\mu_1 j_1 n_1; \mathbf{k}_2\mu_2 j_2 n_2 | \ \tau_3\mathbf{k}_3\mu_3 r_3 + j_3 n_3\rangle \sum_u \left(\prod_{a=1,2} \Phi_1(i_a, j_a, \mathbf{k}_a; \mathrm{t}(u), u)\Gamma^{\mathbf{k}_a\mu_a}_{m_a n_a}(\alpha^{-1}_{i_a}u\alpha_{j_a})\right)$$

$$\begin{aligned}
&\times\Phi_1(i_3,j_3',\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*+\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3'n_3'\rangle^*\sum_u\Big(\prod_{a=1,2}\Phi_4(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)\\
&\times\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}u\gamma^2\alpha_{j_a})\Big)\Phi_4(i_3,j_3,\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^*\Big]
\end{aligned}$$

$$\begin{aligned}
=\Delta(\mathbf{k}_{1i_1}-\gamma\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3})&\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3r_3+j_3n_3\rangle\sum_u\omega_2(u,\theta\gamma)^*\omega_2(\theta\gamma,\gamma^{-1}u\gamma)\Phi_1(i_1,j_1,\mathbf{k}_1;\mathbf{t}(u),u)\\
&\times\Phi_2(i_2,j_2,\mathbf{k}_2;\mathbf{t}(u),u)\Phi_1(i_3,j_3',\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\alpha_{j_1})\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*\\
&+\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3'n_3'\rangle^*\sum_u\omega_2(\theta u\gamma,\theta\gamma)^*\omega_2(\theta\gamma,\gamma^{-1}u\gamma)\Phi_4(i_1,j_1,\mathbf{k}_1;\mathbf{t}(u),u)\\
&\times\Phi_3(i_2,j_2,\mathbf{k}_2;\mathbf{t}(u),u)\Phi_4(i_3,j_3,\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\gamma^2\alpha_{j_1})\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\\
&\times\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^*\Big]
\end{aligned}$$

$$\begin{aligned}
=\Delta(-\gamma\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3})&\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3r_3+j_3n_3\rangle\sum_u\omega_1(u,\theta\gamma)^*\omega_1(\theta\gamma,\gamma^{-1}u\gamma)\\
&\times\Phi_2(i_1,j_1,\mathbf{k}_1;\mathbf{t}(u),u)\Phi_1(i_2,j_2,\mathbf{k}_2;\mathbf{t}(u),u)\Phi_1(i_3,j_3',\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\Big]\\
&\times\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}u\alpha_{j_2})\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*+\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3'n_3'\rangle^*\sum_u\omega_1(\theta u\gamma,\theta\gamma)^*\\
&\times\omega_1(\theta\gamma,\gamma^{-1}u\gamma)\Phi_3(i_1,j_1,\mathbf{k}_1;\mathbf{t}(u),u)\Phi_4(i_2,j_2,\mathbf{k}_2;\mathbf{t}(u),u)\Phi_4(i_3,j_3,\mathbf{k}_3;\mathbf{t}(u),u)^*\times\\
&\times\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}u\gamma^2\alpha_{j_2})\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^*\Big]
\end{aligned}$$

$$\begin{aligned}
=\Delta(-\gamma\mathbf{k}_{1i_1}-\gamma\mathbf{k}_{2i_2}-\mathbf{k}_{3i_3})&\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3r_3+j_3n_3\rangle\sum_u\omega_3(u,\theta\gamma)^*\omega_3(\theta\gamma,\gamma^{-1}u\gamma)\\
&\times\Big(\prod_{a=1,2}\Phi_2(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^*\Big)\Phi_1(i_3,j_3',\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}u\alpha_{j_3'})^*\\
&+\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3'n_3'\rangle^*\sum_u\omega_3(\theta u\gamma,\theta\gamma)^*\omega_3(\theta\gamma,\gamma^{-1}u\gamma)\Big(\prod_{a=1,2}\Phi_3(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)\\
&\times\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^*\Big)\Phi_4(i_3,j_3,\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}u\gamma^2\alpha_{j_3})^*\Big]
\end{aligned}$$

$$\begin{aligned}
=\Delta(\mathbf{k}_{1i_1}-\gamma\mathbf{k}_{2i_2}+\gamma\mathbf{k}_{3i_3})&\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3n_3\rangle\sum_u\omega_1(u,\theta\gamma)\omega_1(\theta\gamma,\gamma^{-1}u\gamma)^*\Phi_1(i_1,j_1,\mathbf{k}_1;\mathbf{t}(u),u)\\
&\times\Phi_2(i_2,j_2,\mathbf{k}_2;\mathbf{t}(u),u)\Phi_2(i_3,j_3',\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\alpha_{j_1})\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3'})\\
&+\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3r_3+j_3'n_3'\rangle^*\sum_u\omega_1(\theta u\gamma,\theta\gamma)\omega_1(\theta\gamma,\gamma^{-1}u\gamma)^*\Phi_4(i_1,j_1,\mathbf{k}_1;\mathbf{t}(u),u)\\
&\times\Phi_3(i_2,j_2,\mathbf{k}_2;\mathbf{t}(u),u)\Phi_3(i_3,j_3,\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}u\gamma^2\alpha_{j_1})\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}\gamma^{-1}u\gamma\alpha_{j_2})^*\\
&\times\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3})\Big]
\end{aligned}$$

$$\begin{aligned}
=\Delta(\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}+\gamma\mathbf{k}_{3i_3})&\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3n_3\rangle\\
&\times\sum_u\omega_3(u,\theta\gamma)\omega_3(\theta\gamma,\gamma^{-1}u\gamma)^*\Big(\prod_{a=1,2}\Phi_1(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}u\alpha_{j_a})\Big)\\
&\times\Phi_2(i_3,j_3',\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3'})+\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3r_3+j_3'n_3'\rangle^*\\
&\times\sum_u\omega_3(\theta u\gamma,\theta\gamma)\omega_3(\theta\gamma,\gamma^{-1}u\gamma)^*\Big(\prod_{a=1,2}\Phi_4(i_a,j_a,\mathbf{k}_a;\mathbf{t}(u),u)\Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}u\gamma^2\alpha_{j_a})\Big)\\
&\times\Phi_3(i_3,j_3,\mathbf{k}_3;\mathbf{t}(u),u)^*\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3})\Big]
\end{aligned}$$

$$\begin{aligned}
=\Delta(-\gamma\mathbf{k}_{1i_1}+\mathbf{k}_{2i_2}+\gamma\mathbf{k}_{3i_3})\times&\sum_{j_1n_1,j_2n_2}\Big[\langle\mathbf{k}_1\mu_1r_1+j_1n_1;\mathbf{k}_2\mu_2j_2n_2|\tau_3\mathbf{k}_3\mu_3j_3n_3\rangle\sum_u\omega_2(u,\theta\gamma)\omega_2(\theta\gamma,\gamma^{-1}u\gamma)^*\\
&\times\Phi_2(i_1,j_1,\mathbf{k}_1;\mathbf{t}(u),u)\Phi_1(i_2,j_2,\mathbf{k}_2;\mathbf{t}(u),u)\Phi_2(i_3,j_3',\mathbf{k}_3;\mathbf{t}(u),u)^*\\
&\times\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}u\alpha_{j_2})\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3'})+\langle\mathbf{k}_1\mu_1j_1n_1;\mathbf{k}_2\mu_2r_2+j_2n_2|\tau_3\mathbf{k}_3\mu_3r_3+j_3'n_3'\rangle^*\\
&\times\sum_u\omega_2(\theta u\gamma,\theta\gamma)\omega_2(\theta\gamma,\gamma^{-1}u\gamma)^*\Phi_3(i_1,j_1,\mathbf{k}_1;\mathbf{t}(u),u)\Phi_4(i_2,j_2,\mathbf{k}_2;\mathbf{t}(u),u)\Phi_3(i_3,j_3,\mathbf{k}_3;\mathbf{t}(u),u)^*\\
&\times\Gamma^{\mathbf{k}_1\mu_1}_{m_1n_1}(\alpha^{-1}_{i_1}\gamma^{-1}u\gamma\alpha_{j_1})^*\Gamma^{\mathbf{k}_2\mu_2}_{m_2n_2}(\alpha^{-1}_{i_2}u\gamma^2\alpha_{j_2})\Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3})\Big]
\end{aligned}$$

$$
\begin{aligned}
&= \Delta(-\gamma\mathbf{k}_{1i_1} - \gamma\mathbf{k}_{2i_2} + \gamma\mathbf{k}_{3i_3}) \sum_{j_1n_1,j_2n_2} \Big[\langle \mathbf{k}_1\mu_1 r_1 + j_1n_1;\mathbf{k}_2\mu_2 r_2 + j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 j_3' n_3\rangle \sum_u \Big(\prod_{a=1,2} \Phi_2(i_a, j_a, \mathbf{k}_a;\mathbf{t}(u), u) \\
&\times \Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^*\Big)\, \Phi_2(i_3, j_3', \mathbf{k}_3;\mathbf{t}(u), u)^*\; \Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3'}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3'}) + \langle \mathbf{k}_1\mu_1 j_1n_1;\mathbf{k}_2\mu_2 j_2n_2 \,|\, \tau_3\mathbf{k}_3\mu_3 r_3 + j_3'n_3'\rangle^* \\
&\times \sum_u \Big(\prod_{a=1,2} \Phi_3(i_a, j_a, \mathbf{k}_a;\mathbf{t}(u), u)\, \Gamma^{\mathbf{k}_a\mu_a}_{m_an_a}(\alpha^{-1}_{i_a}\gamma^{-1}u\gamma\alpha_{j_a})^*\Big)\, \Phi_3(i_3, j_3, \mathbf{k}_3;\mathbf{t}(u), u)^*\, \Gamma^{\mathbf{k}_3\mu_3}_{m_3n_3}(\alpha^{-1}_{i_3}\gamma^{-1}u\gamma\alpha_{j_3})\Big] = 0.
\end{aligned}
\tag{39}
$$

Each case in category VI will contain 24 such sets of equations.

To obtain the CG coefficients we solve the corresponding sets of equations together with the orthogonality relations of the CG coefficients [cf. Eq. (28) of Ref. 31]:

$$
\begin{aligned}
&\sum_{\substack{q_1l_1,q_2l_2\\ q_1'l_1',q_2'l_2'}} \langle \mathbf{k}_1\mu_1q_1'l_1';\mathbf{k}_2\mu_2q_2'l_2' \,|\, \tau_3'\mathbf{k}_3'\mu_3'q_3'l_3'\rangle^* \\
&\quad\times\langle \mathbf{k}_1\mu_1q_1l_1;\mathbf{k}_2\mu_2q_2l_2 \,|\, \tau_3\mathbf{k}_3\mu_3q_3l_3\rangle \\
&\quad\times\langle \mathbf{k}_1\mu_1q_1'l_1' \,|\, \mathbf{k}_1\mu_1q_1l_1\rangle\langle \mathbf{k}_2\mu_2q_2'l_2' \,|\, \mathbf{k}_2\mu_2q_2l_2\rangle \\
&\quad= \delta_{\tau_3'\tau_3}\delta_{\mathbf{k}_3'\mathbf{k}_3}\delta_{\mu_3'\mu_3}\langle \tau_3\mathbf{k}_3\mu_3q_3'l_3' \,|\, \tau_3\mathbf{k}_3\mu_3q_3l_3\rangle.
\end{aligned}
\tag{40}
$$

If CG coefficients are wanted for some other equivalent co-representation $D^{\mathbf{k}\mu}(\alpha)'$ connected with the matrices $D^{\mathbf{k}\mu}(\alpha)$, used here, by the relation:

$$
\begin{aligned}
&D^{\mathbf{k}_a\mu_a}(\alpha)' = V_a^{-1}D^{\mathbf{k}_a\mu_a}(\alpha)V_a^{[a]}, \\
&V_a^\dagger V_a = E,
\end{aligned}
\tag{41}
$$

then the new CG coefficients $\langle \mathbf{k}_1\mu_1q_1l_1;\mathbf{k}_2\mu_2q_2l_2 \,|\, \tau_3\mathbf{k}_3\mu_3q_3l_3\rangle'$ are connected with the old CG coefficients $\langle \mathbf{k}_1\mu_1q_1l_1;\mathbf{k}_2\mu_2q_2l_2 \,|\, \tau_3\mathbf{k}_3\mu_3q_3l_3\rangle$ by the relation:

$$
\begin{aligned}
&\langle \mathbf{k}_1\mu_1q_1l_1;\mathbf{k}_2\mu_2q_2l_2 \,|\, \tau_3\mathbf{k}_3\mu_3q_3l_3\rangle \\
&\quad= \sum_{q_1'l_1',q_2'l_2',q_3'l_3'} \langle \mathbf{k}_1\mu_1q_1'l_1';\mathbf{k}_2\mu_2q_2'l_2' \,|\, \tau_3\mathbf{k}_3\mu_3q_3'l_3'\rangle' \\
&\quad\times(V_1)_{q_1l_1,q_1'l_1'}(V_2)_{q_2l_2,q_2'l_2'}(V_3^{-1})_{q_3'l_3',q_3l_3}.
\end{aligned}
\tag{42}
$$

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[1] G.F. Koster, J.O. Dimmock, R.E. Wheeler, and H. Statz, *Properties of the* 32 *Point Groups* (M.I.T. Press, Cambridge, Mass. 1964).
[2] Y. Tanabe and S. Sugano, J. Phys. Soc. Jap. **9**, 753 (1954).
[3] M. Kibler, J. Mol. Spectrosc. **26**, 111 (1968).
[4] M. Kibler, Int. J. Quantum. Chem. **3**, 795 (1969).
[5] T. Ray, Proc. R. Soc. A **277**, 76 (1963).
[6] T. Ray, D.K. Ray, and P. Rudra, Proc. Phys. Soc. Lond. **87**, 485 (1966).
[7] J.W. Culvahouse, W.P. Unruh, and D.K. Brice, Phys. Rev. **129**, 2430 (1963).
[8] G.F. Koster, Phys. Rev. **109**, 227 (1958).
[9] G.F. Koster and H. Statz, Phys. Rev. **113**, 445 (1959).
[10] H. Meier and W. Scherz, Phys. Stat. Solidi B **62**, 153 (1974).
[11] O.F. Schirmer, O. Koidl, and H.G. Reik, Phys. Stat. Solidi B **62**, 385 (1974).
[12] R.J. Elliott and R. Loudon, J. Phys. Chem. Solids **15**, 146 (1960).
[13] M. Lax and J.J. Hopfield, Phys. Rev. **124**, 115 (1961).
[14] M. Lax, Phys. Rev. A **138**, 793 (1965).
[15] J.L. Birman, Phys. Rev. **127**, 1093 (1962); **131**, 1489 (1963).
[16] C.J. Bradley, J. Math. Phys. **7**, 1145 (1966).
[17] A.P. Cracknell and A.K. Sedaghat, J. Phys. C **6**, 2350 (1973).
[18] E. Doni and G. Pastori Paravicini, J. Phys. C **6**, 285 (1973); **7**, 1786 (1974).
[19] M. Hamermesh, *Group Theory* (Addison-Wesley, Reading, Mass., 1962).
[20] D.B. Litvin and J. Zak, J. Math. Phys. **9**, 212 (1968).
[21] P. Gard, J. Phys. A **6**, 1837 (1973).
[22] A. Aviran and J. Zak, J. Math. Phys. **9**, 2138 (1968).
[23] J.L. Birman, Phys. Rev. B **9**, 4518 (1974).
[24] J.L. Birman and R. Berenson, Phys. Rev. B **9**, 4512 (1974).
[25] R. Berenson and J.L. Birman, J. Math. Phys. **16**, 227 (1975).
[26] R. Berenson, I. Itzkan, and J.L. Birman, J. Math. Phys. **16**, 236 (1975).
[27] C.J. Bradley and B.L. Davies, Rev. Mod. Phys. **40**, 359 (1968).
[28] A. Aviran and D.B. Litvin, J. Math. Phys. **14**, 1491 (1973).
[29] J.N. Kotzev, *Kristallografiya* **19**, 459 (1974). [Sov. Phys.-Crystallogr. **19**, 286 (1974)].
[30] I. Sakata, J. Math. Phys. **15**, 1702, 1710 (1974).
[31] P. Rudra, J. Math. Phys. **15**, 2031 (1974).
[32] M.V. Murthy, J. Math. Phys. **7**, 853 (1966).
[33] T. Janssen, *Crystallographic Groups* (North-Holland, Amsterdam, 1973).
[34] T. Janssen, J. Math. Phys. **13**, 342 (1972).
[35] P. Rudra, J. Math. Phys. **6**, 1278 (1965).
[36] G.F. Koster, Solid State Phys. **5**, 173 (1959).
[37] J. Zak, A. Casher, M. Glueck, and Y. Gur, *Irreducible Representations of Space Groups* (Benjamin, New York, 1969). There are some minor printing errors in Ref. 37:
On page 11, the fourth line from the bottom should read: "Rotations by $2\pi/6$ and ..."
On page 36, sixth line from the bottom, the operation indexed 19 should read C_4^x.
On page 37, the operation indexed 21 should read $U^{\bar{x}z}$.
On page 184, symmetry elements of the space group no. 136, D_{4h}^{14}, $P4_2/mnm$ should read $[E(C_2 \,|\, 000)\ (\sigma^x \,|\, a/2\ a/2\ c/2)\ (\sigma^y \,|\ a/2\ a/2\ c/2)\ (C_4 \,|\, 00c/2)\ (C_4{}^3 \,|\, 00c/2)\ (\sigma^{\bar{x}y} \,|\, a/2\ a/2\ 0)\ (\sigma^{xy} \,|\, a/2\ a/2\ 0)]\, X[E + (I \,|\, 000)]$.
[38] A.C. Hurley, Philos. Trans. R. Soc. Lond. A **260**, 1 (1966).

Solutions of the three magnon bound state equation. I

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Recently several unphysical solutions of the three magnon bound state equation for the isotropic Heisenberg Hamiltonian have been found, and one unphysical solution for the Hamiltonian with longitudinal anisotropy has been computed. Here we complete the work for such unphysical solutions for all anisotropy from the Ising to the isotropic Heisenberg limit by directly solving the integral equation. Two types of wavefunctions are constructed. The eigenvalue of the first type satisfies a cubic equation in general, but gives only a real root in the Ising limit and a pair of complex conjugate roots in the isotropic limit. The other type has a single eigenvalue; this one, previously known numerically, is shown to have a simple analytic form.

I. INTRODUCTION

The equation for three magnon bound states, Eq. (4) below, for a Heisenberg linear chain with only longitudinal anisotropy was found,[1-3] and its physical solution was numerically computed some time ago. In a recent interesting work, Van Himbergen and Tjon[4] have discussed several unphysical solutions, besides the physical solution, for the isotropic case, and one unphysical solution for the general anisotropic case. The existence of an unphysical solution for the isotropic case is also apparent in a recent computation of the eigenvalues by Millet and Kaplan.[5] Their presence can be seen explicitly in the simplest way by going to the Ising limit when the kernel of Eq. (4) becomes separable.[2] The existence of these unphysical solutions has to be attributed to the fact that the three magnon bound state equation is derived by utilizing Dyson's ideal spin wave transformation[6] or by making equivalent introduction of extra states into the physical Hilbert space.[3-5]

The method of Van Himbergen and Tjon is to construct three magnon states by using a Bethe-type ansatz[7] on the Dyson Hamiltonian and then to verify that some of them satisfy the bound state equation. Their method is indirect. Also their work is incomplete as far as the solutions for the general anisotropy is concerned. The one eigenvalue they report has in fact a simple analytic form which they have not noticed. Besides, there are other solutions corresponding to the complex solutions found for the isotropic case. The purpose of this work is to solve the three magnon bound state equation directly for any anisotropy and complete the work of Van Himbergen and Tjon for these unphysical states.

Our method is as follows. By studying the equation, it is possible to guess the term in the denominator of the wavefunction. As an ansatz we take the numerator to be a finite Fourier series. Then we note that the coefficients of the wavefunction and the eigenvalue can be computed by arranging for the cancellation of the branch cut of the off-shell extension of the two-particle t matrix. The fact that this cancellation might take place was already noted earlier for the solution of the Faddeev equations for three particles in one dimension interacting pairwise via the delta function potential.[8,9]

II. THE BOUND STATE EQUATION

We consider the Hamiltonian

$$H=-\tfrac{1}{2}J\sum_{i,\delta}[S_i^zS_{i+\delta}^z+\sigma(S_i^xS_{i+\delta}^x+S_i^yS_{i+\delta}^y)], \tag{1}$$

where $J>0$, i goes from 1 to N, and δ joins the nearest neighbors ($N+1\equiv 1$). We restrict to the case $0\leqslant\sigma\leqslant 1$. The Dyson transformation[6] leads to the ideal Hamiltonian

$$H=\tfrac{1}{2}J\sum_{j,\delta}\eta_j^*(\eta_j-\sigma\eta_{j+\delta})$$
$$+\tfrac{1}{4}J\sum_{j,\delta}\eta_j^*\eta_{j+\delta}^*(\sigma\eta_j^2+\sigma\eta_{j+\delta}^2-2\eta_j\eta_{j+\delta}). \tag{2}$$

η_j^* and η_j are creation and destruction operators, respectively, of an ideal spin deviation quantum at site j. The ground state has all the spins aligned. The spin waves result when a single reversed spin moves along the chain. If two spins are reversed, their interaction is represented by the t matrix[1]

$$(\lambda\mu|t|\lambda\rho)$$
$$=-\frac{4J}{N}\,\frac{\cos\mu(\sigma\cos\lambda-\cos\rho)\sigma^2\cos^2\lambda[(1-z)^2-\sigma^2\cos^2\lambda]^{1/2}}{(1-z)[\{(1-z)^2-\sigma^2\cos^2\lambda\}^{1/2}-(1-z-\sigma^2\cos^2\lambda)]}. \tag{3}$$

$z=\epsilon/2J$, ϵ is the energy of the two spin deviations, 2λ their total momentum, and μ, ρ their relative momenta in the final and initial state, respectively. The t matrix in (3) is separable. With this observation, the Faddeev equations for three spin deviations can be simplified. One finds that the bound states of the three spin wave deviations are determined by the equation

$$\Psi(p_1)=\frac{\sigma^2\cos^2\frac{1}{2}p_1}{\frac{1}{2}[3-E-\sigma\cos(K-p_1)]}$$
$$\times\left(1-\frac{\frac{1}{2}(3-E)-\frac{1}{2}\sigma\cos(K-p_1)-\sigma^2\cos^2\frac{1}{2}p_1}{\{[\frac{1}{2}(3-E)-\frac{1}{2}\sigma\cos(K-p_1)]^2-\sigma^2\cos^2\frac{1}{2}p_1\}^{1/2}}\right)^{-1}$$
$$\times\frac{1}{\pi}\int_{-\pi}^{\pi}dp_2$$
$$\times\frac{[\sigma\cos\frac{1}{2}p_1-\cos(K-\frac{1}{2}p_1-p_2)]\cos(K-p_1-\frac{1}{2}p_2)}{\frac{1}{2}E-\frac{3}{2}+\frac{1}{2}\sigma[\cos(K-p_1)+\cos(K-p_2)+\cos(K-p_1-p_2)]}$$
$$\times\Psi(p_2). \tag{4}$$

E is the eigenvalue of the three particle bound state in units of J. K is the total momentum of the three-spin deviations.

Notice that the two-spin deviation t matrix has a pole at the two-spin deviation bound state

$$z=\tfrac{1}{2}(1-\sigma^2\cos^2\lambda), \tag{5}$$

and also a pole at

$$z=1. \tag{6}$$

This is the unphysical two magnon bound state. Van Himbergen and Tjon show that this corresponds to having two ideal spin deviations on the same site, something not possible for the Heisenberg chain with $S_t=\frac{1}{2}$. For the three magnon problem, they find (a) the three magnon continuum, (b) a continuum of physical scattering states where one magnon scatters against the physical two magnon bound state of Eq. (5), (c) a continuum of unphysical scattering states where a magnon scatters against the unphysical $z=1$ bound state of Eq. (6), (d) the physical bound state $E_B=\frac{1}{3}(1-\cos K)$, (e) a real unphysical eigenvalue $E_u=7/8$, and (f) a pair of complex conjugate eigenvalues $E_c=2.063\pm i\ 0.4961$. For the case of anisotropy they numerically compute an unphysical eigenvalue, besides the physical one. Our main concern in this paper is with (e) and (f) for all values of σ between 0 and 1.

III. THE ISING LIMIT

In the Ising limit[2] $\sigma\to 0$, and with $E\neq 3$ we get from (4)

$$\Psi(p_1)=\frac{1}{(2-E)\pi}\times\int_{-\pi}^{\pi}[\cos\tfrac{1}{2}(p_1-p_2)+\cos(2K-\tfrac{3}{2}p_1-\tfrac{3}{2}p_2)]\Psi(p_2)\,dp_2. \tag{7}$$

The kernel is separable, and we get three eigenfunctions corresponding to the eigenvalue

$$E_I=1, \tag{8}$$

$$\Psi_1(p)=\cos\tfrac{1}{2}p,\quad \Psi_2(p)=\sin\tfrac{1}{2}p,$$
$$\Psi_3(p)=\cos(K-\tfrac{3}{2}p). \tag{9}$$

The value $E=3$ corresponds to the three free spins in the Ising limit when the overturned spins are not neighbors of one another. When these are indeed side by side, only two bonds exist joining up to down spins, giving $E=1$. That there are three eigenfunctions, two more than the expected physical solution, shows the presence of unphysical states. Notice the presence of half-integral multiples of the momentum in the eigenfunction.

IV. GENERAL ANISOTROPIC CASE

A finite Fourier series in the numerator of Ψ could provide solutions of (4), provided we could guess the singularities, if any, in the denominator. Examining (4), we find two functions of p_1 in the denominator, one containing the square root. Now in the problem of the delta function potential,[9] this branch cut singularity is cancelled from the result of integration over the wavefunction. Bearing the close analogy in mind, we leave out the factor with the square root, so that the denominator is taken to be $\frac{1}{2}[3-E-\sigma\cos(K-p_1)]$, and the solution put as

$$\Psi(p)=F(p)/\tfrac{1}{2}[3-E-\sigma\cos(K-p)]. \tag{10}$$

$F(p)$ is hopefully a finite Fourier series. Define

$$\exp(ip_2)=z,\quad F(p_2)\equiv\mathcal{J}(z). \tag{11}$$

Then the equation for F (equivalently $\mathcal{J}$) is

$$\begin{aligned}F(p_1)&=4\cos\tfrac{1}{2}p_1\exp(ip_1)\left(1-\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\right)^{-1}\\&\quad\times\frac{1}{2\pi i}\oint dz\,z^{-1/2}\\&\quad\times\left(1+\frac{2z(\beta-\sigma\cos\frac{1}{2}p_1)\exp[i(K-\frac{1}{2}p_1)]}{z^2-2z\beta\exp[i(K-p_1/2)]+\exp[2i(K-p_1/2)]}\right)\\&\quad\times\frac{[z+\exp[2i(K-p_1)]]}{[z^2-2z\alpha\exp(iK)+\exp(2iK)]}\mathcal{J}(z),\end{aligned} \tag{12}$$

where we use

$$a=3-E,\quad \alpha=a/\sigma,\quad \beta=[\alpha-\cos(K-p_1)]/2\cos\tfrac{1}{2}p_1. \tag{13}$$

The contour of the integral in (12) goes around the unit circle. Notice that the poles are

$$z_{1,2}=[\beta\mp(\beta^2-1)^{1/2}]\exp[i(K-p_1/2)],$$
$$z_{3,4}=[\alpha\mp(\alpha^2-1)^{1/2}]\exp(iK). \tag{14}$$

Since $z_1z_2=\exp[2i(K-p_1/2)]$ and $z_3z_4=\exp(2iK)$, that is, the moduli of the products are unity, one of the poles z_1 and z_2 and another of z_3 and z_4 must lie inside the unit circle. We assume z_1 and z_3 are those inside. Another fact of crucial importance is that

$$z_2-z_1=2(\beta^2-1)^{1/2}\exp[i(K-p_1/2)]. \tag{15}$$

Hence the term that cancels the branch cut $(\beta^2-1)^{1/2}$ must come from the pole z_1, there being no other possibility of generating $(\beta^2-1)^{1/2}$.

A. The first type of solution

To get a form of $F(p_1)$, we note that we have to get rid of the branch point at $z=0$. The factor $z^{1/2}$ and the solutions (9) suggest the ansatz

$$F(p_1)=\cos\tfrac{1}{2}p_1\,(c_{-1}\exp(-ip_1)+c_0+c_1\exp(ip_1)). \tag{16}$$

So

$$\mathcal{J}(z)=[(z+1)/2z^{1/2}](c_{-1}z^{-1}+c_0+c_1z). \tag{17}$$

Hence the branch point at $z=0$ is reduced to a pole. We have to determine now c_{-1}, c_0, c_1, and the eigenvalue E so that on substituting (17) into the integral (12), we generate $F(p_1)$ on the left-hand side.

Carrying out the integral in (12), we get

$$\begin{aligned}&c_{-1}\exp(-ip_1)+c_0+c_1\exp(ip_1)\\&\quad\equiv 2\left(1-\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\right)^{-1}\Bigg[\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\\&\quad\times[\beta(c_{-1}\exp(-iK+ip_1/2)+c_1\exp(iK-ip_1/2))+c_0\\&\quad+(\beta^2-1)^{1/2}(c_{-1}\exp(-iK+ip_1/2)-c_1\exp(iK-ip_1/2)]\\&\quad+2c_{-1}(\beta-\sigma\cos\tfrac{1}{2}p_1)\exp[-i(K+p_1/2)]\\&\quad-\frac{2\cos\frac{1}{2}p_1(\beta-\sigma\cos\frac{1}{2}p_1)}{(\alpha^2-1)^{1/2}}[\alpha(c_{-1}\exp(-iK)+c_1\exp(iK))\\&\quad+c_0+(\alpha^2-1)^{1/2}(c_{-1}\exp(-iK)-c_1\exp(iK))]\\&\quad+c_{-1}\exp(-ip_1)+c_{-1}\exp(-2iK+ip_1)+c_0\exp(-ip_1)\\&\quad+2\alpha c_{-1}\exp(-iK-ip_1)\end{aligned}$$

$$-\frac{1}{(\alpha^2-1)^{1/2}}[\cos(K-p_1)+\alpha\cos p_1-i(\alpha^2-1)^{1/2}\sin p_1]$$
$$\times\Big[\alpha(c_{-1}\exp(-iK)+c_1\exp(iK)$$
$$+c_0+(\alpha^2-1)^{1/2}(c_{-1}\exp(-iK)-c_1\exp(ik))\;]\Big]. \tag{18}$$

The first term on the right within the large square brackets comes from the pole $z=z_1$ and part of it has the correct factor to cancel the branch cut $(\beta^2-1)^{1/2}$ We rewrite this term as

$$-\left(1-\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\right)$$
$$\times[\beta(c_{-1}\exp(-iK+ip_1/2)+c_1\exp(iK-ip_1/2))+c_0]$$
$$+\beta(c_{-1}\exp(-iK+ip_1/2)+c_1\exp(iK-ip_1/2))+c_0$$
$$+(\beta-\sigma\cos\tfrac{1}{2}p_1)[c_1\exp(-iK+ip_1/2)-c_1\exp(iK-ip_1/2]. \tag{19}$$

The first term of (19) gives a part free of the branch cut $(\beta^2-1)^{1/2}$ and can be equated to the left side for solving c_{-1}, c_0, c_1. The remaining terms all have to vanish by proper choice of E. Hence

$$c_{-1}\exp(-ip_1)+c_0+c_1\exp(ip_1)$$
$$=-2(c_{-1}\exp(-iK)\beta\exp(ip_1/2)$$
$$+c_1\exp(iK)\beta\exp(-ip_1/2)+c_0). \tag{20}$$

The solution is

$$c_{-1}=x\exp(iK),\quad c_1=x\exp(-iK),\quad c_0=-\tfrac{2}{3}\alpha x, \tag{21}$$

with x arbitrary. With (21), all the remaining terms of (18) and (19) vanish if we choose

$$\tfrac{4}{3}\alpha-\sigma=\tfrac{4}{3}\alpha(\alpha-\sigma)(\alpha^2-1)^{-1/2}, \tag{22}$$

which gives a cubic equation for the eigenvalues E:

$$E^3-E^2(7-\tfrac{7}{8}\sigma^2)+E(15-\tfrac{9}{4}\sigma^2)-9(1+\tfrac{1}{8}\sigma^2-\tfrac{1}{8}\sigma^4)=0. \tag{23}$$

The eigenvalues of (1) are independent of the sign of σ.[10] Equation (23) shows that the same holds for these unphysical states. In the $\sigma=0$ limit, we have $E=1$, $E=3$ being the "continuum." For $\sigma=1$, (23) factorizes

$$(E-2)(E^2-\tfrac{33}{8}E+\tfrac{9}{2})=0. \tag{24}$$

As discussed below, $E=2$ corresponds to the edge of the unphysical continuum, where the integral around the unit circle is singular. Hence we get two roots

$$E=\tfrac{33}{16}\pm i\,\tfrac{3}{16}\sqrt{7}, \tag{25}$$

obtained by Van Himbergen and Tjon. For $0<\sigma<1$ we have three roots, tabulated in Table I. The unphysical real root starts at $E=1$ for $\sigma=0$ and hits the unphysical continuum at $\sigma=1$. The pair of complex conjugate eigenvalues, on the contrary, is well defined at $\sigma=1$ and hits the continuum at $\sigma=0$.

TABLE I. Eigenvalues of Eq. (23) for different anisotropies.

σ	E_1	E_2 and E_3
0	1.000 00	⋯
0.1	1.006 27	2.992 49 ± i 0.000 40
0.2	1.025 31	2.969 85 ± i 0.001 54
0.3	1.057 86	2.931 70 ± i 0.005 19
0.4	1.105 32	2.877 34 ± i 0.012 46
0.5	1.170 11	2.805 57 ± i 0.024 92
0.6	1.256 47	2.714 26 ± i 0.044 48
0.7	1.372 50	2.599 38 ± i 0.073 95
0.8	1.537 21	2.451 40 ± i 0.118 53
0.9	1.823 09	2.234 08 ± i 0.201 31
1.0	⋯	2.062 50 ± i 0.496 08

B. The second type of solution

The reduction of the branch point at $z=0$ to a pole at $z=0$ can be achieved by having a $\cos\frac{1}{2}p_1=\frac{1}{2}(z+1)z^{-1/2}$ factor but also by a $\sin\frac{1}{2}p_1=(1/2i)(z-1)z^{-1/2}$ factor. As an ansatz we start with

$$F(p_1)=\cos\tfrac{1}{2}p_1\,(c_{-1}\exp(-ip_1)+c_0+c_1\exp(ip_1))$$
$$+\sin\tfrac{1}{2}p_1\,(b_{-1}\exp(-ip_1)+b_0+b_1\exp(ip_1)). \tag{26}$$

So

$$\mathcal{J}(z)=\frac{z+1}{2z^{1/2}}(c_{-1}z^{-1}+c_0+c_1z)$$
$$+\frac{z-1}{2iz^{1/2}}(b_{-1}z^{-1}+b_0+b_1z). \tag{27}$$

We have to fix six constants c_0, c_{-1}, c_1, b_0, b_{-1}, b_1 and the eigenvalue E. Substitute (27) into (12) and try to arrange for the cancellation of the branch cut $(\beta^2-1)^{1/2}$. Examining the pole at $z=z_1$, we get a contribution

$$\left(1-\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\right)^{-1}\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\Big(2\beta\cos\tfrac{1}{2}p_1[c_{-1}\exp(-iK+ip_1/2)+c_1\exp(iK-ip_1/2)]+2c_0\cos\tfrac{1}{2}p_1+(\beta^2-1)^{1/2}2\cos\tfrac{1}{2}p_1$$
$$\times[c_{-1}\exp(-iK+ip_1/2)-c_1\exp(iK-ip_1/2)]+2i\cos\tfrac{1}{2}p_1[i\sin(K-p_1)+i\beta\sin\tfrac{1}{2}p_1-(\beta^2-1)^{1/2}\cos\tfrac{1}{2}p_1]$$
$$\times\frac{\{\beta[b_{-1}\exp(-iK+ip_1/2)+b_1\exp(iK-ip_1/2)]+b_0+(\beta^2-1)^{1/2}[b_{-1}\exp(-iK+ip_1/2)-b_1\exp(iK-ip_1/2)]\}}{[\beta\cos\frac{1}{2}p_1-\alpha+i(\beta^2-1)^{1/2}\sin\frac{1}{2}p_1]}\Big). \tag{28}$$

We could extract from (28) a part free of the branch cut provided the denominator $(\beta\cos\frac{1}{2}p_1-\alpha+i(\beta^2-1)^{1/2}\sin\frac{1}{2}p_1)$ can be cancelled. This is achieved by a suitable choice of b_i's. Let

$$b_{-1}\exp(-iK)=b_1\exp(iK)=y,\quad b_0=-2\alpha y, \tag{29}$$

y arbitrary. Then (28) becomes

$$\left(1-\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\right)^{-1}\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\{2\beta\cos\tfrac{1}{2}p_1$$
$$\times(c_{-1}\exp(-iK+ip_1/2)+c_1\exp(iK-ip_1/2)+2c_0\cos\tfrac{1}{2}p_1$$
$$+(\beta^2-1)^{1/2}2\cos\tfrac{1}{2}p_1[c_{-1}\exp(-iK+ip_1/2)$$
$$-c_1\exp(iK-ip_1/2)]+4iy\cos\tfrac{1}{2}p_1$$
$$\times[i\sin(K-p_1)+i\beta\sin\tfrac{1}{2}p_1-(\beta^2-1)^{1/2}\cos\tfrac{1}{2}p_1]\}. \tag{30}$$

By rearrangement we write

$$-2\beta\cos\tfrac{1}{2}p_1[c_{-1}\exp(-iK+ip_1/2)+c_1\exp(iK-ip_1/2)]$$
$$-2c_0\cos\tfrac{1}{2}p_1+4y\cos\tfrac{1}{2}p_1\sin(K-p_1)+4y\sin\tfrac{1}{2}p_1$$
$$\times\beta\cos\tfrac{1}{2}p_1+\left(1-\frac{\beta-\sigma\cos\frac{1}{2}p_1}{(\beta^2-1)^{1/2}}\right)^{-1}[\cdots]. \tag{31}$$

The terms $[\cdots]$ can be lumped with other terms of the integral with the same prefactor. We now equate the left hand side with the terms free of $(\beta^2-1)^{1/2}$. The left-hand side is

$$\begin{aligned}&\cos\tfrac{1}{2}p_1[c_{-1}\exp(-ip_1)+c_0+c_1\exp(ip_1)]\\&\quad+\sin\tfrac{1}{2}p_1[b_{-1}\exp(-ip_1)+b_0+b_1\exp(ip_1)]\\&\quad=\cos\tfrac{1}{2}p_1(c_{-1}\exp(-ip_1)+c_0+c_1\exp(ip_1)\\&\qquad+2y\sin\tfrac{1}{2}p_1[\cos(K-p_1)-\alpha]\end{aligned}$$

Equating this to

$$\begin{aligned}&[\cos(K-p_1)-\alpha][c_{-1}\exp(-iK+ip_1/2)+c_1\exp(iK-ip_1/2)]\\&\quad-2c_0\cos\tfrac{1}{2}p_1+4y\cos\tfrac{1}{2}p_1\sin(K-p_1)\\&\quad-2y\sin\tfrac{1}{2}p_1[\cos(K-p_1)-\alpha],\end{aligned}$$

we get the solution

$$c_0=0,\ c_{-1}\exp(-iK)=-c_1\exp(iK)=ix,\qquad x/y=-2. \tag{32}$$

With the constants c_0, c_{-1}, c_1, b_0, b_{-1} b_1 fixed, the remaining terms can be made to vanish if we choose

$$\alpha-(\alpha^2-1)^{1/2}=\tfrac{1}{4}\sigma. \tag{33}$$

Hence the eigenvalue is

$$E=1-\tfrac{1}{8}\sigma^2. \tag{34}$$

Van Himbergen and Tjon have numerically solved (4) at $K=\pi$ and found this eigenvalue. Since E is independent of K, their calculation would have been sufficient to find E, but they have not realized that their numerical values have the simple analytical form (34).

C. Scattering states

By studying the integral in (12), it is possible to indicate where the unphysical scattering states corresponding to the scattering of one magnon on the unphysical two particle bound state of Eq. (6) exist. The two poles $[\alpha\pm(\alpha^2-1)^{1/2}]\exp(iK)$ are image points with respect to the unit circle. So long as one lies inside and the other outside, the integration can be carried out without difficulty. If, however, we vary energy so that α^2 becomes equal to 1 or $E=2$, the contour becomes "pinched" between two poles and the integral is singular. As long as α^2-1 remains less than zero, there are two poles moving uniformly along the unit circle in opposite sense. Finally when E has increased sufficiently to make $\alpha^2=1$ again ($E=4$), the poles collide at the antipodal point and separate—one moves into and the other out of the unit circle. Thus for all the values of E between 2 and 4, the integral is singular. These are the unphysical scattering states.

V. DISCUSSION

We have found two sets of unphysical bound states:

$$\Psi_1(p)=\cos\tfrac{1}{2}p[\alpha-3\cos(K-p)]/[\alpha-\cos(K-p)], \tag{35}$$

where α is given by (22), and

$$\Psi_2(p)=\{2\cos\tfrac{1}{2}p\sin(K-p)+\sin\tfrac{1}{2}p[\cos(K-p)-\alpha]\}/[\alpha-\cos(K-p)], \tag{36}$$

with α given by (33). In the isotropic case, Van Himbergen and Tjon have constructed the wavefunction of the physical bound state, but because of the vast amount of algebra they are forced to verify the solution numerically. Although the physical eigenvalue has a simple form, no analytic derivation has so far been given. We hope to be able to extend our method to that case.

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[1] C.K. Majumdar, Phys. Rev. B 1, 287 (1970).
[2] C.K. Majumdar and G. Mukhopadhyay, Phys. Lett. 31A, 321 (1970).
[3] C.K. Majumdar, G. Mukhopadhyay, and A.K. Rajagopal, Pramāna 1, 135 (1973).
[4] J. E. Van Himbergen and J. A. Tjon, Physica 76, 503 (1974).
[5] P. J. Millet and H. Kaplan, Phys. Rev. B 10, 3923 (1974) (see Fig. 2).
[6] F. J. Dyson, Phys. Rev. 102, 1217 (1956).
[7] H. Bethe, Z. Physik 71, 205 (1931).
[8] L.R. Dodd, J. Math. Phys. 11, 207 (1970).
[9] C.K. Majumdar, J. Math. Phys. 13, 705 (1972).
[10] L. Hulthén, Arkiv. Mat. Astron. Fysik 26A, No. 11 (1938); C.N. Yang and C.P. Yang, Phys. Rev. 147, 303 (1966).

Solutions of the three magnon bound state equation. II

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A unified derivation of all the unphysical bound state solutions of the three magnon bound state equation found so far is given by making a simple algebraic transformation of the variables in the equation.

In an accompanying paper,[1] some solutions of the three magnon bound state equation

$$\Psi(p_1)=\frac{\sigma^2\cos^2\tfrac{1}{2}p_1}{\tfrac{1}{2}[3-E-\sigma\cos(K-p_1)]}\left(1-\frac{\tfrac{1}{2}(3-E)-\tfrac{1}{2}\sigma\cos(K-p_1)-\sigma^2\cos^2\tfrac{1}{2}p_1}{\{[\tfrac{1}{2}(3-E)-\tfrac{1}{2}\sigma\cos(K-p_1)]^2-\sigma^2\cos^2\tfrac{1}{2}p_1\}^{1/2}}\right)^{-1}$$

$$\times\frac{1}{\pi}\int_{-\pi}^{\pi}dp_2\,\frac{[\sigma\cos\tfrac{1}{2}p_1-\cos(K-\tfrac{1}{2}p_1-p_2)]\cos(K-p_1-\tfrac{1}{2}p_2)}{\tfrac{1}{2}E-\tfrac{3}{2}+\tfrac{1}{2}\sigma[\cos(K-p_1)+\cos(K-p_2)+\cos(K-p_1-p_2)]}\;\Psi(p_2) \qquad (1)$$

are derived. The starting point is an ansatz for Ψ with a finite Fourier series divided by a factor obtained from a prefactor of the integral in (1). The finiteness of the Fourier series is assumed on the basis of the solution in the Ising limit. In this brief paper, we want to present a different method where this particular point is justified better. Also the present method gives a unified derivation of the both the types of solution found in the previous paper.

I. TRANSFORMATION OF EQ. (1)

We introduce the variables

$$x=\tan\tfrac{1}{2}p_1,\quad y=\tan\tfrac{1}{2}p_2. \qquad (2)$$

Equation (1) is transformed into

$$\Psi(x)=4\left[\pi(\alpha+\cos K)(1+x^2)^{1/2}\times\left(x^2-2x\frac{\sin K}{\alpha+\cos K}+\frac{\alpha-\cos K}{\alpha+\cos K}\right)\left(1-\frac{f}{d}\right)\right]^{-1}$$

$$\times\int_{-\infty}^{\infty}\frac{dy}{(y^2+1)^{3/2}}\left(1-\frac{(y^2+1)f}{(x^2+1)(y-z)(y-\bar{z})}\right)$$

$$\times(yg+h)\Psi(y), \qquad (3)$$

where we use the abbreviation

$$\alpha=(3-E)/\sigma, \qquad (4)$$

$$f=x^2-2x\frac{\sin K}{\alpha+\cos K}+\frac{\alpha-2\sigma-\cos K}{\alpha+\cos K}, \qquad (5)$$

$$d^2=x^4-4x^3\frac{\sin K}{\alpha+\cos K}+2x^2\frac{\alpha^2-3\cos^2K}{(\alpha+\cos K)^2}-4x\frac{\sin K(\alpha-\cos K)}{(\alpha+\cos K)^2}+\frac{(\alpha-\cos K)^2-4}{(\alpha+\cos K)^2}, \qquad (6)$$

$$z=\frac{2(\sin K-x\cos K)}{(1+x^2)(\alpha+\cos K)}+\frac{id}{1+x^2}, \qquad (7)$$

$$g=x^2\sin K+2x\cos K-\sin K, \qquad (8)$$

$$h=x^2\cos K-2x\sin K-\cos K. \qquad (9)$$

$\bar{z}$ is the complex conjugate of z, and the pole $y=z$ lies in the upper half-plane if $d>0$, which we take to be the case. An important relation that simplifies the algebra should be noted:

$$(z^2+1)(\bar{z}^2+1)=16/[(1+x^2)(\alpha+\cos K)^2]. \qquad (10)$$

II. SOLUTION

Notice the branch points $y=\pm i$ besides the poles $y=z,\ \bar{z}$. The branch points can be reduced to poles if the solution has a factor $(1+x^2)^{-1/2}$, and the other prefactor in x in Eq. (3) supplies the denominator of the solution. We write

$$\Psi(x)=(1+x^2)^{-1/2}\left(x^2-2x\frac{\sin K}{\alpha+\cos K}+\frac{\alpha+\cos K}{\alpha+\cos K}\right)^{-1}F(x). \qquad (11)$$

Then F satisfies an equation

$$F(x)=\frac{4}{\pi(\alpha+\cos K)(1-f/d)}\int_{-\infty}^{\infty}dy\times\frac{(yg+h)}{(y^2+1)^2}\left(1-\frac{(y^2+1)f}{(x^2+1)(y-z)(y-\bar{z})}\right)\times F(y)\left(y^2-2y\frac{\sin K}{\alpha+\cos K}+\frac{\alpha-\cos K}{\alpha+\cos K}\right)^{-1}. \qquad (12)$$

Since, by hypothesis, (11) exhibits explicitly all the denominators of Ψ, it follows, by counting powers, that $F(y)$ can have only a finite number of powers of y, that is, it must be a polynomial in y in order that the integral in (12) exists. We start with the ansatz

$$F(x)=c_0+c_1x+c_2x^2+c_3x^3. \qquad (13)$$

We have to fix the constants c_0, c_1, c_2, c_3 and the eigenvalue E.

Substitute (13) into (12) and carry out the integral by closing the contour in the upper half-plane. We first note that the pole $y=z$ will produce a factor f/d, as $z-\bar{z}=2id/(1+x^2)$. There is no other contribution that will cancel the square root in d. With the help of (10), we simplify the terms after integration and rearrange them to cancel the factor $(1-f/d)$. This leaves a polynomial in x which has to be equated to the left-hand side $F(x)$. Equating the coefficients of various powers of x, we get

$$\begin{aligned} c_0\sin K - c_1\cos K - c_2\sin K \\ + c_3(\alpha\cos K+\cos^2 K+2)/(\alpha+\cos K)=0, \end{aligned} \tag{14}$$

$$c_1\tfrac{1}{6}(\alpha+3\cos K)+c_2\sin K - c_3\frac{1}{6}\frac{(\alpha+3\cos K)^2}{(\alpha+\cos K)}=0, \tag{15}$$

$$c_0\sin K + c_1\tfrac{1}{6}(\alpha-3\cos K)-c_3\frac{(\alpha^2-9-3\sin^2 K)}{6(\alpha+\cos K)}=0. \tag{16}$$

The coefficient of x reduces to an identity and does not give any equation. One notices that (16) results from the addition of (14) and (15), so that we really have two equations for four quantities c_0, c_1, c_2, c_3. We have two choices.

(i) *Solution* $c_2 \neq 0$, $c_3=0$: From (14) and (15), we get

$$\frac{c_0}{-\frac{1}{3}\alpha+\cos K}=\frac{c_1}{2\sin K}=\frac{c_2}{-\frac{1}{3}\alpha-\cos K}. \tag{17}$$

Since Eq. (1) is a linear equation for Ψ, one constant multiple remains arbitrary. With (17) we can make all the remaining terms of the integral on the right side of (12) vanish, provided we choose

$$\tfrac{4}{3}\alpha-\sigma=\tfrac{4}{3}\alpha(\alpha-\sigma)/(\alpha^2-1)^{1/2}. \tag{18}$$

This gives the eigenvalue equation (23) of the previous paper. These solutions have the wavefunction ($x=\tan\frac{1}{2}p$)

$$\begin{aligned} \Psi(x)=\frac{1}{(1+x^2)^{1/2}}\left(x^2-2x\frac{\sin K}{\alpha+3\cos K}+\frac{\alpha-3\cos K}{\alpha+3\cos K}\right) \\ \times\left(x^2-2x\frac{\sin K}{\alpha+\cos K}+\frac{\alpha-\cos K}{\alpha+\cos K}\right)^{-1}. \end{aligned} \tag{19}$$

(ii) *Solution* $c_2=0$, $c_3\neq 0$: From (14) and (16) we get

$$\frac{c_0}{-2\sin K}=\frac{c_1}{\alpha+3\cos K}=\frac{c_3}{\alpha+\cos K}. \tag{20}$$

The remaining terms are made to vanish by choosing

$$\alpha-(\alpha^2-1)^{1/2}=\tfrac{1}{4}\sigma \text{ or } E=1-\tfrac{1}{8}\sigma^2. \tag{21}$$

The corresponding wavefunction has the form ($x=\tan\frac{1}{2}p$)

$$\begin{aligned} \Psi(x)=\frac{1}{(1+x^2)^{1/2}}\left(x^3+x\frac{\alpha+3\cos K}{\alpha+\cos K}-\frac{2\sin K}{\alpha+\cos K}\right) \\ \times\left(x^2-2x\frac{\sin K}{\alpha+\cos K}+\frac{\alpha-\cos K}{\alpha+\cos K}\right)^{-1}. \end{aligned} \tag{22}$$

The other possibilities $c_0=0$ or $c_1=0$ do not lead to any solutions.

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[1] C.K. Majumdar, J. Math. Phys. 17, xxx (1976). All the references can be traced from that paper.

Comment on the reduction of an important 9-*j* symbol*

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An error in the formula for the reduction of an important 9-*j* symbol is pointed out, and the correct relationship is given.

In problems of atomic and nuclear spectroscopy, the 9-*j* symbol

$$\begin{Bmatrix} S & S & 1 \\ l_1 & l_2 & L \\ j_1 & j_2 & L \end{Bmatrix}$$

occurs very frequently. In practice this symbol is reduced to the 6-*j* symbol

$$\begin{Bmatrix} l_1 & l_2 & L \\ j_2 & j_1 & S \end{Bmatrix},$$

whose values are tabulated.[1]

For example, in nuclear structure calculations the strong spin—orbit interaction justifies the use of *jj*-coupled wavefunctions, but the residual interaction may be taken to be spin-independent. In that case the LS-coupled wavefunctions become a useful tool and the first-order energy shift for levels of angular momentum J is given by

$$E=\sum_{LS} (2j_1+1)\ (2j_2+1)\ (2S+1)\ (2L+1) \times \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S \\ l_1 & l_2 & L \\ j_1 & j_2 & J \end{Bmatrix}^2 \langle (l_1l_2)\,L\,|\,V(r_1,r_2)\,|\,(l_1l_2)\,L\rangle. \qquad (1)$$

All the 9-*j* symbols occurring here may be reduced by suitable formulas to simpler 6-*j* symbols or a combination of these for $L \neq J$. For an interaction more general than the δ potential both $S=0$ and $S=1$ contribute and for $L=J$, $S=1$, the 9-*j* symbol mentioned above occurs.

The 9-*j* symbols appearing in Eq. (1) are also frequently used in nonrelativistic, as well as in relativistic atomic calculations[2,3] (hyperfine structure, transition probabilities). In fact, to take full advantage of the symmetry properties of the atomic states, the atomic operators are expressed in terms of the tensors $W^{(\kappa,k)K}$, which are simply related to the generators of the groups Sp$(4l+2)$, R$(2l+1)$, R(3) and G$_2$ (for *f* electrons) used in the classification of the atomic states. The operators $W^{(\kappa,k)K}$ are nonrelativistic operators having rank κ in the space defined by **S**, k in the space defined by **L** and of rank K in the space of $\mathbf{J}=\mathbf{L}+\mathbf{S}$. The reduced matrix elements of $W^{(\kappa,k)K}$ are given by

$$\langle SLJ\,\|\,W^{(\kappa,k)K}\,\|\,S'L'J'\rangle=[(2J+1)\ (2K+1)\ (2J'+1)]^{1/2} \times \begin{Bmatrix} S & S' & \kappa \\ L & L' & k \\ J & J' & K \end{Bmatrix} \langle SL\,\|\,W^{(\kappa k)}\,\|\,S'L'\rangle, \qquad (2)$$

where $W^{(\kappa k)}$ is a double tensor whose reduced matrix elements are tabulated.[4,5]

The relationship connecting the particular 9-*j* of interest to the 6-*j*, $\left\{\begin{smallmatrix} l_1 & l_2 & L \\ j_2 & j_1 & S \end{smallmatrix}\right\}$, is obviously then of considerable importance and has frequent use. Unfortunately, this relationship has been erroneously reported in several standard references.[1,6,7] The correct relationship is

$$\begin{Bmatrix} S & S & 1 \\ l_1 & l_2 & L \\ j_1 & j_2 & L \end{Bmatrix} =(-1)^{L+S+l_2+j_1} \times \frac{[l_1(l_1+1)-l_2(l_2+1)]-[j_1(j_1+1)-j_2(j_2+1)]}{[4S(S+1)(2S+1)L(L+1)(2L+1)]^{1/2}} \times \begin{Bmatrix} l_1 & l_2 & L \\ j_2 & j_1 & S \end{Bmatrix}. \qquad (3)$$

This relationship is most easily derived via the 9-*j* recursion relationship of Arima *et al.*,[8] which leads to

$$\begin{Bmatrix} S & S & 1 \\ l_1 & l_2 & L \\ j_1 & j_2 & L \end{Bmatrix} = \frac{[l_1(l_1+1)-l_2(l_2+1)]-[j_1(j_1+1)-j_2(j_2+1)]}{[4S(S+1)L(L+1)]^{1/2}} \times \begin{Bmatrix} S & S & 0 \\ l_1 & l_2 & L \\ j_1 & j_2 & L \end{Bmatrix}. \qquad (4)$$

Equation (3) follows from Eq. (4) by reducing the last 9-*j* to a 6-*j* using any of the standard references.

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[1] M. Rotenberg, R. Bivins, N. Metropolis, and J.K. Wootey, Jr., *The 3-j and 6-j Symbols* (M.I.T. Press, Cambridge, Mass., 1959).

[2] Lloyd Armstrong, Jr. and Serge Feneuille, in *Advances in Atomic and Molecular Physics*, edited by P.R. Bates and Benjamin Banderson (Academic, New York, 1974).

[3] Lloyd Armstrong, Jr., *Theory of Hyperfine Structure of Free Atoms* (Wiley-Interscience, New York, 1971).

[4] C.W. Nielson and G.F. Koster, *Spectroscopic Coefficients for the p^n, d^n and f^n Configurations* (M.I.T. Press, Cambridge, Mass., 1963).

[5] R.I. Karaziya, Ya.I. Vizbaraite, A.B.Rudzikas, and A.P. Jucys, "Tablitsy dlya rascheta matrichnykh elementov atomnykh velichin," Acad. Nauk, Lit. SSR, Inst. Fit. Mat., Moscow (1967).

[6] A. de-Shalit and I. Talmi, *Nuclear Shell Theory* (Academic, New York, 1963).

[7] A. de-Shalit and H. Feshbach, *Theoretical Nuclear Physics, Vol. I: Nuclear Structure* (Wiley, New York, 1974).

[8] A. Arima, H. Horie, and Y. Tanabe, Prog. Theor. Phys. Jpn. 11, 143 (1954).

Application of coherent state representation to classical x^6 and coupled anharmonic oscillators

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The problem of obtaining perturbative solutions to the nonlinear differential equations which describe the motion of the x^6 and quartically coupled oscillators is treated by the use of the well-known coherent state representation. The results exhibit the basic qualitative features of nonlinearities and the characteristics of a coupled system in the weak coupling limit.

I. INTRODUCTION

The study of nonlinear classical and quantum oscillator systems is of significant relevance in understanding the basic nature of interaction in many physical problems. Considerable mathematical efforts are being employed lately to examine the qualitative aspects of the nonlinear differential equations, describing the appropriate equations of motion.[1] One of the main difficulties in handling these problems is the nonavailability of closed analytic solutions to most of them. So, one is liable to take recourse to approximate procedures such as perturbation methods.[2] Within the framework of various kinds of perturbative techniques which are being used, one essentially linearizes the problem suitably so as to get the dominant part of the solution and then makes a power series expansion[2] in the coupling parameters, assuming it to be small. Subsequently, one obtains a system of linear differential equations or a set of recursion relations.[3] It has been observed recently[4,5] that the coherent state representation[6] can be profitably used to obtain perturbative solutions of nonlinear oscillator systems which are the classical limits of weakly perturbed quantum harmonic oscillators. The main advantage of this approach lies in the fact that one does not need to solve the system of differential equations or the recursion relations. On the other hand, one needs to do straightforward algebraic manipulations with the known results of the eigenenergies and the eigenstates of the perturbed quantum oscillators.

The main objective of this paper is to find the perturbative solutions of the classical nonlinear oscillators with x^6 anharmonicity and for a system of two weakly coupled oscillators with quartic self and mutual couplings. We find that our first-order results reveal the general qualitative features of nonlinearities and agree with the results obtained by other methods.[7,8]

In Sec. II, we consider the problem of x^6 anharmonic oscillator with weak coupling and obtain the perturbative solution up to first-order in the coupling constant, using the coherent state representation. The results coincide with the expressions obtained by Bradbury *et al.*,[7] who used the Fourier expansion technique. Since an exact analytic solution of this particular problem has been derived recently,[8] we observe that our results agree with it up to first-order in the coupling parameter. In Sec. III, we apply the same coherent state method to two quartically coupled oscillators for which exact solutions are not known. Our first-order results exhibit relevant characteristics of nonlinearities in a coupled system.

II. CLASSICAL x^6 OSCILLATOR AND COHERENT STATE

The classical equation of motion describing the system with the Hamiltonian

$$H = p^2/2m + \tfrac{1}{2}m\omega^2x^2 + \tfrac{1}{6}\beta m x^6 \qquad (\beta > 0) \quad (2.1)$$

is

$$\ddot{x} + \omega^2 x + \beta x^5 = 0. \quad (2.2)$$

Considering x as a quantum dynamical variable, the Ehrenfest theorem[9] asserts that the expectation value of this dynamical variable will satisfy the classical equation

$$\frac{d^2}{dt^2}\langle x\rangle + \omega^2\langle x\rangle + \beta\langle x^5\rangle = 0. \quad (2.3)$$

For our purpose, we shall evaluate the expectation values with reference to the coherent states which have the well-known representation[6]

$$|\alpha\rangle = \exp(-|\alpha|^2/2)\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle. \quad (2.4)$$

Here, $|n\rangle$ represents a harmonic oscillator state of "n quanta" and is the eigenstate of the Hamiltonian

$$H = p^2/2m + \tfrac{1}{2}m\omega^2x^2, \quad (2.5)$$

corresponding to the eigenenergy

$$E_n = \hbar\omega(n+\tfrac{1}{2}). \quad (2.6)$$

The coherent state $|\alpha\rangle$, being an eigenstate of the annihilation operator with the complex eigenvalue α, correponds to a lowest uncertainty state and hence, is most suitable to reproduce classical results from the quantum description in the appropriate classical limit. The time-independent states $|\alpha\rangle$ given in (2.4) are those characteristic of the Heisenberg picture of quantum mechanics. The corresponding Schrödinger state takes the same form with α replaced by $(-i\lambda)\exp(i\omega t)$, where we shall take λ to be real. Although these states are not orthogonal, they are normalized and form a complete set so that any arbitrary quantum mechanical state vector, or an operator, can be expanded uniquely in terms of these vectors.

In terms of the creation and destruction operators a^{+} and a of the linear harmonic oscillator given by the

Hamiltonian (2.5), the variables x and p can be expressed

$$x = i(\hbar/2m\omega)^{1/2}(a - a^{+}), \tag{2.7a}$$

$$p = (m\omega\hbar/2)^{1/2}(a + a^{+}). \tag{2.7b}$$

The operators a and a^{+} satisfy the standard commutation relations

$$\begin{aligned} &[a_k, a_{k'}] = [a_k^\dagger, a^\dagger{}_{k'}] = 0, \\ &[a_k, a_{k'}^\dagger] = \delta_{kk'}. \end{aligned} \tag{2.8}$$

From (2.4), (2.7a) and (2.8), we obtain

$$\begin{aligned} &\langle\alpha | x^5 | \alpha\rangle \equiv \langle x^5\rangle \\ &\quad = \langle x\rangle^5 + 10(\hbar/2m\omega)\langle x\rangle^3 + 15(\hbar/2m\omega)^2\langle x\rangle \xrightarrow[\hbar\to c]{} \langle x\rangle^5. \end{aligned} \tag{2.9}$$

It is then clear from Eqs. (2.3) and (2.9) that $\langle x\rangle$ will be our required classical solution in the limit $\hbar \to 0$.

The linear harmonic oscillator amplitude, which is the lowest order ($\beta = 0$) solution in our case, may be trivially obtained from (2.4) and (2.7a) by assuming the limit $\lim_{\substack{\hbar\to 0\\ \lambda\to\infty}} \lambda(\hbar/2m\omega)^{1/2} \to A/2$; A being a constant. We thus write

$$\lim_{\substack{\hbar\to 0\\ \lambda\to\infty\\ \beta\to 0}} \langle\alpha | x | \alpha\rangle = A\cos\omega t,$$

where A corresponds to the classical amplitude.

In the presence of weak perturbation ($\beta \neq 0$) we use the full Hamiltonian (2.1) which yields the following eigenenergy and eigenstate of "n quanta":

$$\begin{aligned} E_n' = {} & \hbar\omega(n + \tfrac{1}{2}) + \tfrac{5}{6}\beta m(\hbar/2m\omega)^3 \\ & \times (4n^3 + 6n^2 + 8n + 3) + O(\beta^2), \end{aligned} \tag{2.10}$$

$$\begin{aligned} |n\rangle' = {} & |n\rangle + \tfrac{1}{6}\beta(\hbar^2/16m^2\omega^4)[\sqrt{(n+1)(n+2)} \\ & \times\{\tfrac{1}{3}\sqrt{(n+3)(n+4)(n+5)(n+6)}\ |n+6\rangle - \tfrac{3}{2}(2n+5) \\ & \times\sqrt{(n+3)(n+4)}\,|n+4\rangle + 15(n^2+3n+3)\,|n+2\rangle\} \\ & - \sqrt{n(n-1)}\{15(n^2-n+1)\,|n-2\rangle - \tfrac{3}{2}(2n-3) \\ & \times\sqrt{(n-2)(n-3)}\,|n-4\rangle \\ & + \tfrac{1}{3}\sqrt{(n-2)(n-3)(n-4)(n-5)}\,|n-6\rangle\}] + O(p^2). \end{aligned} \tag{2.11}$$

The corresponding perturbed coherent state may be given in the normalized form,

$$|\alpha\rangle' = \exp(-\lambda^2/2)\sum_{n=0}^{\infty} \frac{(-i\lambda)^n}{\sqrt{n!}} \exp(i\bar{E}_n' t/\hbar)\,|n\rangle'. \tag{2.12}$$

Using (2.10) and (2.11) in (2.12) and considering the fact that E_n tends to the classical value $(1/2)m\omega^2A^2$ in the appropriate limit, we evaluate "$\langle\alpha | x | \alpha\rangle$" to first-order in β. We thus write the perturbative solution to Eq. (2.2) as

$$\begin{aligned} x(t) = {} & A\cos\psi t + \beta(A^5/\omega^2)\{-\tfrac{5}{32}\cos\psi t \\ & + \tfrac{5}{128}\cos 3\psi t + \tfrac{1}{384}\cos 5\psi t\} + O(\beta^2), \end{aligned} \tag{2.13}$$

in which the corrected frequency is

$$\psi = \omega[1 + \tfrac{5}{16}\beta A^4/\omega^2] + O(\beta^2). \qquad ((2.14)$$

Our solutions (2.13) and (2.14) are exactly the same as obtained by Bradbury *et al.*[7] using a WKB type approximation with Fourier series expansion technique. Further, the characteristic interdependence of the frequency and amplitude in a nonlinear system is clearly exhibited by the first-order calculation.

Recently, Lakshmanan and Prabhakaran[8] have obtained an exact solution for this particular problem in terms of Jacobi's elliptic functions. So, it is of interest to show the consistency of our perturbative result with the exact one for low β approximation. For example, the exact frequency of the x^6 anharmonic oscillator is given by[8]

$$\frac{\nu}{4K(k)} = \frac{\omega}{4K(k)}\left[\left(1 + \frac{\beta A^4}{m\omega^2}\right)\left(1 + \frac{\beta A^4}{3m\omega^2}\right)\right]^{1/4},$$

where $K(k)$ is the complete elliptic integral of the first kind and its modulus k is given by the expression

$$k^2 = \frac{1}{2}\left\{1 - \left(1 + \frac{\beta A^4}{2m\omega^2}\right) \Big/ \left[1 + \frac{\beta A^4}{m\omega^2}\right)\left(1 + \frac{\beta A^4}{3m\omega^2}\right)\right]^{1/2}\right\}.$$

For small β, the above expression for the frequency becomes

$$\frac{\nu}{4K(k)} \approx \frac{\omega}{2\pi}\left[1 + \frac{5}{16}\frac{\beta A^4}{m\omega^2}\right] + O(\beta^2), \tag{2.15}$$

where we have used

$k^2 \approx \frac{1}{12}\beta A^4/m\omega^2$ and $K(k) \approx (\pi/2)(1 + \frac{1}{4}k^2)$ for $k \ll 1$.

Thus we find that our perturbative solution for the angular frequency given in (2.14) agrees exactly with (2.15) which is obtained from the exact one in the weak coupling (small β) approximation. As far as the amplitude $x(t)$ is concerned, our expression (2.13) agrees numerically with the exact solution of Ref. 8 for small values of β.

III. THE CASE OF COUPLED NONLINEAR OSCILLATORS

In this section we shall deal with a system of two weakly bound oscillators with quartic couplings. The same problem has been analysed quantum mechanically by Bank, Bender, and Wu.[10]

The Hamiltonian of the system is given by

$$\begin{aligned} H = {} & p_1^2/2m_1 + p_2^2/2m_2 + \tfrac{1}{2}m_1\omega_1^2x_1^2 + \tfrac{1}{2}m_2\omega_2^2x_2^2 \\ & + (\rho/4)[ax_1^4 + bx_2^4 + cx_1^2x_2^2], \end{aligned} \tag{3.1}$$

where the equations of motion are

$$\begin{aligned} &\ddot{x}_1 + \omega_1^2x_1 + (\rho/m_1)[ax_1^2 + \tfrac{1}{2}cx_2^2]x_1 = 0, \\ &\ddot{x}_2 + \omega_2^2x_2 + (\rho/m_2)[bx_2^2 + \tfrac{1}{2}cx_1^2]x_2 = 0. \end{aligned} \tag{3.2}$$

Proceeding as before, we may write the perturbed two-particle coherent state as

$$\begin{aligned} |\alpha\rangle' \equiv |\alpha_1, \alpha_2\rangle' = {} & \exp[-(\lambda_1^2 + \lambda_2^2)/2] \sum_{n_1,n_2=0}^{\infty} \frac{(-i\lambda_1)^{n_1}(-i\lambda_2)^{n_2}}{\sqrt{n_1!n_2!}} \Bigg| \\ & \times\exp(iE'_{n_1,n_2}t/\hbar)\,|n_1, n_2\rangle' \end{aligned} \tag{3.3}$$

in which the perturbed energy and eigenstate of harmonic oscillators are

$$\begin{aligned} E'_{n_1,n_2} = {} & (n_1 + \tfrac{1}{2})\hbar\omega_1 + (n_2 + \tfrac{1}{2})\hbar\omega_2 + \tfrac{3}{4}\rho a(\hbar/2m_1\omega_1)^2 \\ & \times(2n_1^2 + 2n_1 + 1) + \tfrac{3}{4}\rho b(\hbar/2m_2\omega_2)^2(2n_2^2 + 2n_2 + 1) \end{aligned}$$

$$+\tfrac{1}{4}\rho c(\hbar^2/4m_1\omega_1m_2\omega_2)\quad(2n_1+1)(2n_2+1)+O(\rho^2)\,, \tag{3.4}$$

$$\begin{aligned}
|n_1,n_2\rangle' = {}& |n_1,n_2\rangle+\tfrac{1}{4}\rho a(\hbar/4m_1^2\omega_1^3)\\
&\times[-\tfrac{1}{4}\sqrt{(n_1+1)(n_1+2)(n_1+3)(n_1+4)}\;|n_1+4,n_2\rangle\\
&+(2n_1+3)\sqrt{(n_1+1)(n_1+2)}\;|n_1+2,n_2\rangle\\
&-(2n_1-1)\sqrt{n_1(n_1-1)}\;|n_1-2,n_2\rangle\\
&+\tfrac{1}{4}\sqrt{n_1(n_1-1)(n_1-2)(n_1-3)}\;|n_1-4,n_2\rangle]\\
&+\tfrac{1}{4}\rho b(\hbar/4m_2^2\omega_2^3)\\
&\times[-\tfrac{1}{4}\sqrt{(n_2+1)(n_2+2)(n_2+3)(n_2+4)}\;|n_1,n_2+4\rangle\\
&+(2n_2+3)\sqrt{(n_2+1)(n_2+2)}\;|n_1,n_2+2\rangle-(2n_2-1)\\
&\times\sqrt{n_2(n_2-1)}\;|n_1,n_2-2\rangle\\
&+\tfrac{1}{4}\sqrt{n_2(n_2-1)(n_2-2)(n_2-3)}\;|n_1,n_2-4\rangle]\\
&+\tfrac{1}{8}\rho c(\hbar/4m_1\omega_1m_2\omega_2)\\
&\times[-[\sqrt{(n_1+1)(n_1+2)(n_2+1)(n_2+2)}/(\omega_1+\omega_2)]\\
&\times|n_1+2,n_2+2\rangle-[\sqrt{(n_1+1)(n_1+2)n_2(n_2-1)}/(\omega_1-\omega_2)]\\
&\times|n_1+2,n_2-2\rangle\;+[\sqrt{n_1(n_1-1)(n_2+1)(n_2+2)}/(\omega_1-\omega_2)]\\
&\times|n_1-2,n_2+2\rangle\;+[\sqrt{n_1(n_1-1)n_2(n_2-1)}/(\omega_1+\omega_2)\\
&\times|n_1-2,n_2-2\rangle]+O(\rho^2).
\end{aligned}\tag{3.5}$$

Substituting (3.4) and (3.5) in (3.3), and retaining terms up to the first-order in ρ in the algebraic calculation in which we have taken appropriate classical limits, we obtain the perturbative solutions:

$$\begin{aligned}
x_1(t)={}&A_1\cos\psi_1t+(\rho a/m_1)A_1^3/32\omega_1^2(\cos3\psi_1t\\
&-6\cos\psi_1t)-(\rho c/m_1)(A_1A_2^2/32\omega_1)\{(\omega_1+\omega_2)^{-1}\\
&\times\cos(\psi_1+2\psi_2)t\\
&+(\omega_1-\omega_2)^{-1}\cos(\psi_1-2\psi_2)t\}+O(\rho^2),
\end{aligned}\tag{3.6a}$$

$$\begin{aligned}
x_2(t)={}&A_2\cos\psi_2t+(\rho^6/m_2)(A_2^3/32\omega_2^2)(\cos3\psi_2t\\
&-6\cos\psi_2t)-(\rho c/m_2)(A_2A_1^2/32\omega_2)\\
&\times\{(\omega_1+\omega_2)^{-1}\cos(\psi_2+2\psi_1)t\\
&-(\omega_1-\omega_2)^{-1}\cos(\psi_2-2\psi_1)t\}+O(\rho^2),
\end{aligned}\tag{3.6b}$$

in which

$$\psi_1=\omega_1[1+(\rho/8m_1\omega_1^2)(3aA_1^2+cA_2^2)]+O(\rho^2), \tag{3.7a}$$

$$\psi_2=\omega_2[1+(\rho/8m_2\omega_2^2)(3bA_2^2+cA_1^2)]+O(\rho^2). \tag{3.7b}$$

The expressions in (3.6) have a resonance form that is easy to interpret. Considering the first oscillator, we may think that the second coordinate oscillating with a time dependence given by $\cos\psi_2t$ results in a forced motion on the first coordinate, and hence, the denominator is of the usual resonance form. The same argument is applicable to the second oscillator as well. Further, the effect of the nonlinearity in the coupled system has been manifested through the interdependence of the amplitudes and frequencies of both the oscillators.

As a special case, we recover the well-known Duffing equation

$$\ddot{x}+\omega^2x+\epsilon x^3=0,$$

from Eqs. (3.2) in the limit $b=c=0$. In this limit, solutions given in (3.6a) and (3.7a) coincide exactly with the result recently obtained by Bhaumik and Dutta-Roy.[4]

Finally, we remark that the same procedure can be extended with much computational labor to evaluate higher order terms in the perturbation series. However, we shall not do this here because the general features of the nonlinearities as well as the characteristics of a coupled system are contained in our first-order results or amplitudes and the modified frequencies in the weak coupling limit.

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[1] See for example: H. T. Davis, *Introduction to Nonlinear Differential and Integral Equations* (Dover, New York, 1962), N. Minorsky, *Nonlinear Oscillations* (Van Nostrand, Princeton, New Jersey, 1962).

[2] For a comprehensive review we may refer to A. H. Nayfeh, *Perturbation Methods* (Wiley, New York, 1973).

[3] R. H. G. Hellman and E. W. Montroll, Physica 74, 22 (1974).

[4] K. Bhaumik and B. Dutta-Roy, J. Math. Phys. 16, 1131 (1975).

[5] I. A. Malkin, J. Math. Phys. 14, 576 (1973); F. T. Hioe, J. Math. Phys. 15, 445, 1174 (1974).

[6] J. R. Kaluder and E. C. G. Sudarshan, *Fundamentals of Quantum Optics* (Benjamin, New York, 1968); R. J. Glauber, *Quantum Optics and Electronics* (Gordon and Breach, New York, 1964).

[7] T. C. Bradbury and A. Brintzenhoff, J. Math. Phys. 12, 1269 (1971).

[8] M. Lakshmanan and J. Prabhakaran, Lett. Nuovo Cimento 7, 689 (1973); P. M. Mathews and M. Lakshmanan, Ann. Phys. (N.Y.) 79, 171 (1973).

[9] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968).

[10] T. Banks, C. M. Bender, and T. T. Wu, Phys. Rev. 8, 3346 (1973).

On the Majorana transformation

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Some properties of the Dirac equation in its four- and two-component forms suggested by the Majorana representation of Dirac matrices are derived. Extension of the ideas to higher spin is also given.

INTRODUCTION

In 1937, Majorana[1] proposed a representation of Dirac matrices with

$$\alpha_{1,3}=\begin{pmatrix}\sigma_{1,3} & 0\\ 0 & -\sigma_{1,3}\end{pmatrix},\quad \alpha_2=\begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix},\quad \beta=\begin{pmatrix}\sigma_2 & 0\\ 0 & -\sigma_2\end{pmatrix}, \tag{1}$$

where the σ_i are a representation of Pauli matrices.[2] This leads to[3]

$$\gamma_i^\dagger=\gamma_i, \quad \text{and} \quad \gamma_4^\dagger=-\gamma_4, \tag{2}$$

and for solutions ψ of the Dirac equation

$$H\psi(x)=\{\boldsymbol{\alpha}\cdot\mathbf{P}+m\beta\}\psi(x)=i\frac{\partial}{\partial t}\psi(x), \tag{3}$$

where m is the mass, $\mathbf{P}$ the momentum operator, and where x stands collectively for the space coordinates $\mathbf{x}$ and the time coordinate t, one has the simple charge conjugation property, that $\psi^c=\psi^*$. The representation of Eq. (1) is only one of several equivalent representations of the Dirac matrices,[4] all of which have particular utility in that they exhibit aspects of Dirac theory more clearly than can representation independent arguments. As particularly emphasized in Ref. 4, different representations also suggest unitary transformations of the theory to forms of the operators and wavefunctions useful for particular applications.

The purpose of this paper is to explore in some detail particular unitary transformations of Eq. (3), utilizing a modified Majorana representation with[5]

$$\alpha_\perp=\begin{pmatrix}\sigma_\perp & 0\\ 0 & -\sigma_\perp\end{pmatrix},\quad \alpha_3=\begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix},\quad \beta=\begin{pmatrix}\sigma_3 & 0\\ 0 & -\sigma_3\end{pmatrix}, \tag{4}$$

the change from Eq. (1) being convenient for discussions relevant to elementary particle physics. In the next section the unitary trasformations of the Dirac equation will be derived, followed by a discussion of the two-component form in this representation and the extension of the spin one-half results to higher spin.

UNITARY TRANSFORMATIONS

A general unitary transformation $U(\mathbf{R}, \hat{\mathbf{e}}, \theta)$ is defined by

$$U(\mathbf{R}, \hat{\mathbf{e}}, \theta)=\exp[\tfrac{1}{2}\mathbf{R}\cdot\hat{\mathbf{e}}\theta] \tag{5}$$

where θ and $\hat{\mathbf{e}}$ are, respectively, a real number and a real unit vector and $\mathbf{R}$ is a 4×4 matrix made from the Pauli matrices and the 2×2 identity, subject to the restriction[6]

$$\mathbf{R}^\dagger=-\mathbf{R} \tag{6}$$

so that $U^\dagger=U^{-1}$.

A well-known example of Eq. (5) is the Foldy–Wouthuyson (FW) transformation[7] with $\mathbf{R}=\beta\boldsymbol{\alpha}$, $\hat{\mathbf{e}}=\hat{\mathbf{P}}$, and $\tan\theta=P/m$ leading to the transformed Dirac equation

$$E\beta\phi_{\mathrm{FW}}=i\frac{\partial}{\partial t}\phi_{\mathrm{FW}}, \tag{7}$$

with $E=(m^2+P^2)^{1/2}$, and

$$E\beta=U_{\mathrm{FW}}HU_{\mathrm{FW}}^\dagger, \quad \varphi_{\mathrm{FW}}=U_{\mathrm{FW}}\psi. \tag{8}$$

Another well-known example of Eq. (5) is the Cini–Touschek (CT) transformation[8] with $\mathbf{R}=\boldsymbol{\alpha}\beta$, $\hat{\mathbf{e}}=\hat{\mathbf{P}}$, and $\tan\theta=m/P$ leading to the equation

$$E\boldsymbol{\alpha}\cdot\hat{\mathbf{P}}\phi_{\mathrm{CT}}=i\frac{\partial}{\partial t}\varphi_{\mathrm{CT}} \tag{9}$$

with

$$E\boldsymbol{\alpha}\cdot\hat{\mathbf{P}}=U_{\mathrm{CT}}HU_{\mathrm{CT}}^\dagger,$$
$$\phi_{\mathrm{CT}}=U_{\mathrm{CT}}\psi. \tag{10}$$

Both of these transformations can be motivated by particular representations of Dirac matrices, the FW transformation by the representation in which $\beta=\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$, and the CT transformation by the representation in which $\boldsymbol{\alpha}=\left(\begin{smallmatrix}\sigma & 0\\ 0 & -\sigma\end{smallmatrix}\right)$, and which has $\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)=i\alpha_1\alpha_3\alpha_2=-\gamma_5$. Both of these transformations, also, have the property that $\mathbf{R}\cdot\hat{\mathbf{e}}\mathbf{R}\cdot\hat{\mathbf{e}}=-1$ so that a form for the exponential operator in terms of $\sin(\theta/2)$ and $\cos(\theta/2)$ is possible as for the rotation operator, and this property will be maintained in the operators discussed below.

One can look at the modified Majorana representation Eq. (4), as an exchange of the roles of P_3 and m by comparison to the representation with $\alpha=\left(\begin{smallmatrix}\sigma & 0\\ 0 & -\sigma\end{smallmatrix}\right)$, useful in the high energy limit when $m/P\ll1$. So the modified Majorana representation will be useful to describe the physical situation in which $P_3/(m^2+P_1^2)^{1/2}\ll1$, that is, when the transverse momentum of the particle is large compared to it longitudinal momentum. Corresponding to γ_5 in the high-energy representation, the chirality operator, there is an operator $K=i\alpha_1\beta\alpha_2$ which in the modified Majorana representation has the form

$$K=i\alpha_1\beta\alpha_2=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{11}$$

In the Majorana limit, when only the transverse momentum is important, one expects to have simultaneous eigenfunctions of K and the Hamiltonian, and perhaps to make interactions with projection operators $\frac{1}{2}(1\pm K)$ in analogy to chirality projection operators $\frac{1}{2}(1\pm\gamma_5)$.

The first unitary operator to construct is the one that brings the Dirac Hamiltonian into a form E times an operator that commutes with K. It is clear that $\mathbf{R}$ must be some other matrix than $\beta\boldsymbol{\alpha}$ since

$$\begin{aligned}\exp(\tfrac{1}{2}\boldsymbol{\alpha}\cdot\hat{\mathbf{e}}\beta\theta)H\exp(-\tfrac{1}{2}\boldsymbol{\alpha}\cdot\hat{\mathbf{e}}\beta\theta) &= \boldsymbol{\alpha}\cdot\mathbf{P}+(m\cos\theta-\hat{\mathbf{e}}\cdot\mathbf{P}\sin\theta)\beta \\ &\quad +(m\sin\theta+\hat{\mathbf{e}}\cdot\mathbf{P}\cos\theta-\hat{\mathbf{e}}\cdot\mathbf{P})\,\boldsymbol{\alpha}\cdot\hat{\mathbf{e}}\end{aligned} \tag{12}$$

and the desired transformation cannot be given by this simple form. In fact, the result requires the product of two transformations of the type shown in Eq. (12). Such a product has the general form

$$\begin{aligned}e^{A}e^{B}=\exp\Bigg[A+B-\frac{\cos\theta_1}{(\theta_1)^2}[A,B]_- \\ +\frac{1}{(\theta_1)^2}\left(1-\frac{\sin\theta_1}{\theta_1}\right)[A,[A,B]_-]_-\Bigg],\end{aligned} \tag{13}$$

with

$$\begin{aligned}&A=\tfrac{1}{2}\boldsymbol{\alpha}\cdot\hat{\mathbf{e}}_1\beta\theta_1,\\ &B=\tfrac{1}{2}\boldsymbol{\alpha}\cdot\hat{\mathbf{e}}_2\beta\theta_2,\\ &[\hat{\mathbf{e}}_1\theta_1,\hat{\mathbf{e}}_2\theta_2]_-=0.\end{aligned} \tag{14}$$

This form may be derived by letting $f(z)=\exp(Az)\times\exp(Bz)$, taking the derivative, then integrating and choosing $z=1$. Since only commutators of σ are involved, the results is true for all spins by defining α and β for general spin. A double transformation like Eq. (13) is seen to introduce a rotation, in addition to a unitary transformation of the FW and CT type. In detail, one finds the transformation

$$E\mathbf{R}\cdot\hat{\mathbf{b}}\alpha_3\phi_{\mathrm{MAJ}}=i\frac{\partial}{\partial t}\phi_{\mathrm{MAJ}}, \tag{15}$$

with

$$\begin{aligned}&H_{\mathrm{MAJ}}=E\mathbf{R}\cdot\hat{\mathbf{b}}\alpha_3=U_{\mathrm{MAJ}}HU^{\dagger}_{\mathrm{MAJ}},\\ &\phi_{\mathrm{MAJ}}=U_{\mathrm{MAJ}}\psi,\end{aligned} \tag{16}$$

where

$$U_{\mathrm{MAJ}}=\exp[\tfrac{1}{2}\mathbf{R}\cdot\hat{\mathbf{b}}\tan^{-1}(P_3/b)], \tag{17}$$

$$\mathbf{R}_{\perp}=\boldsymbol{\alpha}_{\perp}\alpha_3,\quad R_3=\beta\alpha_3, \tag{18}$$

$$\mathbf{b}=(P_1,P_2,m). \tag{19}$$

The new Hamiltonian H_{MAJ} is a linear combination of $\boldsymbol{\alpha}_{\perp}$ and β with the matrix form

$$H_{\mathrm{MAJ}}=E\begin{pmatrix}\sigma\cdot\hat{\mathbf{b}} & 0\\ 0 & -\sigma\cdot\hat{\mathbf{b}}\end{pmatrix}. \tag{20}$$

As noted previously, this form ought to be useful when the longitudinal momentum is small. It commutes with K and so the eigenstates can be simultaneous eigenstates of H_{MAJ} and K.

There are, of course, other unitary transformations of H that commute with K. In fact, any transformation that eliminates α_3 from the Hamiltonian and leaves a linear combination of $\boldsymbol{\alpha}_{\perp}$ and β, give an H' that commutes with K. For example, the result for the transformed Hamiltonian in Eq. (12) when $\hat{\mathbf{e}}=\hat{\mathbf{P}}_3$, in order to eliminate α_3, is that $\tan\theta=P_3/m$, $\mathbf{R}=\beta\boldsymbol{\alpha}$ to give

$$\begin{aligned}\exp[\tfrac{1}{2}\beta\alpha_3\tan^{-1}(P_3/m)]\exp[-\tfrac{1}{2}\beta\alpha_3\tan^{-1}(P_3/m) \\ =\boldsymbol{\alpha}_{\perp}\cdot\mathbf{P}_{\perp}+(m^2+P_3^2)^{1/2}\beta.\end{aligned} \tag{21}$$

It is often simpler to look at the unitary transformations of H from the point of view in which the desired forms are obtained by the transformation of $E\beta=H_{\mathrm{FW}}$. In this case one has the following results:

$E\beta\to\boldsymbol{\alpha}\cdot\mathbf{P}+m\beta$: $\mathbf{R}=\boldsymbol{\alpha}\beta$, $\hat{\mathbf{e}}=\hat{\mathbf{P}}$, $\tan\theta=P/m$;

$E\beta\to E\boldsymbol{\alpha}\cdot\mathbf{P}$: $\mathbf{R}=\boldsymbol{\alpha}\beta$, $\hat{\mathbf{e}}=\hat{\mathbf{P}}$, $\theta=\pi/2$;

$E\beta\to\boldsymbol{\alpha}_{\perp}\cdot\mathbf{P}_{\perp}+\sqrt{m^2+P_3^2}\,\beta$: $\mathbf{R}=\boldsymbol{\alpha}\beta$, $\hat{\mathbf{e}}=\hat{\mathbf{P}}_{\perp}$,
$\tan\theta=P_{\perp}/(m^2+P_3^2)^{1/2}$;

$E\beta\to E/b\{\boldsymbol{\alpha}_{\perp}\cdot\mathbf{P}_{\perp}+m\beta\}$: $\mathbf{R}=\boldsymbol{\alpha}\beta$, $\hat{\mathbf{e}}=\hat{\mathbf{P}}_{\perp}$, $\tan\theta=P_{\perp}/b$;

$E\beta\to P_3\alpha_3+b\beta$: $\mathbf{R}=\boldsymbol{\alpha}\beta$, $\hat{\mathbf{e}}=\hat{\mathbf{P}}_3$, $\tan\theta=P_3/b$.

Another way of finding particular unitary transformations of the Dirac equation when the method shown in Eq. (13) would prove cumbersome is to construct the transformation by analogy with a simpler one, looking at the Pauli matrix structure for guidance. For example, the only differences between Eq. (10) in the representation of Dirac matrices with $\boldsymbol{\alpha}=\left(\begin{smallmatrix}\sigma & 0\\ 0 & -\sigma\end{smallmatrix}\right)$, and Eq. (20) which is in the modified Majorana representation, are the substitutions $m\to-P_3$, $P\to b$, and $\hat{\mathbf{P}}\to\hat{\mathbf{b}}$. With these replacements, the CT transformation becomes the Majorana transformation and the Dirac Hamiltonian in the $\boldsymbol{\alpha}=\left(\begin{smallmatrix}\sigma & 0\\ 0 & -\sigma\end{smallmatrix}\right)$, $\beta=\left(\begin{smallmatrix}0 & 1\\ 1 & 0\end{smallmatrix}\right)$ representation becomes the Dirac Hamiltonian in the modified Majorana representation.

TWO-COMPONENT FORM

As an alternative to unitary transformations of the Dirac equation, one can decouple the upper two components of the Dirac wavefunction from the lower two components and obtain Hamiltonian equations for each pair of components, such equations again exhibiting aspects of the theory, that are less obvious in the four-component formulation. The exact separation using the modified Majorana representation will be carried out in this section.

Carrying out the matrix operations of Eq. (3), using the representation of Dirac matrices in Eq. (4) one has

$$\begin{aligned}&\sigma\cdot\mathbf{P}_{\perp}\psi_u-P_3\psi_L+m\sigma_3\psi_u=E_{\mathrm{op}}\psi_u,\\ &-\sigma\cdot\mathbf{P}_{\perp}\psi_L-P_3\psi_u-m\sigma_3\psi_L=E_{\mathrm{op}}\psi_L,\end{aligned} \tag{22}$$

where

$$E_{\mathrm{op}}=\frac{i\partial}{\partial t}\quad\text{and}\quad\psi=\begin{pmatrix}\psi_u\\ \psi_L\end{pmatrix}.$$

Note that

$$\begin{pmatrix}\psi_u\\ 0\end{pmatrix}=\tfrac{1}{2}(1+K)\psi,\quad\begin{pmatrix}0\\ \psi_L\end{pmatrix}\tfrac{1}{2}(1-K)\psi. \tag{23}$$

Using $\mathbf{b}$, defined in Eq. (19), Eqs. (22) can be written more compactly as

$$\begin{aligned}&\sigma\cdot\mathbf{b}\psi_u-P_3\psi_L=E_{\mathrm{op}}\psi_u,\\ &-\sigma\cdot\mathbf{b}\psi_L-P_3\psi_u=E_{\mathrm{op}}\psi_L,\end{aligned} \tag{24}$$

so that

$$\psi_L = -P_3 O \psi_u, \tag{25}$$

with

$$O = (E_{\text{op}} + \sigma \cdot \mathrm{b})^{-1}. \tag{26}$$

Substituting Eq. (25) into the first of Eqs. (24) yields

$$(\sigma \cdot \mathrm{b} + P_3^2 O)\psi_u = E_{\text{op}}\psi_u. \tag{27}$$

Solving Eq. (26) for E_{op} and substituting the result in Eq. (27) gives a quadratic equation for O with solutions

$$O = [-\sigma \cdot \mathrm{b} \pm ((\sigma \cdot \mathrm{b})^2 + P_3^2)^{1/2}]/P_3^2, \tag{28}$$

so that

$$\pm((\sigma \cdot \mathrm{b})^2 + P_3^2)^{1/2}\psi_u = E_{\text{op}}\psi_u. \tag{29}$$

If the original wavefunction ψ is normalized to unity, then ψ_u and ψ_L are not normalized. However, one may take as the normalized two-component wavefunction, ϕ_u, defined by

$$\phi_u = (1 + P_3^2 O^\dagger O)^{1/2}\psi_u. \tag{30}$$

Expanding this equation when P_3 is small compared to b, one has

$$\phi_u \approx \sqrt{2}\left[1 + \frac{b^2}{P_3^2} \mp \frac{b^2}{P_3^2}\left(1 + \frac{P_3^2}{2b^2} + \cdots\right)\right]^{1/2}\psi_u \tag{31}$$

which only makes sense if the upper sign is chosen in Eqs. (28) and (29).

The two-component equation for the normalized lower components may be derived in a similar way, the results being identical except for an additional minus sign in the results corresponding to Eqs. (25) and (29).

In all the above considerations, care has been taken to explicitly exhibit the $\sigma \cdot \mathrm{P}$ matrices. This proves important when an interacting Dirac particle is considered.

This kind of reduction to two-component forms using the modified Majorana representation is analogous to the separation into large and small components when the Dirac—Pauli representation[9] of the matrices is used, and, in fact, can be readily related to the Majorana transformation of the Dirac equation just as the Dirac—Pauli reduction is related to the FW transformation.

HIGHER SPIN

To discuss the higher spin realizations of the Majorana transformations, one requires a Hamiltonian formulation of the wave equation. The description due to Weaver, Hammer and Good[10] will be used here. In this description, the wavefunction ψ is $2(2s+1)$-component, representing a particle and antiparticle with spin s, and satisfies the wave equation

$$H_s\psi = \frac{i\partial}{\partial t}\psi, \tag{32}$$

where $(H_s)^2 = E^2$. H_s depends on E, m, P, and four $2(2s+1)$ square matrices $\boldsymbol{\alpha}$ and β. In general, H_s is a nonlocal operator. There is a well-defined prescription for finding H_s, and the spin $\frac{3}{2}$ result is shown below and will be studied as a typical example of higher spin, showing all the complications, i.e.,

$$\begin{aligned} H_{3/2}^{\text{WHG}} = [&(2E^2 + 7P2)m\beta + (6E^2 + 2\text{op}^2)\boldsymbol{\alpha} \cdot \mathrm{P} \\ &- 9m(\boldsymbol{\alpha} \cdot \mathrm{P})^2\beta - 18(\boldsymbol{\alpha} \cdot \mathrm{P})^3]/2(E^2 + P^2). \end{aligned} \tag{33}$$

The problems with higher spin occur because the characteristic equation for the spin matrices becomes more complicated as the spin increases.[11] The simple equation $(\mathbf{s} \cdot \hat{\mathrm{e}} + \frac{1}{2})(\mathbf{s} \cdot \hat{\mathrm{e}} - \frac{1}{2}) = 0$ for spin one-half, leading to $(\sigma \cdot \hat{\mathrm{e}})^2 = 1$, becomes $(\mathrm{s} \cdot \hat{\mathrm{e}} + \frac{3}{2})(\mathrm{s} \cdot \hat{\mathrm{e}} + \frac{1}{2})(\mathrm{s} \cdot \hat{\mathrm{e}} - \frac{1}{2})(\mathrm{s} \cdot \hat{\mathrm{e}} - \frac{3}{2}) = 0$ for spin three-halves leaving cubes of spin matrices in a particular direction as the maximum spin matrix powers, rather than the first power as for spin-one-half. This leads, as discussed in Ref. 4, to a more complicated general form of the unitary operator required to make transformations analogous to Eqs. (16) and (21).

To explicitly discuss the transformations of $H_{3/2}$ requires a definition of $\boldsymbol{\alpha}$ and β, i.e.,

$$\boldsymbol{\alpha} = \frac{2}{3}\begin{pmatrix} \mathrm{s} & 0 \\ 0 & -\mathrm{s} \end{pmatrix}, \quad \beta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{34}$$

so that $\boldsymbol{\alpha}$ and β anti-commute. In place of Eq. (5) a more general form is required with the structure

$$U_{3/2}(\mathrm{R}, \hat{\mathrm{e}}, \phi_0, \phi_1) = \exp[\tfrac{3}{2}\mathrm{R} \cdot \hat{\mathrm{e}}\phi_0 + (\tfrac{3}{2}\mathrm{R} \cdot \hat{\mathrm{e}})^3\phi_1], \tag{35}$$

suggested by the above discussion of the characteristic equation. Again ϕ_0 and ϕ_1 are real, as is $\hat{\mathrm{e}}$, and $\mathrm{R}^\dagger = -\mathrm{R}$. In view of the spin complications, it is particularly simple to investigate the connection between the spin three-halves Foldy—Wouthuyson form of the Hamiltonian $E\beta$ and other forms. Some results arising from the equation

$$\begin{aligned} &U_{3/2}(\boldsymbol{\alpha}\beta, \hat{\mathrm{e}}, \phi_0, \phi_1)E\beta U_{3/2}^\dagger(\boldsymbol{\alpha}\beta, \hat{\mathbf{e}}, \phi_0, \phi_1) \\ &\quad = [\cos N + \tfrac{1}{2}(\cos Q - \cos N)(\tfrac{9}{4}(\boldsymbol{\alpha} \cdot \hat{\mathrm{e}})^2 - \tfrac{1}{4})]\beta E \\ &\qquad + [2\sin N + (\tfrac{1}{3}\sin Q - \sin N)(\tfrac{9}{4}(\boldsymbol{\alpha} \cdot \hat{\mathrm{e}})^2 - \tfrac{1}{4})]\tfrac{3}{2}\boldsymbol{\alpha} \cdot \hat{\mathrm{e}}E, \end{aligned} \tag{36}$$

where

$$\begin{aligned} N &= \phi_0 - \phi_1/4, \\ Q &= 3\phi_0 - \tfrac{27}{4}\phi_1, \end{aligned} \tag{37}$$

are listed below:

$$\begin{aligned} &E\beta \to H_{3/2}^{\text{WHG}}\text{: } \hat{\mathrm{e}} = \hat{\mathrm{P}},\ \tan N = P/m,\ \tan Q = [(3E^2 + P^2)/m^2]P/m; \\ &E\beta \to E\boldsymbol{\alpha} \cdot \hat{\mathrm{P}}[\tfrac{13}{4} - \tfrac{9}{4}(\boldsymbol{\alpha} \cdot \hat{\mathrm{P}})^2]\text{: } \hat{\mathrm{e}} = \hat{\mathrm{P}},\ N = Q = \pi/2; \\ &E\beta \to m\beta + \boldsymbol{\alpha} \cdot \hat{\mathrm{P}}[\tfrac{13}{4} - \tfrac{9}{4}(\boldsymbol{\alpha} \cdot \hat{\mathrm{P}})^2]P\text{: } \hat{\mathrm{e}} = \hat{\mathrm{P}},\ \tan N = \tan Q = P/m; \\ &E\beta \to P_3\alpha_3(\tfrac{13}{4} - \tfrac{9}{4}\alpha_3^2) + b\beta\text{: } \hat{\mathrm{e}} = \hat{\mathrm{P}}_3,\ \tan N = \tan Q = P_3/b; \\ &E\beta \to \boldsymbol{\alpha} \cdot \mathrm{P}_\perp[\tfrac{13}{4} - \tfrac{9}{4}(\boldsymbol{\alpha} \cdot \hat{\mathrm{P}}_\perp)^2] + (m^2 + P_3^2)^{1/2}\beta\text{:} \\ &\qquad \hat{\mathrm{e}} = \hat{\mathrm{P}}_\perp,\ \tan N = \tan Q = P_\perp/(m^2 + P_3^2); \\ &E\beta \to E/b\{\boldsymbol{\alpha} \cdot \mathrm{P}_\perp[\tfrac{13}{4} - \tfrac{9}{4}(\boldsymbol{\alpha} \cdot \hat{\mathrm{P}}_\perp)^2] + m\beta\}\text{: } \hat{\mathrm{e}} = \hat{\mathrm{P}}_\perp, \\ &\qquad\qquad \tan N = \tan Q = P_\perp/b. \end{aligned} \tag{38}$$

One sees that replacing $\boldsymbol{\alpha} \cdot \hat{\mathrm{k}}$ for spin one-half, the projection of $\boldsymbol{\alpha}$ in the $\hat{\mathrm{k}}$ direction, by the spin three-halves expression $\boldsymbol{\alpha} \cdot \hat{\mathrm{k}}[\frac{13}{4} - \frac{9}{4}(\boldsymbol{\alpha} \cdot \hat{\mathrm{k}})^2]$, all the spin one-half forms of the transformed Dirac Hamiltonian can be obtained for spin three-halves, and that the corresponding unitary transformations are well-defined, and completely analogous to the spin one-half results. This result has been discussed previously, in Ref. 4, in connection with the generalization of the Melosh transformation[12] to higher spin, but it is seen here to apply to all forms of the transformed Hamiltonian and the related spin projection directions.

It is much more difficult in the spin three-halves case to construct the unitary transformation from $H_{3/2}^{\mathrm{WHG}}$ to the forms in Eqs. (38) because of the greatly increased algebraic manipulations. One can, in principle, however, work out all the transformation operators using the form

$$\begin{aligned}\exp[\tfrac{3}{2}\mathrm{R}\cdot\hat{\mathrm{e}}\phi_0+(\tfrac{3}{2}\mathrm{R}\cdot\hat{\mathrm{e}})^3\phi_1]\\ =\cos(N/2)-\tfrac{1}{2}[\cos(Q/2)-\cos(N/2)][-\tfrac{9}{4}(\mathrm{R}\circ\hat{\mathrm{e}})^2+\tfrac{1}{4}]\\ +\tfrac{3}{2}\mathrm{R}\cdot\hat{\mathrm{e}}\{2\sin(N/2)-[\tfrac{1}{3}\sin(Q/2)-\sin(N/2)]\\ \times[-\tfrac{9}{4}(\mathrm{R}\cdot\hat{\mathrm{e}})^2+\tfrac{1}{4}]\},\end{aligned} \tag{39}$$

where R must be $\boldsymbol{\alpha}\beta$ with $\boldsymbol{\alpha}$ and β as given in Eq. (34) or the alternate form with $\boldsymbol{\alpha}=\frac{2}{3}\begin{pmatrix}0&\mathbf{s}\\ \mathbf{s}&0\end{pmatrix}$, and $\beta=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$, or any other definitions such that $\mathrm{R}^\dagger=-\mathrm{R}$ and R has the eigenvalue spectrum of the spin three-halves matrices so that the characteristic equation causing closure of the products of the matrices holds.

DISCUSSION

Many aspects of the Majorana representation of the Dirac matrices $\boldsymbol{\alpha}$ and β have been discussed in detail, including transformation of the Dirac Hamiltonian to useful forms, and the complementary reduction to two-component equations for the positive and negative energy eigenstates. Of course, one can equally well convert other physical operators to transformed forms using the same methods, well-known in the case of the FW transformation. In addition to the spin one-half results, many of the ideas can be extended to higher spins as noted in Ref. 4 and carried out in some detail here for the spin three-halves case.

In many respects the Majorana transformation and aspects of the Melosh transformation[12] are complementary. In the latter case one deals with the set of Dirac matrices that has $\alpha_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$, and one has in a limited way interchanged P_3 and m with respect to the Dirac—Pauli representation and the FW transformation. This leads to discussions appropriate when the longitudinal momentum is large compared to $(m^2+P_\perp^2)^{1/2}$, whereas in the Majorana case it is the inverse ratio that is appropriate for consideration.

All of the results derived in the preceeding sections have pertained to the free particle. This has allowed exact results to be obtained both for the unitary transformations and for the reduction of the four-component Dirac theory to a two-component form. It is, of course, very important to investigate the same problems with some external potential. In general, exact results can no longer be obtained, but there are some special kinds of interactions which permit exact results, for example, a constant magnetic field with or without an anomalous magnetic moment interaction, as well as other kinds of additive interactions that commute with the unitary transformations or still allow exact reduction to be carried out.[13] Looking at the reduction to two-component form, for example, in the presence of a constant, external magnetic field B in the z direction, and with an anomalous magnetic moment interaction of the form $(iq\kappa/4m)\beta\mathrm{B}\cdot(\boldsymbol{\alpha}\times\boldsymbol{\alpha})/2$ with q and κ the charge and anomalous g factor, one finds the two-component equation

$$\pm[P_3^2+(\sigma\circ\pi_\perp+m\sigma_3-q\kappa B/4m)^2]^{1/2}\phi_u=E_{\mathrm{op}}\phi_u. \tag{40}$$

Although this is an exact result, it is almost as complicated as the four-component form. One can, however, carry out a unitary transformation of Eq. (40) with the operator

$$V=\exp[\tfrac{1}{2}\sigma_3\sigma\circ\pi_\perp\tan^{-1}(|\pi_\perp|/m)] \tag{41}$$

useful because

$$V(\sigma\circ\pi_\perp+m\sigma_3)V^\dagger=(m^2+(\sigma\cdot\pi_\perp)^2)^{1/2}\sigma_3. \tag{42}$$

The result is

$$\begin{aligned}\pm\{P_3^2+[(m^2+(\sigma\circ\pi_\perp)^2)^{1/2}\sigma_3-q\kappa B/4m]^2\}^{1/2}V\phi_u\\ =E_{\mathrm{op}}\phi_u,\end{aligned} \tag{43}$$

a form which is diagonal when one takes $V\phi_u$ to be a simultaneous eigenstate of P_3, $(\sigma\circ\pi_\perp)^2$, and σ_3. This affords a simple way of getting the exact energy eigenvalues compared to the usual methods.[14] It is not clear, of course, how far one wishes to pursue such a two-component formalism since the separation of the four-component wavefunction into two-component functions is broken by a special Lorentz transformation in the z direction.

One may, in the spin one-half case, note that the transformed Hamiltonian's of Eqs. (20) and (21) are invariant to the general K transformation $\psi'=\exp(iK\delta/2)\psi$ with δ a real number. This is the Majorana equivalent of γ_5-invariance and it also holds for the free particle Dirac equation when $P_3=0$, since the formal result of the unitary transformations is to eliminate operators (e.g., α_3) that do not commute with K. The corresponding invariance in the representation that has $\alpha_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ is to the transformation $\exp(i\alpha_3\delta/2)$, and the Melosh and related unitary transformations are constructed to remove operators that do not commute with α_3.

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[1] E. Majorana, Nuovo Cimento 14, 171 (1937).

[2] The particular representation to be used in this paper is the standard one with $\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix}$, $\sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix}$, $\sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$.

[3] Gamma matrices are defined by $\gamma_i=-i\beta\alpha_i$, $\gamma_4=\beta$, and * indicates complex conjugation.

[4] See, for example, D.L. Weaver, Phys. Rev. (to be published).

[5] Here ⊥ refers to the components transverse to the third component.

[6] The symbol † means Hermitian conjugation.

[7] L.L. Foldy and S.A. Wouthuyson, Phys. Rev. 78, 29 (1950).

[8] M. Cini and B. Touschek, Nuovo Cimento 7, 422 (1958).

[9] P.A.M. Dirac, Proc. R. Soc. 117, 610 (1928); W. Pauli,

Encycl. Phys. **5**, 142 (1958). See R. E. Moss, Am. J. Phys. **39**, 1169 (1971) for a good discussion.

[10] D. L. Weaver, C. L. Hammer, and R. H. Good, Jr., Phys. Rev. B **135**, 241 (1964).

[11] For a general discussion, see S. A. Williams, J. P. Draayer, and T. A. Weber, Phys. Rev. **152**, 1207 (1966).

[12] H. J. Melosh, Phys. Rev. D **9**, 1095 (1974). This is the transformation which is different from the FW transformation, rather than the FW transformation specialized to "good" components as discussed by J. S. Bell, Acta Phys. Austriaca, Suppl. **13**, 395 (1974).

[13] D. L. Weaver, Tufts University preprint.

[14] See, for example, W. Tsai and A. Yildiz, Phys. Rev. D **4**, 3643 (1971); W. Tsai, Phys. Rev. D **7**, 1945 (1973).

Canonical transformations and phase space path integrals

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A previous discussion of canonical transformations and path integrals is extended to the phase space path integral method. Within this approach a broader class of canonical transformations can be introduced than within the Lagrangian approach, including coordinate transformations and essentially all infinitesimal tranformations.

1. INTRODUCTION

The great importance of unitary transformations in quantum mechanics and their correspondence with classical canonical transformations is something which need hardly be stressed. Consequently the definition and employment of these transformations in the context of the path integral formulations of quantum mechanics is of interest. Although unitary matrices can be easily used to transform path integrals, the problem has been the identification of the transformed variables with the correspondingly transformed classical variables.

In a previous article[1] the author has exploited Dirac's discussion of the classical limit of a path integral in order to make the identification. The discussion was limited to the Lagrangian path integral method and only a limited class of canonical transformations could be defined and carried out.

In the following, the same kind of analysis is applied to the more general phase-space path-integral method. We find that essentially all of the infinitesimal canonical transformations can be applied to path integrals with a clear correspondence between the classical and quantum generators. Those finite transformations that can be built up from repeated applications of infinitesimal transformations follow obviously. As for intrinsically finite transformations, it is found that a limited but somewhat more general class than that of Ref. 1 can be defined. The ordering problem—that is, the ambiguity inherent in all known quantization procedures[2]—is discussed at several points, particularly as it complicates the consistent carrying out of quantization with different sets of canonical variables.

In Sec. 2, aspects of the phase-space path-integral method are reviewed briefly. The discussion parallels one of Pearle's[3] somewhat, but is given here to establish our notation and point of view. In Sec. 3, infinitesimal transformations are discussed, and finite transformations in Sec. 4.

2. PHASE-SPACE PATH-INTEGRALS

In this section we discuss the phase-space path-integral in terms appropriate to the sections that follow. We consider a nonrelativistic system with m degrees of freedom and begin with the propagator $K(q_f, q_0, t_f, t_0)$ so that

$$\psi(q_f, t_f) = \int K(q_f, q_0, t_f, t_0)\psi(q_0, t_0)\, d^m q_0. \tag{1}$$

Three properties of the propagator are of concern to us. First, it must be a unitary matrix. Second, it must have at least the semigroup property

$$K(q'', q, t'', t) = \int K(q'', q', t'', t')K(q', q, t', t)\, d^m q', \tag{2}$$

where $t'' > t' > t$. Third, it must approach the identity as the time interval vanishes, i. e.,

$$\lim_{t' \to t} K(q', q, t', t) = \delta^m(q' - q). \tag{3}$$

From (2) we can construct the lattice expression for a general path integral

$$\psi(q_f, t_f) = \lim_{N \to \infty} \int \psi(q_0, t_0) \prod_{n=0}^{N=1} K(q_{n+1}, q_n, t_{n+1}, t_n)\, d^m q_n, \tag{4}$$

where $q_N = q_f$, $t_N = t_f$, $t_{n+1} = t_n + \epsilon$ and $\epsilon = (t_f - t_0)/N$. Now we seek a first-order approximation for the propagator in (4) for ϵ small. We write the propagator in the form

$$K(q', q, t+\epsilon, t) = (2\pi\hbar)^{-m} \int \mathcal{K}(p, q', q, t+\epsilon, t) \times \exp[(i/\hbar) p_i (q'_i - q_i)]\, d^m p\,. \tag{5}$$

The function $\mathcal{K}$ is not uniquely defined by (5) but can be expressed, for example, as a line integral in the $2m$-dimensional q, q' space, i. e.,

$$\mathcal{K}(p, q', q, t+\epsilon, t) = \int_c K(q', q, t+\epsilon, t) \exp[-(i/\hbar) p_i (q'_i - q_i)]\, d^m(q' - q), \tag{6}$$

where c denotes that some function $f_c(q', q)$ is held constant. The limit in (3) becomes

$$\lim_{\epsilon \to 0} \mathcal{K}(p, q', q, t+\epsilon, t) = 1, \tag{7}$$

which is, unlike (3), a continuous limit. Now we can approximate $\mathcal{K}$ to first-order as

$$\mathcal{K}(p, q', q, t+\epsilon, t) \approx 1 - (i/\hbar)H(p, q', q, t)\epsilon \approx \exp[-(i/\hbar)H(p, q', q, t)\epsilon]. \tag{8}$$

Unitarity of K then determines that, if $\mathcal{K}$ is chosen so that H is a symmetric function of q_i and q'_i, H must be real. From here on we assume that this is always the choice that is made. H is still not specified uniquely, however. The propagator now takes the form

$$K(q', q, t+\epsilon, t) = (2\pi\hbar)^{-m} \int \exp\{(i/\hbar)[p_i(q'_i - q_i) - H(p, q', q, t)\epsilon]\}\, d^m p \tag{9}$$

and (4) becomes

$$\psi(q_f, t_f) = \lim_{t\to\infty} \int \psi(q_0, t_0) \exp\left((i/\hbar) \sum_{n=0}^{N-1} [p_{ni}(q_{n+1\,i} - q_{ni}) - H(p_n, q_{n+1}, q_n, t)\epsilon]\right)(2\pi\hbar)^{-Nm} \prod_{n=0}^{N-1} d^m p_n d^m q_n. \tag{10}$$

Formally taking the limit, we obtain the usual phase-space path-integral

$$\psi(q_f, t_f) = \int \exp\{(i/\hbar) \int_{t_0}^{t_f} [p_i\, dq_i - H_0(p, q, t)\, dt]\} \times Dp Dq\, \psi(q_0, t_0)\, d^m q_0 \tag{11}$$

with

$$H_0(p, q, t) = \lim_{q'\to q} H(p, q', q, t). \tag{12}$$

The classical limit argument of Dirac[4] can now be used to identify H_0 with the classical Hamiltonian function. If desired, the Hamiltonian operator can be reconstructed from H in the usual manner.[2] The ambiguity in H mentioned above corresponds to the different ways in which the p and q operators can be ordered in the expression for the (unique) Hamiltonian operator. Note that we have taken the $\epsilon\to 0$ limit before the $\hbar \to 0$ limit. A brief discussion of why this is done and what is meant by it is given in the Appendix.

Path integral quantization may be regarded as an attempt to reverse the procedure discussed above. The well-known operator-ordering problem[2] manifests itself in the ambiguity of the passage from H_0 to H where different choices can lead to different propagators. We thus have two closely related operator-ordering ambiquities.

As is well known the p integrations in (9) can often be carried out explicitly, and if H is quadratic in the p's the usual Lagrangian path integral is obtained.

3. INFINITESIMAL TRANSFORMATIONS

Since the Hamiltonian is the generator of an infinitesimal unitary (canonical) transformation, we expect that we can use the phase-space path-integral as a model for the expression of such transformations in a form suitable for use with path integral propagators.[3] Let us consider a one parameter group of unitary transformations with s labeling the parameter. The corresponding unitary matrices are the $U(Q, q, s)$ so that

$$\chi(Q) = \int U(Q, q, s)\psi(q)\, d^m q. \tag{13}$$

They have the group property

$$U(Q, q, s_1 + s_2) = \int U(Q, q', s_2)\, U(q', q, s_1)\, d^m q' \tag{14}$$

and the limit

$$\lim_{s\to 0} U(Q, q, s) = \delta^m(Q - q). \tag{15}$$

The finite transformations can be built up from the infinitesimal ones, i. e.,

$$\chi(Q) = \lim_{N\to\infty} \int \psi(q) \prod_{n=0}^{N-1} U(q_{n+1}, q_n, \Delta s)\, d^m q_n, \tag{16}$$

where $q_{0i} = q_i$, $q_{Ni} = Q_i$, and $\Delta s = s/N$. The clear analogy with Sec. 2 allows us to immediately write

$$U(Q, q, \Delta s) \approx (2\pi\hbar)^{-m} \int \exp\{(i/\hbar)[P_i(Q_i - q_i) - G(P, Q, q)\Delta s]\} \times d^m P \tag{17}$$

for the infinitesimal case, and

$$\chi(Q) = \lim_{N\to\infty} \int \psi(q) \exp\left((i/\hbar) \sum_{n=0}^{N-1} [P_{ni}(q_{n+1\,i} - q_{ni}) - G(P_n, q_{n+1}, q_n)\Delta s]\right)(2\pi\hbar)^{-Nm} \prod_{n=0}^{N-1} d^m P_n d^m q_n \tag{18}$$

for the finite case. We can again take the formal limit, obtaining

$$\chi(Q) = \int \exp\{(i/\hbar) \int_0^s [P_i(s')\, dq_i'(s') - G_0(P, q')\, ds']\} DPDq' \psi(q)\, d^m q, \tag{19}$$

with $q_i'(s) = Q_i$, $q_i'(0) = q_i$, and

$$G_0(P, q) = \lim_{Q\to q} G(P, Q, q). \tag{20}$$

Thus a unitary transformation that can be built out of repeated applications of an infinitesimal transformation can be represented as an abstract "path integral."

Now we wish to consider the transformed path integral and, by repeating the classical limit argument, identify G_0 with the classical generator of the corresponding canonical transformation. When doing this we must use (19) even if we are only concerned with the infinitesimal case, since a transformation of the form (17) will not remain infinitesimal as $\hbar$ approaches zero independently of Δs. The transformed propagator

$$\begin{aligned}\tilde{K}(Q_f, Q_0, t_f, t_0) &= \int U(Q_f, q_f, s) K(q_f, q_0, t_f, t_0) U^*(Q_0, q_0, s)\, d^m q_0\, d^m q_f \\ &= \int \exp\{(i/\hbar)[\int_0^s (P_{fi}(s')\, dq_{fi}'(s') - G_0(P_f, q_f')\, ds' \\ &\quad + \int_{t_0}^{t_s} (p_i\, dq_i - H_0\, dt) - \int_0^s (P_{0i}(s')\, dq_{0i}'(s') \\ &\quad - G_0(P_0, q_0')\, ds')]\} DP_f Dq_f' Dp Dq DP_0 Dq_0',\end{aligned} \tag{21}$$

where $q_{fi}'(0) = q_f$, $q_{fi}'(s) = Q_f$, etc. If $\hbar$ becomes very small we get phase cancellation unless the real and the abstract paths satisfy

$$\delta\{\int_0^s [P_{fi}\, dq_{fi}' - G_0(P_f, q_f')\, ds'] + \int_{t_0}^{t_f} [p_i\, dq_i - H_0(p, q, t)\, dt] - \int_0^s [P_{0i}\, dq_{0i}' - G_0(P_0, q_0')\, ds']\} = 0. \tag{22}$$

At this point we can let $s = \Delta s$ and consider it small on a macroscopic scale so that, to first-order in Δs,

$$\delta\{P_{fi}(Q_{fi} - q_{fi}) - G_0(P_f, q_f)\Delta s + \int_{t_0}^{t_f} [p_i\, dq_i - H_0(p, q, t)\, dt] - P_{0i}(Q_{0i} - q_{0i}) + G_0(P_0, q_0)\Delta s\} = 0, \tag{23}$$

where $\delta Q_{fi} = \delta Q_{0i} = 0$. The variation yields, in addition to the usual Hamilton equations,

$$Q_{fi} - q_{fi} = \frac{\partial G_0(P_f, q_f)}{\partial P_{fi}} \Delta s, \quad P_{fi} - p_{fi} = -\frac{\partial G_0(P_f, q_f)}{\partial q_{fi}} \Delta s,$$

$$Q_{0i} - q_{0i} = \frac{\partial G_0(P_0, q_0)}{\partial P_{0i}} \Delta s, \quad P_{0i} - p_{0i} = -\frac{\partial G_0(P_0, q_0)}{\partial q_{0i}} \Delta s. \tag{24}$$

Since the endpoints are arbitrary, Eqs. (24) give essentially the usual transformation equations. We could of course have carried out the variation (23) first and then let s become small with the same results. Thus we can identify $G_0(P,q)$ with the classical generator of the transformation. We note that there may be many G's corresponding to a particular G_0, thus confirming the well-known many-to-one relationship between unitary and canonical transformations.

4. FINITE TRANSFORMATIONS

Now we wish to consider intrinsically finite unitary transformations. We hope to be able to express them in terms of the generating functions $F_1(Q,q)$, $F_2(P,q)$, $F_3(Q,p)$, and $F_4(P,p)$. Starting with F_1, which is simplest, we look for a transformation matrix of the form

$$U_1(Q,q)=R_1(Q,q)\exp[-(i/\hbar)F_1(Q,q)] \tag{25}$$

which is a slight generalization of the form considered in Ref. 1. Such a matrix will be unitary if

$$\begin{aligned}&F_1(Q,q)=A_{1i}(Q)a_{1i}(q)+B_1(Q)+b_1(q),\\&R_1(Q,q)=(2\pi\hbar)^{-m/2}D_1^{1/2}(Q,q)\end{aligned} \tag{26}$$

where

$$D_1(Q,q)=\det\left(\frac{\partial^2F_1}{\partial q_i\,\partial Q_i}\right),$$

analogous to the Van Vleck determinant.[5] In addition, the A_i and a_i must be unbounded, single-valued functions of the Q_i and q_i respectively, as if they defined point transformations.

As before we identify our F_1 with the corresponding classical generating function by considering the classical limit of the transformed propagator. The new propagator is

$$\begin{aligned}&\widetilde{K}(Q_f,Q_0,t_f,t_0)\\&\quad=(2\pi\hbar)^{-m}\int\exp\Big\{(i/\hbar)\Big[-F_1(Q_f,q_f)+\int_{t_0}^{t_f}(p_i\,dq_i-H_0\,dt)\\&\qquad+F_1(Q_0,q_0)\Big]\Big\}D_1^{1/2}(Q_f,q_f)D_1^{1/2}(Q_0,q_0)DpDq\,d^mq_f\,d^mq_0.\end{aligned} \tag{27}$$

If $D_1^{1/2}$ is a reasonably smooth function, by considering the classical limit and carrying out the resulting variation as before, we are led in a straightforward way to the appropriate transformation equations

$$p_i=\frac{\partial F_1}{\partial q_i}\,,\quad P_i=-\frac{\partial F_1}{\partial Q_i}\,. \tag{28}$$

We note that, as in Ref. 1, a special case of U_1 is the transformation to the momentum representation

$$U_1(p,q)=(2\pi\hbar)^{-m/2}\exp[-(i/\hbar)p_iq_i]. \tag{29}$$

This notation, though perhaps slightly confusing, is unambiguous and will be useful in what follows.

We now consider the transformation matrix $U_2(P,q)$ defined by

$$\varphi(P)=\int U_2(P,q)\psi(q)\,d^mq. \tag{30}$$

As before we look for matrices of the form

$$U_2(P,q)=R_2(P,q)\exp[-(i/\hbar)F_2(P,q)] \tag{31}$$

and again find that R_2 and F_2 take forms equivalent to (26). The transformed propagator, however, must have the form

$$\begin{aligned}&\widetilde{K}(Q_f,Q_0,t_f,t_0)\\&\quad=\int U_1^*(P_f,Q_f)U_2(P_f,q_f)K(q_f,q_0,t_f,t_0)\\&\qquad\times U_2^*(P_0,q_0)U_1(P_0,Q_0)\,d^mP_f\,d^mq_f\,d^mP_0\,d^mq_0\\&\quad=(2\pi\hbar)^{-2m}\int\exp\Big\{(i/\hbar)\Big[P_{fi}Q_{fi}-F_2(P_f,q_f)\\&\qquad+\int_{t_0}^{t_f}(p_i\,dq_i-H_0\,dt)+F_2(P_0,q_0)-P_{0i}Q_{0i}\Big]\Big\}\\&\qquad\times D_2^{1/2}(P_f,q_f)D_2^{1/2}(P_0,q_0)DpDq\,d^mP_f\,d^mq_f\,d^mP_0\,d^mq_0.\end{aligned} \tag{32}$$

Considering the classical limit yields

$$Q_2=\frac{\partial F_2}{\partial P_i}\,,\quad P_i=\frac{\partial F_2}{\partial q_i} \tag{33}$$

as expected. The same reasoning can be applied to obtain matrices $U_3(Q,p)$ and $U_4(P,p)$. Among the U_2 class of transformations are the coordinate transformations for which

$$A_{2i}(P)=P_i,\quad B_2(P)=b_2(q)=0. \tag{34}$$

Once we have drawn the correspondence between a class of unitary transformations of the path integral and the appropriate classical transformations, we can ask whether one can now carry out path integral quantization with different sets of canonical variables and obtain consistent results. If the conventional canonical quantization procedure is attempted naively, inconsistencies appear which are due to the operator-ordering ambiguity.[6] We naturally expect an analogous situation with the path integral method. We will illustrate this with a very simple example—a coordinate transformation applied to a free particle moving in one dimension. We will compare the results obtained by quantizing in the transformed representation with those obtained by directly transforming the original propagator.

It is sufficient to work with the propagator for an infinitesimal time interval which is

$$\begin{aligned}&K(q',q,t+\epsilon,t)\\&\quad=(2\pi\hbar)^{-1}\int\exp\{(i/\hbar)[p(q'-q)-(p^2/2m)\epsilon]\}\,dp.\end{aligned} \tag{35}$$

Using this and the transformation matrix

$$U_2(P,q)=(2\pi\hbar)^{-1/2}\left[\frac{\partial a(q)}{\partial q}\right]^{1/2}\exp\left[-\frac{i}{\hbar}a(q)P\right] \tag{36}$$

in (32), we obtain

$$\begin{aligned}&\widetilde{K}(Q',Q,t+\epsilon,t)\\&\quad=(2\pi\hbar)^{-1}\int\exp\{(i/\hbar)[P(Q'-Q)-\widetilde{H}(P,Q',Q)\epsilon]\}\,dP\end{aligned} \tag{37}$$

with

$$\begin{aligned}&\widetilde{H}(P,Q',Q)\\&\quad=\tfrac{1}{2}[d^{-3/2}(Q)\,d^{-1/2}(Q')+d^{-1/2}(Q)\,d^{-3/2}(Q')]\frac{P^2}{2m}\\&\qquad+\frac{\hbar^2}{4m}\,d^{-1}(Q)\frac{d^2d^{-1}(Q)}{dQ^2}\;,\end{aligned} \tag{38}$$

where $d(Q)=dq/dQ$ if $Q=a(q)$. To get this result, the expression $\exp(-i\epsilon p^2/2m\hbar)$ has been approximated to first-order in ϵ in intermediate steps. There are of course other equivalent forms for $\widetilde{H}(P,Q,Q')$ but all contain some sort of "extra" term such as the last term in (38). This is due to the awkwardness of expressing propagators corresponding to Hamiltonian operators containing terms such as $\hbar^2 f(q)(d/dq)g(q) \times (d/dq)h(q)$ in path integral form. The "extra" terms proportional to the curvature scalar R that appear when path integral quantization is carried out in curved spaces[5,7] are of similar origin.

Path integral quantization in the new canonical variables can be carried out, but leads to the question of which form of $\widetilde{H}(P, Q, Q')$ corresponding to

$$\widetilde{H}_0(P, Q) = d^{-2}(Q)P^2/2m \tag{39}$$

is to be used in (37). Equation (38) is a far from obvious guess. By comparison, in the canonical quantization procedure one would have to guess at the operator

$$-\frac{\hbar^2}{2m}\left[d(Q)^{-1/2}\frac{d}{dQ}\, d(Q)^{-1/2}\right]^2$$

to correspond to $\widetilde{H}_0$.

There remain many canonical transformations which cannot be put into the forms we have discussed. We should mention a notable example, the transformation of a harmonic oscillator to the energy representation. This can be accomplished classically by an F_2 proportional to $q^2 \cot(P)$ but the corresponding U_2 is not unitary, failing to satisfy the requirements for (26). This corresponds to the fact that P would be a phase variable which cannot be observable (Hermitian) due to the boundedness of H. It is probable that a much wider range of canonical transformations can be dealt with in a path integral context, but accomplishing this requires a discussion of the classical limit that is more general than our quite straightforward one.

APPENDIX

The invoking of Dirac's classical limit argument in Sec. 2 must be regarded as merely suggestive for various reasons and we give here a more careful analysis. To begin with, one cannot merely take the limit $\hbar \to 0$ in (10) while holding ϵ fixed since approximation (8) would be violated. On the other hand, if one takes the limit $\epsilon \to 0$ first, one cannot really regard (11) as a well-defined expression for the propagator, since it does not distinguish between the various choices for $H(p, q', q, t)$ which would give different propagators but the same H_0. As a result, we argue in the following fashion.

We begin with (10) and let $\hbar$ and ϵ become small, ϵ shrinking at a faster rate, so that each term $H(p_n, q_{n+1}, q_n, t)\epsilon/\hbar$ remains small. The number N becomes correspondingly very large so that the sum over n becomes large. Then when the entire set of p_n's and q_n's are varied, there are large variations in the total phase of the exponential except near the set that gives stationary phase. This set is defined by

$$\delta\left\{\sum_{n=0}^{N-1}\left[p_{ni}(q_{n+1\,i} - q_{ni}) - H(p_n, q_{n+1}, q_n, t)\epsilon\right]\right\} = 0, \tag{40}$$

with $\delta q_{0i} = \delta q_{Ni} = 0$. On a macroscopic scale, where $\hbar$ can be considered negligible, ϵ can be considered negligible *a fortiori*, and so we make the lowest-order approximation in (40), giving

$$\delta \int \left[p_i\, dq_i - H_0(p, q, t)\, dt\right] = 0 \tag{41}$$

as desired. At other points in this article where the Dirac argument is invoked, it can be understood in the same way.

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[1] R. Fanelli, J. Math. Phys. **16**, 1729 (1975).
[2] L. Cohen, J. Math. Phys. **11**, 3296 (1970).
[3] P. Pearle, Phys. Rev. D **8**, 2503 (1973).
[4] P.A.M. Dirac, *Principles of Quantum Mechanics* (Oxford U.P., New York/London, 1958), Fourth ed.
[5] B.S. DeWitt, Rev. Mod. Phys. **29**, 377 (1957).
[6] See for example A. Messiah, *Quantum Mechanics* (Wiley, New York, 1966) Vol. I, pp. 69, 70.
[7] K.S. Cheng, J. Math. Phys. **13**, 1723 (1972), **14**, 980 (1973); I.W. Mayes and J.S. Dowker, J. Math. Phys. **14**, 434 (1973); G.S. Um, J. Math. Phys. **15**, 220 (1974).

Numerical experiments on the Calogero lattice*

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This paper presents the results of computer experiments performed on one-dimensional, classical mechanical, N-body systems whose point particles interact pairwise via the potential $V(r)=ar^2+br^{-2}$, where r is interparticle distance and where a and b are positive constants. When each particle interacts with all other particles, the numerical experiments indicate that the system is mathematically integrable for either free-end or fixed-end boundary conditions. On the other hand, when each particle interacts with only its nearest neighbors, the computer detects a transition from near-integrable to stochastic behavior again for either free-end or fixed-end boundary conditions. Our results thus support the conjecture that integrability is highly sensitive to changes in the total interaction potential but insensitive to modification of boundary conditions.

I. INTRODUCTION

In this paper, we investigate two related one-dimensional, classical, N-particle, Hamiltonian systems. In both systems, the particles interact pairwise via the potential

$$V(r)=ar^2+br^{-2}, \tag{1}$$

where r is interparticle separation distance and where a and b are positive constants. In one system, each particle interacts with all other particles, yielding the Hamiltonian

$$H=\sum_{j=1}^{N}\left(\frac{P_j^{\,2}}{2m}\right)+\sum_{j>k=1}^{N-1}[a(X_j-X_k)^2+b(X_j-X_k)^{-2}], \tag{2}$$

where the X_j and P_j denote particle coordinates and momenta and where all particles have mass m. In the other system, each particle interacts with only its nearest neighbors, yielding the Hamiltonian

$$H=\left(\sum_{j=1}^{N}\left(\frac{P_j^{\,2}}{2m}\right)+\left(\frac{1}{8a}\right)\sum_{j=1}^{N-1}\left\{a\left[Q_{j+1}-Q_j+\left(\frac{b}{a}\right)^{1/4}\right]^2\right.\right.$$
$$\left.\left.+b\left[Q_{j+1}-Q_j+\left(\frac{b}{a}\right)^{1/4}\right]^{-2}\right\}\right)-\left(\frac{(N-1)}{4}\right)\left(\frac{b}{a}\right)^{1/2}, \tag{3}$$

where the Q_j in Eq. (3) are related to the X_j in Eq. (2) via $X_j=Q_j+j(b/a)^{1/4}$, with $(b/a)^{1/4}$ being the equilibrium distance between particles when only nearest neighbors interact. The last term in Eq. (3) appears in order that $H=0$ when all Q_j and P_j are zero; the factor $(8a)^{-1}$ is introduced in order that the second sum reduce to $\frac{1}{2}\sum(Q_{j+1}-Q_j)^2$ in the low energy, harmonic approximation. As written, Hamiltonians (2) and (3) are for systems having free ends; however, we may easily convert to fixed ends by setting $Q_1\equiv Q_N\equiv 0$.

Calogero[1] was the first to suggest studying Hamiltonian systems having the pair interaction given by Eq. (1); for this reason we here refer to either Hamiltonians (2) or (3) as a Calogero lattice. In particular, Calogero[1] and later Calogero and Marchioro[2] studied the quantum mechanical behavior of the free-end Hamiltonian (2). Their results led them to conjecture that Hamiltonian (2), considered classically, should be mathematically integrable which means that all system trajectories lie on smooth, invariant, integral surfaces; indeed Marchioro[3] earlier proved integrability for the case $N=3$. Pursuant to a request from Calogero that we use a computer to test the integrability of Hamiltonian (2) in the classical case for $N>3$, we investigated Hamiltonian (2) using both free-end and fixed-end boundary conditions; in addition, we chose to examine Hamiltonian (3) using the same boundary conditions in order to determine the affect on integrability of changing the interaction range. After concluding our numerical work, we learned that Moser[4] had rigorously proved integrability for Hamiltonian (2) with free ends using a method due to Lax.[5] We nonetheless present our results for this rigorously integrable case in order that the computer results for the rigorously solved case can be compared with the results obtained for the mathematically undecided cases.

In this paper, a computer is used to produce evidence in support of integrability or its lack by numerically integrating initially close trajectory pairs and establishing whether the phase space distance between the two trajectories of a pair grows linearly or exponentially with time. Although this particular computer test is currently the most sensitive method known when the number of particles is greater than three,[6] it must nonetheless be applied with great care. In general when initially close trajectories separate linearly with time, the system is either precisely integrable[7] or it is near-integrable in the sense that most trajectories,[8] neglecting sets of small measure, lie on smooth, invariant, integral surfaces. However, it is possible, as appears to occur for the unequal-mass, hard point gas,[9] for an ergodic and mixing system to exhibit linear separation of initially close trajectories. We here rule out this latter possibility for Hamiltonians (2) and (3) by computing the time average single particle kinetic energies and demonstrating that equipartition of energy does not occur (as required for ergodicity and mixing) when trajectory-pair separation is linear. Finally, we distinguish integrable from near-integrable behavior by increasing the system energy and observing whether or not a transition (the so-called stochastic transition[6])

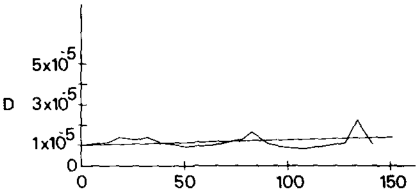

FIG. 1. A graph showing the linear growth with time of separation distance $D(t)$ between two initially close $[D(0)=10^{-5}]$ trajectories of Hamiltonian (2) for free ends and $N=4$. The solid straight line is a least squares line fit of the data points.

from linear to exponential separation occurs. If such a transition is observed, it is overwhelmingly likely[10] that the system is near-integrable rather than precisely integrable at low energy. If the linear to exponential transition does not occur as the energy becomes extremely large, then one has strong evidence for integrability at all energies. Certainly such evidence does not constitute a mathematical proof; however, this test has, before the fact, correctly predicted integrability for both the Toda Hamiltonian[7] and for Hamiltonian (2), as we show here. Thus a linear separation of initially close trajectories which persists as the energy increases to high values must be considered as a quite strong argument for integrability. Indeed for both Hamiltonian (2) and the Toda lattice, we continued to obtain linear separation between members of trajectory pairs even when the energy was so large that our numerical integration scheme was no longer providing accurate integration.

In regard to computer accuracy, we performed all our numerical integrations using a standard, double precision, fourth-order, Runge—Kutta subroutine with a variable integration step size which usually ran 0.05 or less. The total system energy was observed to remain constant to at least eight decimals. Several of our longest runs were time reversed regaining the initial state to at least four or five digit accuracy. Finally, the linear or exponential separation of initially close trajectory pairs themselves directly measure loss in integration accuracy with time.

In the following section, we present the results of our computer experiments, and, in the last section, we briefly state our conclusions.

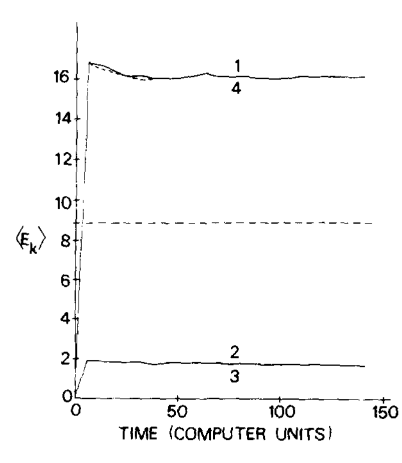

FIG. 2. A graph of the time average, single particle kinetic energies $\langle E_K\rangle$ versus time for one member of the trajectory pair investigated in Fig. 1. Here the time average, total system kinetic energy is approximately 35.5. The dotted, Horizontal line represents the equipartition value of single particle kinetic energy. No tendency toward equipartition is observed.

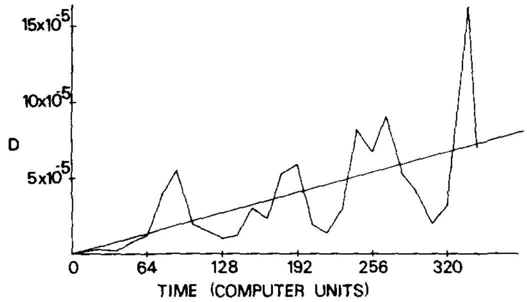

FIG. 3. A graph showing the linear growth with time of separation distance $D(t)$ between two initially close $[D(0)=10^{-7}]$ trajectories of Hamiltonian (2) for fixed ends and $N=5$.

II. PRESENTATION OF COMPUTER RESULTS

We have investigated Hamiltonian (2) for free boundaries using $N=3, 4$, and 10 and for fixed boundaries using $N=5$ and 10 (3 and 8 moving particles, respectively, since particles 1 and N are fixed). In all our calculations, we numerically set $a=b=m=1$. We performed numerical integrations for many different initial conditions at each of many distinct energies. All our experiments yielded the same results; namely, each phase space trajectory we investigated separated linearly with time from an initially close neighbor and each trajectory exhibited no tendency toward equipartition of single particle kinetic energy. Typical results are presented in Figs. 1—4. Figure 1 shows the typical linear growth of trajectory-pair separation distance D, given by

$$D=\sum_{j=1}^{N}\left[(P_j'-P_j)^2+(X_j'-X_j)^2\right]^{1/2}, \qquad (4)$$

versus time for free ends with $N=4$. Here the initial separation distance was set equal to 10^{-5} and the time average of the total kinetic energy was found to be approximately 35.5. Figure 2 presents a graph of the time average of single particle kinetic energy $E_j=(P_j^2/2m)$ versus time for one member of the trajectory pair shown in Fig. 1; no tendency toward equipartition is observed

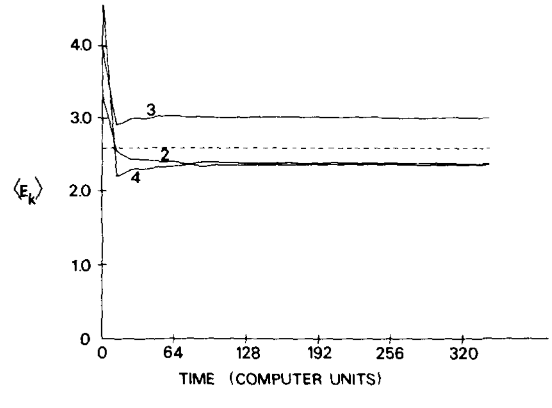

FIG. 4. A graph of the time average single particle kinetic energies $\langle E_K\rangle$ versus time for one member of the trajectory pair investigated in Fig. 3. Here the time average, total system kinetic energy is approximately 7.78, making the equipartition value approximately 2.59 for this fixed-end, $N=5$, three moving particles system. As in Fig. 2, there is no tendency toward equipartition.

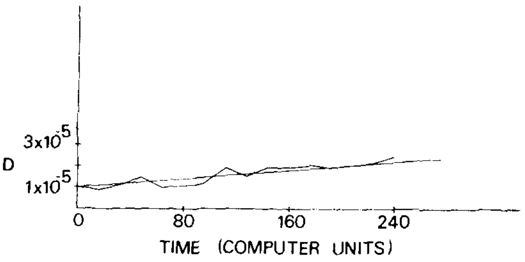

FIG. 5. A graph showing the linear growth with time of separation distance $D(t)$ between two initially close trajectories $[D(0)=10^{-5}]$ of Hamiltonian (3) using $\lambda=5$, fixed ends and a total system energy $E=1.42$.

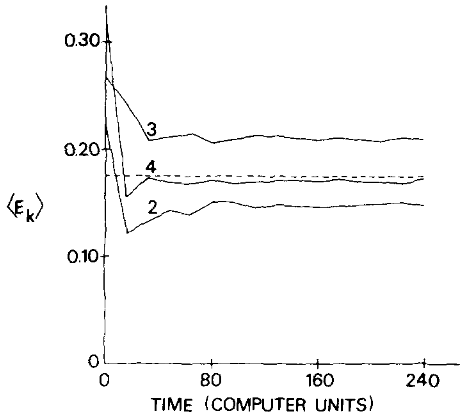

FIG. 6. A graph showing that equipartition of single particle kinetic energies $\langle E_k \rangle$ does not occur for one member of the trajectory pair investigated in Fig. 5. Here the average total kinetic energy was approximately 0.53, making the equipartition value approximately 0.176.

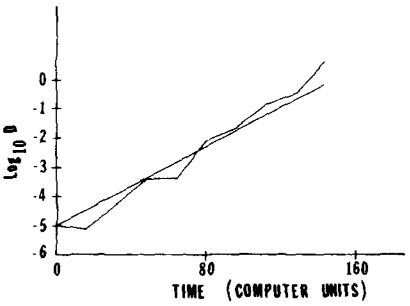

FIG. 7. By increasing the total system energy to $E=3.46$ for the system described in Fig. 5, we obtained the exponential growth of separation distances $D(t)$ shown here, indicating that Hamiltonian (3) with fixed ends is nonintegrable.

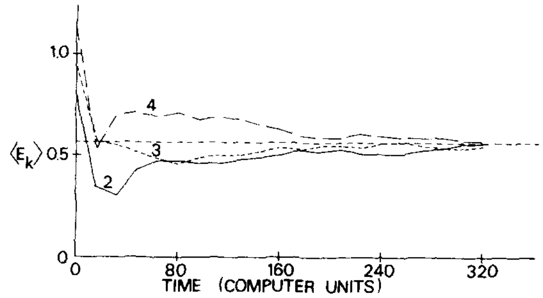

FIG. 8. For one member of the exponentially separating trajectory pair investigated in Fig. 7, we obtained the approach to equipartition of single particle kinetic energies $\langle E_k \rangle$ shown here. The equipartition value is approximately 0.563.

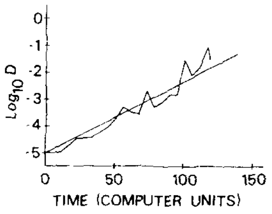

FIG. 9. This graph shows that exponential separation of initially close trajectories can also occur for Hamiltonian (3), using free ends and $N=10$. Here the total system energy $E=20$ while the average total kinetic energy is approximately 10.

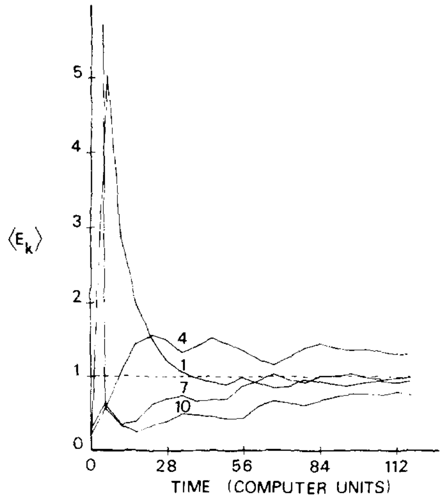

FIG. 10. The trend toward equipartition of single particle kinetic energies $\langle E_k \rangle$ for one member of the trajectory pair investigated in Fig. 9. For this ten particle system, we show curves only for particles 1, 4, 7, and 10. The equipartition value is approximately unity.

although the average kinetic energies of the end particles 1 and 4 tend toward the same value as also happens for the two interior particles 2 and 3. In Fig. 3, we show typical linear growth of trajectory pair separation distance for fixed ends with $N=5$ ($X_1 \equiv X_1' \equiv X_5 \equiv X_5' \equiv 0$). Here the initial separation distance was chosen to be 10^{-7} while the time average of the total kinetic energy was found to be approximately 7.78. The time average of single particle kinetic energy for one member of the trajectory pair shown in Fig. 3 appears in Fig. 4, where, again, equipartition is not observed. These results were found to persist even for values of the total system energy so large that our integration subroutine was unable to provide accurate trajectory integrations. These results indicate that Hamiltonian (2) is integrable for either free-end or fixed-end boundary conditions.

Our investigation of Hamiltonian (3) exposed the existence of a transition from linear to exponential separation of initially close trajectories as the total system energy is increased. In Fig. 5, we show typical linear growth of the distance D, given by

$$D=\left(\sum_{j=1}^{N}\left[(P_j'-P_j)^2+(Q_j'-Q_j)^2\right]\right)^{1/2}, \tag{5}$$

using fixed ends, $N=5$, and total energy $E=1.42$. Figure 6 shows that equipartition does not occur for either member of the trajectory pair shown in Fig. 5. However, in Fig. 7, we see that exponential separation between initially close trajectories does occur for the system of Fig. 5 when the total system energy is increased to $E=3.46$. Moreover, at this increased energy, one member of the trajectory-pair shown in Fig. 7 yields the equipartition of single particle kinetic energy shown in Fig. 8. Finally, in Fig. 9, we show that exponential separation also occurs for Hamiltonian (3) using free ends, $N=10$, and a total system energy $E=20$. The trend toward equipartition is shown in Fig. 10 for one member of the trajectory pair shown in Fig. 9.

III. CONCLUSIONS

Our computer experiments indicate that the Calogero Hamiltonian (2) is integrable for either free or fixed ends. The correctness of this computer prediction, at least for the free-end case, has been confirmed by a completely independent, rigorous analysis due to Moser. On the other hand, the computer experiments indicate that the Calogero Hamiltonian (3) is nonintegrable and that it exhibits a stochastic transition for either free or fixed ends. Clearly these computer results do not constitute a proof; however, in view of the accuracy of past computer predictions, the evidence presented here must be regarded as quite strong indeed.

The Calogero lattice of Hamiltonian (2) thus joins the equal-mass Toda lattice[7] in being an integrable nonlinear system having both attractive and repulsive interparticle forces; indeed this Calogero lattice has long range attractive forces. The Calogero lattice of Hamiltonian (3), on the other hand, joins the unequal-mass Toda lattice[11] as a nonintegrable system exhibiting a stochastic transition. These two models will likely prove significant for both mathematics and physics. The integrable models illuminate new methods for exactly solving nonlinear systems while the stochastic models provide insights into the nature of thermodynamic irreversibility. In particular, a study of energy transport in these systems may greatly increase our understanding of thermal conductivity.

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[1] F. Calogero, J. Math. Phys. 12, 419 (1971).
[2] F. Calogero and C. Marchioro, J. Math. Phys. 15, 1425 (1974).
[3] C. Marchioro, J. Math. Phys. 11, 2193 (1970).
[4] J. Moser, Advan. Math. (to be published).
[5] P.D. Lax, Comm. Pure Appl. Math. 21, 467 (1968).
[6] B.V. Chirikov, "Research Concerning the Theory of Non-Linear Resonances and Stochasticity," Report No. 267, Institute of Nuclear Physics, Novosibirsk, USSR, 1969 (unpublished). An English translation of this report is available as Translation 71-40, CERN, Geneva, 1971.
[7] J. Ford, S.D. Stoddard, and J.S. Turner, Prog. Theor. Phys. 50, 1547 (1973).
[8] V.I. Arnold and A. Avez, *Ergodic Problems of Classical Mechanics* (Benjamin, New York, 1968), Chap. 4,
[9] G. Casati and J. Ford, J. Comput. Phys. (to be published).
[10] E. Zehnder, Comm. Pure Appl. Math. 25, 131 (1973).
[11] G. Casati and J. Ford, Phys. Rev. A 12. 1702 (1975).

Stationary scattering for N-body systems involving Coulomb potentials

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A stationary Hilbert space scattering theory is derived for N-body systems involving Coubomb-like potentials. The derivation is based on stationary representations of the α-channel renormalized wave operators, $\Omega_{\pm}^{(a)}$, having the form $\Omega_{\pm}^{(a)} = \text{s-lim}_{\epsilon\to+\infty} W_{\pm\epsilon}^{(a)} P^{(a)} F_{\pm\epsilon}^{(a)*}$, where $W_{\pm\epsilon}^{(a)} P^{(a)}$ are the stationary operators which form the basis of short-range stationary scattering theory and $F_{\pm\epsilon}^{(a)*}$ are appropriate stationary "renormalization" terms.

I. INTRODUCTION

A general time-dependent potential scattering theory can be based on the "modified" or "renormalized" α-channel wave operators, $\Omega_{\pm}^{(\alpha)}$, defined as follows:

$$\Omega_{\pm}^{(\alpha)} = \operatorname*{s-lim}_{t\to\pm\infty} W^{(\alpha)}(t)\exp[-iG^{(\alpha)}(t)]P^{(\alpha)},$$
$$W^{(\alpha)}(t) = \exp(iHt)\exp(-iH_\alpha t), \tag{1.1}$$

where H denotes the full Hamiltonian, H_α the α-channel Hamiltonian, $P^{(\alpha)}$ the projector onto the α-channel subspace $\mathcal{H}^{(\alpha)}$ and the "renormalization" term $G^{(\alpha)}(t)$ is an appropriate function of the time and center-of-mass momenta of the n_α fragments making up the channel α. The renormalized wave operators were first shown to exist by Dollard[1] for the case of Coulomb-like scattering with $G^{(\alpha)}(t)$ given by

$$G^{(\alpha)}(t) = \epsilon(t)\sum_{j<k}^{n_\alpha} \frac{M_j M_k e_j e_k}{|M_j\mathbf{p}_k - M_k\mathbf{p}_j|} \times\log\left(\frac{2|t|\,|M_j\mathbf{p}_k - M_k\mathbf{p}_j|^2}{M_j M_k(M_j + M_k)}\right),$$
$$\epsilon(t) = \begin{cases} 1, & t>0, \\ -1, & t<0, \end{cases} \tag{1.2}$$

where M_j, e_j, and $\mathbf{p}_j$ denote respectively the mass, charge, and center-of-mass momenta of the jth fragment.

For time-dependent theories for which $G^{(\alpha)}(t)$ can be chosen to be zero, i.e., scattering via short-range potentials, a mathematically rigorous stationary formalism can be developed in terms of the following strong[2] or weak[3] Riemann–Stieltjes integral representations for $\Omega_{\pm}^{(\alpha)}$

$$\Omega_{\pm}^{(\alpha)} = \operatorname*{s-lim}_{\epsilon\to+0} W_{\pm\epsilon}^{(\alpha)} P^{(\alpha)} \tag{1.3}$$

where

$$W_{\pm\epsilon}^{(\alpha)} = \pm\int_0^{\pm\infty} du\,\exp(\mp u)W^{(\alpha)}(u/\epsilon)$$
$$= \int_{-\infty}^{+\infty} \frac{\pm i\epsilon}{H-\lambda\pm i\epsilon}\, d_\lambda E_\lambda^{H_\alpha} \tag{1.4}$$
$$= \int_{-\infty}^{+\infty} d_\lambda E_\lambda^H \frac{\mp i\epsilon}{H_\alpha - \lambda \mp i\epsilon},$$

with $E_\lambda^{H_\alpha}$ and E_λ^H denoting the spectral families corresponding to H_α and H respectively.

When long-range potentials are present, i.e., when $G^{(\alpha)}(t)$ cannot be chosen to be zero, the stationary representations (1.3) are no longer valid. In particular, since (1.3) leads to the well-known relationship between the complex energy distorted waves and the physical distorted waves this relationship will not be valid when long-range forces are present.

Recently, the following stationary representations of the renormalized wave operators for Coulomb-like scattering have been derived,[4]

$$P_{\Delta_\alpha}\Omega_{\pm}^{(\alpha)*} = \operatorname*{s-lim}_{\epsilon\to+0} P_{\Delta_\alpha} F_{\pm\epsilon}^{(\alpha)} W_{\pm\epsilon}^{(\alpha)*} R_{\pm}^{(\alpha)}, \tag{1.5}$$

where $R_{\pm}^{(\alpha)}$ denote the ranges of $\Omega_{\pm}^{(\alpha)}$, P_{Δ_α} projects onto functions of the form $\phi = \phi_1 \Pi_{j=1}^{\alpha} \chi_j \in \mathcal{H}^{(\alpha)}$ where χ_j, $j=1,\ldots,n_\alpha$, denote the bound states which make up the channel α and $\hat{\phi}_1$, where $\hat{\phi}_1$ denotes the $3n_\alpha$-dimensional Fourier transform of ϕ_1, satisfies $\chi_{\Delta_\alpha}\hat{\phi}_1 = \hat{\phi}_1$ where for an arbitrary fixed $\eta>0$,

$$\Delta_\alpha = \{\mathbf{p}_j,\ j=1,\ldots,n_\alpha:\ |M_j\mathbf{p}_k - M_k\mathbf{p}_j| > \eta \text{ for each } k>j\} \tag{1.6}$$

and the stationary renormalization term is given by

$$F_{\pm\epsilon}^{(\alpha)*} = \Gamma\left(1 \pm i\sum_{j<k}^{n_\alpha} \frac{M_j M_k e_j e_k}{|M_j\mathbf{p}_k - M_k\mathbf{p}_j|}\right)^{-1} \times\exp\left(\pm i\sum_{j<k}^{n_\alpha} \frac{M_j M_k e_j e_k}{|M_j\mathbf{p}_k - M_k\mathbf{p}_j|}\log\frac{\epsilon M_j M_k(M_j+M_k)}{2|M_j\mathbf{p}_k - M_k\mathbf{p}_j|^2}\right). \tag{1.7}$$

The stationary representations (1.5) have been used[4,5] to derive the relationship between the complex energy distorted waves and off-energy-shell "T matrix," and the corresponding physical distorted waves and on-energy-shell S matrix for two-body Coulomb-like scattering. This derivation was restricted to two-body scattering due to the explicit occurrence of the ranges $R_{\pm}^{(\alpha)}$ in the stationary representations (1.5).

In this paper we will show that stationary representations for $\Omega_{\pm}^{(\alpha)}$, similar to (1.5), however without the ranges $R_{\pm}^{(\alpha)}$, are valid [Theorem (2.1)]. In Sec. III we apply these stationary representations to derive a stationary Hilbert space scattering formalism for general N-body Coulomb-like scattering.

II. STATIONARY REPRESENTATIONS OF THE COULOMB-LIKE RENORMALIZED WAVE OPERATORS

The scattering systems considered in this paper will be assumed to consist of N distinguishable spinless particles described by the self-adjoint Hamiltonian H of the form

$$
\begin{aligned}
&H=H_0+V, \quad H_0=-\sum_{i=1}^{N}(2m_i)^{-1}\nabla_i^2,\\
&V=\sum_{i<i'}^{N} V_{ii'}(\mathbf{x}_i-\mathbf{x}_{i'}),\\
&V_{ii'}(\mathbf{x})=\hat{e}_i\hat{e}_{i'}\,|x|^{-1}+V_{ii'}^{(s)}(\mathbf{x}_i-\mathbf{x}_{i'}),
\end{aligned}
\tag{2.1}
$$

with domain $\mathcal{D}(H_0)$ and each $V_{ii'}$ symmetric on $\mathcal{D}(V_{ii'})\supset\mathcal{D}(H_0)$ where $m_i(\hat{e}_i)$ denote the mass (charge) of the ith particle and $V_{ii'}^{(s)}$ are short range potentials, i.e.,

$$
V_{ii'}^{(s)}(\mathbf{x})=O(|\mathbf{x}|^{-1-\epsilon_0}), \quad \epsilon_0>0, \quad |\mathbf{x}|\to\infty. \tag{2.2}
$$

We will further assume that for each channel α the α-channel Hamiltonian, H_α, is self-adjoint on $\mathcal{D}(H_\alpha)=\mathcal{D}(H_0)$. In addition, H_α will be assumed to have the decomposition

$$
H_\alpha=H_\alpha^{\text{kin}}+H_\alpha^{\text{int}} \tag{2.3}
$$

where H_α^{kin} depends only on the center-of-mass momentum variables of the fragments making up the channel α and H_α^{int} depends only on the internal coordinates of the α-channel fragments and has a pure point spectrum on $\mathcal{H}^{(\alpha)}$.

The above general requirements will be implicitly assumed hereafter.

In the following we will denote by $\mathcal{D}^{(\alpha)}$ the set of functions, dense in $\mathcal{H}^{(\alpha)}$, having the form $\phi=\phi_1\Pi_{j=1}^{n_\alpha}\chi_j\in\mathcal{H}^{(\alpha)}$ where χ_j, $j=1,\ldots,n_\alpha$, denote the bound state wave functions making up the channel α and $\phi_1\in L^2(\mathbb{R}^{3n_\alpha})$ is such that

$$
\Gamma\left(1\pm i\sum_{j<k}^{n_\alpha}\frac{M_jM_ke_je_k}{|M_j\nabla_k-M_k\nabla_j|}\right)^{-1}\phi_1\in L^2(\mathbb{R}^{3n_\alpha}).
$$

Theorem (2.1): Assume that the renormalized wave operators, $\Omega_\pm^{(\alpha)}$, for Coulomb-like scattering exist. Then $\Omega_\pm^{(\alpha)}$ have the following stationary representations

$$
\Omega_\pm^{(\alpha)}\psi=\operatorname*{s-lim}_{s\to+0}W_{\pm\epsilon}^{(\alpha)}F_{\pm\epsilon}^{(\alpha)*}\psi \tag{2.4}
$$

valid for each $\psi\in\mathcal{D}^{(\alpha)}$ with $W_{\pm\epsilon}^{(\alpha)*}$ and $F_{\pm\epsilon}^{(\alpha)}$ given by (1.4) and (1.7) respectively.

Proof: We use the Bochner integral representations of $W_{\pm\epsilon}^{(\alpha)}$ given by (1.4) to write for $\psi\in\mathcal{D}^{(\alpha)}$,

$$
\begin{aligned}
&W_{\pm\epsilon}^{(\alpha)}F_{\pm\epsilon}^{(\alpha)*}\psi\\
&\quad=\pm\int_0^{\pm\infty}du\exp(\mp u+iHu/\epsilon)\exp(-iH_\alpha u/\epsilon)F_{\pm\epsilon}^{(\alpha)*}\psi.
\end{aligned}
$$

Using the explicit form of $F_{\pm\epsilon}^{(\alpha)*}$ given by (1.6) allows us to rewrite the above as follows

$$
\begin{aligned}
&W_{\pm\epsilon}^{(\alpha)}F_{\pm\epsilon}^{(\alpha)*}\psi\\
&\quad=\int_0^{\pm\infty}du\exp(\mp u+iHu/\epsilon)\exp[-iH_\alpha u/\epsilon-iG^{(\alpha)}(u/\epsilon)]\\
&\qquad\times\exp\left(\pm i\sum_{j<k}^{n_\alpha}\frac{M_jM_ke_je_k}{|M_j\nabla_k-M_k\nabla_j|}\log|u|\right)\\
&\qquad\times\Gamma\left(1\pm i\sum_{j<k}^{n_\alpha}\frac{M_jM_ke_je_k}{|M_j\nabla_k-M_k\nabla_j|}\right)^{-1}\psi
\end{aligned}
\tag{2.5}
$$

where $G^{(\alpha)}$ is given by (1.2). By the Lebesgue dominated convergence theorem for Bochner integrals (Ref. 6, Theorem 3.7.9) the strong limit $\epsilon\to+0$ of (2.5) can be taken under the integral for each $\psi\in\mathcal{D}^{(\alpha)}$ to obtain

$$
\begin{aligned}
&\operatorname*{s-lim}_{\epsilon\to+\infty}W_{\pm\epsilon}^{(\alpha)}F_{\pm\epsilon}^{(\alpha)*}\psi\\
&\quad=\Omega_\pm^{(\alpha)}(\pm1)\int_0^{\pm\infty}du\exp\left(\mp u\pm i\sum_{j<k}^{n_\alpha}\frac{M_jM_ke_je_k}{|M_j\nabla_k-M_k\nabla_j|}\right.\\
&\qquad\left.\times\log|u|\right)\;\Gamma\left(1\pm i\sum_{j<k}^{n_\alpha}\frac{M_jM_ke_je_k}{|M_j\nabla_k-M_k\nabla_j|}\right)^{-1}\psi=\Omega_\pm^{(\alpha)}\psi,
\end{aligned}
$$

which proves (2.4).

The above proof of the stationary representations (2.4) depends explicitly on the logarithmic dependence on $|t|$ of the renormalization term $G^{(\alpha)}(t)$. In the case of two-body scattering via potentials satisfying $V(x)=O(|\mathbf{x}|^{-\gamma})$, $\frac{1}{2}<\gamma<1$ as $|\mathbf{x}|\to\infty$, the time-dependent renormalization term[7] leads (via a similar argument as given in Ref. 4 to obtain $F_{\pm\epsilon}^{(\alpha)}$) to the following stationary renormalization terms,

$$
\left[(\pm\epsilon)\int_0^{\pm\infty}dt\exp\left(\mp\epsilon t\pm i\frac{q(\gamma)M^\gamma}{(1-\gamma)p^\gamma}t^{1-\gamma}\right)\right]^{-1} \tag{2.6}
$$

where $q(\gamma)$ is a real constant, M denotes the reduced mass, and $p=|\mathbf{p}|$, where $\mathbf{p}$ is the relative momenta. We note that the techniques used to prove (1.5) and (2.4) are not immediately applicable since the stationary renormalization terms (2.6) are infinite in the limit $\epsilon\to+0$.

III. STATIONARY HILBERT SPACE FORMALISM

In this section, we derive a stationary Hilbert space formalism for N-body Coulomb-like scattering from the stationary representations (2.4) for the renormalized wave operators.

It follows from the Riemann–Stieltjes integral representations (1.4) that the following equalities are valid for each $\epsilon>0$ and each $\psi\in\mathcal{D}^{(\alpha)}$,

$$
\begin{aligned}
W_{\pm\epsilon}^{(\alpha)}F_{\pm\epsilon}^{(\alpha)*}\psi&=\int_{-\infty}^{+\infty}\frac{\pm i\epsilon}{H-\lambda\pm i\epsilon}d_\lambda E_\lambda^{H_\alpha}F_{\pm\epsilon}^{(\alpha)*}\psi.\\
&=\int_{-\infty}^{+\infty}d_\lambda E_\lambda^{H}\frac{\mp i\epsilon}{H_\alpha-\lambda\mp i\epsilon}F_{\pm\epsilon}^{(\alpha)*}\psi.
\end{aligned}
\tag{3.1}
$$

Furthermore, for $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$ where $\tilde{\mathcal{D}}^{(\alpha)}$ is defined as follows,

$$
\tilde{\mathcal{D}}^{(\alpha)}=\left\{\psi\in\mathcal{D}^{(\alpha)}\,\middle|\,\Gamma\left(1\pm i\sum_{j<k}^{n_\alpha}\frac{M_jM_ke_je_k}{|M_j\nabla_k-M_k\nabla_j|}\right)^{-1}\psi\in\mathcal{D}(H_\alpha)\right\},
$$

we can apply Lemma 5 of Ref. 2 to rewrite the first equality in (3.1) as follows for each $\epsilon>0$,

$$
\begin{aligned}
&W_{\pm\epsilon}^{(\alpha)}F_{\pm\epsilon}^{(\alpha)*}\psi\\
&\quad=F_{\pm\epsilon}^{(\alpha)*}\psi-\int_{-\infty}^{+\infty}\frac{1}{H-\lambda\pm i\epsilon}\\
&\qquad\times V^{(\alpha)}d_\lambda E_\lambda^{H_\alpha}F_{\pm\epsilon}^{(\alpha)*}\psi,
\end{aligned}
\tag{3.2}
$$

where $V^{(\alpha)}=H-H_\alpha$.

The equalities (3.1) and (3.2) together with (2.4) allow us to state the following theorem which provides solution integral equations in Hilbert space for the Coulomb-like renormalized wave operators.

Theorem (3.1): Assume that the stationary representations (2.4) for the Coulomb-like renormalized wave operators are valid. Then for each $\psi\in\mathcal{D}^{(\alpha)}$ we have

$$\begin{aligned}\Omega_\pm^{(\alpha)}\psi&=\operatorname*{s-lim}_{\epsilon\to+0}\int_{-\infty}^{+\infty}\frac{\pm i\epsilon}{H-\lambda\pm i\epsilon}\,d_\lambda E_\lambda^{H_\alpha}F_{\pm\epsilon}^{(\alpha)*}\psi\\&=\operatorname*{s-lim}_{\epsilon\to+0}\int_{-\infty}^{+\infty}d_\lambda E_\lambda^{H}\frac{\mp i\epsilon}{H_\alpha-\lambda\pm i\epsilon}\,F_{\pm\epsilon}^{(\alpha)*}\psi.\end{aligned}\tag{3.3}$$

Furthermore, the following solution integral equations are valid,

$$\begin{aligned}\Omega_\pm^{(\alpha)}\psi=\operatorname*{s-lim}_{\epsilon\to+0}\Bigg\{F_{\pm\epsilon}^{(\alpha)*}\psi-\int_{-\infty}^{-\infty}\frac{1}{H-\lambda\pm i\epsilon}\\\times V^{(\alpha)}d_\lambda E_\lambda^{H_\alpha}F_{\pm\epsilon}^{(\alpha)*}\psi\Bigg\}\text{ for each }\psi\in\tilde{\mathcal{D}}^{(\alpha)}.\end{aligned}\tag{3.4}$$

In order to derive stationary Riemann—Stieltjes integral representations for the S operator, we will require the following lemma.

Lemma (3.2): Assume that the Coulomb-like renormalized wave operators exist. Then for all channels α and β we have

$$\lim_{\epsilon\to+0}\langle F_{+\epsilon}^{(\beta)*}\phi\,|\,W_{-\epsilon}^{(\beta)*}\Omega_-^{(\alpha)}\psi\rangle=0\tag{3.5}$$

for all $\phi\in\mathcal{D}^{(\beta)}$ $\psi\in\mathcal{H}^{(\alpha)}$ and

$$\operatorname*{w-lim}_{\epsilon\to+0}\Omega_+^{(\beta)*}W_{+\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*}\psi=0\tag{3.6}$$

for $\psi\in\mathcal{D}^{(\alpha)}$.

Proof: From the integral representation (1.4) for $W_{-\epsilon}^{(\beta)*}$ we have for $\phi\in\mathcal{D}^{(\beta)}$ and $\psi\in\mathcal{H}^{(\alpha)}$,

$$\begin{aligned}&\langle F_{+\epsilon}^{(\beta)*}\phi\,|\,W_{-\epsilon}^{(\beta)*}\Omega_-^{(\alpha)}\psi\rangle\\&\quad=-\int_0^{-\infty}du\exp(u)\langle F_{+\epsilon}^{(\beta)*}\phi\,|\,\exp(iH_\beta u/\epsilon)\exp(-iHu/\epsilon)\Omega_-^{(\alpha)}\psi\rangle.\end{aligned}$$

We now note that due to the existence of the renormalized wave operators the following equality is valid,

$$\begin{aligned}\lim_{\epsilon\to+0}\{\langle F_{+\epsilon}^{(\beta)*}\phi\,|\,W_{-\epsilon}^{(\beta)*}\Omega_-^{(\alpha)}\psi\rangle+\int_0^{-\infty}du\exp(u)\\\times\langle F_{+\epsilon}^{(\beta)*}\phi\,|\exp(iH_\beta u/\epsilon)\exp[-iH_\alpha u/\epsilon-iG^{(\alpha)}(u/\epsilon)]\psi\rangle\}=0.\end{aligned}$$

Thus from the above equality, (3.5) will be valid if for each $\phi\in\mathcal{D}^{(\beta)}$ and $\psi\in\mathcal{H}^{(\alpha)}$ we have

$$\begin{aligned}\lim_{\epsilon\to+0}(-1)\int_0^{-\infty}du\exp(u)\\\times\ \langle F_{+\epsilon}^{(\beta)*}\phi\,|\ \exp[-i(H_\alpha-H_\beta)u/\epsilon-iG^{(\alpha)}(u/\epsilon)]\psi\rangle=0.\end{aligned}\tag{3.7}$$

We first note that if α and β are two channels which have in common a complex fragment whose bound state wavefunctions correspond to different energy eigenvalues, then (3.7) is immediately valid due to the orthogonality of the bound state wavefunctions.

In order to prove (3.7) and hence (3.5) for general channels α and β we can apply the Lebesgue dominated convergence theorem to see that (3.7) will be valid if the limit $\epsilon\to+0$ of the following expression is zero,

$$\langle F_{+\epsilon}^{(\beta)*}\phi\,|\exp[-i(H_\alpha-H_\beta)u/\epsilon-iG^{(\alpha)}(u/\epsilon)]\psi\rangle,\tag{3.8}$$

for all ϕ contained in a dense subset of $\mathcal{D}^{(\beta)}$ and all ψ contained in a dense subset of $\mathcal{H}^{(\alpha)}$.

In the case $\alpha=\beta$, we can transform expression (3.8) to the momentum representation and choose as the dense set of functions $\phi=\phi_1\Pi_{j=1}^{n_\alpha}\chi_j$, where ϕ_1 is a Schwartz function with $\operatorname{supp}\phi_1\subset\Delta_\alpha$, where Δ_α is defined by (1.6) with $\eta=0$. By an appropriate integration by parts the limit $\epsilon\to+0$ of (3.8) can be shown to be zero and thus (3.5) is valid for the case $\alpha=\beta$.

We finally consider the case $\alpha\neq\beta$ with α and β different arrangement channels. Thus we have, $H_\alpha-H_\beta=\sum_{l=1}^N\gamma_lk_l^2+\gamma_0$, where the $\mathbf{k}_i$, $i=1,\ldots,N$, denote the momentum variables of the N particles and at least one of the constants γ_l, $l=0,\ldots,N$, say γ_1, is nonzero. The functions ϕ and ψ in (3.8) will be chosen from $\kappa^{(\alpha)}$ and $\kappa^{(\beta)}$ respectively, where $\kappa^{(\gamma)}$ consists of functions $\tilde{\chi}(\mathbf{k}_1,\ldots,\mathbf{k}_N)$, where $\tilde{\chi}$ denotes the $3N$-dimensional Fourier transform of χ, with $\tilde{\chi}$ a Schwartz function which is zero in a neighborhood of $M_j\sum_iC_i^{(k)}\mathbf{k}_i-M_k\sum_iC_i^{(j)}\mathbf{k}_i=0$, for each $j<k$, $j,k=1,\ldots,n_\gamma$, where $\mathbf{p}_l=\sum_iC_i^{(l)}\mathbf{k}_i$, and in addition $\tilde{\chi}$ is zero in a neighborhood of $\mathbf{k}_1=0$. Thus, by an appropriate integration by parts in the first component k_{11} of $\mathbf{k}_1$, the limit $\epsilon\to+0$ of (3.8) is zero, which concludes the proof of (3.5).

The proof of the relation (3.6) is analogous to the proof of (3.5) given above and thus will be omitted.

The S operator $S_{\alpha\beta}$, corresponding to an incoming channel α and outgoing channel β, is defined in terms of the renormalized wave operators as follows:

$$S_{\alpha\beta}=(1/2\pi i)\Omega_+^{(\beta)*}\Omega_-^{(\alpha)}.\tag{3.9}$$

We will now apply Lemma (3.2) to derive stationary representations of $S_{\alpha\beta}$.

Theorem (3.3): Assume that the renormalized wave operators for Coulomb-like scattering exist. Then $S_{\alpha\beta}$ has the following strong Riemann—Stieltjes integral representations:

$$\begin{aligned}&\langle\phi\,|\,S_{\alpha\beta}\psi\rangle\\&\quad=-(1/\pi)\lim_{\epsilon\to+0}\Bigg\langle F_{+\epsilon}^{(\beta)*}\phi\,\Bigg|\\&\qquad\times\int_{-\infty}^{+\infty}d_\lambda E_\lambda^{H_\beta}V^{(\beta)}\Omega_-^{(\alpha)}\frac{\epsilon}{(H_\alpha-\lambda)^2+\epsilon^2}\psi\Bigg\rangle,\end{aligned}\tag{3.10}$$

valid for $\phi\in\mathcal{D}^{(\beta)}$ and $\psi\in\mathcal{H}^{(\alpha)}$ and

$$\begin{aligned}S_{\alpha\beta}\psi=-(1/\pi)\operatorname*{w-lim}_{\epsilon\to+0}\int_{-\infty}^{+\infty}\frac{\epsilon}{(H_\beta-\lambda)^2+\epsilon^2}\\\times\Omega_+^{(\beta)*}V^{(\alpha)}d_\lambda E_\lambda^{H_\alpha}F_{-\epsilon}^{(\alpha)*}\psi,\end{aligned}\tag{3.11}$$

where $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$.

Proof: It follows from (2.4) that

$$\langle\phi\,|\,\Omega_{\pm}^{(\beta)*}\psi\rangle=\lim_{\epsilon\to+0}\langle F_{\pm\epsilon}^{(\beta)*}\phi\,|\,W_{\pm\epsilon}^{(\beta)*}\psi\rangle \tag{3.12}$$

for $\phi\in\mathcal{D}^{(\beta)}$ and $\psi\in\mathcal{H}$, where $W_{\pm}^{(\beta)*}$ are given by the following strong Riemann–Stieltjes integrals:

$$W_{\pm\epsilon}^{(\beta)*}=\int_{-\infty}^{+\infty}d_{\lambda}E_{\lambda}^{H}{}_{\beta}\,\frac{\mp i\epsilon}{H-\lambda\mp i\epsilon}. \tag{3.13}$$

Thus from (3.12) and (3.5) we have for $\phi\in\mathcal{D}^{(\beta)}$ and $\psi\in\mathcal{H}^{(\alpha)}$,

$$\langle\phi\,|S_{\alpha\beta}\psi\rangle=(1/2\pi i)\lim_{\epsilon\to+0}\,\langle F_{+\epsilon}^{(\beta)*}\phi\,|\,\{W_{+\epsilon}^{(\beta)*}-W_{-\epsilon}^{(\beta)*}\}\Omega_{-}^{(\alpha)}\psi\rangle.$$

Inserting the explicit Riemann–Stieltjes integral representations (3.13) for $W_{\pm\epsilon}^{(\beta)*}$ and using the interwining properties [cf. Theorem (4.1) Ref. 8] yields

$$\begin{aligned}\langle\phi\,|\,S_{\alpha\beta}\psi\rangle&\\ =-(1/\pi)\lim_{\epsilon\to+0}&\Big\langle F_{+\epsilon}^{(\beta)*}\phi\,\Big|\\ &\times\int_{-\infty}^{+\infty}d_{\lambda}\,E_{\lambda}^{H}{}_{\beta}(H-\lambda)\Omega_{-}^{(\alpha)}\frac{\epsilon}{(H_{\alpha}-\lambda)^{2}+\epsilon^{2}}\,\psi\Big\rangle.\end{aligned} \tag{3.14}$$

In order to complete the proof of (3.10) we must show

$$\begin{aligned}&\int_{\infty}^{+\infty}d_{\lambda}\,E_{\lambda}{}^{H}{}_{\beta}(H-\lambda)\Omega_{-}^{(\alpha)}\frac{\epsilon}{(H_{\alpha}-\lambda)^{2}+\epsilon^{2}}\,\psi\\ &\quad=\int_{-\infty}^{+\infty}d_{\lambda}\,E_{\lambda}^{H}{}_{\beta}V^{(\beta)}\Omega_{-}^{(\alpha)}\frac{\epsilon}{(H_{\alpha}-\lambda)^{2}+\epsilon^{2}}\,\psi\end{aligned} \tag{3.15}$$

for all $\psi\in\mathcal{H}^{(\alpha)}$. We first note that if the above equality is valid for finite intervals of integration then it is valid for infinite intervals of integration. Thus, for an arbitrary subdivision $\pi_{n}=\{a=\lambda_{1}<\circ\circ\cdot<\lambda_{n}=b\}$ of (a,b) with $|\pi_{n}|=\sup_{k}|\lambda_{k}-\lambda_{k-1}|$ and $\lambda_{k}'\in(\lambda_{k-1},\lambda_{k})$ we consider

$$\begin{aligned}&\left\|\sum_{k=1}^{n}(E_{\lambda_{k}}^{H}{}_{\beta}-E_{\lambda_{k-1}}^{H}{}_{\beta})\{(H-\lambda_{k}')-V^{(\beta)}\}\Omega_{-}^{(\alpha)}\,\frac{\epsilon}{(H_{\alpha}-\lambda_{k}')^{2}+\epsilon^{2}}\,\psi\right\|^{2}\\ &\quad=\sum_{k=1}^{n}\left\|\,(E_{\lambda_{k}}^{H}{}_{\beta}-E_{\lambda_{k-1}}^{H}{}_{\beta})(H_{\beta}-\lambda_{k}')\Omega_{-}^{(\alpha)}\frac{\epsilon}{(H_{\alpha}-\lambda_{k}')^{2}+\epsilon^{2}}\,\psi\right\|^{2}.\\ &\quad\leqslant|\pi_{n}|^{2}\left\|\sum_{k=1}^{n}(E_{\lambda_{k}}^{H}{}_{\beta}-E_{\lambda_{k-1}}^{H}{}_{\beta})\Omega_{-}^{(\alpha)}\frac{\epsilon}{(H_{\alpha}-\lambda_{k}')^{2}+\epsilon^{2}}\,\psi\right\|^{2}.\end{aligned}$$

Since the last expression above converges to zero as $|\pi_{n}|\to+0$, the equality (3.15) is valid.

In order to prove representation (3.11) we use (2.4) together with (3.6), which yields

$$S_{\alpha\beta}\psi=(1/2\pi i)\,\mathrm{w}\text{-}\lim_{\epsilon\to+0}\Omega_{+}^{(\beta)*}\{W_{-\epsilon}^{(\alpha)}-W_{+\epsilon}^{(\alpha)}\}F_{-\epsilon}^{(\alpha)*}\psi$$

for all $\psi\in\mathcal{D}^{(\alpha)}$. It is easy to see by an analogous argument as given for (3.10) together with Lemma 5 of Ref. 2, that (3.11) follows from the above equality.

The stationary representation (3.10) relates $V^{(\beta)}\Omega_{-}^{(\alpha)}$ to the scattering operator $S_{\alpha\beta}$. We will now derive the relation between the operators $V^{(\beta)}W_{-\epsilon_2}^{(\alpha)}$, $\epsilon_2>0$, and $S_{\alpha\beta}$. In the case of short range potential scattering this relationship has been derived and is provided by Lemma 4 of Ref. 2 and Theorem 2 of Ref. 9. The proof of the following Lemma (3.4) and Theorem (3.5) is a generalization of the proof of Theorem 1 of Ref. 9 and Lemma 4 of Ref. 2 respectively, which takes into account the stationary renormalization term $F_{-\epsilon}^{(\alpha)*}$.

Lemma (3.4): Assume that the stationary representations (2.4) of the Coulomb-like renormalized wave operators are valid. Then for each $\epsilon>0$, $W_{\pm\epsilon}^{(\alpha)}F_{\pm\epsilon}^{(\alpha)*}$ map $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$ into $\mathcal{D}(H)$. Furthermore, there exists nonnegative constants α, β, γ, δ and ω such that for each $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$ we have

$$\begin{aligned}\|V^{(\beta)}(\Omega_{-}^{(\alpha)}-W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*})\psi\|&\leqslant\alpha\,\|\psi\|+\beta\|H_{\alpha}\psi\|\\ &+\gamma\left\|H_{\alpha}\Gamma\left(1-i\sum_{j<k}^{n_{\alpha}}\frac{M_{j}M_{k}e_{j}e_{k}}{|M_{j}\nabla_{k}-M_{k}\nabla_{j}|}\right)^{-1}\psi\right\|\\ &+(\delta+\epsilon\omega)\left\|\Gamma\left(1-i\sum_{j<k}^{n_{\alpha}}\frac{M_{j}M_{k}e_{j}e_{k}}{|M_{j}\nabla_{k}-M_{k}\nabla_{j}|}\right)^{-1}\psi\right\|.\end{aligned} \tag{3.16}$$

In addition, the following equality is valid;

$$\mathrm{s}\text{-}\lim_{\epsilon\to+0}V^{(\beta)}(\Omega_{-}^{(\alpha)}-W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*})\psi=0, \tag{3.17}$$

for each $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$.

Proof: It has been shown in Theorem 1 of Ref. 9 that $W_{\pm\epsilon}^{(\alpha)}$ maps $\mathcal{D}(H_{\alpha})$ into $\mathcal{D}(H)$. Since $F_{\pm\epsilon}^{(\alpha)*}\psi\in\mathcal{D}(H_{\alpha})$ for each $\psi\in\mathcal{D}^{(\alpha)}$ we have $W_{\pm\epsilon}^{(\alpha)}F_{\pm\epsilon}^{(\alpha)*}\psi\in\mathcal{D}(H)$ for each $\epsilon>0$.

As a consequence of Lemma 1 of Ref. 2 there exists nonnegative constants a and b such that the following bound is valid,

$$\begin{aligned}&\|\exp(iHu/\epsilon)H\exp(-iH_{\alpha}u/\epsilon)F_{-\epsilon}^{(\alpha)*}\psi\|\\ &\quad\leqslant a\left\|H_{\alpha}\Gamma\left(1-i\sum_{j<k}^{n_{\alpha}}\frac{M_{j}M_{k}e_{j}e_{k}}{|M_{j}\nabla_{k}-M_{k}\nabla_{j}|}\right)^{-1}\psi\right\|\\ &\quad\quad+b\left\|\Gamma\left(1-i\sum_{j<k}^{n_{\alpha}}\frac{M_{j}M_{k}e_{j}e_{k}}{|M_{j}\nabla_{k}-M_{k}\nabla_{j}|}\right)^{-1}\psi\right\|\end{aligned}$$

for each $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$. Thus, the following Bochner integrals exist and the following equality is satisfied,

$$\begin{aligned}&(HW_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*}-W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*}H_{\alpha})\psi\\ &\quad=-\int_{0}^{-\infty}dt\exp(u+iHu/\epsilon)(H-H_{\alpha})\exp(-iH_{\alpha}u/\epsilon)\,F_{-\epsilon}^{(\alpha)*}\psi\end{aligned}$$

for each $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$. Integrating the above Bochner integral by parts, which can be justified via Lemma 2 of Ref. 2, yields the following equality:

$$\begin{aligned}&(HW_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*}-W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*}H_{\alpha})\psi\\ &\quad=i\epsilon(W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*}-F_{-\epsilon}^{(\alpha)*})\psi,\end{aligned} \tag{3.18}$$

valid for each $\epsilon>0$ and each $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$.

We now consider for $\psi\in\tilde{\mathcal{D}}^{(\alpha)}$,

$$\begin{aligned}&V^{(\beta)}(\Omega_{-}^{(\alpha)}-W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*})\psi\\ &\quad=C(\zeta)(\zeta-H)(\Omega_{-}^{(\alpha)}-W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*})\psi,\end{aligned}$$

where $C(\zeta)=(H-H_{\beta})\,(\zeta-H)^{-1}$, $\mathrm{Im}\zeta>0$. Since, by Lemma 2 of Ref. 9, $C(\zeta)$ is bounded, there exists a constant $B>0$ independent of ϵ such that

$$\begin{aligned}&\|V^{(\beta)}(\Omega_{-}^{(\alpha)}-W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*})\psi\|\\ &\quad\leqslant B\,\|(\zeta-H)(\Omega_{-}^{(\alpha)}-W_{-\epsilon}^{(\alpha)}F_{-\epsilon}^{(\alpha)*})\psi\|.\end{aligned} \tag{3.19}$$

Furthermore, by the intertwining properties

$$(\zeta - H)(\Omega_-^{(\alpha)} - W_{-\epsilon}^{(\alpha)} F_{-\epsilon}^{(\alpha)*})\psi = (\Omega_-^{(\alpha)} - W_{-\epsilon}^{(\alpha)} F_{-\epsilon}^{(\alpha)*})$$
$$\times (\zeta - H_\alpha)\psi + (H W_{-\epsilon}^{(\alpha)} F_{-\epsilon}^{(\alpha)*} - W_{-\epsilon}^{(\alpha)} F_{-\epsilon}^{(\alpha)*} H_\alpha)\psi. \qquad (3.20)$$

From (3.19), (3.20), (3.18) and the explicit forms of $W_{-\epsilon}^{(\alpha)}$ and $F_{-\epsilon}^{(\alpha)*}$ we obtain

$$\| V^{(\beta)}(\Omega_-^{(\alpha)} - W_{-\epsilon}^{(\alpha)} F_{-\epsilon}^{(\alpha)*})\psi \|$$
$$\leqslant B \Big\{ \| (\Omega_-^{(\alpha)} - W_{-\epsilon}^{(\alpha)} F_{-\epsilon}^{(\alpha)*})(\zeta - H_\alpha)\psi \|$$
$$+ 2\epsilon \left\| \Gamma \left(1 - i \sum_{j<k}^{n_\alpha} \frac{M_j M_k e_j e_k}{|M_j \nabla_k - M_k \nabla_j|}\right)^{-1} \psi \right\| \Big\}, \qquad (3.21)$$

valid for each $\psi \in \tilde{D}^{(\alpha)}$ and each $\epsilon > 0$. Relations (3.16) and (3.17) follow immediately from (3.21).

Theorem (3.5): Assume that the Coulomb-like renormalized wave operators exist. Then the following stationary representation of $S_{\alpha\beta}$ is valid:

$$\langle \phi | S_{\alpha\beta}\psi \rangle = \lim_{\epsilon_1 \to +0} \lim_{\epsilon_2 \to +0} (-1/\pi) \Big\langle F_{+\epsilon_1}^{(\beta)*}\phi \Big|$$
$$\times \int_{-\infty}^{-\infty} d_\lambda E_\lambda^{H_\beta} V^{(\beta)} W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*} \frac{\epsilon_1}{(H_\alpha - \lambda)^2 + \epsilon_1^2} \psi \Big\rangle \qquad (3.22)$$

for all $\phi \in D^{(\beta)}$ and $\psi \in \tilde{D}^{(\alpha)}$.

Proof: We have from Theorem (3.3)

$$\langle \phi | S_{\alpha\beta}\psi \rangle = \lim_{\epsilon_1 \to +0} (1/2\pi i) \Big\langle F_{+\epsilon_1}^{(\beta)*}\phi \Big| \int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_\beta} V^{(\beta)} \Omega_-^{(\alpha)}$$
$$\times \left(\frac{1}{H_\alpha - \lambda + i\epsilon_1} - \frac{1}{H_\alpha - \lambda - i\epsilon_1} \right) \psi \Big\rangle,$$

for all $\phi \in D^{(\beta)}$ and $\psi \in H^{(\alpha)}$. Thus, in order to prove (3.22) we are required to show that the strong limit $\epsilon_2 \to +0$ of the following expression is zero,

$$\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_\beta} V^{(\beta)} \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\}$$
$$\times \left\{ \frac{1}{H_\alpha - \lambda + i\epsilon_1} - \frac{1}{H_\alpha - \lambda - i\epsilon_1} \right\} \psi \qquad (3.23)$$

for each $\epsilon_1 > 0$ and all $\psi \in \tilde{D}^{(\alpha)}$.

We first note that

$$\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_\beta} V^{(\beta)} \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\} \frac{(\mp 1)}{H_\alpha - \lambda \mp i\epsilon_1} \psi$$
$$= (\pm i) \int_0^{\mp\infty} dt \exp(\pm \epsilon_1 t - iH_\beta t) V^{(\beta)}$$
$$\times \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\} \exp(iH_\alpha t)\psi \qquad (3.24)$$

is valid for each $\psi \in \tilde{D}^{(\beta)}$ and all $\epsilon_1 > 0$, $\epsilon_2 > 0$. In order to show the above equality we rewrite the resolvent contained in the above Riemann—Stieltjes integral in terms of Bochner integrals over t, which yields

$$\int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_\beta} V^{(\beta)} \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\} \frac{(\mp 1)}{H_\alpha - \lambda \mp i\epsilon_1} \psi$$
$$= (\pm i) \int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_\beta} V^{(\beta)} \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\}$$
$$\times \int_0^{\mp\infty} dt \exp[(\pm \epsilon_1 - i\lambda + iH_\alpha)t]\psi. \qquad (3.25)$$

By the inequalities (3.16), the following Bochner integrals exist for $\psi \in \tilde{D}^{(\alpha)}$:

$$\int_0^{\mp\infty} dt \exp[(\pm \epsilon_1 - i\lambda)t] V^{(\beta)}$$
$$\times \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\} \exp(iH_\alpha t)\psi.$$

Thus we can rewrite the last expression in (3.25) as follows:

$$(\pm i) \int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_\beta} \int_0^{\mp\infty} dt \exp[(\pm \epsilon_1 - i\lambda)t]$$
$$\times V^{(\beta)} \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\} \exp(iH_\alpha t)\psi.$$

Applying Theorem 3′ of Ref. 2 together with the inequalities (3.16) allows us to interchange the above λ and t integrals which verifies (3.24).

The relations (3.24) allow us to rewrite (3.23) as follows:

$$(-i) \int_0^{+\infty} dt \exp(-\epsilon_1 t - iH_\beta t) V^{(\beta)} \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\}$$
$$\times \exp(iH_\alpha t)\psi + (+i) \int_0^{-\infty} dt \exp(+\epsilon_1 t - iH_\beta t) V^{(\beta)}$$
$$\times \{\Omega_-^{(\alpha)} - W_{-\epsilon_2}^{(\alpha)} F_{-\epsilon_2}^{(\alpha)*}\} \exp(iH_\alpha t)\psi. \qquad (3.26)$$

That the strong limit $\epsilon_2 \to +0$ of the above expression is zero, follows by an application of the Lebesgue dominated convergence theorem for Bochner integrals, whose hypothesis can be verified from the inequalities (3.16), together with the relation (3.17). Thus the stationary representation (3.22) is valid.

IV. DISCUSSION

In this paper we have derived a natural generalization of the short range stationary scattering theory which is valid for general Coulomb-like potentials. In particular, we have shown that all the essential results contained in Refs. 2 and 3 for short range scattering have a generalization to scattering via Coulomb-like potentials.

It is easy to see in a heuristic manner that the stationary scattering formalism of Sec. III leads to the relationship between the complex energy distorted waves and off-energy-shell "T matrices" and the corresponding physical distorted waves and on-energy-shell S matrix for N-body Coulomb-like scattering. We hope to provide a concrete derivation of this relationship in a future publication.

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[1] J. Dollard, "Non-relativistic time-dependent scattering theory and the Coulomb interaction," thesis, Princeton University (1963); J. Math. Phys. 5, 729 (1964).

[2] W.O. Amrein, V. Georgescu, and J.M. Jauch, Helv. Phys. Acta 44, 407 (1971).

[3] E. Prugovečki, *Quantum Mechanics in Hilbert Space* (Academic, New York, 1971).

[4] J. Zorbas, Nuovo Cimento Lett. 10, 121 (1974). Note that the signs in the gamma and exponential functions of Eq. 16 should be interchanged.

[5] J. Zorbas, "The Gell-Mann—Goldberger formula for long-range potential scattering," to appear, Rep. Math. Phys. (1976).

[6] E. Hille and R.S. Phillips, *Functional analysis and semi-groups* (Am. Math. Soc. Coll. Publ. 31, 1957).

[7] W.O. Amrein, Ph.A. Martin, and B. Misra, Helv. Phys. Acta 43, 313 (1970); E.B. Manoukian and E. Prugovečki, Can. J. Phys. 49, 102 (1971).

[8] E. Prugovečki, Nuovo Cimento B 4, 105 (1971).

[9] C. Chandler and A.G. Gibson, Helv. Phys. Acta 45, 734 (1972).

A class of field theories with unique well-defined functional integration

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A class of field theories is considered where the codomain of the field is taken to be a compact Hausdorff topological group G. The product space G^{R^n} is then a compact Hausdorff topological group G^{R^n} and as such there exists a unique measure on this space.

I. INTRODUCTION

The quantum nonrelativistic mechanics of a point particle in n dimensional Euclidian space R^n can be set in the framework of the Hilbert space $L^2(R^n, \mathbb{C})$, the equivalance classes of Lebesque square integrable functions on R^n. It would be natural to try and formulate quantum field theory in a similar setting, but infinite-dimensional integrals are difficult to define. The definition is usually made by taking the limit of finite-dimensional integrations as in Wiener integration or as in the following brief argument due to Rosen.[1]

Consider a linear n-tuble field with topology given by the norm

$$\|\mathbf{u}-\mathbf{v}\| = \sup_{\mathbf{x}\in R^n} \{[\mathbf{u}(\mathbf{x})-\mathbf{v}(\mathbf{x})]\cdot[\mathbf{u}(\mathbf{x})-\mathbf{v}(\mathbf{x})]\}^{1/2}.$$

In this topology the finite-dimensional linear normed subspaces are locally compact Abelian topological groups, and as such for each finite-dimensional subspace there exists an invariant Haar measure. The measure on the whole space is then defined as the limit $m \rightarrow \infty$ of the measures on the m-dimensional subspaces.

In recent years interest has been aroused in nonlinear field theories and in particular field theories in which the range of the field is taken to be a Lie group (Dowker[2]). It is shown below that when any compact topological group is used for the codomain of the field, there is a unique well-defined integration, without the problem of a limit over finite-dimensional subspaces, and an associated L^2 space. Path integrals are also well defined in this class of field theories, and so could be a perfect setting for the Feynman approach to quantum field theory.

II. THE FUNCTION SPACE

In what is to follow the field will be defined to be the space of functions

$$f: R^n \rightarrow G.$$

In usual theories G is taken to be a linear vector space R^m or $\mathbb{C}^m$, but in the theories considered here G will be taken to be a compact topological group. The function space will be denoted G^{R^n}. (It is to be noted that some authors use this notation to mean only continuous functions, but here it will be used to denote all functions.)

As a general reference for point set topology, Dugundji[3] is recommended, but some definitions are important in the following arguments and will be stated for completeness. A topological group relates its algebraic and topological structure in the following way:

Definition 1: G is a topological group if G is an algebraic group and the function

$$P: G\times G \rightarrow G \quad \text{given by} \quad P(g_1, g_2) = g_1 g_2^{-1}$$

is continuous. (Here juxtaposition denotes group multiplication). An algebraic group structure can be defined point-wise in the space G^{R^n} as follows. Given any f_1, f_2, there exists f_3 defined by $f_3(\mathbf{x}) = f_1(\mathbf{x}) f_2(\mathbf{x})$. A topology may be defined on G^{R^n}, which makes it a topological group. The point topology is the smallest topology such that the evaluation functions $E_{\mathbf{x}}(f) = f(\mathbf{x})$ are continuous. This topology can be built up from basic open sets of the form $\Pi_{\mathbf{x}\in R^n} O_{\mathbf{x}}$, where $O_{\mathbf{x}}$ is open in G and $O_{\mathbf{x}} = G$ for all but a finite number of values of R^n. Since the mapping has continuous coordinates with this topology, G^{R^n} is a topological group. The group G is endowed with two other properties namely:

Definition 2: A topological space (G, T) is said to be Hausdorff if given any two points g_1, $g_2 \in G$ there exists two elements of the topology τ_1, $\tau_2 \in T$ such that $g_1 \in \tau_1$, $g_2 \in \tau_2$ and $\tau_1 \cap \tau_2 = \phi$.

Definition 3: A topological space is said to be compact if given any open covering there exists a finite subcovering. With the point topology G^{R^n} inherits these two properties from G.

Theorem 1: If G is Hausdorff, G^{R^n} is Hausdorff.

Theorem 2: If G is compact, G^{R^n} is compact.

These two theorems are proved in Dugundji; note that the proof of the last theorem depends on the axiom of choice.

III. MEASURE AND THE HILBERT SPACE

The nice feature of compact topological groups is that there exists a unique finite measure. The proof of this is given in Dunford and Schwarz.[4] (Note that in Dunford and Schwarz topological groups are by definition Hausdorff.)

Theorem 3: Given any compact Hausdorff topological group G there exists a unique nonnegative countably additive regular measure μ, the Haar measure, defined on the Borel sets β of G such that $\mu(G) = 1$ and $\mu(gE) = \mu(E)$ for each $g \in G$, $E \in \beta$, and furthermore

$$\mu(Ef) = \mu(E^{-1}) = \mu(E).$$

Since G^{R^n} inherits the properties of being Hausdorff and compact from G, it also inherits the property of the existence of a unique measure. This can be seen more clearly as follows: A basic open set in G^{R^n} may be prescribed by $\Pi_{i=1}^n O_{\mathbf{x}_i}$ for a finite number of points $\mathbf{x}_i$ in R^n, where $O_{\mathbf{x}_i}$ is strictly contained in G^{R^n}, the points of R^n for which $O_{\mathbf{x}} = G$ are suppressed. A set function ρ from these basic open sets into the positive reals may be defined as follows:

$$\rho\left(\prod_{i=1}^{n} O_{\mathbf{x}_i}\right) = \prod_{i=1}^{n} \nu(O_{\mathbf{x}_i}), \tag{3.1}$$

where ν is the Haar measure in G. The function ρ may be extended to an outer measure and can be shown to satisfy the properties of Theorem 3 and since the Haar measure μ is unique, it must coincide with the extension of ρ.

The equivalence classes of square integrable functions $L^2(G^{R^n}, \beta^{R^n}, \mu, \mathbb{C})$, abbreviated $L^2(G^{R^n})$, form a Hilbert space (Dunford and Schwarz) and so a framework for quantum mechanics is present in this field theory. An additional feature of the use of compact topological groups is contained in the following theorem (Dunford and Schwarz).

Theorem 4: Let $\{R^\alpha\}$ be a maximal set of unitary finite dimensional representations of G^{R^n} ($\alpha \in \mathcal{A}$ some index set) no two of which are equivalent. Let $\{R_{ij}^\alpha\}$ be the corresponding family of matrix elements. Then $\{R_{ij}^\alpha\}$ is a complete set of orthogonal functions in $L_2(G^{R^n})$.

IV. CONTINUOUS FUNCTION SPACES AND BOUNDARY CONDITIONS

Interest is not always in G^{R^n}, but in some subset of it, in particular $C(R^n, G)$, the space of continuous functions, or $C(R^n, G, \infty, e)$, the space of continuous functions, such that, as $|\mathbf{x}| \to \infty$, $f(\mathbf{x}) \to e$ the identity element of G. This space will be abbreviated $C_0(R^n, G)$. The latter space is of interest in kink theory (Williams[5]), where because of the boundary conditions the space divides naturally into homotopy classes which for suitable choice of G, for example SU(2), correspond to half-integral spin conserved particle structures. In this case it is the class of trivial maps $\Pi(e)$ of $C_0(R^n, G)$ which is of particular interest. [The class $\Pi(e)$ is the subset of maps of $C_0(R^n, G)$ which can be continuously deformed into the identity.]

It can be seen that $C(R^n, G)$, $C_0(R^n, G)$, and $\Pi(e)$ are algebraic subgroups of G^{R^n}, and, because every basic open set will contain one element of each, they are all dense in G^{R^n}, since R^n is Hausdorff. The following theorem (Halmos[6]) shows that none of these subsets contain measurable sets in G^{R^n}.

Theorem 5: Every Borel set A of finite positive measure in a locally compact group G has the property that AA^{-1} contains an open neighborhood of the identity.

The reason for this is as follows: The Borel sets β^{R^n} of G^{R^n} are the class of subsets of the form β^E, where E is a countable subset of R^n. Thus β^{R^n} contains no set in which a noncountable set of coordinates is restricted (Kingman[7]). This means that $C(R^n, G)$, $C_0(R^n, G)$, and $\Pi(e)$ are thick subsets of G^{R^n} (Halmos[6]). The following theorem (Kingman[7]) shows how these three subspaces may be made into measure spaces.

Theorem 6: If Ω' is a thick subset of a finite measure space Ω, β, μ; $\beta' = \Omega' \cap \beta$ and $\mu'(F \cap \beta') = \mu(F)$ for any $F \in \beta$ then Ω', β', μ', is a measure space.

This may be seen alternatively as follows. A measure can be defined on $C(R^n, G)$ [and similarly on $C_0(R^n, G)$ and $\Pi(e)$] in the following way. With the topology induced by G^{R^n} the basic open sets of $C(R^n, G)$ are $C(R^n, G) \cap \Pi_{\mathbf{x}} O_{\mathbf{x}}$. It is clear that if

$$C(R^n, G) \cap \prod_{\mathbf{x}} O_{\mathbf{x}} = C(R^n, G) \cap \prod_{\mathbf{x}'} O'_{\mathbf{x}'},$$

then $\mathbf{x} = \mathbf{x}'$, $O_{\mathbf{x}} = O'_{\mathbf{x}'}$ so that the set function on the basic open sets defined by

$$\rho'(C(R^n, G) \cap \prod_{\mathbf{x}} O_{\mathbf{x}}) = \prod_{\mathbf{x}} \gamma(O_{\mathbf{x}}),$$

where ν is the measure in G, is unambiguous. This can be extended to an outer measure and then reduced to a measure on the measurable sets.

V. TIME DEVELOPMENT AND PATH INTEGRATION

In the Feynman formulation of nonrelativistic quantum mechanics the time development of a system is prescribed by a propagator which can be derived from a "sum" over all possible histories of a system G. (The following arguments will be restricted to a system G but apply equally well to G^{R^n}.) The space of all possible dynamics $C([t, t'], G)$, $[t, t'] \subset R$, satisfies the same properties as $C(R^n, G)$ above. That is, $C([t, t'], G)$ is a thick subset of a compact Hausdorff topological group $G^{[t, t']}$.

The Feynman "sum" is an integration over the subspace $C([t, t'], G) \cap O_t \times O'_{t'}$; here O_t is an open neighborhood of $g \in G$ and $O'_{t'}$ an open neighborhood of $g' \in G$. This subspace can be assigned a measure of total weight unity defined by $[\nu(O_t) \cdot \nu(O'_{t'})]^{-1} \mu'$, where μ' is the measure in $C([t, t'], G)$ and ν the measure in G. The Feynman propagator from an open set $O'_{t'}$ to an open set O_t is given by

$$\tilde{K}(O_t, O'_{t'}) = [\nu(O_t) \cdot \nu(O'_{t'})] \int_{O_t \times O'_{t'}} d\mu' \exp[iS(f)], \tag{5.1}$$

where S is the action function

$$S : C([t, t'], G) \to R$$

If the limit $\nu(O_t)$, $\nu(O'_{t'}) \to 0$ of (5.1) is well defined, this will be the usual Feynman propagator

$$\lim_{\substack{\nu(O_t) \\ \nu(O'_{t'}) \to 0}} \tilde{K}(O_t, O'_{t'}) = K(g, g'; t, t').$$

If the action is independent of translations,

$$S(gf) = S(f) \;\forall\; g \in G,$$

because the measure is also translationally invariant,

$$K(g, g'; t, t') = K(g(g')^{-1}, e; t, t).$$

This corresponds to the usual translational invariance of point particle mechanics.

VI. CONCLUSION

The class of field theories investigated here do give the possibility of a useful well-defined functional integration without the problem of limit of finite-dimensional integrations. The existence of a finite measure stems from the compact Hausdorff nature of G and the uniqueness from the group property of G.

The measure μ is by construction invariant under the group action of G^{R^n}, but it can also be seen to be invariant under another set of transformations. Let T be any combination of rotations and translations in R^n, $T\mathbf{x}=\mathbf{x}'$. The action of $\hat{T}$ on $f\in G^{R^n}$ may be defined

$$\hat{T}f(\mathbf{x})=f(T^{-1}\mathbf{x}).$$

The action of $\hat{T}$ on the basic open sets is then

$$\hat{T}\prod_{i=1} O_{\mathbf{x}_i}=\prod_{i=1}^{n} O_{\mathbf{x}'_i}, \quad \text{where } T^{-1}\mathbf{x}_i=\mathbf{x}'_i,\ O_{\mathbf{x}'_i}=O_{\mathbf{x}_i}$$

That is $\hat{T}$ transforms the basic open sets into basic open sets. From the definition of measure on the basic open sets it can easily be seen that

$$\mu\left(\hat{T}\prod_{i=1}^{n} O_{\mathbf{x}_i}\right)=\mu\left(\prod_{i=1}^{n} O_{\mathbf{x}_i}\right)$$

so that the measure is invariant under this transformation. In fact T can be any transformation $R^n \rightarrow R^n$, that is, a one-to-one and onto function.

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[1] G. Rosen, *Formulations of Classical and Quantum Dynamical Theories* (Academic, New York, 1969).

[2] J. S. Dowker, J. Phys. A 5, 936 (1972).

[3] J. Dugundji, *Topology* (Allyn and Bacon, Boston, 1966).

[4] N. Dunford and J. T. Schwarz, *Linear Operators* (Interscience, New York, 1957).

[5] J. G. Williams, J. Math. Phys. **11**, 2611 (1970).

[6] P. R. Halmos, *Measure Theory* (Van Nostrand, Princeton, N. J., 1950).

[7] J. F. C. Kingman and S. J. Taylor, *Introduction to Measure and Probability* (Cambridge U. P., Cambridge, 1966).

Solution of the Dirac equation with Coulomb and magnetic moment interactions

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The Dirac equation for a charged spin 1/2 particle with an anomalous magnetic moment in the Coulomb field is solved. A new phenomenon of formation of very narrow resonances of very high mass at small distances is demonstrated.

I. INTRODUCTION

We solve in this paper the Dirac equation with the Coulomb potential plus the additional interaction due to the anomalous magnetic moment of the electron in the Coulomb field. To our knowledge, this problem has not been solved before. Aside from this, the result shows a remarkable new phenomenon of resonance formation at short distances which is the real motivation of presenting this investigation. The anomalous magnetic moment of the electron is small relative to the normal magnetic moment (which is taken care of by the Dirac equation), but is of the same order of magnitude as the whole magnetic moment of the proton. We show that the magnetic interactions play the dominant role at small distances.

II. THE WAVE EQUATION

We consider a relativistic spin $\frac{1}{2}$ particle of charge e_2 possessing an anomalous magnetic moment a (in units of $e_2\hbar/2mc$) in the Coulomb field of a fixed center. The normal magnetic moment is already taken into account by the Dirac equation. The equation we study is thus

$$\begin{aligned}\{\gamma^\mu[p_\mu - (e_2/c)A_\mu] - m_r c\}\Psi \\ = -a(e^2\hbar/4mc^2)\gamma^\mu\gamma^\nu F_{\mu\nu}\Psi.\end{aligned} \tag{1}$$

Here A_μ and $F_{\mu\nu}$ refer to the Coulomb field of the fixed source e_1 at the origin. Thus

$$A_\mu = (e_1/r),\ \sigma). \tag{2}$$

Passing to the Dirac α, β matrices and evaluating the right-hand side of (1) with the help of (2), we obtain

$$\begin{aligned}\left[c\boldsymbol{\alpha}\cdot\mathbf{p} - \left(E - \frac{e_1e_2}{r}\right) + \beta m_r c^2\right]\Psi \\ = -a\frac{e_1e_2\hbar}{2mc}\frac{1}{r^2}i\beta\alpha_r\Psi,\end{aligned} \tag{3}$$

where $\alpha_r = \boldsymbol{\alpha}\cdot\mathbf{r}/r$. Note that we have put the reduced mass m_r in the Dirac equation, but the anomalous magnetic moment is measured in units of $e\hbar/2mc$, m = mass of the particle. We shall consider both cases $e_1e_2 = \alpha$ and $e_1e_2 = -\alpha$, corresponding to two leptons or lepton–antilepton systems, respectively.

III. SEPARATION OF ANGULAR COORDINATES AND THE REDUCED RADIAL EQUATION

We study now Eq. (3). Having exhibited all the magnitudes, we shall take from now on $\hbar = c = 1$.

Using the relation

$$\boldsymbol{\alpha}\cdot\mathbf{p} = \alpha_r p_r + i(\alpha_r/r)\boldsymbol{\sigma}\cdot\mathbf{L},\ [\alpha_r, p_r] = 0, \tag{4}$$

we rewrite (3) as

$$\begin{aligned}\left[\alpha_r p_r + i\frac{\alpha_r}{r}\boldsymbol{\sigma}\circ\mathbf{L} + a\frac{e_1e_2}{2m}\frac{1}{r^2}i\beta\alpha_r\right. \\ \left. + \beta m_r - \left(E - \frac{e_1e_2}{r}\right)\right]\Psi = 0.\end{aligned} \tag{5}$$

We see from (5) immediately that

$$J^2,\ J_z,\ \text{and}\ K = \beta(\boldsymbol{\sigma}\cdot\mathbf{L} + 1) \tag{6}$$

are still constants of the motion as in the ordinary Coulomb problem, because $\boldsymbol{\sigma}\cdot\mathbf{L} = \beta K - 1$. We therefore look for simultaneous eigenfunctions of the Hamiltonian and J^2, J_z, K, which we label by $\Psi^\kappa_{jj_z}$ with

$$K\Psi^\kappa_{jj_z} = -\kappa\Psi^\kappa_{jj_z}. \tag{7}$$

It follows from (7) that the four-component equation can be split into two coupled two-component equations by putting

$$\Psi^\kappa_{jj_z} = \begin{pmatrix}\phi \\ \chi\end{pmatrix}, \tag{8}$$

such that ϕ and χ are eigenfunctions of $(\boldsymbol{\sigma}\cdot\mathbf{L} + 1)$:

$$(\boldsymbol{\sigma}\cdot\mathbf{L} + 1)\phi = -\kappa\phi,\quad (\boldsymbol{\sigma}\cdot\mathbf{L} + 1)\chi = \kappa\chi. \tag{9}$$

Because on angular momentum states $|l\rangle$ we have

$$\begin{aligned}(\boldsymbol{\sigma}\circ\mathbf{L} + 1)|l = j + \tfrac{1}{2}\rangle = -(j + \tfrac{1}{2})|l = j + \tfrac{1}{2}\rangle, \\ (\boldsymbol{\sigma}\cdot\mathbf{L} + 1)|l = j - \tfrac{1}{2}\rangle = (j + \tfrac{1}{2})|l = j - \tfrac{1}{2}\rangle.\end{aligned} \tag{10}$$

we can separate the angular and radial parts of ϕ and χ by writing

$$\begin{aligned}\phi = g(r)|l = j + \tfrac{1}{2}\rangle, \\ \chi = if(r)|l = j - \tfrac{1}{2}\rangle.\end{aligned} \tag{11}$$

Inserting these into (8) and (7), we find

$$K\Psi^\kappa_{jj_z} = -(j + \tfrac{1}{2})\Psi^\kappa_{jj_z}; \tag{12}$$

hence

$$\kappa = j + \tfrac{1}{2}. \tag{13a}$$

If we consider the other possibility, where ϕ and χ are interchanged in (8), we get the same equation as (12) with $\kappa = -(j + \frac{1}{2})$. Therefore,

$$\kappa = \pm(j + \tfrac{1}{2}). \tag{13b}$$

Returning now to our Eq. (5), we note that

$$\alpha_r = \begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix} = \rho_1 \begin{pmatrix} \sigma_r & 0 \\ 0 & \sigma_r \end{pmatrix} \tag{14}$$

and

$$\sigma_r \,|\, l = j - \tfrac{1}{2}\rangle = - \,|\, l = j + \tfrac{1}{2}\rangle . \tag{15}$$

Consequently, the angular parts separate, and we obtain the following two coupled equations for the radial parts,

$$\begin{aligned} \frac{df}{dr} &= \left(\frac{\kappa - 1}{r} + a\frac{e_1 e_2}{2mr^2}\right) f(r) \\ &\quad + \left(m_r - E + \frac{e_1 e_2}{r}\right) g(r), \\ \frac{dg}{dr} &= \left(-\frac{\kappa + 1}{r} - a\frac{e_1 e_2}{2mr^2}\right) g(r) \\ &\quad + \left(m_r + E - \frac{e_1 e_2}{r}\right) f(r) \end{aligned} \tag{16}$$

or, letting

$$g(r) = (1/r) u_1(r), \quad f(r) = (1/r) u_2(r), \tag{17}$$

$$\begin{aligned} \frac{du_2}{dr} &= \left(\frac{\kappa}{r} + a\frac{e_1 e_2}{2mr^2}\right) u_2 \\ &\quad + \left(m_r - E + \frac{e_1 e_2}{r}\right) u_1, \\ \frac{du_1}{dr} &= -\left(\frac{\kappa}{r} + a\frac{e_1 e_2}{2mr^2}\right) u_1 \\ &\quad + \left(m_r + E - \frac{e_1 e_2}{r}\right) u_2. \end{aligned} \tag{18}$$

One can try to solve these coupled first order equations as a matrix equation, or, as we shall do, decouple them by going to a second order equation. We first introduce a dimensionless variable x by letting

$$r \equiv a r_0 x, \quad r_0 = \alpha / m, \tag{19}$$

and

$$\epsilon = \operatorname{sgn}(e_1 e_2). \tag{20}$$

Then

$$\begin{aligned} \frac{du_2}{dx} &= \left(\frac{\kappa}{x} + \frac{\epsilon}{2x^2}\right) u_2 + B(x) u_1, \\ \frac{du_1}{dx} &= -\left(\frac{\kappa}{x} + \frac{\epsilon}{2x^2}\right) u_1 + A(x) u_2, \\ &\quad 0 < x \leqslant \infty, \end{aligned} \tag{21}$$

where

$$\begin{aligned} A(x) &\equiv a r_0 (m_r + E) - \epsilon \alpha / x, \\ B(x) &\equiv a r_0 (m_r - E) + \epsilon \alpha / x. \end{aligned} \tag{22}$$

Differentiating the second of Eqs. (21), and using the first, we obtain

$$\begin{aligned} \frac{d^2 u_1}{dx^2} &= \left(\frac{\kappa}{x^2} + \frac{\epsilon}{x^3}\right) u_1 - \left(\frac{\kappa}{x} + \frac{\epsilon}{2x^2}\right) \frac{du_1}{dx} \\ &\quad + A'(x) u_2 + A(x) \left[\left(\frac{\kappa}{x} + \frac{\epsilon}{2x^2}\right) u_2 + B(x) u_1\right]. \end{aligned}$$

Here we insert for u_2 its value obtained from (21)

$$u_2 = \frac{1}{A}\left[u_1' + \left(\frac{\kappa}{x} + \frac{\epsilon}{2x^2}\right) u_1\right]$$

and obtain an equation in u_1 only:

$$\begin{aligned} &\left(\frac{d^2 u_1}{dx^2} - \frac{A'}{A}\frac{du_1}{dx}\right) - \left[\frac{\kappa(\kappa+1)}{x^2} + \frac{\epsilon(\kappa+1)}{x^3} + \frac{1}{4x^4}\right. \\ &\quad \left. + \frac{A'}{A}\left(\frac{\kappa}{x} + \frac{\epsilon}{2x^2}\right) + AB\right] u_1 = 0. \end{aligned} \tag{23}$$

The first order derivative term du_1/dx can be eliminated by the transformation

$$u_1 = \sqrt{A}\,\psi_1. \tag{24}$$

Then

$$\begin{aligned} \frac{du_1}{dx} &= \frac{1}{2}\frac{A'}{\sqrt{A}}\psi_1 + \sqrt{A}\psi_1', \\ \frac{d^2 u_1}{dx^2} &= \frac{1}{2}\frac{A''\sqrt{A} - \frac{1}{2}A'A'/\sqrt{A}}{A}\psi_1 \\ &\quad + \frac{A'}{\sqrt{A}}\frac{d\psi_1}{dx} + \sqrt{A}\frac{d^2\psi_1}{dx^2}. \end{aligned}$$

We insert these expressions into (23), observing from (22) that

$$AB = -k^2 + 2\epsilon\, a r_0 \alpha E / x - \alpha^2 / x_2,$$

where

$$k^2 \equiv -a^2 r_0^2 (m_r^2 - E^2) \tag{25}$$

and evaluate and insert A', A'' as well, and obtain finally after some algebra the eigenvalue equation

$$\left(\frac{d^2}{dx^2} + k^2 - V_1(x)\right)\psi_1 = 0, \tag{26}$$

where the energy-dependent dynamical "potential" $V_1(x)$ is given by

$$\begin{aligned} V_1(x) &\equiv \frac{\kappa(\kappa+1)}{x^2} + 2\epsilon a r_0 \alpha E \frac{1}{x} \\ &\quad + \frac{1}{x^2}\left[\frac{\epsilon(\kappa+1)}{h_1(x)} + \frac{3}{4}\frac{1}{h_1^2(x)} - \alpha^2\right] \\ &\quad + \frac{1}{x^3}\left[\epsilon(\kappa + 1) + \frac{1}{2}\frac{1}{h_1(x)}\right] + \frac{1}{4x^4}, \end{aligned} \tag{27}$$

with

$$h_1(x) \equiv -\epsilon + \frac{\alpha}{2\pi}\frac{m_r + E}{m} x.$$

In the transformation (24) leading to (27) we assumed $A(x) > 0$ which is fulfilled for $\epsilon = -1$. For $\epsilon = +1$ there is, however, a region with $A(x) < 0$ and in this case one has to transform according to

$$u_1 = \sqrt{-A}\,\psi_1 \tag{24'}$$

which leads exactly to the same equation (27).

In a similar fashion, if we eliminate u_1 from the two equations (18) and set

$$u_2 = \sqrt{B(x)}\,\psi_2, \tag{28}$$

we obtain

$$\left(\frac{d^2}{dx^2} + k^2 - V_2(x)\right)\psi_2 = 0, \tag{29}$$

where

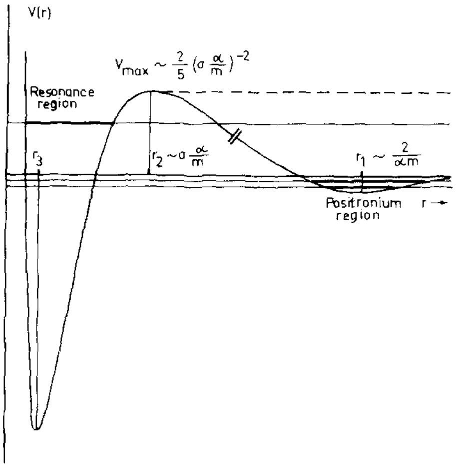

FIG. 1. The effective dynamical "potential" for $\kappa = j + \frac{1}{2} = 1$. The positronium levels are indicated schematically at Bohr radius and the resonance levels at $r \sim a(\alpha/m)$, $V_{\max} \sim (35\ \mathrm{GeV})^2$.

$$V_2(x) \equiv \frac{\kappa(\kappa-1)}{x^2} + 2\epsilon a r_0 \alpha E \frac{1}{x} + \frac{1}{x^2}\left[-\frac{\epsilon(\kappa-1)}{h_2(x)} + \frac{3}{4}\frac{1}{h_2^2(x)} - \alpha^2\right] + \frac{1}{x^3}\left[\epsilon(\kappa-1) - \frac{1}{2}\frac{1}{h_2(x)}\right] + \frac{1}{4x^4}, \tag{30}$$

with

$$h_2(x) \equiv -\epsilon + \frac{\alpha}{2\pi}\frac{E - m_r}{m}x.$$

IV. STUDY OF THE EIGENVALUE EQUATION AND SUPERPOSITRONIUM RESONANCES

The dynamical potentials $V_i(x)$, Eqs. (27) and (30), are rather complicated, but for $E/m \gg 1$ they become essentially independent of E. For a fixed value of $\kappa = 1$, $\epsilon = -1$, i.e., $e_1 = -e_2$, $V_1(x)$ has the behavior shown schematically in Fig. 1.

We see from Fig. 1 that the new terms of the interaction proportional to the anomalous magnetic moment $a = \alpha/2\pi$ only very slightly change the potential in the positronium region, and these changes are taken into account in quantum electrodynamics. However, at distances of the order of $a\alpha/m$ the structure of the potential is entirely changed, and we obtain a new region, which we call the superpositronium resonance region. Clearly the spectrum of the Hamiltonian is continuous for $k^2 > 0$, and we can only locate the position of the resonances. For this purpose we first truncate the potential along the dotted line so that we have a potential well. Let

$$\tilde{V}(x) = V(x) - V_{\max}(x). \tag{31}$$

There are exact upper and lower bounds for the number of bound states[1] in such a potential $\tilde{V}(x)$:

$$n \leq \frac{2}{\pi}\int_0^\infty |\tilde{V}(x)|^{1/2}dx, \qquad n \geq \left\{\left\{\frac{1}{2} - \frac{1}{\pi}\int_0^\infty dx \frac{\tilde{V}(x)}{\sqrt{-\tilde{V}_{\min}}}\right\}\right\}, \tag{32}$$

where $\{\{\cdots\}\}$ indicates the integral part of the quantity inside the parentheses.

By numerical integration we find

$$\{\{0.9\}\} \leq n \leq 1.2, \quad \text{for } \kappa = +1. \tag{33}$$

We thus expect one resonance for each fixed value of κ. For the truncated potential we have indeed located the position of the bound state by numerical integration. The actual location of the resonances will be done by a numerical phase-shift analysis and will be reported elsewhere.

V. DISCUSSION AND CONSEQUENCES

(1) There are no new parameters in the present calculation, the value of the anomalous magnetic moment being fixed as $a = \alpha/2\pi$ from the lowest radiative corrections.

(2) For $\epsilon = +1$, i.e., $e_1 = e_2$, the Coulomb interaction is repulsive and bound states in the positronium region no longer exist. In the superpositronium resonance region there is, however, an approximate symmetry of the "potential," and the change of sign in ϵ can be compensated by a change in the quantum number κ. This can be seen as follows. Under the assumption $E/m \gg 1$ we have $1/h_i \ll 1$. Since the Coulomb interaction $2\epsilon a r_0 \alpha E/x$ is also negligible at distances $x \lesssim a\alpha/m$, the relevant potential is approximately given from (27) by

$$V_1(x) \sim \frac{\kappa(\kappa+1)}{x^2} + \frac{\epsilon(\kappa+1)}{x^3} + \frac{1}{4x^4}.$$

Comparing (27) and (30), we see that $V_1(x)$ goes over into $V_2(x)$ under the replacement

$$\epsilon \to -\epsilon \quad \text{and} \quad \kappa \to -\kappa.$$

We therefore expect similar resonances in the lepton—lepton system if they have high masses. However, the potential for $\epsilon = 1$ can be quite different if E is small as seen from Eq. (27).

(3) In order to ascertain that the new resonances are indeed realistic, for example, for the e^+e^- system, many further effects have to be considered.[2] These include the magnetic moment of the other particle, recoil effects, and other higher order radiative corrections. Unfortunately, there is no close relativistic theory of a two-body bound state even for a pure Coulomb interaction. These effects have to be considered step by step, and some are being investigated. But in view of the recent discovery of very narrow high mass resonances in the e^+e^- system a dynamical model such as the present one obviously opens up remarkable new possibilities and further directions of research.

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[1] F. Calogero, Comm. Math. Phys. 1, 80 (1965).

[2] A.O. Barut and J. Kraus, Phys. Lett. B 59 175 (1975).

Comultiplicator of finite magnetic groups

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A matrix algebraic method for constructing the comultiplicator group for any finite magnetic group is given. Each element of this comultiplicator group corresponds to an inequivalent factor system of the magnetic group.

1. INTRODUCTION

Projective representations[1,2] of groups belonging to a factor system are useful for representations of nonsymmorphic space groups[3,4] and other problems of physics.[5] For magnetic groups which contain the antilinear time reversal operator[6] either singly or in conjunction with space rotations (proper or improper) and translations, the corresponding theory of projective corepresentations belonging to a factor system are used.[3,7,8]

Schur[8-10] showed that for a group G of linear operators the nonassociated factor systems can be obtained from the multiplicator group K. The multiplicator group is defined like this. For every group G there exists a smallest extension $\hat{G}$, such that the factor group $\hat{G}/K \approx G$, where the multiplicator group $K \subseteq C(\hat{G})$, the center of $\hat{G}$. Schur also gave the algebraic method of constructing K.

Janssen[8] has extended Schur's results to magnetic groups. The multiplicator group $K(M, G)$ of a magnetic group $M(G)$ (in the notation of Ref. 3), termed the comultiplicator group, is shown to be isomorphic to the factor group $Z_G^2(M)/B_G^2(M)$, where $Z_G^n(M)$ is the group of n cocylces with arguments in M and values in the unimodular complex group U(1), and $B_G^n(M)$ is the corresponding group of n coboundaries. Thus the problem of obtaining the classes of factor systems reduces to the problem of algebraic topology.

Since the majority of the solid state physicists work with matrix methods, we have explained here the matrix methodical procedure of constructing the comultiplicator $K(M, G)$. In this we follow the original method of Schur[9,11] for linear groups. No proof has been given, since Janssen has already proved[8] the necessary theorems in a rigorous way. In Sec. 2 we have explained Schur's original method of constructing K for any linear group G and we have extended it for a finite magnetic group. In Sec. 3 we have given examples of some particular cases.

2. FACTOR SYSTEMS AND COMULTIPLICATOR GROUP

The magnetic group is defined as

$$M = G \cup a_0 G \tag{1}$$

where a_0 is a fixed antilinear operator.

$$a_0 = \theta v_0, \quad v_0^2 \in G \tag{2}$$

where θ is the time reversal operator and v_0 is a fixed linear operator. We also define the associated linear group

$$M' = G \cup v_0 G. \tag{3}$$

A representation $D(\alpha)$, $\alpha \in M$, will belong to the factor system $\omega(\alpha, \beta)$, $\alpha, \beta \in M$ if

$$D(\alpha)\, D(\beta)^{[\alpha]} = \omega(\alpha, \beta)^{[\alpha\beta]}\, D(\alpha\beta). \tag{4}$$

We have used the following notation

$$A^{[\alpha]} \begin{cases} A & \text{if } \alpha \in G, \\ A^* & \text{if } \alpha \in M - G, \end{cases} \tag{5}$$

where A is either a matrix or a complex number. The set of complex numbers $\omega(\alpha, \beta)$ satisfy these relations

$$\begin{aligned} &\omega(\alpha, \beta)^{[\gamma]}\omega(\alpha\beta, \gamma) = \omega(\alpha, \beta\gamma)\, \omega(\beta, \gamma), \\ &|\omega(\alpha, \beta)| = 1. \end{aligned} \tag{6}$$

We first mention Schur's method[9,11,12] of constructing the multiplicator K. Let $(a_1, a_2, \ldots, a_k)$ be the generators of G and the defining relations be

$$\begin{aligned} &a_i^{n(i)} = e, \quad i = 1, 2, \ldots, k; \\ &a_i a_j = a_1^{n_1(i,j)}\, a_2^{n_2(i,j)} \cdots a_i^{n_i(i,j)}, \quad j < i = 2, 3, \ldots, k. \end{aligned} \tag{7}$$

The exponents are all positive integers. We extend G to $\hat{G}$ by defining new group elements with the relations

$$\begin{aligned} &A_i^{n(i)} = E, \quad i = 1, 2, \ldots, k, \\ &A_i A_j = J(i, j)\, A_1^{n_1(i,j)}\, A_2^{n_2(i,j)} \cdots A_i^{n_i(i,j)}, \quad j < i = 2, 3, \ldots, k, \\ &J(i, j)\, A_m = A_m\, J(i, j), \quad m = 1, 2, \ldots, k, \quad j < i = 2, 3, \ldots, k, \\ &J(i, j)\, J(m, n) = J(m, n)\, J(i, j), \quad n < m = 2, 3, \ldots, k, \\ &\qquad\qquad\qquad\qquad\qquad\qquad j < i = 2, 3, \ldots, k. \end{aligned} \tag{8}$$

From this set of relations we obtain positive integers $n(i, j)$ such that

$$J(i, j)^{n(i,j)} = E, \quad j < i = 2, 3, \ldots, k. \tag{9}$$

One then obtains the derived group $[\hat{G}, \hat{G}]$, the group generated by the elements $\hat{g}_i \hat{g}_j \hat{g}_i^{-1} g_j^{-1}$, $\hat{g}_i, \hat{g}_j \in \hat{G}$, and the group $\mathcal{J}$, generated by the elements $J(i, j)$. Schur has shown that

$$K = [\hat{G}, \hat{G}] \cap \mathcal{J}. \tag{10}$$

K contains elements of the form $J(i, j)^{b_1(i,j)}$, $J(i, j)^{b_2(i,j)}, \ldots, J(i, j)^{b_{\Phi(i,j)}(i,j)}$, where the $b_m(i, j)$ are positive integers. If $e(i, j)$ are the $n(i, j)$th primitive root of unity, then the allowed sets of factor systems are obtained by substituting $e(i, j)^{b_m(i,j)}$ for $\omega(i, j)$.

We extend this method to finite magnetic groups. Two cases arise.

(i) $v_0^2 = e$, so that M is generated by $(a_1, a_2, \ldots, a_k, \theta v_0 = a_{k+1})$;

(ii) $v_0^2 = a_k$, so that M is generated by $(a_1, a_2, \ldots, a_{k-1}, \theta v_0)$.

We treat these two cases separately. In the first case we define a matrix group extension $\hat{M}$ of M:

$$
\begin{aligned}
&A_iA_j = J(i,j)\,A_1^{n_1(i,j)}A_2^{n_2(i,j)}\cdots A_i^{n_i(i,j)}, \quad j<i=2,3,\ldots,k,\\
&A_i^{n(i)} = E, \quad i=1,2,3,\ldots,k,\\
&A_{k+1}A_j^* = J(k+1,j)^*A_1^{n_1(k+1,j)}A_2^{n_2(k+1,j)}\cdots A_{k+1}^{n_{k+1}(k+1,j)},\\
&\qquad\qquad j=1,2,\ldots,k,\\
&A_{k+1}A_{k+1}^* = J(k+1)\,E,\\
&A_mJ(i,j) = J(i,j)\,A_m, \quad j<i=2,3,\ldots,k, \quad m=1,2,3,\ldots,k,\\
&A_mJ(k+1,j)^* = J(k+1,j)^*A_m, \quad j=1,2,3,\ldots,k,\\
&\qquad\qquad m=1,2,3,\ldots,k,\\
&A_mJ(k+1) = J(k+1)\,A_m, \quad m=1,2,3,\ldots,k,\\
&A_{k+1}J(i,j)^* = J(i,j)^{-1}A_{k+1}, \quad j<i=2,3,\ldots,k,\\
&A_{k+1}J(k+1,j) = J(k+1,j)^{*-1}A_{k+1}, \quad j=1,2,3,\ldots,k,\\
&A_{k+1}J(k+1)^* = J(k+1)^{-1}A_{k+1},\\
&J(i,j)\,J(m,n) = J(m,n)\,J(i,j), \quad j<i=2,3,\ldots,k,\\
&\qquad\qquad n<m=2,3,\ldots,k,\\
&J(i,j)\,J(k+1,n)^* = J(k+1,n)^*\,J(i,j), \quad j<i=2,3,\ldots,k,\\
&\qquad\qquad n=1,2,3,\ldots,k,\\
&J(i,j)\,J(k+1) = J(k+1)\,J(i,j), \quad j<i=2,3,\ldots,k,\\
&J(k+1,j)^*\,J(k+1,n)^* = J(k+1,n)^*J(k+1,j)^*,\\
&\qquad\qquad j=1,2,3,\ldots,k,\\
&\qquad\qquad n=1,2,3,\ldots,k,\\
&J(k+1,j)^*\,J(k+1) = J(k+1)\,J(k+1,j)^*, \quad j=1,2,3,\ldots,k.
\end{aligned}
\tag{11}
$$

It should be noted that the positive integers $n_i(k+1,j)$ are obtained from the structure of M'.

$$
v_0a_j = a_1^{n_1(k+1,j)}a_2^{n_2(k+1,j)}\cdots a_k^{n_k(k+1,j)}v_0^{n_{k+1}(k+1,j)}, \quad j=1,2,3,\ldots,k.
$$

Manipulations of these relations give us

$$
\begin{aligned}
&J(i,j)^{n(i,j)} = E, \quad j<i=2,3,\ldots,k,\\
&J(k+1,j)^{*n(k+1,j)} = E, \quad j=1,2,3,\ldots,k,\\
&J(k+1)^{n(k+1)} = E.
\end{aligned}
\tag{12}
$$

We construct the derived group $[\hat{M},\hat{M}]$ as the group generated by the elements

$$
\hat{M}_i\hat{M}_j^{[\hat{m}_i]}\hat{M}_{i'}^{[\hat{m}_i\hat{m}_j]}M_{j'}^{[\hat{m}_i\hat{m}_j\hat{m}_i^{-1}]}, \tag{13}
$$

where $\hat{M}_i$ is the matrix corresponding to the element $\hat{m}_i \in \hat{M}$, and $\hat{M}_{i'}$ is the matrix corresponding to the element $\hat{m}_i^{-1}$. If $\hat{m}_i$ is any of the elements $J(i,j)$, $J(k+1,j)^*$, or $J(k+1)$, then $\hat{M}_{i'}$ is simply inverse of the corresponding matrix. $\mathcal{J}$ is defined as the group generated by $J(i,j)$, $J(k+1,j)^*$, and $J(k+1)$. Then

$$
K(M,G) = [\hat{M},\hat{M}] \cap \mathcal{J}. \tag{14}
$$

$K(M,G)$ contains elements of the form $J(i,j)^{b_m(i,j)}$, $J(k+1,j)^{*b_m(i,j)}$, $J(k+1)^{b_m(k+1)}$ with integral $b_m(i,j)$, $b_m(k+1,j)$, $b_m(k+1)$. If $e(i,j)$ is the $n(i,j)$th root of unity and $e(k+1)$ the $n(k+1)$th root of unity, then the different sets of factor systems of $M(G)$ will be obtained by substituting $e(i,j)^{b_m(i,j)}$ and $e(k+1)^{b_m(k+1)}$ for $\omega(i,j)$ and $\omega(a_{k+1},a_{k+1})$. It can be shown with the help of Eq. (6) that $J(k+1)^2 = E$.

In the second case $\hat{M}$ is constructed by the following prescription. We start with the structure of M', whose generators are $(a_1, a_2, \ldots, a_{k-1}, v_0)$:

$$
\begin{aligned}
&a_i^{n(i)} = e, \quad i=1,2,3,\ldots,k-1, \quad v_0^2 = a_k, \quad v_0^{2n(k)} = e,\\
&a_ia_j = a_1^{n_1(i,j)}a_2^{n_2(i,j)}\cdots a_{k-1}^{n_{k-1}(i,j)}, \quad j<i=2,3,\ldots,k-1,\\
&v_0a_j = a_1^{n_1(0,j)}a_2^{n_2(0,j)}\cdots a_{k-1}^{n_{k-1}(0,j)}, \quad j=1,2,3,\ldots,k-1.\\
&\qquad\qquad v_0^{n_0(0,j)},
\end{aligned}
\tag{15}
$$

We construct $\hat{M}$ by the following relations:

$$
\begin{aligned}
&A_iA_j = J(i,j)\,A_1^{n_1(i,j)}A_2^{n_2(i,j)}\cdots A_{k-1}^{n_{k-1}(i,j)},\\
&\qquad\qquad j<i=2,3,\ldots,k-1,\\
&A_i^{n(i)} = E, \quad i=1,2,3,\ldots,k-1,\\
&A_0A_j^* = J(0,j)^*A_1^{n_1(0,j)}A_2^{n_2(0,j)}\cdots A_{k-1}^{n_{k-1}(0,j)}A_0^{n_0(0,j)},\\
&\qquad\qquad j=1,2,\ldots,k-1,\\
&A_0A_0^* = J(0)\,A_k, \quad A_k^{n(k)} = E,\\
&A_mJ(i,j) = J(i,j)\,A_m, \quad j<i=2,3,\ldots,k-1,\\
&\qquad\qquad m=1,2,3,\ldots,k-1,\\
&A_mJ(0,j)^* = J(0,j)^*A_m, \quad j=1,2,3,\ldots,k-1,\\
&\qquad\qquad m=1,2,3,\ldots,k-1,\\
&A_mJ(0) = J(0)\,A_m, \quad m=1,2,3,\ldots,k-1,\\
&A_0J(i,j)^* = J(i,j)^{-1}A_0, \quad j<i=2,3,\ldots,k-1,\\
&A_0J(0,j) = J(0,j)^{*-1}A_0, \quad j=1,2,3,\ldots,k-1,\\
&A_0J(0)^* = J(0)^{-1}A_0,\\
&J(i,j)J(m,n) = J(m,n)J(i,j), \quad j<i=2,3,\ldots,k-1,\\
&\qquad\qquad n<m=2,3,\ldots,k-1,\\
&J(i,j)\,J(0,n)^* = J(0,n)^*J(i,j), \quad j<i=2,3,\ldots,k-1,\\
&\qquad\qquad n=1,2,3,\ldots,k-1,\\
&J(i,j)\,J(0) = J(0)\,J(i,j), \quad j<i=2,3,\ldots,k-1,\\
&J(0,j)^*\,J(0,n)^* = J(0,n)^*\,J(0,j)^*, \quad j=1,2,3,\ldots,k-1,\\
&\qquad\qquad n=1,2,3,\ldots,k-1,\\
&J(0,j)^*\,J(0) = J(0)\,J(0,j)^*, \quad j=1,2,3,\ldots,k-1.
\end{aligned}
\tag{16}
$$

Afterwards the method of procedure is the same as that in case (i). In the next section we give examples of this procedure in some special cases.

3. SOME EXAMPLES

A. $M(G) = C_{n\,i}\,(C_n)$

The defining relations of M' are

$$a_1^n = e, \quad a_2^2 = e, \quad a_2a_1 = a_1a_2.$$

$\hat{M}$ is defined by

$$
\begin{aligned}
&A_1^n = E, \quad A_2A_2^* = J(2)E, \quad A_2A_1^* = J(2,1)^*A_1A_2,\\
&A_1J(2) = J(2)A_1, \quad A_1J(2,1)^* = J(2,1)^*A_1,\\
&A_2J(2)^* = J(2)^{-1}A_2, \quad A_2J(2,1) = J(2,1)^{*-1}A_2,\\
&J(2)\,J(2,1)^* = J(2,1)^*\,J(2).
\end{aligned}
$$

We get $J(2)^2 = E$, $J(2,1)^{*n} = E$. $[\hat{M}, \hat{M}]$ is generated by $J(2)$ and $J(2,1)^*$, the generators of $\mathcal{J}$. Hence $K(M, G)$ is generated by $J(2)$ and $J(2,1)^*$.

B. $M(G) = D_n(C_n)$

The defining relations of M' are

$$a_1^n = e, \quad a_2^2 = e, \quad a_2 a_1 = a_1^{n-1} a_2.$$

$\hat{M}$ is defined by

$$A_1^n = E, \quad A_2 A_2^* = J(2)E, \quad A_2 A_1^* = J(2,1)^* A_1^{n-1} A_2,$$

$$A_1 J(2) = J(2) A_1, \quad A_1 J(2,1)^* = J(2,1)^* A_1,$$

$$A_2 J(2)^* = J(2)^{-1} A_2, \quad A_2 J(2,1) = J(2,1)^{*-1} A_2,$$

$$J(2)\, J(2,1)^* = J(2,1)^*\, J(2).$$

We get $J(2,1)^{*n} = E$, $J(2)^2 = E$.

$[\hat{M}, \hat{M}]$ is generated by the elements $J(2)$, $J(2,1)^{*\,n-2}$, $J(2,1)^{*2}$, $J(2,1)^* A_1^{n-2}$, $J(2,1)^{*\,n-1} A_1^2$. If $n =$ odd or $4m + 2$, then $J(2,1)^* \in [\hat{M}, \hat{M}]$. If $n = 4m$, then $J(2,1)^* \notin [\hat{M}, \hat{M}]$, but $J(2,1)^{*2} \in [\hat{M}, \hat{M}]$.

Thus, for $n = 4m$, $K(M, G)$ is generated by $J(2)$ and $J(2,1)^{*2}$; and for $n =$ odd or $4m + 2$, $K(M, G)$ is generated by $J(2)$ and $J(2,1)^*$.

C. $M(G) = D_n \otimes I(D_n)$

The defining relations of M' are

$$a_1^n = e, \quad a_2^2 = e, \quad e_3^2 = e, \quad a_2 a_1 = a_1^{n-1} a_2,$$
$$a_3 a_1 = a_1 a_3, \quad a_3 a_2 = a_2 a_3.$$

$\hat{M}$ is defined by

$$A_1^n = E, \quad A_2^2 = E, \quad A_3 A_3^* = J(3)\, E,$$

$$A_2 A_1 = J(2,1)\, A_1^{n-1} A_2, \quad A_3 A_1^* = J(3,1)^* A_1 A_3,$$

$$A_3 A_2^* = J(3,2)^* A_2 A_3, \quad A_1 J(3) = J(3)\, A_1,$$

$$A_1 J(2,1) = J(2,1)\, A_1, \quad A_1 J(3,1)^* = J(3,1)^* A_1,$$

$$A_1 J(3,2)^* = J(3,2)^* A_1, \quad A_2 J(3) = J(3)\, A_2,$$

$$A_2 J(2,1) = J(2,1)\, A_2, \quad A_2 J(3,1)^* = J(3,1)^* A_2,$$

$$A_2 J(3,2)^* = J(3,2)^* A_2, \quad A_3 J(3)^* = J(3)^{-1} A_3,$$

$$A_3 J(2,1)^* = J(2,1)^{-1} A_3, \quad A_3 J(3,1) = J(3,1)^{*-1} A_3,$$

$$A_3 J(3,2) = J(3,2)^{*-1} A_3, \quad J(3)\, J(2,1) = J(2,1)\, J(3),$$

$$J(3)\, J(3,1)^* = J(3,1)^*\, J(3), \quad J(3)\, J(3,2)^* = J(3,2)^*\, J(3),$$

$$J(2,1)\, J(3,1)^* = J(3,1)^*\, J(2,1),$$

$$J(2,1)\, J(3,2)^* = J(3,2)^*\, J(2,1),$$

$$J(3,1)^*\, J(3,2)^* = J(3,2)^*\, J(3,1)^*.$$

We get $J(3)^2 = E$, $J(2,1)^n = E$, $J(3,1)^{*n} = E$, $J(3,2)^{*2} = E$. $[\hat{M}, \hat{M}]$ contains $J(2)$, $J(3,1)^*$, $J(3,2)^*$, $J(2,1)\, A_1^{n-2}$, $J(2,1)\, A_1^2$. Hence if $n = 2m$, $K(M, G)$ is generated by $J(2)$, $J(2,1)^m$, $J(3,1)^*$, $J(3,2)^*$; and if $n = 2m + 1$, $K(M, G)$ is generated by $J(2)$, $J(2,1)$, $J(3,1)^*$, $J(3,2)^*$.

D. $M(G) = C_{2n}(C_n)$

$\hat{M}$ is defined by

$$A_1^n = E, \quad A_0 A_0^* = J(0)\, A_1, \quad A_0 J(0) = J(0)^{-1} A_0.$$

We obtain $J(0)^{2n} = E$. $[\hat{M}, \hat{M}]$ and hence $K(M, G)$ are generated by $J(0)$.

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[1] M. Hamermesh, *Group Theory* (Addison-Wesley, Reading, Mass., 1962).

[2] H. Boerner, *Representations of Groups* (North-Holland, Amsterdam, 1970).

[3] C.J. Bradley and B.L. Davies, Rev. Mod. Phys. **40**, 359 (1968).

[4] P. Rudra, J. Math. Phys. **6**, 1273, 1278 (1965).

[5] R. Warren and W.H. Klink, J. Math. Phys. **13**, 306 (1972).

[6] E.P. Wigner, *Group Theory* (Academic, New York, 1959).

[7] M.V. Murthy, J. Math. Phys. **7**, 853 (1966).

[8] T. Janssen, J. Math. Phys. **13**, 342 (1972).

[9] I. Schur, J. Reine Angew. Math. **127**, 20 (1904); **132**, 85 (1907).

[10] C.W. Curtis and I. Reiner, *Representation Theory of Finite Groups and Associative Algebra* (Interscience, New York, 1962).

[11] W. Döring, Z. Naturforsch. **14**, 343 (1959).

[12] A.C. Hurley, Phil. Trans. Roy. Soc. (London) A **240**, 1 (1966).

Spinor representations and projective factor systems of crystallographic point groups

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We have given the correspondence between the factor system of the spinor representations of the different crystallographic point groups and the factor system given by Doering and Hurley. It turns out that for the groups C_1, C_i, C_2, C_s, C_{2h}, C_4, S_4, C_{4h}, C_3, C_{3i}, C_{3v}, D_3, D_{3d}, C_6, C_{6h}, C_{3h} the factor system of the spinor representations are associated with that of the vector representations.

1. INTRODUCTION

It is well known that the spinor representations[1] of the rotation group and the Lorentz group can be looked upon as projective representations[2,3] of the respective groups. The equivalence of them has been emphasized by many authors.[4-9] For the Lorentz group and the rotation group there is just one factor system (other than the trivial factor system of the vector representations) to which the spinor representations are associated.[1] For the crystallographic point groups the nonassociative factor systems and the corresponding representations have been worked out by Doering[10] and Hurley.[11] Here we have given the factor systems of the different crystallographic point groups (in Hurley's notation) to which the spinor representations of the groups are associated. For the spinor representations we use the factor system given by Zak *et al.*[12] For the groups C_1, C_i, C_2, C_s, C_{2h}, C_4, S_4, C_{4h}, C_3, C_{3i}, C_{3v}, D_3, D_{3d}, C_6, C_{6h}, C_{3h} the factor system of the spinor representations are associated with that of the vector representations.

TABLE I. The factor systems of the crystallographic point groups to which their spinor representations are associated and the corresponding $\alpha(g)$'s defined in Eq. (4). $\rho=\exp(\pi i/4)$. $\xi=\exp(\pi i/6)$.

Serial number	Point group	Doering and Hurley's notation of factor system and identification with point group operations	Factor system to which the spinor representation belongs	The numbers $\alpha(g)$ and their interrelations
1.	C_i	$A^2=E,\ A=I$	Vector	$\alpha(E)=1,\ \alpha(I)=1$
2.	C_2, C_s	$A^2=E,\ A=C_2, IC_2$	Vector	$\alpha(E)=1,\ \alpha(A)=\pm i$
3.	C_{2h}	$A^2=E,\ B^2=E,\ BA=\alpha AB$ $\alpha=\pm 1,\ A=C_2,\ B=I$	Vector $\alpha=1$	$\alpha(E)=1,\ \alpha(C_2)=\pm i,\ \alpha(I)=\pm 1$ $\alpha(IC_2)=\alpha(I)\ \alpha(C_2)$
4.	D_2, C_{2v}	$A^2=E,\ B^2=E,\ BA=\alpha AB$ $\alpha=\pm 1,\ A=U^z,\ B=U^x,\ IU^x$	Projective $\alpha=-1$	$\alpha(E)=1,\ \alpha(A)=\pm i,\ \alpha(B)=\pm i$ $\alpha(AB)=\alpha(A)\ \alpha(B)$
5.	D_{2h}	$A^2=E,\ B^2=E,\ BA=\gamma AB$ $C^2=E,\ CA=\beta AC,\ CB=\alpha BC$ $\alpha,\beta,\gamma=\pm 1.$ $A=U^z,\ B=U^x,\ C=I$	Projective $\alpha,\ \beta=1$ $\gamma=-1$	For the elements $g\in D_2$, $\alpha(g)$ are the same as in the case 4 $\alpha(I)=\pm 1,\ \alpha(Ig)=\alpha(I)\alpha(g)$
6.	C_4, S_4	$A^4=E\ A=C_4^z, IC_4^z$	Vector	$\alpha(E)=1,\ \alpha(A)=\pm\rho,\ \pm\rho^3$ $\alpha(A^m)=[\alpha(A)]^m,\ m=2,3$
7.	C_{4h}	$A^4=E,\ B^2=E,\ BA=\alpha AB$ $\alpha=\pm 1,\ A=C_4^z,\ B=I$	Vector $\alpha=1$	For the elements $g\in C_4$, $\alpha(g)$ are the same as in the case 6 $\alpha(I)=\pm 1,\ \alpha(Ig)=\alpha(I)\alpha(g)$
8.	D_4	$A^4=\alpha E,\ B^2=E,\ BA=A^3B$ $\alpha=\pm 1,\ A=C_4^z,\ B=U^x$	Projective $\alpha=-1$	$\alpha(E)=1,\ \alpha(C_4^z)=\pm i,\ \alpha(U^x)=\pm i$ $\alpha(C_4^{mz})=(\alpha(C_4^z))^m,\ m=2,3$ $\alpha(U^y)=\alpha(U^x)\alpha(C_4^{2z})$ $\alpha(U^{xy})=\alpha(U^x)\alpha(C_4^z)$ $\alpha(U^{\bar{x}y})=\alpha(U^x)\alpha(C_4^{3z})$
9.	D_{4h}	$A^4=\alpha E,\ B^2=E,\ BA=A^3B$ $C^2=E,\ CA=\beta AC,\ CB=\gamma BC$ $\alpha,\beta,\gamma=\pm 1$ $A=C_4^z,\ B=U^x,\ C=I$	Projective $\alpha=-1,\beta,\ \gamma=1$	For elements $g\in D_4$, $\alpha(g)$ are the same as in the case 8 $\alpha(I)=\pm 1,\ \alpha(Ig)=\alpha(I)\alpha(g)$

TABLE I. (*Continued*).

10.	C_3	$A^3=E,\ A=C_3^z$ (hexagonal axes)	Vector	$\alpha(E)=1,\ \alpha(C_3^z)=-1,\ \exp(\pm\pi i/3)$ $\alpha(C_3^{2z})=[\alpha(C_3^z)]^2$
11.	C_{3i}	$A^3=E,\ B^2=E,\ BA=AB$ $A=C_3^z,\ B=I$ (hexagonal axes)	Vector	For elements $g\in C_3$, $\alpha(g)$ are the same as in the case 10 $\alpha(I)=\pm1,\ \alpha(Ig)=\alpha(I)\alpha(g)$
12.	D_3, C_{3v}	$A^3=E,\ B^2=E,\ BA=A^2B$ $A=C_3^z,\ B=U^x,\ IU^x$ (hexagonal axes)	Vector	$\alpha(E)=1,\ \alpha(C_3^z)=-1,\ \alpha(C_3^{2z})=1$ $\alpha(U^x)=\pm i,\ \alpha(U^{xy})=\alpha(C_3^z)\alpha(U^x)$ $\alpha(U^y)=-\alpha(C_3^z)\alpha(U^x)$
13.	D_{3d}	$A^6=E,\ B^2=E,\ BA=\alpha A^5B$ $\alpha=\pm1,\ A=IC_3^z,\ B=U^x$ (hexagonal axes)	Vector $\alpha=1$	$\alpha(E)=1,\ \alpha(IC_3^z)=\pm1$ $\alpha(I^mC_3^{mz})=[\alpha(C_3^zI)]^m,\ m=2,3,4,5$ $\alpha(U^x)=\alpha(U^y)=\alpha(U^{xy})=\pm i,$ $\alpha(IU^x)=\alpha(IU^y)=\alpha(IU^{xy})$ $=-\alpha(IC_3^z)\alpha(U^x)$
14.	C_6	$A^6=E,\ A=C_6^z$ (hexagonal axes)	Vector	$\alpha(E)=1, \alpha(C_6^z)=\pm\xi, \pm i, \pm\xi^5$ $\alpha(C_6^{mz})=(\alpha(C_6^z))^m, m=2,3,4,5$
15.	C_{6h}	$A^6=E,\ B^2=E,\ BA=\alpha AB$ $\alpha=\pm1,\ A=C_6^z,\ B=I$ (hexagonal axes)	Vector $\alpha=1$	For elements $g\in C_6$, $\alpha(g)$ are the same as in the case 14. $\alpha(I)=\pm1, \alpha(Ig)=\alpha(I)\alpha(g)$
16.	C_{3h}	$A^6=E,\ A=IC_6^z$ (hexagonal axes)	Vector	$\alpha(E)=1,\ \alpha(IC_6^z)=\pm\xi,\ \pm i, \pm\xi^5$ $\alpha(I^mC_6^{mz})=[\alpha(IC_6^z)]^m,\ m=2,3,4,5$
17.	D_6, D_{3h}	$A^6=E,\ B^2=E,\ BA=\alpha A^5B$ $\alpha=\pm1$ $A=C_6^z,\ IC_6^z,\ B=U^x$ (hexagonal axes)	Projective $\alpha=-1$	$\alpha(E)=1,\ \alpha(A)=\pm i,\ \alpha(B)=\pm i$ $\alpha(A^m)=(\alpha(A))^m, m=2,3,4,5$ $\alpha(AB)=\alpha(A^3B)=\alpha(A^5B)=\alpha(A)\alpha(B),$ $\alpha(A^2B)=\alpha(A^4B)=\alpha(B)$
18.	D_{6h}	A,B and their multiplication laws as in 17 $I^2=E,\ IB=\beta BI,\ IA=\gamma AI$ $\alpha,\beta,\gamma=\pm1$ (hexagonal axes)	Projective $\alpha=-1, \beta, \gamma=1$	For the elements $g\in D_{6h}$, $\alpha(g)$ are the same as in case 17 $\alpha(I)=\pm1,\ \alpha(Ig)=\alpha(I)\alpha(g)$
19.	T	$A^2=\alpha E,\ B^2=\alpha E,\ BA=\alpha AB$ $C^3=E,\ CA=BC,\ CB=ABC$ $\alpha=\pm1,\ A=U^z,\ B=U^x$ $C=C_3^{xyz}$	Projective $\alpha=-1$	$\alpha(E)=\alpha(U^z)=\alpha(U^x)=\alpha(U^y)=1,$ $\alpha(C_3^{xyz})=\alpha(C_3^{\bar{x}yz})=\alpha(C_3^{x\bar{y}z})=\alpha(C_3^{xy\bar{z}})$ $=\xi^2, -1, -\xi^4$ $\alpha(C_3^{2xyz})=\alpha(C_3^{2x\bar{y}z})=-\alpha(C_3^{2xy\bar{z}})$ $=-\alpha(C_3^{2\bar{x}yz})=[\alpha(C_3^{xyz})]^2$
20.	T_h	A,B,C and their multiplication laws as in 19 $I^2=E,\ IA=AI,\ IB=BI$ $IC=CI$	Projective $\alpha=-1$	For the elements $g\in T$, $\alpha(g)$ are the same as in case 19. $\alpha(I)=\pm1,\ \alpha(Ig)=\alpha(I)\alpha(g)$
21.	O	A,B,C and their multiplication laws as in 19 $D^2=E,\ DA=\alpha BD,\ DB=\alpha AD,$ $DC=C^2D,\ \alpha=\pm1$ $D=U^{zx}$	Projective $\alpha=-1$	$\alpha(E)=\alpha(U^z)=\alpha(U^x)=\alpha(U^y)$ $=\alpha(C_3^{2xyz})=\alpha(C_3^{2x\bar{y}z})=1,$ $\alpha(C_3^{xyz})=\alpha(C_3^{\bar{x}yz})=\alpha(C_3^{x\bar{y}z})=\alpha(C_3^{xy\bar{z}})$ $=\alpha(C_3^{2\bar{x}yz})=\alpha(C_3^{2xy\bar{z}})=-1,$ $\alpha(U^{xz})=\alpha(U^{\bar{x}z})=\alpha(U^{yz})=\alpha(U^{\bar{y}z})$ $=\alpha(U^{xy})=\alpha(C_4^{3x})=-\alpha(U^{\bar{x}y})$ $=-\alpha(C_4^y)=-\alpha(C_4^x)=-\alpha(C_4^z)$ $=-\alpha(C_4^{3y})=-\alpha(C_4^{3z})=\pm i$
22.	O_h	A,B,C,D and their multiplication laws as in 21. $I^2=E,\ IA=AI, IB=BI,$ $IC=CI, ID=\beta DI$ $\alpha,\beta=\pm1$	Projective $\alpha=-1$ $\beta=1$	For the elements $g\in O$, $\alpha(g)$ are the same as in case 21 $\alpha(I)=\pm1,\ \alpha(Ig)=\alpha(I)\alpha(g)$

2. PROJECTIVE REPRESENTATIONS OF FINITE GROUPS

For any finite group G, the projective representations $D^\lambda(g_i)$ belonging to the factor system $\lambda(g_i, g_j)$, $g_i, g_j \in G$, satisfy the relation[2]

$$D^\lambda(g_i)D^\lambda(g_j) = \lambda(g_i,g_j)D^\lambda(g_ig_j), \quad |\lambda(g_i,g_j)| = 1. \tag{1}$$

The $\lambda(g_i,g_j)$'s satisfy

$$\lambda(g_i,g_j)\lambda(g_ig_j,g_k) = \lambda(g_i,g_jg_k)\lambda(g_j,g_k). \tag{2}$$

Conversely,[2] any set of complex numbers $\lambda(g_i,g_j)$ with moduli 1 satisfying Eq. (2) will form a factor system. Another such set $\lambda(g_i,g_j)'$ will be a factor system associated with $\lambda(g_i,g_j)$ if there exist numbers $\alpha(g_i)$, $g_i \in G$, such that

$$\lambda(g_i,g_j)' = \alpha(g_i)\alpha(g_j)\alpha(g_ig_j)^{-1}\lambda(g_i,g_j), \quad |\alpha(g_i)| = 1. \tag{3}$$

If the operator O_{g_i} corresponding to the group element g_i gives rise to the representation belonging to the factor system $\lambda(g_i,g_j)$, then

$$O'_{g_i} = \alpha(g_i)O_{g_i} \tag{4}$$

will give rise to the representation $D^\lambda(g_i)' = \alpha(g_i)D^\lambda(g_i)$ which belongs to the factor system $\lambda(g_i,g_j)'$.

The distinct classes of nonassociated factor systems for a finite group can be obtained from Schur's multiplicator group.[13,14] For the crystallographic point groups Doering[10] has given the nonassociated factor systems and the character tables for each group. Hurley[11] has given all the irreducible matrices. For the spinor representations of the crystallographic point groups we have taken the representations given by Zak *et al.*,[12] which are not all associated with some nontrivial factor system of the corresponding groups. We have tabulated in Table I the complex numbers $\alpha(g_i)$ so that O'_{g_i} will belong to a factor system given by Doering and Hurley, and O_{g_i} will belong to the factor system of the spinor representations.

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[1] H. Weyl, *Theory of Groups and Quantum Mechanics* (Dover, New York, 1950).

[2] M. Hamermesh, *Group Theory* (Addison-Wesley, Reading, Mass., 1962).

[3] H. Boerner, *Representations of Groups* (North-Holland, Amsterdam, 1970).

[4] E. Brown, Amer. J. Phys. 38, 704 (1970).

[5] D. Koelling, Q. Prog. Rep. Solid State Mol. Theory Group, M.I.T., no. 66, 40 (1967).

[6] R. Gilmore, Q. Prog. Rep., Solid State Mol. Theory Group, M.I.T., no. 69, 101 (1968).

[7] S. Mase, J. Phys. Soc. (Japan) 14, 1538 (1959).

[8] A. Kitz, Phys. Stat. Sol. B 8, 813 (1965); 10, 455 (1965).

[9] M. Glueck, Y. Gur, and J. Zak, J. Math. Phys. 8, 787 (1967).

[10] W. Doering, Z. Naturforsch. 14, 343 (1959).

[11] A.C. Hurley, Phil. Trans. Roy. Soc. (London) A 260, 1 (1966).

[12] J. Zak, A. Casher, M. Glueck, and Y. Gur, *Irreducible Representations of Space Groups* (Benjamin, New York, 1969).

[13] I. Schur, J. Reine Angew. Math. 127, 20 (1904); 132, 85 (1907).

[14] P. Rudra, J. Math. Phys. 17, 509 (1976).

Removal of the nodal singularity of the C-metric

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The charged C-metric is transformed into another exact solution of the Einstein–Maxwell field equations corresponding to a massive charged particle accelerated by an electric field. When the appropriate equations of motion are satisfied, the nodal singularity associated with the C-metric disappears.

A nodal singularity associated with the charged C-metric[1] is indeed a manifestation of the neglect of the force necessary to accelerate a massive charged particle, as has been suggested[2] by Kinnersley and Walker. By transforming the charged C-metric into another exact solution of the Einstein–Maxwell field equations with an additional parameter E_0 representing an electric field, the nodal singularity can be eliminated by choosing the value of E_0 appropriately. For example, in the case of small acceleration A, the requisite condition is found to be $eE_0 = mA$, in accord with Newton's second law.

I. TRANSFORMATION OF THE CHARGED C-METRIC

In terms of the retarded null coordinates employed in Ref. 2, the charged C-metric can be expressed in the form

$$ds^2 = -H\,du^2 - 2\,du\,dr - 2Ar^2\,du\,dx + r^2(G^{-1}\,dx^2 + G\,dz^2),$$

where

$$G = 1 - x^2 - 2mAx^3 - e^2A^2x^4,$$

$$H = -A^2r^2G + ArG' + (1 + 6mAx + 6e^2A^2x^2) - 2(m + 2e^2Ax)r^{-1} + e^2r^{-2}.$$

As in Ref. 3, where we transformed the Reissner–Nordstrom metric ($A = 0$) into another solution of the Einstein–Maxwell field equations with an additional magnetic field, we introduce complex electromagnetic and gravitational potentials associated with the spacelike Killing vector $\mathbf{a}_z$. In the present example

$$\Phi = -iex, \quad \mathcal{E} = -[r^2G(x) + e^2x^2].$$

The field equations are left invariant under a group of transformations which were discussed by Kinnersley.[4] In particular, we shall employ the Harrison-type transformation

$$\Phi' = \Lambda^{-1}(\Phi + \tfrac{1}{2}iE_0\mathcal{E}), \quad \mathcal{E}' = \Lambda^{-1}\mathcal{E},$$

where

$$\Lambda = 1 + iE_0\Phi - \tfrac{1}{4}E_0{}^2\mathcal{E}.$$

From the reality of $\mathcal{E}'$ it is clear that the transformed metric is static rather than stationary. Because Λ is real, we may write the transformed metric as follows:

$$ds^2 = \Lambda^2(-H\,du^2 - 2\,du\,dr - 2Ar^2\,du\,dx + r^2G^{-1}\,dx^2) + \Lambda^{-2}r^2G\,dz^2.$$

Applied to Minkowski space, where $A = m = e = 0$, this transformation produces the electric analog of Melvin's magnetic universe,[5] with the electric field in the direction opposite to the polar axis (cf. Ref. 3). Applied to the general charged C-metric, the transformation yields a solution which resembles the electric universe asymptotically, but which also has a black hole accelerating in the direction opposite to the polar axis.

II. EMBEDDING OF $\Sigma^+(u,r)$

We may embed the 2-surface $\Sigma^+(u, r)$ defined by $u = \text{const}$, $r = \text{const}$ as a surface of revolution in Euclidean space. The induced metric on Σ^+ is simply

$$d\sigma^2 = r^2(\mathcal{G}^{-1}\,dx^2 + \mathcal{G}\,dz^2),$$

where $\mathcal{G} = \Lambda^{-2}G(x) = G(x)/[(1 + \frac{1}{2}eE_0x)^2 + \frac{1}{4}E_0{}^2r^2G(x)]^2$.

There are two zeroes of $G(x)$ between which $G(x)$ is positive. The function $\mathcal{G}(x)$ has the same properties in the interval $x_2 \leqslant x \leqslant x_1$. We introduce the angular coordinates

$$\theta = \int_x^{x_1} \mathcal{G}^{-1/2}\,dx, \quad \phi = kz,$$

where, to avoid a node at the north pole $\theta = \theta_1 = 0$, we choose

$$k = -\frac{1}{2}\frac{d\mathcal{G}}{dx}\bigg|_{x_1},$$

$$\rho(\theta) = k^{-1}[\mathcal{G}(x(\theta))]^{1/2}.$$

Then the induced metric on Σ^+ can be expressed in the form

$$d\sigma^2 = r^2(d\theta^2 + \rho^2(\theta)\,d\phi^2).$$

To avoid a node at the south pole, one requires that

$$\epsilon = -\frac{d\rho}{d\theta}\bigg|_{\theta_2} = 1.$$

Explicitly, this equation (which does not involve r) reads as follows:

$$x_2(1 + 3mAx_2 + 2e^2A^2x_2{}^2)/(1 + \tfrac{1}{2}eE_0x_2)^4 = -x_1(1 + 3mAx_1 + 2e^2A^2x_1{}^2)/(1 + \tfrac{1}{2}eE_0x_1)^4.$$

For sufficiently small values of the acceleration A, the zeroes of $G(x)$ are located at $x_2 = -1 - mA$ and $x_1 = 1 - mA$, respectively. One concludes, therefore, that in this regime the constants e, E_0, m, and A must satisfy

$$eE_0 = mA,$$

which is precisely the same relation one might expect on the basis of classical mechanics.

While the replacement of the charged C-metric by our solution with an appropriately chosen value of E_0 permits one to avoid the problem of the nodal singularity, it remains to be seen whether the proposed physical interpretation of the solution can be fully justified.

[1] T. Levi-Civita, Atti Accad. Naz. Lincei Cl. Sci. Fis. Mat. Nat. Rend. 27, 343 (1918).

[2] W. Kinnersley and M. Walker, Phys. Rev. D 2, 1359 (1970).

[3] F. J. Ernst, J. Math. Phys. (to appear).

[4] W. Kinnersley, J. Math. Phys. 14, 651 (1973).

[5] W. B. Bonnor, Proc. Phys. Soc. London, Sect. A 67, 225 (1953); M. A. Melvin, Phys. Rev. 139, B225 (1965).

Probability measures on fuzzy events in phase space*

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The notion of fuzzy sample point is introduced, and generalized probability measures on fuzzy events are defined. This leads to the concept of spectral measure on fuzzy events. It is shown that such measures can be associated with quantum-mechanical states when the fuzzy elementary events are represented by Gaussian distributions on phase space.

1. INTRODUCTION

The modern approach to probability theory dating back to Kolmogorov's formulation is based on the concept of probability space, defined as a triple $(\mathcal{X},\mathcal{A},P)$ consisting of the sample space $\mathcal{X}$, a Boolean σ-algebra $\mathcal{A}$ of events in $\mathcal{X}$, and the probability measure P, characterized by its property of σ-additivity and normalization to unity on $\mathcal{X}$. Underlying the empirical interpretation of P is the assumption that given an event Δ, any experiment ultimately provides data which can be unambiguously described by elements of $\mathcal{X}$ even when $\mathcal{X}$ has a cardinality equal to that of the continuum.

In this note we investigate the possibility of generalizing basic probabilistic concepts to the case when the sample points are "fuzzy." The obtained formalism is then considered in the context of quantum mechanics, with the aim of arriving at a stochastic description of measurements of noncommuting observables.

In Sec. 2 we examine the operational meaning of fuzzy sample points by relating them to the calibration procedure of instruments used in measurement. In Sec. 3 we formulate the concept of fuzzy event and introduce probability measures on such events. This leads in a natural manner to a generalization of the concept of spectral measure associated with two or more observables. After treating this concept in a general context in Sec. 4, we turn to the special case of generalized spectral measures associated with simultaneous measurement of position and momentum of quantum-mechanical particles. Thus we arrive at a specific proposal for assigning probability measures in phase space to every quantum mechanical state.

Basically, there have been two types of attempts at a stochastic formulation of quantum mechanics. The first type had been advocated by Moyal[1] and was based on an interpretation of the Wigner transform $w_\rho(q,p)$ of a statistical operator ρ as a probability density in phase space. It ran, however, into the problem of interpreting negative probabilities since $w_\rho(q,p)$ is not positive definite. The other type had been introduced by Dirac[2] and led to complex probabilities. It was later independently considered[3] within the context of complex probability measures. It was shown[4] that an empirical meaning can be assigned to this concept, but when the formalism was applied to quantum mechanics, this interpretation ran into the difficulty[4] of having the family of events in phase space dependent on the considered state ρ.

In contradistinction with the above attempts, the probability measures in phase space considered in Sec. 5 are positive-definite, being actually derivable from the Husimi transform[5] of ρ. However, they are probability measures on "fuzzy" events of the type introduced in Sec. 3 and are not derivable from conventional probability measures[6] on "sharp" events; in view of the uncertainty principle, this fact is not surprising. On the other hand, they do reduce to the conventional probability distributions in position or momentum in the limiting case of infinitely precise position and infinitely precise momentum measurements, respectively.

2. FUZZY SAMPLE POINTS

The conceptual framework for probability theory advocated in the next section rests on the observation that the outcome of any realistic simultaneous measurement of n real stochastic quantities $A_1, \ldots, A_n$ cannot be exhaustively described by only n numbers $(\alpha_1, \ldots, \alpha_n)$, except in those cases when the respective sets $\sigma(A_1), \ldots, \sigma(A_n)$ of values in $\mathbb{R}^1$ which these variables can assume are all finite or at most countably infinite discrete subsets of $\mathbb{R}^1$. In general, however, one should specify to what degree of certainty is some $\lambda_k \neq \alpha_k$ and not α_k itself the actual value of A_k. This stipulation is essential in objectifying the measurement process at least in the minimal sense of securing concurrence between different measurements carried out on the same sample with different instruments of varying accuracy.[7]

We adopt the attitude that an *exhaustive* description of the measurement outcome can be achieved by providing in addition to the n-tuple $\alpha = (\alpha_1, \ldots, \alpha_n)$ also a nonnegative function $\chi(\lambda)$, $\lambda \in \mathbb{R}^n$, with a maximum at α. This function $\chi(\lambda)$ provides a measure for the relative certitude that $\lambda \in \sigma(A_1) \times \circ\circ\circ \times \sigma(A_n)$ and not α is the actual value of the extracted sample point. We shall refer to the pair $\hat{\alpha} = (\alpha, \chi)$ as a *fuzzy sample point* and to χ as the *confidence function* of $\hat{\alpha}$. For a given instrument $\mathcal{I}$ supposed to measure values from some subset Δ of the joint range $\sigma(A_1, \ldots, A_n)$ of $A_1, \ldots, A_n$, we shall call the procedure of attaching to each $\alpha \in \Delta$ a confidence function χ, the *accuracy calibration* of $\mathcal{I}$. In view of the probabilistic interpretation of calibration that we shall promptly advocate, we require that

$$\int_{\mathbb{R}^n} \chi(\lambda)\, d\lambda = 1. \tag{2.1}$$

Since the applications considered in this note relate to quantum-mechanical observables with continuous spectra, let us specialize our treatment to independent stochastic variables $A_1, \ldots, A_n$ for which $\sigma(A_1), \ldots, \sigma(A_n)$ are closed intervals on $\mathbb{R}^1$ and which can assume any value from the n-dimensional closed interval $\sigma = \sigma(A_1, \ldots, A_n) = \sigma(A_1) \times \cdots \times \sigma(A_n)$. Under these circumstances we request that $\chi \in C^\infty(\sigma)$, i.e., that it be infinitely many times differentiable on σ. We shall also talk of a *sharp sample point* α, which in analogy with a fuzzy sample point can be represented by the pair (α, δ_α), where $\delta_\alpha(\lambda)$ is the Dirac function $\delta^{(n)}(\alpha - \lambda)$ in $\mathbb{R}^n$. Such terminology suggests an obvious operational meaning for the confidence function χ of $\hat{\alpha}$.

Let us discuss first the case of a single stochastic quantity A_k measured by a given instrument $\mathcal{I}_k$. For some reading $\alpha_k \in \mathbb{R}^1$ of $\mathcal{I}_k$, the value $\chi_k(\lambda_k)$ at λ_k of the confidence function of $\hat{\alpha}_k$ could be taken[8] to be the probability density for the actually determined value of A_k having been in reality λ_k when a reading of $\mathcal{I}_k$ yielded α_k. Thus, assuming that sharp sample points could be prepared, a calibration of $\mathcal{I}_k$ could be carried out by comparing readings of $\mathcal{I}_k$ against perfectly accurate instruments which prepare sharp sample points. Naturally, since in reality such ideal absolutely precise apparata do not exist, the calibration procedure has to rely on results obtained by checking each imperfectly accurate instrument against some other such instruments. Nevertheless, as long as we admit at least the possibility of indefinitely increasing the precision of the instruments preparing or measuring samples of A_k, we can view the concept of sharp sample point as a limiting process in analogy to viewing the δ "function" as a δ sequence of actual functions.

Such an interpretation of a fuzzy sample point $\hat{\alpha}_k$ leads to the expression

$$r(\hat{\alpha}_k) = \int_{-\infty}^{+\infty} r(\lambda_k) \chi_k(\lambda_k)\, d\lambda_k, \quad \hat{\alpha}_k = (\alpha_k, \chi_k) \tag{2.2}$$

for the probability density of $\hat{\alpha}_k$ derivable from the probability density $r(\beta_n)$ for sharp sample points $(\beta_k, \delta_{\beta_k})$. Indeed, (2.2) is the only expression compatible with the request that $\chi(\beta_k) = r(\hat{\alpha}_k)$ when a δ distribution $r(\lambda_k) = \delta(\lambda_k - \beta_k)$ of sharp sample points $(\beta_k, \delta_{\beta_k})$ had been prepared.

In case of two or more stochastically independent quantities $A_1, \ldots, A_n$ it is not necessary to assume that arbitrarily precise simultaneous measurements of these n quantities can be performed in order to give an analogous operational meaning to a confidence function of the form

$$\chi(\lambda_1, \ldots, \lambda_n) = \chi_1(\lambda_1) \cdots \chi_n(\lambda_n). \tag{2.3}$$

If the fuzzy point $\hat{\alpha} = (\alpha, \chi)$ with the above confidence function is the outcome of the calibration of an apparatus $\mathcal{I}$ for the simultaneous measurement of $A_1, \ldots, A_n$, when when the reading of $\mathcal{I}$ is $\alpha = (\alpha_1, \ldots, \alpha_n)$ we give each $\chi_k(\lambda_k)$, $k = 1, \ldots, n$, the same meaning as in the calibration of the instrument $\mathcal{I}_k$ measuring only A_k. In other words, we adopt the principle (cf. Ref. 8, E-principle) that if a family $\mathcal{J}$ of samples with sharp values β_k of A_k has been prepared with a totally random distribution in those values, then the simultaneous measurements of $A_1, \ldots, A_k, \ldots, A_n$ which yield the value α_k for A_k correspond to a subfamily $\mathcal{J}_k$ of $\mathcal{J}$ in which the distribution of the β_k values is described by $\chi_k(\beta_k)$. Naturally, the impossibility of actually producing absolutely sharp values for A_k necessitates the same type of concurrence approach to the calibration of $\mathcal{I}$ as used in the calibration of an instrument $\mathcal{I}_k$ measuring A_k exclusively.[7]

3. FUZZY PROBABILITY SPACES

Let us generalize now the concept of probability space $(\mathbb{R}^n, \mathcal{B}^n, P)$ over the family $\mathcal{B}^n$ of Borel sets in $\mathbb{R}^n$ to the case when the samples are fuzzy rather than sharp. We start from the assumption that a family $\mathcal{S}^n$ is given which consists of fuzzy sample points that can be obtained by the simultaneous measurement of $A_1, \ldots, A_n$ with a certain class of instruments.

We define a *fuzzy event* $\hat{\Delta}$ as a family

$$\hat{\Delta} = \{\hat{\alpha} \mid \alpha \in \Delta, \chi_\alpha(\lambda) \in L^1(\Delta)\}, \quad \Delta \in \mathcal{B}^n, \tag{3.1}$$

of fuzzy sample points, a unique fuzzy point $\hat{\alpha}$ being attached to each α from a Borel set $\Delta \in \mathcal{B}^n$, i.e., $\hat{\Delta}$ is determined by the function $\chi_\alpha(\lambda)$ on $\Delta \times \mathbb{R}^n$; in addition, we impose on $\chi_\alpha(\lambda)$ the condition that it be Lebesgue integrable on Δ for each fixed λ. We shall refer to the $L^1(\Delta)$ (inα) nonnegative function $\chi_\alpha(\lambda)$ as the *characteristic function of the fuzzy event* $\hat{\Delta}$. If Δ consists of only one point, i.e., $\Delta = \{\alpha\}$, then we shall say that $\hat{\Delta}$ is an *elementary fuzzy event*. Obviously the family of elementary fuzzy events coincides with the family $\mathcal{S}^n$ of fuzzy sample points.

Two fuzzy events $\hat{\Delta}_k = \{\chi_\alpha^{(k)} \mid \alpha \in \Delta^{(k)}\}$, $k = 1, 2$, will be said to be *compatible* if and only if $\chi_\alpha^{(1)}(\lambda) \equiv \chi_\alpha^{(2)}(\lambda)$ for all $\alpha \in \Delta^{(1)} \cap \Delta^{(2)}$. In particular, we note that $\hat{\Delta}_1$ and $\hat{\Delta}_2$ are compatible whenever the Borel sets Δ_1 and Δ_2 are disjoint.

We denote by $\mathcal{E}^n$ the family of all fuzzy events (3.1). A fuzzy event $\hat{\Delta}$ can be viewed as the outcome of the calibration of an instrument $\mathcal{I}$ for the simultaneous measurement of $A_1, \ldots, A_n$ on the section Δ of its scale $S(\mathcal{I}) \subset \mathbb{R}^n$. Thus, compatible fuzzy events $\hat{\Delta}_1$ and $\hat{\Delta}_2$ are either the outcome of measurements with one instrument or with replicas of the same instruments $\mathcal{I}$, or with two distinct instruments $\mathcal{I}_1$ and $\mathcal{I}_2$ of identical calibration on that part of their overlapping scales $S(\mathcal{I}_1) \cap S(\mathcal{I}_2)$ which contains the Borel set $\Delta_1 \cap \Delta_2$.

If $\hat{\Delta}_1, \hat{\Delta}_2 \in \mathcal{E}$ are compatible we shall write $\hat{\Delta}_1 \leftrightarrow \hat{\Delta}_2$ and define

$$\hat{\Delta}_1 \wedge \hat{\Delta}_2 = \{\hat{\alpha} \mid \alpha \in \Delta_1 \cap \Delta_2\}, \tag{3.2}$$

$$\hat{\Delta}_1 \vee \hat{\Delta}_2 = \{\hat{\alpha} \mid \alpha \in \Delta_1 \cup \Delta_2\} \tag{3.3}$$

as their intersection and union respectively. It is easy to check that the family $\mathcal{E}$ is a partial Boolean ring[9] under the operations $\leftrightarrow$, $\wedge$, and $\vee$; i.e., $\hat{\Delta} \leftrightarrow \hat{\Delta}$ for all $\Delta \in \mathcal{E}$, $\hat{\Delta}_1 \leftrightarrow \hat{\Delta}_2$ implies $\hat{\Delta}_2 \leftrightarrow \hat{\Delta}_1$; and if $\hat{\Delta}_1, \hat{\Delta}_2, \hat{\Delta}_3 \in \mathcal{E}$ are mutually compatible, then $\hat{\Delta}_1 \wedge \hat{\Delta}_2 \leftrightarrow \hat{\Delta}_3$, $\hat{\Delta}_1 \vee \hat{\Delta}_2 \leftrightarrow \hat{\Delta}_3$.

When $\hat{\Delta}_1 \leftrightarrow \hat{\Delta}_2$, we can define their difference

$$\hat{\Delta}_1 \setminus \hat{\Delta}_2 = \{\hat{\alpha} \mid \alpha \in \Delta_1 \setminus \Delta_2\}. \tag{3.4}$$

If $\hat{\Delta}_2 = \hat{\Delta}_1 \wedge \hat{\Delta}_2$ we shall say that $\hat{\Delta}_2$ is contained in $\hat{\Delta}_1$ and write $\hat{\Delta}_2 \prec \hat{\Delta}_1$.

In analogy to an ordinary probability measure on $\mathcal{B}^n$, we define a *probability measure* $P(\hat{\Delta})$, $\hat{\Delta} \in \mathcal{E}^n$, *on fuzzy events* as a not identically vanishing and nonnegative function on $\mathcal{E}^n$ which vanishes on the empty set $\emptyset$, i.e., $P(\emptyset)=0$, and is σ-additive in the sense that whenever $\hat\Delta\in\mathcal{E}^n$ is the union of disjoint fuzzy events,

$$\hat\Delta=\hat\Delta_1\vee\hat\Delta_2\vee\cdots,\quad \hat\Delta_i\wedge\hat\Delta_j=\emptyset \text{ for } i\neq j,$$

we have

$$P(\hat\Delta)=P(\hat\Delta_1)+P(\hat\Delta_2)+\cdots. \tag{3.5}$$

Furthermore, since a small change in calibration should produce only a small change in the probability $P(\hat\Delta)$ of a given fuzzy event, we impose the additional condition that

$$\lim_{\hat\Delta^{(k)}\to\hat\Delta} P(\hat\Delta^{(k)})=P(\hat\Delta),\quad \forall\,\hat\Delta\in\mathcal{E}^n, \tag{3.6}$$

for any sequence $\hat\Delta^{(k)}=\{(\alpha,\chi_\alpha^{(k)})\mid\alpha\in\Delta\}$, $k=1,2,\cdots$, for which at each $\alpha\in\Delta$ the confidence functions $\chi_\alpha^{(k)}$ converge to the confidence function χ_α in (3.1) (in a topology related to the particular nature of the instruments used in measurements of $A_1,\ldots,A_n$).

We easily see that if $(\mathbb{R}^n,\mathcal{E}^n,P)$ is a fuzzy probability space, then for any compatible $\hat\Delta_1,\hat\Delta_2\in\mathcal{E}^n$

$$P(\hat\Delta_1\backslash\hat\Delta_2)=P(\hat\Delta_1)-P(\hat\Delta_2)\ \text{ if } \Delta_2\prec\Delta_1, \tag{3.7}$$

$$P(\hat\Delta_1\vee\hat\Delta_2)=P(\hat\Delta_1)+P(\hat\Delta_2)-P(\hat\Delta_1\wedge\hat\Delta_2). \tag{3.8}$$

As a matter of fact (3.7) follows from the fact that $\hat\Delta_1=\hat\Delta_2\vee(\hat\Delta_1\backslash\hat\Delta_2)$ and $\hat\Delta_2\wedge(\hat\Delta_1\backslash\hat\Delta_2)=\emptyset$, while (3.8) is a consequence of (3.7) and the relation

$$P(\hat\Delta_1\backslash\hat\Delta_2)+P(\hat\Delta_2\backslash\hat\Delta_1)+P(\hat\Delta_1\wedge\hat\Delta_2)=P(\hat\Delta_1\vee\hat\Delta_2).$$

Since no normalization condition $P(\hat{\mathbb{R}}^n)=1$ has been imposed on P, the numbers $P(\hat\Delta)$ have to be interpreted as relative probabilities. The reason for avoiding a normalization condition becomes obvious if we consider the simplest of the fuzzy probability space $(\mathbb{R}^n,\mathcal{E}^n,P)$ derivable from an ordinary probability density $\omega(\lambda)$ in accordance to (2.2):

$$P(\hat\Delta)=\int_\Delta d^n\alpha\int_{\mathbb{R}^n}\omega(\lambda)\chi_\alpha(\lambda)\,d^n\lambda,\quad \hat\Delta=\{\chi_\alpha\mid\alpha\in\Delta\}. \tag{3.9}$$

For a fuzzy

$$\hat{\mathbb{R}}^n=\{\chi_\alpha\mid\alpha\in\mathbb{R}^n\}\in\mathcal{E}^n \tag{3.10}$$

we have

$$P(\hat{\mathbb{R}}^n)=\int_{\mathbb{R}^n}d^n\lambda\,\omega(\lambda)\int_{\mathbb{R}^n}\chi_\alpha(\lambda)\,d^n\alpha, \tag{3.11}$$

which in view of the normalization condition

$$\int_{\mathbb{R}^n}\omega(\lambda)\,d^n\lambda=1 \tag{3.12}$$

can be equal to one for any distribution $\omega(\lambda)$ if and only if

$$\int_{\mathbb{R}^n}\chi_\alpha(\lambda)\,d^n\alpha\equiv1. \tag{3.13}$$

Comparison with (2.1) shows that (3.13) can be expected to hold in the special case when

$$\chi_\eta(\xi)=\chi_0(\xi-\eta),\quad \forall\,\eta\in\mathbb{R}^1, \tag{3.14}$$

i.e., when $\hat{\mathbb{R}}^1$ corresponds to instruments which have congruent calibrations at all points on their reading scales, but not in general.

Many of the basic concepts of probability theory can be generalized to fuzzy probability spaces as long as one heeds the compatibility condition. For example, with any specific global fuzzy event $\hat{\mathbb{R}}^n$ presented in (3.10) we can associate a nonnegative normalized measure

$$P(\hat{\mathbb{R}}^n;\Delta)=P(\hat\Delta)/P(\hat{\mathbb{R}}^n),\quad \hat\Delta\prec\hat{\mathbb{R}}^n, \tag{3.15}$$

on the Borel sets $\Delta\in\mathcal{B}^n$ and then define means, medians, moments, etc., with respect to this measure. Naturally, the values of the quantities will be dependent on the choice of $\hat{\mathbb{R}}^n$, namely, from the empirical point of view, on the choice of the class of instruments (with compatible calibrations) used in performing the measurements yielding the fuzzy sample points. If arbitrarily accurate measurements are feasible, then $\mathcal{E}^n$ would contain for each $\alpha\in\mathbb{R}^n$ elementary events χ_α of arbitrarily narrow spread[8] and $P(\hat\Delta)$, $\hat\Delta\in\mathcal{E}^n$, would be derivable from an ordinary probability density $\omega(\xi)$ in accordance to (3.9). Thus the case of a probability measure

$$P_\delta(\Delta)=\int_\Delta\omega(\lambda)\,d^n\lambda,\quad \Delta\in\mathcal{B}^n \tag{3.16}$$

on "perfectly sharp" events $\Delta\in\mathcal{B}^n$ can be regarded as idealized case of $P(\hat\Delta)$. Then $P_\delta(\Delta)$ is conceived only in the limit of constructing more and more accurate instruments $\mathcal{I}^{(1)},\mathcal{I}^{(2)},\ldots$ leading to δ sequences $\chi_\alpha^{(1)},\chi_\alpha^{(2)},\cdots$ for the corresponding $\hat{\mathbb{R}}^n_{(1)},\hat{\mathbb{R}}^n_{(2)},\cdots$ defined as in (3.10); in this limit the fuzzy sample point at each $\alpha\in\mathbb{R}^n$ becomes sharp, so that (3.9) reduces (3.16).

On the other hand, when arbitrarily precise measurements are impossible—as is the case in measurements of noncommuting observables in quantum mechanics—we do not have instrument-independent notions of mean value, moments, etc., and these concepts have a meaning only within the context of a given class of instruments with congruent calibrations.

4. SPECTRAL MEASURES ON FUZZY SETS

Let now $A_1,\ldots,A_n$ be n independent observables of a quantum-mechanical system. In order to avoid cumbersome notation we consider only the case when all the spectra $\sigma(A_k)$, $k=1,\ldots,n$, coincide with the entire real line $\mathbb{R}^1$.

If $A_1,\ldots,A_n$ commute (to avoid confusion with compatibility of events, we avoid the term "compatible" when applied to observables) the conventional probability distribution for the simultaneous measurement of $A_1,\ldots,A_n$ can be expressed by means of their spectral measure (Ref. 10, Chap. IV, Sec. 1) $E^{A_1,\ldots,A_n}(\Delta)$ by the relation

$$P_\rho^{A_1,\ldots,A_n}(\Delta)=\mathrm{Tr}\{\rho E^{A_1,\ldots,A_n}(\Delta)\} \tag{4.1}$$

for the state represented by the density operator ρ. If a partial Boolean ring $\mathcal{E}(A_1,\ldots,A_n)$ is given (corresponding to a certain class of instruments), then the values of the probability measure on $\mathcal{E}^n$ should be related to its values (4.1) on $\mathcal{B}^n$ in accordance to (3.9) and (3.16). If we introduce for each $\hat\Delta=\{\chi_\alpha\mid\alpha\in\Delta\}\in\mathcal{E}^n$ the operator

$$E^{A_1,\dots,A_n}(\hat{\Delta}) = \int_{\Delta} d^n\alpha \int_{\mathbb{R}^n} \chi_\alpha(\lambda)\, dE_\lambda^{A_1,\dots,A_n}, \tag{4.2}$$

then we can express this extension of $P_\rho^{A_1,\dots,A_n}$ to $\mathcal{E}^n$ by (4.1) with $\Delta \in \mathcal{B}^n$ replaced by $\hat{\Delta} \in \mathcal{E}^n$, i.e.,

$$\begin{aligned} P_\rho^{A_1,\dots,A_n}(\hat{\Delta}) &= \int_{\Delta} d^n\alpha \int_{\mathbb{R}^n} \chi_\alpha(\lambda)\, d_\lambda \operatorname{Tr}\{\rho E_\lambda^{A_1,\dots,A_n}\} \\ &= \operatorname{Tr}\{\rho E^{A_1,\dots,A_n}(\hat{\Delta})\}. \end{aligned} \tag{4.3}$$

The interchange of the trace operation and the operation of integration that leads to (4.3) can be easily justified by using Tonelli's and Fubini's theorems and the standard calculus of functions on spectral measures.[10]

Generalizing from (4.2), we define a *spectral measure on fuzzy events* $\mathcal{E}(A_1, \dots, A_n)$ as a family of nonnegative operators $E(\hat{\Delta}) \geq 0$ which equals zero on the empty set and for which

$$E(\hat{\Delta}) = \operatorname*{s-lim}_{N\to\infty} \sum_{k=1}^{N} E(\hat{\Delta}_k) \tag{4.4}$$

on any $\hat{\Delta} \in \mathcal{E}^n$ which can be decomposed as in (3.5). We note that no further generalization would be achieved by requiring only a weak limit in (4.4) since $E(\hat{\Delta}_1) + \cdots + E(\hat{\Delta}_N) \geq 0$, and therefore the existence of a weak limit implies that of a strong limit.

If we accept now the premise that spectral measures $E^{A_1,\dots,A_n}(\hat{\Delta})$ can be attached to the fuzzy events corresponding to measurements of noncommuting observables $A_1, \dots, A_n$, then clearly $\mathcal{E}^n$ is not expected to contain elementary events of arbitrarily narrow spread and $E^{A_1,\dots,A_n}(\hat{\Delta})$ cannot be constructed as in (4.2) from its values on $\mathcal{B}^n$. To what extent are we then limited in the choice of $E^{A_1,\dots,A_n}(\hat{\Delta})$ on *a priori* grounds, i.e., due to intrinsic features of the operational interpretation of $P_\rho^{A_1,\dots,A_n}(\hat{\Delta})$?

One set of preconditions follows from the observation that any measurement of $A_1, \dots, A_n$ is also a measurement of $A_1, \dots, A_{n-1}$. Thus, for probability measures on sharp events we have for all $\Delta_{n-1} \in \mathcal{B}^{n-1}$

$$P_\rho^{A_1,\dots,A_{n-1},A_n}(\Delta_{n-1} \times \mathbb{R}^1) = P_\rho^{A_1,\dots,A_{n-1}}(\Delta_{n-1}). \tag{4.5}$$

We expect that a similar relation could hold on the extensions

$$P_\rho^{A_1,\dots,A_n}(\hat{\Delta}) = \int_{\Delta} d^n\alpha \int_{\mathbb{R}^n} \chi_\alpha(\lambda)\, dP_\rho^{A_1,\dots,A_n} \tag{4.6}$$

to fuzzy events $\hat{\Delta}$. It is easy to see that this is indeed the the case for fuzzy sets in which at any fixed $\alpha_{n-1} \in \mathbb{R}^{n-1}$ we have

$$\begin{aligned} &\chi_{\alpha_{n-1}\times\beta}(\lambda_{n-1}, \mu) = \chi_{\alpha_{n-1}}(\lambda_{n-1})\chi_\beta(\mu), \\ &\int \chi_\beta(\mu)\, d\beta \equiv \chi_{\sigma(A_n)}(\mu), \end{aligned} \tag{4.7}$$

for all $\beta \in \sigma(A_n)$. In that case we shall say that the calibration in the measurement of A_n is *spectrum-normalized*. We shall denote fuzzy events having the property (4.7) by $\hat{\Delta}_{n-1} \times \hat{\mathbb{R}}^1$.

Our conclusion is that the relation (4.5) extends to fuzzy events of the form $\hat{\Delta}_{n-1} \times \hat{\mathbb{R}}^1$, and consequently

$$E^{A_1,\dots,A_n}(\hat{\Delta}_{n-1} \times \hat{\mathbb{R}}^1) = E^{A_1,\dots,A_{n-1}}(\hat{\Delta}_{n-1}). \tag{4.8}$$

We expect (4.8) to hold even when the values of the spectral measure on fuzzy events are not derivable in accordance to (4.2) from its values on sharp events.

Naturally, similar relations hold for the case when A_n is replaced by any A_k, $k = 1, \dots, n-1$. After n reductions of this type we find that $E^{A_1,\dots,A_n}(\hat{\Delta}_n)$ is related to each $E^{A_k}(\hat{\Delta}_1)$, which in turn is related by

$$\begin{aligned} &E^{A_k}(\hat{\Delta}_1) = \int_{\Delta_1} d\eta \int_{-\infty}^{+\infty} \chi_\eta(\xi)\, dE_\xi^{A_k}, \\ &\hat{\Delta}_1 = \{\chi_\eta \mid \eta \in \Delta_1\} \end{aligned} \tag{4.9}$$

to the spectral measure $E^{A_k}(\Delta_1)$ on Borel sets $\Delta_1 \in \mathcal{B}^1$.

5. SPECTRAL MEASURES IN PHASE SPACE

Let us consider the simple case of a particle without spin moving in one dimension and described quantum-mechanically in the Hilbert space $L^2(\mathbb{R}^1)$. If the position Q and momentum P were commuting observables, the probability distribution for their simultaneous measurement on the system in the state ρ would be derivable from a probability density on sharp elementary events, which would correspond to optimally precise measurements of Q and P. In actuality, however, uncertainty relations hold and it is not the δ eigenfunctions of Q and P, respectively, but the Gaussian wavepackets (we take $\hbar = 1$)

$$\phi_{q,p}^{(s)}(x) = (\pi s^2)^{-1/4} \exp\{-[(x-q)^2/2s^2] + ipx\} \tag{5.1}$$

that have the minimum standard derivations in Q and P compatible with these relations. This suggests that fuzzy sample points $(q, p; \chi)$ with confidence functions

$$\chi_{q,p}^{(s)}(x, y) = \pi^{-1} \exp\{-[(x-q)^2/s^2] - s^2(y-p)^2\} \tag{5.2}$$

represent the outcome of simultaneous measurements of Q and P with optimally accurate instruments, and that it is for probability densities on such sample points rather than on sharp sample points that one should search.

Thus we assume that

$$\mathcal{S}(Q, P) = \{(q, p; \chi_{q,p}^{(s)}) \mid q, p \in \mathbb{R}^1, 0 < s < \infty\} \tag{5.3}$$

is the family of all fuzzy sample points corresponding to the calibration of optimally accurate instruments. We associate with each elementary event (q, p, s) described by $\chi_{q,p}^{(s)}$ the operator $F^{Q,P}(q, p, s)$, constructed from the spectral measures $E^Q(\Delta)$ and $E^P(\Delta)$, $\Delta \in \mathcal{B}^1$, of the observables Q and P, respectively, by means of the following weak cross-iterated integrals[10]:

$$F(q, p; s) = \int_{-\infty}^{+\infty} d_x E_x^Q \int_{-\infty}^{+\infty} d_y\, E_y^P \hat{\chi}_{q,p}^{(s)}(x, y). \tag{5.4}$$

In (5.4) $\hat{\chi}_{q,p}^{(s)}$ is derived from the Fourier transform $\tilde{\chi}_{q,p}^{(s)}$ of $\chi_{q,p}^{(s)}$:

$$\begin{aligned} \hat{\chi}_{q,p}^{(s)}(x, y) = (2\pi)^{-1} \int_{\mathbb{R}^2} &\exp[i(\tfrac{1}{2}uv + xu + yv)] \\ &\times \tilde{\chi}_{q,p}(u, v)\, du\, dv. \end{aligned} \tag{5.5}$$

It is interesting to note that if it were not for the factor $\exp(\frac{1}{2}iuv)$ in (5.5) the function $\hat{\chi}_{q,p}^{(s)}$ would be identical to $\chi_{q,p}^{(s)}(x, y)$.

With $\mathcal{S}(Q, P)$ given by (5.3), the family $\mathcal{E}(Q, P)$ of fuzzy events in the phase space $\mathbb{R}^2$ is unambiguously determined in accordance to the procedure depicted in Sec. 3. Hence a fuzzy event $\hat{\Delta} \in \mathcal{E}(Q,P)$ can be specified by providing a value $s(q,p)$ for each $(q,p) \in \Delta$:

$$\hat{\Delta} = \{\chi_{q,p}(x,y) = \chi_{q,p}^{s(q,p)}(x,y) \,|\, (q,p) \in \Delta\}, \quad \Delta \in \mathcal{B}^2. \qquad (5.6)$$

It is clear that $s(q,p)$ has to be a Borel-measurable function in order that the characteristic function $\chi_{q,p}(x,y)$ of $\hat{\Delta}$ be Lebesgue integrable on Δ in q and p.

We define the spectral measure $E^{Q,P}(\hat{\Delta})$ on $\mathcal{E}(Q;P)$ by the following Bochner integral[10]:

$$E^{Q,P}(\hat{\Delta}) = \int_{\Delta} F(q,p;s(q,p))\, dq\, dp. \qquad (5.7)$$

It remains to show that $E^{Q,P}(\hat{\Delta})$ is indeed a spectral measure on the fuzzy events of $\mathcal{E}(Q,P)$ and that it satisfies the conditions (4.8) and (4.9).

We shall prove first that $E^{Q,P}(\hat{\Delta}) \geqslant 0$ by showing that $F(q,p;s) > 0$ for every $(q,p;s) \in \mathcal{S}(Q,P)$.

We insert (5.5) into (5.4) and reverse[10] the orders of integration. The integration in the weak sense with respect to the two spectral functions E_x^Q and E_y^P can be performed explicitly and yields

$$F(q,p;s) = (2\pi)^{-1} \int_{\mathbb{R}^2} S(u,v) \tilde{\chi}_{q,p}^{(s)}(u,v), \qquad (5.8)$$

$$S(u,v) = \exp(\tfrac{1}{2}iuv) \exp(iQu) \exp(iPv).$$

The operator-valued function $S(u,v)$ that enters the above Bochner integral is the function von Neumann used in his proof of the uniqueness of canonical commutation relations (cf. Ref. 10) and can be rewritten in the form

$$\begin{aligned} S(u,v) &= \exp(\tfrac{1}{2}iPv) \exp(iQu) \exp(\tfrac{1}{2}iPv) \\ &= \exp(\tfrac{1}{2}iQu) \exp(iPv) \exp(\tfrac{1}{2}iQv) \qquad (5.9) \end{aligned}$$

by using the Weyl relations. If we express $\tilde{\chi}_{q,p}^{(s)}(u,v)$ in (5.8) as the product $\tilde{\chi}_q^{(s)}(u) \tilde{\chi}_p'^{(s)}(v)$, where

$$\begin{aligned} &\chi_{q,p}^{(s)}(x,y) = \chi_q^{(s)}(x) \chi_p^{(s)}(y), \\ &\chi_q^{(s)}(x) = (\pi s^2)^{-1/2} \exp[-(x-q)^2/s^2], \qquad (5.10) \\ &\chi_p'^{(s)}(y) = \pi^{-1/2} s \exp[-s^2(y-p)^2], \end{aligned}$$

and take into account that

$$\begin{aligned} \int_{-\infty}^{-\infty} \chi_q^{(s)}(x)\, dE_x^Q &= (2\pi)^{-1/2} \Big(\int_{-\infty}^{+\infty} \tilde{\chi}_q^{(s)}(v) \exp(ixv)\, dv \Big)\, dE_x^Q \\ &= (2\pi)^{-1/2} \int_{-\infty}^{+\infty} \tilde{\chi}_q^{(s)}(v) \exp(iQv)\, dv, \qquad (5.11) \end{aligned}$$

we obtain by performing in (5.8) the integration in $u \in \mathbb{R}^1$:

$$\begin{aligned} F(q,p;s) = (2\pi)^{-1/2} &\int_{-\infty}^{+\infty} dv\, \tilde{\chi}_p'^{(s)}(v) \exp(\tfrac{1}{2}iPv) \\ &\times \Big(\int_{-\infty}^{+\infty} \chi_q^{(s)}(x)\, dE_x^Q \Big) \exp(\tfrac{1}{2}iPv). \qquad (5.12) \end{aligned}$$

Similarly, by inserting the second expression for $S(u,v)$ from (5.9) into (5.8) and integrating in $v \in \mathbb{R}^1$ we arrive at

$$\begin{aligned} F(q,p;s) = (2\pi)^{-1/2} &\int_{-\infty}^{+\infty} du\, \tilde{\chi}_q^{(s)}(u) \exp(\tfrac{1}{2}iQu) \\ &\times \Big(\int_{-\infty}^{+\infty} \chi_p'^{(s)}(y)\, dE_y^P \Big) \exp(\tfrac{1}{2}iQu). \qquad (5.13) \end{aligned}$$

Let ρ be any density operator with the configuration representation $\rho(x,x')$. By observing that[10]

$$[\exp(\tfrac{1}{2}iPv) \rho \exp(\tfrac{1}{2}iPv)](x,x') = \rho(x + \tfrac{1}{2}v, x' - \tfrac{1}{2}v)$$

and inserting in (5.12) the actual values for $\chi_q^{(s)}(x)$ and $\tilde{\chi}_p'^{(s)}(v)$, we get

$$\begin{aligned} \mathrm{Tr}\{\rho F(q,p;s)\} = (2\pi s)^{-1} &\int_{\mathbb{R}^2} dv\, dx\, \rho\left(x + \frac{v}{2},\, x - \frac{v}{2}\right) \\ &\times \pi^{-1/2} \exp\left(-\frac{(x-q)^2}{s^2} - \frac{v^2}{4s^2} - ivp\right). \qquad (5.14) \end{aligned}$$

After performing the substitution $\xi = x + v/2$, $\xi' = x - v/2$, (5.14) yields in terms of (5.1)

$$\begin{aligned} \mathrm{Tr}\{\rho F(q,p;s)\} &= (2\pi s)^{-1} \int_{\mathbb{R}^2} d\xi\, d\xi'\, \rho(\xi, \xi') \\ &\quad \times \pi^{-1/2} \exp\left(-\frac{(\xi-q)^2}{2s^2} - \frac{(\xi'-q)^2}{2s^2} - ip(\xi - \xi')\right) \\ &= (2\pi)^{-1} \mathrm{Tr}\{\rho \,|\, \phi_{q,p}^{(s)} \rangle \langle \phi_{q,p}^{(s)} \,|\,\} \geqslant 0. \qquad (5.15) \end{aligned}$$

This establishes that $F(q,p;s)$ is a positive-definite operator for all $q,p \in \mathbb{R}^1$ and $s > 0$.

The fact $E^{Q,P}(\emptyset) = 0$ is true by definition. Furthermore, the weak σ-additivity of $E^{Q,P}$ on $\mathcal{E}(Q,P)$ is a trivial consequence of (5.7) and, as noted in Sec. 4, in conjunction with the positive-definiteness it implies strong σ-additivity.

It remains to verify the relations (4.8) and (4.9). Since in accordance with (4.7) and (5.3)

$$\hat{\Delta}_1 \times \hat{\mathbb{R}}^1 = \{\chi_q^{(s)}(x) \chi_0'^{(s)}(y-p) \,|\, q \in \Delta_1\}, \qquad (5.16)$$

this task is reduced to proving that

$$\begin{aligned} \int_{\Delta_1} dq \int_{-\infty}^{+\infty} \chi_q^{(s)}(x)\, dE_x^Q = E^Q(\hat{\Delta}_1) &= E^{Q,P}(\hat{\Delta}_1 \times \hat{\mathbf{R}}^1) \\ &= \int_{\Delta_1 \times \mathbb{R}^1} F(q,p;s)\, dq\, dp, \qquad (5.17) \end{aligned}$$

which in turn is established by showing that

$$\int_{-\infty}^{+\infty} \chi_q^{(s)}(x)\, dE_x^Q = \int_{-\infty}^{+\infty} F(q,p;s)\, dp \qquad (5.18)$$

for all $q \in \mathbf{R}^1$ and all $s > 0$.

By integrating the expression (5.13) for $F(q,p;s)$ over $\mathbb{R}^1$ in the p variable and noting that

$$\int_{-\infty}^{+\infty} \chi_p'^{(s)}(y)\, dp \equiv 1 \qquad (5.19)$$

we arrive at the result

$$\int_{-\infty}^{+\infty} F(q,p;s)\, dp = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} du\, \tilde{\chi}_q^{(s)}(u) \exp(iQu), \qquad (5.20)$$

which according to (5.11) is indeed equal to the left-hand side of (5.18).

The counterpart relation

$$\int_{-\infty}^{+\infty} \chi_p'^{(s)}(y)\, dE_y^P = \int_{-\infty}^{+\infty} F(q,p;s)\, dq, \tag{5.21}$$

in which the roles of Q and P are reversed, can be obtained in exactly the same manner from (5.12). This concludes the proof that (5.7) has all the expected properties of a spectral measure on the fuzzy events $\mathcal{E}(Q,P)$ in phase space.

It is interesting to note that the only point in the entire derivation where we used the specific form (5.2) of the fuzzy sample points was in deriving (5.14) and (5.15), i.e., the positivity condition. The linearity in $\hat{\chi}$ of (5.4) implies that there are other distributions $\chi_{q,p}(x,y)$ in $\mathbb{R}^2$ besides Gaussians of minimal spread for which this condition can be satisfied, and which therefore could play the role of elementary fuzzy events. In fact, in general a fuzzy sample point $(p,q;\chi_{q,p})$ can have a confidence function of the form

$$\chi_{q,p}(x,y) = \int \chi_{q',p'}^{(s)}(x,y)\, d\mu(q',p',s), \tag{5.22}$$

where μ is a normalized measure on $\mathbb{R}^2 \times (0,\infty)$.

6. CONCLUSION

The results of the preceding section can be extended only at the price of increased complexity in the notation to the general case of n particles moving in three-dimensional space. Thus they provide a framework for analyzing the motion of such a general system in its phase space $\mathbb{R}^{6n}$. According to (5.7) and (5.15), in the Schrödinger picture such a study reduces to studying the time-evolution of the Husimi transform[5] of the state of the system. The analysis of Secs. 2 and 3 provides an empirical interpretation to the mathematical information that any such study yields.

If we turn our attention to the asymptotic behavior in time of the system, then we can apply to the two-dimensional spectral measures (5.7), or their $6n$-dimensional counterparts, all the techniques used in studying the asymptotic behavior of ordinary spectral measures for commuting observables. In particular, the physical asymptotic conditions[10,11] formulated for commuting observables can be extended without change to the spectral measures associated with simultaneous measurements of position and momentum. Moreover, the very existence of operators representing spectral measures on fuzzy events in phase space implies that if the wave operators exist in the strong sense, then these conditions would be satisfied not only by the position *or* the momentum probability distributions taken separately, but also by the position *and* momentum probability distribution of the interacting state and its free incoming and outgoing asymptotic states.

We should emphasize that the family $\mathcal{S}(Q,P)$ of fuzzy sample points in (5.3) represents the outcomes of simultaneous measurement of Q and P with *optimally accurate* apparatus. If it were not for the uncertainty relations, any such optimally accurate apparatus would yield sharp sample points. However, in the present case the optimally accurate instruments are provided by those Heisenberg arrangements for gedanken experiments, which yield the *minimum* $\Delta p = 2^{-1/2}s^{-1}$ spread in momentum p compatible with a given spread $\Delta q = 2^{-1/2}s$ in position q, i.e., for which $\Delta q \Delta p = \frac{1}{2}$. A typical such setup would consist of a filtering device allowing through only particles of given momentum p, a source emanating photons of a certain wavelength λ and a microscope with a prism for observing the recoil of a photon off the particle whose position and momentum is being measured (cf. Ref. 4, Sec. 4). If the filtering device is ideal (in the sense of not affecting at all the system, if it lets it pass through) the parameter s in (5.2) can be expected to be proportional to the resolving power of the microscope.[4]

We note in this context that probability measures on fuzzy events have been previously considered by Zadeh,[12] but only for the case when the sample points themselves were not fuzzy. Consequently, Zadeh's approach is not at all suited to the quantum-mechanical problem considered in this note.

If we compute the mean values $\bar{Q}(\rho;s)$ of Q and $\bar{P}(\rho;s)$ of P in Sec. 5 for the probability distribution functions $\mathrm{Tr}\{\rho E^{Q,P}(\hat{\Delta}[q] \times \hat{\mathbb{R}}^1)\} = \mathrm{Tr}\{\rho E^Q(\hat{\Delta}[q])\}$ and $\mathrm{Tr}\{\rho E^{Q,P}(\hat{\mathbb{R}}^1 \times \Delta[p])= \mathrm{Tr}\{\rho E^P(\hat{\Delta}[p])\}$, respectively, where

$$\hat{\Delta}[q] \times \hat{\mathbb{R}}^1 = \{\chi_{q'}^{(s)}(x)\chi_{p'}'^{(s)}(y) \mid -\infty < q' \leqslant q, p' \in \mathbb{R}^1\}, \tag{6.1}$$

$$\hat{\mathbb{R}}^1 \times \hat{\Delta}[p] = \{\chi_{q'}^{(s)}(x)\chi_{p'}'^{(s)}(y) \mid q' \in \mathbb{R}^1, -\infty < p' \leqslant p\}, \tag{6.2}$$

we get in view of (5.17) and (5.21)

$$\begin{aligned}\bar{Q}(\rho;s) &= \int_{-\infty}^{+\infty} q d_q\, \mathrm{Tr}\{\rho E^{Q,P}(\hat{\Delta}[q] \times \hat{\mathbb{R}}^1)\}\\ &= \int_{-\infty}^{+\infty} q\, d_q \int_{-\infty}^{+\infty} \chi_q^{(s)}(x)\, d_x\, \mathrm{Tr}\{\rho E_x^Q\},\end{aligned} \tag{6.3}$$

$$\begin{aligned}\bar{P}(\rho;s) &= \int_{-\infty}^{+\infty} p\, d_p\, \mathrm{Tr}\{\rho E^{Q,P}(\hat{\mathbb{R}}^1 \times \hat{\Delta}[p])\}\\ &= \int_{-\infty}^{+\infty} p\, d_p \int_{-\infty}^{+\infty} \chi_p'^{(s)}(y)\, d_y\, \mathrm{Tr}\{\rho E_y^P\}.\end{aligned} \tag{6.4}$$

These quantities represent the mean values of position and momentum, respectively, for measurements carried out on the system in the state ρ with instruments $\mathcal{J}(Q;s)$ and $\mathcal{J}(P;s)$ having the calibrations $\chi_q^{(s)}$ and $\chi_p'^{(s)}$, respectively, at all $q,p \in \mathbb{R}^1$. They do not coincide, however, with the expectation values $\bar{Q}(\rho)$ of Q and $\bar{P}(\rho)$ of P, respectively, in the state ρ:

$$\bar{Q}(\rho) = \int_{-\infty}^{+\infty} q\, d_q\, \mathrm{Tr}\{\rho E_q^Q\}, \tag{6.5}$$

$$\bar{P}(\rho) = \int_{-\infty}^{+\infty} p\, d_p\, \mathrm{Tr}\{\rho E_p^P\}. \tag{6.6}$$

This is to be expected, since $\bar{Q}(\rho)$ is in fact the mean value of Q for measurements of position carried out on the system in state ρ with a *perfectly precise* instrument $\mathcal{J}(Q)$, i.e., an instrument with calibration $\delta_q(x)$ at all $q \in \mathbb{R}^1$; similarly, $\bar{P}(\rho)$ is the mean value of P when the employed instrument $\mathcal{J}(P)$ has calibration function $\delta_p(y)$, $p \in \mathbb{R}^1$. On the other hand, given this interpretation, we expect that $\bar{Q}(\rho;s) \approx \bar{Q}(\rho)$ when $\mathcal{J}(Q;s)$ is very accurate, i.e., s is very small, and that $\bar{P}(\rho;s) \approx \bar{P}(\rho)$ when $\mathcal{J}(P;s)$ is very accurate, i.e., s is very large. Comparison of (6.5) with (6.3) and of (6.6) with (6.4) shows that this is indeed the case; that, in fact,

$\bar{Q}(\rho;s) \to \bar{Q}(\rho)$ when $s \to +0$ while $\bar{P}(\rho;s) \to \bar{P}(s)$ when $s \to +\infty$.

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[1] E. J. Moyal, Proc. Camb. Phil. Soc. 45, 99 (1949).
[2] P. A. M. Dirac, Rev. Mod. Phys. 17, 195 (1945).
[3] E. Prugovečki, J. Math. Phys. 7, 1054 (1966).
[4] E. Prugovečki, Can. J. Phys. 45, 2173 (1967).
[5] K. Husimi, Proc. Phys. Math. Soc. Japan 22, 264 (1940).
[6] A. Kolmogorov, *Foundations of the Theory of Probability* (Chelsea, New York, 1956).
[7] E. Prugovečki, Found. Phys. 6, 557 (1975).
[8] E. Prugovečki, Found. Phys. 4, 9 (1973).
[9] S. Kochen and E. P. Specker, J. Math. Mech. 17, 59 (1967).
[10] E. Prugovečki, *Quantum Mechanics in Hilbert Space* (Academic, New York and London, 1971).
[11] E. Prugovečki, Nuovo Cimento B 4, 105 (1971).
[12] L. A. Zadeh, J. Math. Anal. Appl. 23, 421 (1968).

Hilbert spaces of analytic functions and generalized coherent states

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Generalized coherent states which are associated with a generalization of the harmonic oscillator commutation relation are investigated. It is shown that these states form an overcomplete basis in a Hilbert space of analytic functions. The generalized creation and annihilation operators are bounded except in a limit in which they reduce to the usual boson creation and annihilation operators. In this limit the Hilbert space of analytic functions reduces to the Bargmann–Segal Hilbert space of entire functions and in another limit it reduces to the Hardy–Lebesgue space.

1. INTRODUCTION

In this paper, we investigate generalized coherent states which are associated with a generalization of the harmonic oscillator commutation relation.[1] It is shown that these states form an overcomplete basis in a Hilbert space of analytic functions. The generalized creation and annihilation operators are bounded except in a limit in which they reduce to the usual Boson creation and annihilation operators.[1] In this limit, the Hilbert space of analytic functions reduces to the Bargmann–Segal Hilbert space of entire functions[2] and in another limit it reduces to the Hardy–Lebesgue space.

In the mathematical literature there exists a class of functions which are one parameter generalizations of the hypergeometric functions.[3] These functions are related to the elliptic theta functions and are called "basic hypergeometric functions." Their properties are remarkably similar to those of the usual hypergeometric functions. Here we will investigate the corresponding one-parameter generalization of coherent states,[4] the harmonic oscillator commutation relation, and the Bargmann–Segal Hilbert space of entire functions. Through its dependence on the parameter, the generalized commutation relation continuously interpolates between a commutation and an anticommutation relation.[1] The covariant multidimensional generalization of the harmonic oscillator commutation relation and its connection with dual resonance models in high energy physics have been discussed in Ref. 5.

2. THE HILBERT SPACE H_q

The Hilbert space H_q, where $0 < q < 1$ is a real parameter, is spanned by the vectors $|n\rangle$, generated from the vacuum $|0\rangle$ by the creation operator a^+. The Hermitian conjugate of a^+ is annihilation operator a, and the following relations hold:

$$\begin{aligned} &aa^+ = qa^+a + 1, \\ &\langle 0|0\rangle = 1, \\ &|n\rangle = (a^+)^n|0\rangle, \\ &a|0\rangle = 0. \end{aligned} \tag{1}$$

The following can be proven using the relations (1):

$$\begin{aligned} &a^+|n\rangle = |n+1\rangle, \\ &a|n\rangle = [n]|n-1\rangle, \\ &\langle m|n\rangle = \langle 0|a^m(a^+)^n|0\rangle = [n]!\,\delta_{nm}, \end{aligned} \tag{2}$$

where

$$[n] \equiv (1-q^n)/(1-q) = 1 + q + \cdots + q^{n-1}$$

is the "basic number n"[6] and

$$\begin{aligned} &[n]! \equiv [1][2]\cdots[n], \\ &[0]! \equiv 1. \end{aligned}$$

We will also use $[\infty] = (1-q)^{-1}$.

The vectors $([n]!)^{-1/2}|n\rangle$ form an orthonormal basis and the Hilbert space H_q consists of all vectors $|f\rangle \equiv \equiv \sum_{n=0}^{\infty} f_n|n\rangle$ with complex f_n such that $\langle f|f\rangle \equiv \sum_{n=0}^{\infty} |f_n|^2[n]!$ is finite. If $|g\rangle \equiv \sum_{n=0}^{\infty} g_n|n\rangle$ is also a vector in the Hilbert space then $\langle f|g\rangle \equiv \sum_{n=0}^{\infty} \bar{f}_n g_n [n]!$ where the bar denotes the complex conjugate.

Using Eq. (2), it can be shown that the operators a and a^+ are bounded with

$$\|a\| = \|a^+\| = (1-q)^{-1/2} = [\infty]^{1/2}.$$

As $q \to 1$, $[\infty] \to \infty$ and a and a^+ become the usual harmonic oscillator operators which are unbounded.

3. COHERENT STATES

The vectors $|z\rangle \equiv \sum_{n=0}^{\infty} (z^n/[n]!)|n\rangle$ belong to the Hilbert space for $|z| < (1-q)^{-1/2} = [\infty]^{1/2}$ and they satisfy

$$a|z\rangle = z|z\rangle. \tag{3}$$

They are analogous to the coherent states of quantum optics[4] and we will call them by the same name. These generalized coherent states reduce to the coherent states of quantum optics in the limit $q \to 1$.

Let $|\omega\rangle$ denote a coherent state with eigenvalue ω. Then

$$\langle \omega|z\rangle = \sum_{n=0}^{\infty} \frac{(\bar{\omega}z)^n}{[n]!} = E(\bar{\omega}z) \tag{4}$$

where $E(z)$ is the basic exponential function[6] defined by

$$E(z) \equiv \sum_{n=0}^{\infty} \frac{z^n}{[n]!} \quad \text{for } |z|^2 < [\infty]. \tag{5a}$$

Another representation which exhibits the meromorphy of $E(z)$ is

$$E(z)=\frac{1}{G((1-q)z)} \quad \text{with } G(z)=\prod_{n=0}^{\infty}(1-q^n z). \tag{5b}$$

$G(z)$ is an entire function and $\lim_{q\to 1} E(z)=e^z$.

Using the coherent states, to every vector $|f\rangle \equiv \sum_{n=0}^{\infty} f_n|n\rangle$ of the Hilbert space there corresponds a function $f(z)$ analytic in the region $|z|^2<[\infty]$ by

$$f(z)\equiv\langle\bar{z}|f\rangle=\sum_{n=0}^{\infty} f_n z^n. \tag{6}$$

It follows that

$$\langle\bar{z}|a^+|f\rangle=\sum_{n=0}^{\infty}[n]f_n z^{n+1}=zf(z) \tag{7}$$

and

$$\langle\bar{z}|a|f\rangle=\sum_{n=0}^{\infty}[n]f_n z^{n-1}=\frac{D}{Dz}f(z),$$

where D/Dz is the q-difference operator[6,7] defined by

$$\frac{D}{Dz}f(z)\equiv\frac{f(z)-f(qz)}{z-qz}. \tag{8}$$

In the limit $q\to 1$, $D/Dz\to d/dz$.

The relations (7) show that the representation of a and a^+ in the analytic function space coincides with the q-difference operation, and the "multiplication by the variable z" operation respectively.

4. THE SCALAR PRODUCT

We will now show that by using the notion of "basic integration,"[6,8] the scalar product in H_q can be expressed in closed form in terms of the analytic functions corresponding to the vectors. The basic integral of a function F of a real variable x is defined by

$$\mathbf{S}_0^b F(x)\,Dx\equiv(1-q)b\sum_{l=0}^{\infty}q^l F(q^l b). \tag{9}$$

In the limit $q\to 1$ the basic integral becomes the Riemann integral.

The scalar product can be written as

$$\langle f|g\rangle=\frac{1}{\pi}\mathbf{S}\,\frac{D^2z}{E(q|z|^2)}\overline{f(z)}g(z), \tag{10}$$

where $\mathbf{S}\,D^2z$ consists of an ordinary integration over the argument ϕ of the complex variable $z=|z|e^{i\phi}$, and a basic integration over the modulus squared, i.e.,

$$\mathbf{S}\,D^2zF(z,\bar{z})\equiv\tfrac{1}{2}\mathbf{S}_0^{[\infty]}D(|z|^2)\int_0^{2\pi}d\phi\,F(z,\bar{z}) \tag{11}$$

We note that

$$\lim_{q\to 1}\mathbf{S}\,D^2z\,F(z,\bar{z})=\int d^2z\,F(z,\bar{z})$$
$$=\int_{-\infty}^{+\infty}dx\int_{-\infty}^{+\infty}dy\,F(x+iy,x-iy).$$

Hence the notation $\mathbf{S}\,D^2z$.

Also, the weight function $[E(q|z|^2)]^{-1}$ is zero on the circles $|z|^2=q^{-l}[\infty]$, $(l=1,2,\cdots)$ and taking any one of these circles as the upper limit is equivalent to taking $[\infty]$ as the upper limit for the scalar product defined by (10).

We now demonstrate that the scalar product as given by (10) yields the same result as (2) for the scalar product of two basis vectors.

We have

$$\langle\bar{z}|m\rangle=z^m,\quad\langle\bar{z}|n\rangle=z^n$$

and

$$\frac{1}{\pi}\mathbf{S}\,\frac{D^2z}{E(q|z|^2)}\overline{z^m}z^n$$

$$=\frac{1}{2\pi}\mathbf{S}_0^{[\infty]}\frac{D(|z|^2)}{E(q|z|^2)}\int_0^{2\pi}d\phi\,|z|^{m+n}\exp[i(n-m)\phi]$$

$$=\mathbf{S}_0^{[\infty]}\frac{D(|z|^2)}{E(q|z|^2)}(|z|^2)^m\delta_{mn}$$

$$=\delta_{mn}\sum_{l=0}^{\infty}q^l\left[E\left(\frac{q^{l+1}}{1-q}\right)\right]^{-1}\left(\frac{q^{l+1}}{1-q}\right)^m,$$

where we have used (9) and (11).

From (5),

$$G(q)/G(q^{l+1})=(1-q)(1-q^2)\cdots(1-q^l)$$
$$=(1-q)^l[l]! \tag{12}$$

and

$$\sum_{l=0}^{\infty}q^l\left[E\left(\frac{q^{l+1}}{1-q}\right)\right]^{-1}\left(\frac{q^l}{1-q}\right)^m$$

$$=\sum_{l=0}^{\infty}q^lG(q^{l+1})\frac{q^{lm}}{(1-q)^m}=\frac{G(q)}{(1-q)^m}\sum_{l=0}^{\infty}\frac{q^{(m+1)l}}{(1-q)^l[l]!}$$

$$=\frac{G(q)}{(1-q)^m}E\left(\frac{q^{m+1}}{1-q}\right)$$

$$=\frac{G(q)}{(1-q)^m}\frac{1}{G(q^{m+1})}=[m]!\,.$$

Thus we have shown that

$$\mathbf{S}\,[D^2z/E(q|z|^2)]\overline{z^m}z^n=\delta_{mn}[m]!=\langle m|n\rangle. \tag{13}$$

It follows from the completeness of basis vectors that the scalar product for any two vectors in the Hilbert space is given by (10).

By explicit manipulation of the scalar product (10) we can now show that the operators "multiplication by z" and D/Dz acting on functions in the Hilbert space are indeed Hermitian conjugates. That is,

$$\mathbf{S}\,\frac{D^2z}{E(q|z|^2)}\overline{f(z)}\frac{D}{Dz}g(z)=\mathbf{S}\,\frac{D^2z}{E(q|z|^2)}(\overline{zf(z)})g(z) \tag{14}$$

First we treat z and $\bar{z}$ as independent variables and generalize the definition (5) of the q-difference operator to analytic functions of two variables,

$$\frac{D}{Dz}F(z,\bar{z})\equiv\frac{F(z,\bar{z})-F(qz,\bar{z})}{z-qz}, \tag{15}$$

and we note that following property of D/Dz:

$$\frac{D}{Dz}(F(z)G(z))=\left(\frac{D}{Dz}F(z)\right)G(z)+F(qz)\frac{D}{Dz}G(z), \quad (16)$$

where the dependence of the functions (if any) on **z** is suppressed.

Second we mention that if $f(z)$ is an analytic function of z alone, then $\overline{f(z)}$ is an analytic function of $\bar{z}$ alone and we can write $\overline{f(z)}\equiv\overline{f(\mathbf{z})}$, where $\bar{f}$ is analytic function of its argument.

Using (5), (15), and (16), we have

$$\frac{1}{E(q|z|^2)}\overline{f(z)}\frac{D}{Dz}g(z)=G(q(1-q)z\bar{z})\bar{f}(\bar{z})\frac{D}{Dz}g(z)$$

$$=\frac{D}{Dz}[G((1-q)z\bar{z})\bar{f}(\bar{z})g(z)]$$

$$-\frac{D}{Dz}G((1-q)z\bar{z})\Big)\bar{f}(\bar{z})g(z),$$

$$\frac{D}{Dz}G((1-q)z\bar{z})=-\bar{z}G(q(1-q)|z|^2)=-\frac{\bar{z}}{E(q|z|^2)},$$

so that

$$\mathbf{S}\frac{D^2z}{E(q|z|^2)}\overline{f(z)}\frac{D}{Dz}g(z)=\mathbf{S}D^2z\frac{D}{Dz}$$

$$\times[G((1-q)|z|^2)\bar{f}(\bar{z})g(z)]+\mathbf{S}\frac{D^2z}{E(q|z|^2)}\bar{z}f(\bar{z})g(z).$$

The first term on the right-hand side is a boundary term. To show that it vanishes, we choose $|z|^2$ and $\bar{z}$ as independent variables and consider the term is square brackets as a function of these variables.

We have

$$\frac{D}{Dz}=\bar{z}\frac{D}{D(|z|^2)},$$

$$d\phi=i\frac{d\bar{z}}{\bar{z}},$$

$$\mathbf{S}D^2z\frac{D}{Dz}[G((1-q)|z|^2)\bar{f}(\bar{z})g(z)]$$

$$=\frac{i}{2}\overset{[\infty]}{\underset{0}{\mathbf{S}}}D(|z|^2)\frac{D}{D(|z|^2)}\oint d\bar{z}[G((1-q)|z|^2)\bar{f}(\bar{z})g(z)]$$

$$=\frac{i}{2}\oint d\bar{z}\left[G((1-q)|z|^2)f(\bar{z})g\left(\frac{|z|^2}{\bar{z}}\right)\quad\right|_{|z|^2=0}^{|z|^2=[\infty]}=0,$$

where we have used the fact that

$$\overset{b}{\underset{0}{\mathbf{S}}}\frac{D}{Dx}F(x)\,Dx=F(b)-F(0) \quad (17)$$

and that at the upper limit $G(1)=0$, and at the lower limit $|z|^2=0$; the $\bar{z}$ integration is over a circle with zero radius whereas the integrand is nonsingular at the origin so that the integral is zero and Eq. (14) follows.

5. PROPERTIES OF FUNCTIONS BELONGING TO H_q

The mapping of vectors belonging to H_q, into functions analytic in the region $|z|^2<[\infty]$ is injective, i.e., to different vectors of the Hilbert space H_q, correspond different functions analytic in the region $|z|^2<[\infty]$ but it is not true that to every function analytic in the region $|z|^2<[\infty]$ there corresponds a vector in H_q. For functions belonging to H_q, only certain types of singularities are allowed on the boundary of the region $|z|^2<[\infty]$. For example, one can show that the function $[1-(1-q)^{1/2}z]^{-\alpha}$ belongs to the Hilbert space H_q if and only if $\alpha<\frac{1}{2}$. The Hilbert space H_q is identical with the space of functions analytic in the region $|z|^2<[\infty]$ for which the norm defined in terms of the scalar product (10) is finite.

6. THE LIMITS $q\rightarrow 1$ AND $q\rightarrow 0$

Considered as sets of analytic functions, $H_q\subset H_{q'}$ if $q'<q$. Let f and g be entire functions satisfying

$$\int d^2z\exp(-|z|^2)|f(z)|^2<\infty$$

and

$$\int d^2z\exp(-|z|^2|g(z)|^2<\infty.$$

Then

$$\lim_{q\rightarrow 1}\mathbf{S}\frac{D^2z}{E(q|z|^2)}\overline{f(z)}g(z)=\int d^2z\exp(-|z|^2)\overline{f(z)}g(z). \quad (18)$$

The rhs is the scalar product introduced by Bargmann in his work on a Hilbert space of entire functions. Thus H_q becomes the Bargmann—Segal space in the "limit" $q\rightarrow 1$.

Let f and g be two functions belonging to some H_q. Then

$$\lim_{q\rightarrow 0}\mathbf{S}\frac{D^2(z)}{E(q|z|^2)}\overline{f(z)}g(z)=\int_0^{2\pi}d\phi\,\overline{f(\exp(i\phi))}g(\exp(i\phi)). \quad (19)$$

The rhs is the scalar product used in defining the Hilbert space of functions on the circle $|z|=1$. Thus H_q becomes the Hardy—Lebesgue space[9] in the limit $q\rightarrow 0$.

7. OVERCOMPLETENESS OF THE COHERENT STATES

The fact that the scalar product can be defined by (10) allows us to write down a completeness relation for the coherent states, i.e.,

$$\frac{1}{\pi}\mathbf{S}\frac{D^2z}{E(q|z|^2)}|\bar{z}\rangle\langle\bar{z}|=I \quad (20)$$

where the I on the rhs denotes the identity operator. Because of the discrete nature of the basic integral, not all coherent states contribute to the completeness relation (20). Hence the coherent states form an overcomplete set. Moreover, since the basis vectors $|n\rangle$ can be expressed in terms of coherent states on a single closed contour,

$$|n\rangle=\frac{[n]!}{2\pi i}\oint\frac{|z\rangle}{z^{n+1}}dz.$$

Even the set of states contributing to the completeness relation (20) is overcomplete.

8. THE INTEGRATION REGION

Eqs. (9) and (11) show that $\mathbf{S}\,D^2z$ consists of integrations over circles with radii $(q^l[\infty])^{1/2}$, $l=0,1,2\cdots$. The integration over the lth circle is weighed by a factor of q^l. The integrand of Eq. (11) is a function of z and $\bar{z}$ and can be re-expressed as a function of z and $|z|^2$,

$$\mathbf{S}\, D^2z\, F=\tfrac{1}{2}\overset{[\infty]}{\underset{0}{\mathbf{S}}}\, D(|z|^2)\int d\phi\, F$$

$$=-\frac{i}{2}\overset{[\infty]}{\underset{0}{\mathbf{S}}}\, D(|z|^2)\oint_{|z|=\text{fixed}}\frac{dz}{z}\,F(z,|z|^2)$$

$$=-\frac{i}{2}\sum_{l=0}^{\infty}q^l\oint_{|z|^2=q^l[\infty]}\frac{dz}{z}\,F\left(z,\frac{q^l}{1-q}\right).$$

If the function $F(z,q^l/(1-q))$ has only poles as its singularities inside the region $|z|^2<q[\infty]$, then the Cauchy integral formula can be used to evaluate the contour integral around the lth circle.

It is remarkable that in the limit $q\rightarrow 1$, the countably infinite set of circles moving outward from the origin covers the entire complex plane, and thus the infinite set of contour integrals becomes Bargmann's area integral. This happens because the ratio of the radii of neighboring circles is $q^{1/2}$ which approaches 1 and the radius of the outermost circle is $[\infty]^{1/2}=(1-q)^{-1/2}$ which approaches infinity in this limit. In the limit $q\rightarrow 0$, $[\infty]\rightarrow 1$ and the infinite set of circles moving inward toward the origin all disappear into the origin except the outermost circle which becomes the unit circle.

Thus, we see that in some sense H_q provides a rather remarkable interpolation between the Bargmann–Segal space and the Hardy–Lebesgue space.

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[1] P. Jordan and O. Klein, Z. Phys. 45, 751 (1927); P. Jordan and E. Wigner, Z. Phys. 47, 631 (1928). For a general discussion, see E.M. Henley and W. Thirring, *Elementary Quantum Field Theory* (McGraw-Hill, New York, 1962).

[2] V. Bargmann, Commun. Pure Appl. Math. 14, 187 (1961); 20, 1 (1967); Rev. Mod. Phys. 34, 829 (1962); I.E. Segal, Ill. J. Math. 6, 500 (1962); *Mathematical Problems of Relativistic Physics* (Am. Math. Soc., Providence, R.I., 1963).

[3] W.N. Bailey, *Generalized Hypergeometric Series* (Cambridge University Press, London, 1935); L.J. Slater, *Generalized Hypergeometric Functions* (Cambridge U.P., London, 1966).

[4] J.R. Klauder and E.C.G. Sudarshan, *Quantum Optics* (Benjamin, New York, 1968).

[5] D.D. Coon, M. Baker, and S. Yu, Phys. Rev. D 5, 1429 (1972).

[6] F.H. Jackson, Q. J. Pure. Appl. Math. 41, 193 (1910). For additional references see L.J. Slater, Ref. 3.

[7] R. Boas and R. Buck, *Polynomial Expansions of Analytic Functions* (Academic, New York, 1964), and references contained therein.

[8] F.H. Jackson, Q. J. Math., Oxford Ser. 2, 1 (1951).

[9] K. Hoffman, *Banach Spaces of Analytic Functions* (Prentice-Hall, Englewood Cliffs, New Jersey, 1962); V.P. Khavin, *Spaces of Analytic Functions*, Progress in Mathematics 1 (Plenum, New York, 1968).

Critical-exponent inequalities in the Ornstein–Zernike theory

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A recent generalization of the classical Ornstein–Zernike theory of critical scattering is used to derive inequalities for the critical-point exponents which characterize a first-order phase transition. These inequalities for fluids are found to differ from the corresponding Buckingham–Gunton inequalities for Ising ferromagnets and the Josephson inequality.

In the absence of a general theory for the calculation of critical-point exponents, the derivation of inequalities for critical exponents has proved rather useful for both experimental results and theoretical works. The more fundamental inequalities—the Rushbrooke and the Griffiths inequalities—are common both to ferromagnets and to fluids.[1] There are, however, several inequalities for ferromagnets which have not been proved for fluid systems. In this note we derive inequalities which differ from their counterparts for ferromagnets by using the recently extended theory of Ornstein–Zernike[2] which entails $\eta = 0$.

In Ref. 2 the inequality

$$\gamma \leqslant 2\nu \tag{1}$$

was derived. However, it is clear that the analysis does not single out a particular approach to the critical point. Hence, in particular, for an approach along the coexistence curve one has that

$$\gamma' \leqslant 2\nu'. \tag{2}$$

(Strictly speaking we have $\gamma'_L \leqslant 2\nu'_L$ and $\gamma'_G \leqslant 2\nu'_G$. However, in agreement with available experimental data, we consider equal exponents on the saturated liquid and saturated gas side of the critical point, that is, $\nu' \equiv \nu'_L = \nu'_G$ and $\gamma' \equiv \gamma'_L = \gamma'_G$.)

Consider the energy in terms of the net correlation function $G(r)$ and the pair potential $u(r)$:

$$U = \tfrac{1}{2}k_B TNd + \tfrac{1}{2}V \int [1 + G(r)]u(r)\, d\mathbf{r}, \tag{3}$$

where d is the spatial dimensionality of the system. In terms of Fourier transforms the caloric equation of state (3) becomes

$$U = \tfrac{1}{2}k_B TNd + \tfrac{1}{2}V\hat{u}(\mathbf{k}=0) + [V/2(2\pi)^d] \int \hat{G}(k)\,\hat{u}(k)\, d\mathbf{k}, \tag{4}$$

where we suppose that $0 < |\hat{u}(\mathbf{k}=0)| < \infty$. This assumption should be quite general for fluid systems.

In the Ornstein–Zernike theory,[2] near the critical point, $d > 2$, and for k^2 small, $\hat{G}(k)$ is given by

$$\hat{G}(k) \approx \tfrac{1}{2} \sum_{j=1}^{l} [L_j/(k^2 + A_j) + L_j^*/(k^2 + A_j^*)], \tag{5}$$

where $|A_j| \to t^{2\nu_j}$ as $t \to 0$, where $\nu_j > 0$, $j = 1, 2, \ldots, l$, with $t \equiv |(T - T_c)/T_c|$. The exponent ν_j, of course, depends on the direction of approach to the critical point. From (4) and (5) we have for the specific heat at constant volume C_V as the critical point is approached along the critical isochore for $T > T_c$,

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V \approx -\frac{V_c \pi^{d/2}}{(2\pi)^d} \frac{\Gamma(2 - d/2)}{(d-2)} \hat{u}(\mathbf{k}=0) \times \left(\frac{\partial}{\partial T} \sum_{j=1}^{l} \mathrm{Re}(L_j A_j{}^{d/2-1})\right)_V, \quad 2 < d < 4$$

$$\approx (V_c/32\pi^2)\,\hat{u}(\mathbf{k}=0) \left(\frac{\partial}{\partial T} \sum_{j=1}^{l} \mathrm{Re}(L_j A_j \ln A_j)\right)_V, \quad d = 4$$

and (6)

$$\approx -[V_c/2(2\pi)^d] \left(\int \frac{\hat{u}(k)\, d\mathbf{k}}{k^4}\right) \left(\frac{\partial}{\partial T} \sum_{j=1}^{l} \mathrm{Re}(L_j A_j)\right)_V, \quad d > 4$$

when the residue L_j is essentially constant.

From $|A_j(T, \rho_c)| \sim (T - T_c)^{2\nu_j}$ as $T \to T_c$ from above one has that $\mathrm{Re}[L_j A_j{}^{d/2-1}(T, \rho_c)] \sim (T - T_c)^{\omega_j}$ with $\omega_j \geqslant \nu_j(d-2) \geqslant \bar{\nu}(d-2)$, where $\bar{\nu} \equiv \min\{\nu_1, \ldots, \nu_l\}$. [Recall that $\nu \equiv \max\{\nu_1, \ldots, \nu_l\}$.] Since $C_V \sim (T - T_c)^{-\alpha}$, we have from (6) that

$$\begin{aligned} &\alpha \leqslant 1 - \bar{\nu}(d-2), \quad 2 < d \leqslant 4, \\ &\alpha \leqslant 1 - 2\bar{\nu}, \qquad d > 4. \end{aligned} \tag{7}$$

The study of the behavior of C_V along the critical isochore and for $T < T_c$ is somewhat more complicated. In the two-phase region the specific heat at constant total volume is related to the properties of the system in its liquid and gaseous phases separately[3] by

$$C_V(T) = x_L C_V^L + x_G C_V^G + \frac{x_L T}{\rho_L^3 K_T^L}\left(\frac{\partial \rho_L}{\partial T}\right)^2 + \frac{x_G T}{\rho_G^3 K_T^G}\left(\frac{\partial \rho_G}{\partial T}\right)^2, \tag{8}$$

where $x_L(x_G)$ represents the mole fraction of the liquid (gas). If $\alpha' > 2(1 - \beta) - \gamma'$, then the first two positive terms of (8) are the leading terms. Therefore, from (6) and (8) we have that

$$\alpha' \leqslant 1 - \bar{\nu}'(d-2), \quad 2 < d \leqslant 4,$$

and (9)

$$\alpha' \leqslant 1 - 2\bar{\nu}', \qquad d > 4,$$

where $\bar{\nu}' \equiv \min\{\nu'_1, \ldots, \nu'_l\}$. (We suppose that $\bar{\nu}' \equiv \bar{\nu}'_L = \bar{\nu}'_G$, $\beta \equiv \beta_L = \beta_G$, and $\alpha' \equiv \alpha'_L = \alpha'_G$.)

The similarity between (7) and (9) suggests that (9) should be true even for the case when the Rushbrooke inequality holds as an equality. One would not expect the direction of the inequality (9) to reverse (with > replacing $\leqslant$) just when $\alpha' = 2(1-\beta) - \gamma'$, however, this has not been shown rigorously.

In order to relate (7) and (9) to existing inequalities, we suppose that $\nu = \bar{\nu}$ and $\nu' = \bar{\nu}'$, where $\nu' \equiv \max\{\nu_1', \ldots, \nu_l'\}$. That is, the finite number of simple poles which characterize the first-order phase transition are such that $|A_j(T, \rho_c)| \sim (T - T_c)^{2\nu}$ and $|A_j(T, \rho_{\text{coex}})| \sim (T_c - T)^{2\nu'}$ as $t \to 0$ for $j = 1, 2, \ldots, l$. (The number of poles for each approach to the critical point, of course, need not be the same.) Therefore, (7) and (9) become

$$\begin{aligned} &\alpha \leqslant 1 - \nu(d-2), \quad 2 < d \leqslant 4, \\ &\alpha \leqslant 1 - 2\nu, \qquad\quad d > 4, \end{aligned} \tag{10}$$

and

$$\begin{aligned} &\alpha' \leqslant 1 - \nu'(d-2), \quad 2 < d \leqslant 4, \\ &\alpha' \leqslant 1 - 2\nu' \qquad\quad d > 4. \end{aligned} \tag{11}$$

Results (10) and (11) should be contrasted to the Josephson inequalities[4] $(2-\alpha) \leqslant \nu d$ and $(2-\alpha') \leqslant \nu' d$ respectively. The Josephson inequalities are consistent with (10) and (11) for $2 < d \leqslant 4$ only if $\nu \geqslant \frac{1}{2}$ and $\nu' \geqslant \frac{1}{2}$. Note, however, that whereas (10) and (11) are satisfied by the classical values $\nu = \nu' = \frac{1}{2}$ and $\alpha = \alpha' = 0$ for $2 < d \leqslant 4$, the Josephson inequalities fail for the classical theories for $d < 4$.

From (2), (11), the Rushbrooke inequality,[3] $(2 - \alpha') \leqslant 2\beta + \gamma'$, the Griffiths inequality,[5] $(2-\alpha') \leqslant \beta(\delta+1)$, and the Liberman inequality,[6] $\beta(\delta - 1) \leqslant \gamma'$, for fluids we have

$$\begin{aligned} &\frac{1}{2} + \frac{1}{d}\,\frac{(1-\gamma')}{\gamma'} \leqslant \frac{2\beta+\gamma'}{\gamma' d}, \quad 2 < d \leqslant 4, \\ &\qquad\qquad \beta \geqslant \tfrac{1}{2}, \qquad\qquad d > 4, \end{aligned} \tag{12}$$

and

$$\begin{aligned} &d\,\frac{(\delta-1)}{\delta+1} + \frac{2(1-\gamma')}{\gamma'}\left(\frac{\delta-1}{\delta+1}\right) \leqslant 2, \quad 2 < d \leqslant 4, \\ &\left(\frac{1+\gamma'}{\gamma'}\right)\left(\frac{\delta-1}{\delta+1}\right) \leqslant 1, \qquad\qquad d > 4. \end{aligned} \tag{13}$$

Results (12) and (13) should be compared to the Buckingham–Gunton inequalities[7,8] with $\eta = 0$, $(2\beta + \gamma')/\gamma' d \leqslant \frac{1}{2}$ and $2 \leqslant d(\delta - 1)/(\delta + 1)$ respectively. Consistency between the Buckingham–Gunton inequalities and those of (12) and (13) for $2 < d \leqslant 4$ demands $\gamma' \geqslant 1$. One should point out, however, that the assumption of positivity of the spin–spin correlation functions used in deriving the Buckingham–Gunton inequalities—valid for Ising ferromagnets—is certainly false for fluids.

If one supposes, as is usually done when obtaining the fundamental Rushbrooke and Griffiths inequalities, that $\alpha \geqslant 0$ and $\alpha' \geqslant 0$, one obtains from (1), (2), (10), and (11) that $\gamma \leqslant 2\nu \leqslant 2/(d-2)$ and $\gamma' \leqslant 2\nu' \leqslant 2/(d-2)$ for $2 < d \leqslant 4$. Therefore, if $\gamma \geqslant 1$ and $\gamma' \geqslant 1$, then for $d \geqslant 4$ we must have that $\gamma = \gamma' = 1$, $\alpha = \alpha' = 0$, and $\nu = \nu' = \frac{1}{2}$. Also, from (12) and (13), we obtain that for $d \geqslant 4$, $\beta \geqslant \frac{1}{2}$ and $\delta \leqslant 3$. Therefore, the classical values for the critical-point exponents may be realized for fluid systems with $d \geqslant 4$.

In closing it may be interesting to point out that whereas the Fisher[8] inequality, $\gamma \leqslant (2-\eta)\nu$, agrees with our result (1) for $\eta = 0$, the Buckingham–Gunton inequalities with $\eta = 0$ differ from our results (12) and (13). Nevertheless, the Fisher and the Buckingham–Gunton inequalities are derived under the same assumptions,[8] which can all be justified for Ising models with ferromagnetic interactions. Also, it has been shown recently[9] that if $\eta = 0$, then the results of the Ornstein–Zernike theory of Ref. 2 for $d > 2$ still apply, and hence also those presented in this note.

[1] R.B. Griffiths, in *Phase Transitions and Critical Phenomena*, *Vol.* 1, edited by C. Domb and M.S. Green (Academic, New York, 1972).

[2] M. Alexanian and M. Medina-Noyola, Phys. Rev. A **11**, 1414 (1975).

[3] M.E. Fisher, J. Math. Phys. 5, 944 (1964).

[4] B.D. Josephson, Proc. Phys. Soc. (London) 92, 269, 276 (1967).

[5] R.B. Griffiths, J. Chem. Phys. 43, 1958 (1965).

[6] D.A. Liberman, J. Chem. Phys. 44, 419 (1966).

[7] M.J. Buckingham and J.D. Gunton, Phys. Rev. 178, 848 (1969).

[8] M.E. Fisher, Phys. Rev. **180**, 594 (1969).

[9] M. Alexanian, Phys. Rev. A **12**, 1609 (1975).

L_p-space techniques in potential scattering

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We consider potential scattering of structureless particles for potentials $V(\mathbf{x})$ contained in certain L_p-spaces. In particular we study the compactness properties of $K(t)=V^{1/2}\exp(-iH_0t)V^{1/2}$, H_0 being the free Hamiltonian. By interpreting $\tilde{K}(z)=\int_0^\infty dt\exp(izt)K(t)$, $\operatorname{Im}z\geq 0$, as a Bochner integral, we find the following property for the total cross section $\sigma_{\text{tot}}(\omega)$ (ω is the energy variable): If $V\in L_1(\mathbb{R}^3)\cap L_p(\mathbb{R}^3)$, $3/2\leq p\leq 2$, then $\int_{\omega_0}^\infty d\omega[\omega^{1/2}\sigma_{\text{tot}}(\omega)]^q$ is finite for some suitable $\omega_0\geq 0$ and $2p/(2p-3)<q<\infty$.

1. INTRODUCTION

In the present work we study the properties of certain operators which play a role in the quantum mechanical scattering of structureless particles. In the past much attention has been paid to the operator

$$\tilde{K}(z)=iV^{1/2}(z-H_0)^{-1}V^{1/2},\quad z\in\mathbb{C}, \tag{1.1}$$

especially with respect to its compactness and behavior for large z (see Ref. 1 for a survey). Here denotes $H_0=\mathrm{p}^2$ the free Hamiltonian and $V(\mathbf{x})$ the potential, $H=H_0+V$ being the full Hamiltonian. Although the corresponding time-dependent operator

$$K(t)=V^{1/2}\exp(-iH_0t)V^{1/2} \tag{1.2}$$

has been considered in the literature,[2] not so much seems to be known about its compactness properties. Here we consider the latter in some detail (Sec. 3) and also (Sec. 4) the implied properties for $\tilde{K}(z)$, where the latter is interpreted as a Bochner integral

$$\tilde{K}(z)=\begin{cases}\int_0^\infty dt\exp(izt)K(t), & 0\leqslant\arg z\leqslant\pi,\\ -\int_0^\infty dt\exp(-izt)K(-t), & \pi<\arg z<2\pi.\end{cases} \tag{1.3}$$

One result is that $\tilde{K}(\omega)$, ω real, is contained in some L_p-space of vector-valued (actually compact operator-valued) functions under suitable conditions on V. In Sec. 5 it is shown how this leads to corresponding integrability properties for the total cross section.

2. MATHEMATICAL PRELIMINARIES

In this section we establish our notation and discuss a few background results to be used in the sequel.

We denote by $L_p(\mathbf{R}^n)$, or simply L_p, the L_p-space of complex-valued functions on $\mathbf{R}^n$, the underlying measure space being S, Σ, μ with $S=\mathbf{R}^n$, $\Sigma=\mathcal{B}$, the Borel sets in $\mathbf{R}^n$, and μ Lebesgue measure. In the following we shall also encounter L_p-spaces of functions which take their value in a *complex* Banach space $\mathcal{X}$; notation $L_p(\mathbb{R}^n,\mathcal{X})=L_p(\mathcal{X})$. For reflexive $\mathcal{X}$ the dual of $L_p(\mathcal{X})$ is $L_q(\mathcal{X}^*)$, $1<p<\infty$, $p^{-1}+q^{-1}=1$.[3]

In the present work all integrals will be of the Lebesgue type and standard theorems such as those of Fubini and Tonelli will be used without explicit mention. Fourier transforms will play an important role. As is well known the Fourier transform $\tilde{f}=Ff$, or more explicitly

$$\tilde{f}(k)=(Ff)(k)=(2\pi)^{-n/2}\int dx\exp(ikx)f(x) \tag{2.1}$$

exists as an element of $L_q(\mathbf{R}^n)$, $p^{-1}+q^{-1}=1$ if $1\leqslant p\leqslant 2$ (but not necessarily if $p>2$). In this case F can be interpreted as a bounded transformation from L_p into L_q, its bound obeying

$$\|F\|_{p,q}\leqslant(2\pi)^{-(2/p-1)n/2},\quad 1\leqslant p\leqslant 2,\ p^{-1}+q^{-1}=1. \tag{2.2}$$

We denote the L_p-norm of $f\in L_p(\mathbf{R}^n,\mathcal{X})$ by $\|f\|_p$;

$$\begin{aligned}\|f\|_p&=[\textstyle\int_{\mathbf{R}^n}dx\,|f(x)|^p]^{1/p},\quad 1\leqslant p<\infty,\\ \|f\|_\infty&=\operatorname*{ess\,sup}_{x\in\mathbf{R}^n}|f(x)|.\end{aligned} \tag{2.3}$$

If $\mathcal{X}=\mathbb{C}$, $|f(x)|$ denotes the absolute value of $f(x)$, in the Banach space case $|f(x)|$ is the norm of $f(x)\in\mathcal{X}$. Let $f(x)\in L_1(\mathcal{X})$. Then $f(x)$ is (by definition) strongly measureable (i.e., its measurability is defined with respect to the open sets in the norm topology of $\mathcal{X}$).

Thus $\exp(ikx)f(x)$ is Bochner integrable[4,5] so that the Fourier transform $\tilde{f}(k)=Ff(x)$ exists. In the same way as in the scalar-valued case one can prove:

Proposition 2.1: Let $f\in L_1(\mathcal{X})$. Then $\tilde{f}(k)\in L_\infty(\mathcal{X})$ is strongly continuous in k, $\|\tilde{f}\|_\infty\leqslant\|f\|_1$, and (Riemann–Lebesgue)

$$\lim_{k\to\infty}|\tilde{f}(k)|=0. \tag{2.4}$$

We also have

Proposition 2.2: Let $\mathcal{X}$ be a complex Hilbert space. Then the Fourier transform constitutes a unitary mapping of the Hilbert space $L_2(\mathcal{X})$ onto itself.

The proof proceeds again along the same lines as in the scalar-valued case, i.e., by considering sequences of simple functions and their limits in $L_2(\mathcal{X})$.

Corollary 2.1: Let $\mathcal{X}$ be a complex Hilbert space. Then the Fourier transform F defines a bounded linear transformation from $L_p(\mathcal{X})$, $1\leqslant p\leqslant 2$, to $L_q(\mathcal{X})$, $p^{-1}+q^{-1}=1$. Its bound obeys (2.2).

The proof is evident from an application of the Riesz–Thorin convexity theorem for L_p-spaces of vector-valued functions (see Ref. 6., pp. 536, 537). Let $x=(x_1,\ldots,x_n)\in\mathbf{R}^n$ and let $\lambda\in\mathbf{R}$ so that $\lambda x=(\lambda x_1,\ldots,\lambda x_n)\in\mathbf{R}^n$ and let, furthermore, f be a function from $\mathbf{R}^n$ into the Banach space $\mathcal{X}$. We define the dilatation operator D_λ through

$$(D_\lambda f)(x)=f(\lambda x). \tag{2.5}$$

Evidently $D_1=1$, $D_\lambda D_\mu=D_{\lambda\mu}$, $D_{\lambda^{-1}}=(D_\lambda)^{-1}$ for $\lambda\neq 0$, and if g is scalar-valued, $D_\lambda(fg)=(D_\lambda f)(D_\lambda g)$. For $f\in L_p(\mathcal{X})$,

$1 \leqslant p < \infty$, we have $\|D_\lambda f\|_p = |\lambda|^{-n/p}\|f\|_p$, $\lambda \neq 0$, and this relation also holds for $p = \infty$ if we define $|\lambda|^{-n/p} = 1$ for this case. Denoting the class of bounded operators on a Banach space $\mathcal{Y}$ by $\mathcal{B}(\mathcal{Y})$ and by $\|T\|_{p,q}$ the norm of a bounded operator T from $L_p(\mathcal{X})$ into $L_q(\mathcal{X})$, we have

$$D_\lambda \in \mathcal{B}(L_p(\mathcal{X})), \quad \|D_\lambda\|_{p,p} = |\lambda|^{-n/p}, \quad \lambda \neq 0, 1 \leqslant p \leqslant \infty. \tag{2.6}$$

Proposition 2.3: D_λ, considered as an operator function in $L_p(\mathcal{X})$, $1 \leqslant p < \infty$, is strongly continuous in each $\lambda \neq 0$.

Proof: Let $\lambda_0 \neq 0$ be real and let λ range through the interval $[\lambda_0 - \Lambda, \lambda_0 + \Lambda]$, disjunct from zero. Let $f \in L_p(\mathcal{X})$, $1 \leqslant p < \infty$. Then, for given $\epsilon > 0$, there is an $f_0 \in L_p(\mathcal{X})$, f_0 continuous and vanishing outside a hypersphere with radius $\rho = \rho(\epsilon)$ about the origin in $\mathbf{R}^n$, such that $\|f - f_0\|_p < \epsilon$. Now

$$\|(D_\lambda - D_{\lambda_0})f\|_p \leqslant (\|D_\lambda\|_p + \|D_{\lambda_0}\|_p)\|f - f_0\|_p + \|(D_\lambda - D_{\lambda_0})f_0\|_p$$
$$\leqslant 2\epsilon A^{-n/p} + \|(D_\lambda - D_{\lambda_0})f_0\|_p,$$

where $A = \min\{|\lambda_0 - \Lambda|, |\lambda_0 + \Lambda|\}$. Since

$$\|(D_\lambda - D_{\lambda_0})f_0\|_p = [\int_{|x| \leqslant \rho} dx\, |f_0(\lambda x) - f_0(\lambda_0 x)|^p]^{1/p}$$

and $f_0(x)$ is uniformly continuous in the domain $|x| \leqslant \rho \cdot \max\{|\lambda_0 - \Lambda|, |\lambda_0 + \Lambda|\}$, we can make the right-hand side of this expression arbitrarily small by making $|\lambda - \lambda_0|$ sufficiently small. Thus it follows that

$$\lim_{\lambda \to \lambda_0}\|(D_\lambda - D_{\lambda_0})f\|_p = 0. \qquad \blacksquare$$

Before we proceed let us introduce some further notation. We will denote $L_2(\mathbf{R}^n) = \mathcal{H}$. For an element f of $\mathcal{H}$ we have the alternative expressions $|f|$ and $\|f\|_2$ for its norm. The class of bounded operators on a Banach space $\mathcal{X}$ will be denoted by $\mathcal{B}(\mathcal{X})$. The various Carlemann classes of compact operators on $\mathcal{H}$ will be denoted by $\mathcal{B}_p(\mathcal{H}) = \mathcal{B}_p$, $1 \leqslant p \leqslant \infty$. For $A \in \mathcal{B}_p$ its $\mathcal{B}_p$-norm is $|||A|||_p = \mathrm{tr}[A^*A]^{p/2}$ for $1 \leqslant p < \infty$ and $|||A|||_\infty = |A|$, the (supremum) norm of A as a bounded operator on $\mathcal{H}$. As is well known $\mathcal{B}_p$ is a Banach space under the corresponding $\mathcal{B}_p$-norm. Examples are the trace class $\mathcal{B}_1$ and the Schmidt class $\mathcal{B}_2$, the latter being a Hilbert space, $\mathcal{B}_\infty$ is the uniformly closed subspace of all compact operators in $\mathcal{B}(\mathcal{H})$.

3. PROPERTIES OF $K(t)$

Theorem 3.1: Let $\phi, \psi \in L_p(\mathbf{R}^n)$, $p \geqslant 2$. Then $K(t)$, defined by

$$(K(t)f)(x) = (4\pi i t)^{-n/2}\phi(x) \int dy \exp[i(x-y)^2/(4t)]$$
$$\times \psi(y)f(y), \quad t \neq 0, \ f \in L_2(\mathbf{R}^n) = \mathcal{H} \tag{3.1}$$

exists as a bounded linear operator on $L_2(\mathbf{R}^n)$ and is strongly continuous in each $t \neq 0$. Its norm obeys the estimate

$$|K(t)| \leqslant |4\pi t|^{-n/p}\|\phi\|_p\|\psi\|_p, \quad t \neq 0. \tag{3.2}$$

Proof: For the existence and norm estimate see Ref. 6, Sec. 6. With $\hat{F}$ ($\hat{F}$ is essentially the Fourier transform) defined by

$$(\hat{F}f)(x) = (2\pi)^{-n/2} \int dy \exp[i(x-y)^2/2]f(y) \tag{3.3}$$

we have for $t > 0$ (the case $t < 0$ goes similarly)

$$K(t)f = (i)^{-n/2}\phi D_{(2t)^{-1/2}} \hat{F} D_{(2t)^{1/2}}(\psi f)$$

and the continuity follows from the strong continuity of D_t (Proposition 2.3). $\blacksquare$

Remark: It follows from Corollary 2.1 and the validity of Proposition 2.3 for the general Banach space case that Theorem 3.1 remains true with $L_2(\mathbf{R}^n)$ replaced by $L_2(\mathbf{R}^n, \mathcal{X})$, $\mathcal{X}$ being a Hilbert space.

Lemma 3.1: Let, in Theorem 3.1, $\phi, \psi \in L_2(\mathbf{R}^n)$, respectively $L_p(\mathbf{R}^n)$, $2 \leqslant p \leqslant 4$. Then for $t \neq 0$, $K(t)$ is contained in $\mathcal{B}_2(\mathcal{H})$, respectively $\mathcal{B}_4(\mathcal{H})$ and $|||K(t)|||_2 = |4\pi t|^{-n/2}\|\phi\|_2\|\psi\|_2$, respectively $|||K(t)|||_4 \leqslant |4\pi t|^{-n/p} \times \|\phi\|_p\|\psi\|_p$, whereas $|||K(t)|||_2$, respectively $|||K(t)|||_4$ is continuous in each $t \neq 0$.

Proof: The first case is obvious, whereas in the second case we have for $t \neq 0$

$$|||K(t)|||_4^4 = \mathrm{tr}[K^*(t)K(t)]^2$$
$$= |4\pi t|^{-2n} \int dx_1\, dx_2\, dy_1\, dy_2\, |\phi(y_1)\phi(y_2)\psi(x_1)\psi(x_2)|^2$$
$$\times \exp\{(i/2t)[(x_1 - x_2)y_1 - (x_1 - x_2)y_2]\}$$
$$= |4\pi t|^{-2n} \cdot (2\pi)^n \int dx_1\, dx_2\, |\psi(x_1)\psi(x_2)|^2$$
$$\times |D_{(2t)^{-1}}\Phi(x_1 - x_2)|^2. \tag{3.4}$$

Here Φ is the Fourier transform of $|\phi|^2$, an element of $L_{q/2}$, $2/p + 2/q = 1$ so that $|\phi|^2 \in L_{q/4}$ (note that $1 \leqslant q/4 \leqslant \infty$). Since $|\psi|^2 \in L_{p/2}$, the convolution $(|\psi|^2 * |D_{(2t)^{-1}}\Phi|^2)(x_1) = \int dx_2 |\psi(x_2)|^2 |\Phi(x_1 - x_2)/(2t)|^2$ is contained in L_r; $r^{-1} = 2p^{-1} + 4q^{-1} - 1 = 1 - 2p^{-1}$ (for convolution in L_p-spaces see Ref. 6). Thus

$$|\psi|^2 \cdot (|\psi|^2 * |D_{(2t)^{-1}}\Phi|^2) \in L_s, \quad s^{-1} = 2p^{-1} + r^{-1} = 1,$$

i.e., is contained in L_1. Hence (3.13) is finite, i.e., $K(t) \in \mathcal{B}_4(\mathcal{H})$, $t \neq 0$, and

$$|||K(t)|||_4^4 \leqslant |4\pi t|^{-2n} \cdot (2\pi)^n \cdot \||\psi|\|_{p/2}^2 \||\psi|^2 * |D_{(2t)^{-1}}\Phi|^2\|_r$$
$$\leqslant |4\pi t|^{-2n} \cdot (2\pi)^n \|\psi\|_p^4 \||\psi|^2\|_{p/2} \||D_{(2t)^{-1}}\Phi|^2\|_{q/4}$$
$$\leqslant |4\pi t|^{-2n} \cdot (2\pi)^n \|\psi\|_p^4 \|D_{(2t)^{-1}}\Phi\|_{q/2}^2$$
$$\leqslant |4\pi t|^{-2n} \cdot (2\pi)^n \|\psi\|_p^4 \|D_{(2t)^{-1}}\|_{q/2,q/2}^2 \|F\|_{p/2,q/2}^2 \|\phi\|_p^4$$
$$\leqslant |4\pi t|^{-4n/p} \cdot \|\phi\|_p^4 \|\psi\|_p^4.$$

The continuity of $\|K(t)\|_4$ for $t \neq 0$ follows from the strong continuity of D_t and can easily be made explicit, for instance, by starting from the expression (3.4). $\blacksquare$

Theorem 3.2: Let ϕ, ψ and $K(t)$ be as defined before. We distinguish the following cases:

(a) $\phi, \psi \in L_p(\mathbf{R}^n)$, $2 \leqslant p \leqslant \infty$.

Then for $t \neq 0$, $K(t) \in \mathcal{B}(\mathcal{H})$ and is continuous in the strong operator topology on $\mathcal{B}(\mathcal{H})$ in each $t \neq 0$, while

$$|K(t)| \leqslant |4\pi t|^{-n/p}\|\phi\|_p\|\psi\|_p, \quad t \neq 0.$$

(b) $\phi, \psi \in L_p(\mathbf{R}^n)$, $2 < p \leqslant 4$.

Then for $t \neq 0$, $K(t) \in \mathcal{B}_4(\mathcal{H})$ and is continuous in the norm topology of $\mathcal{B}_4(\mathcal{H})$ in each $t \neq 0$, while

$$\| K(t) \|_4 \leqslant |4\pi t|^{-n/p} \|\phi\|_p \|\psi\|_p, \quad t \neq 0.$$

(c) $\phi, \psi \in L_2(\mathbf{R}^n)$.

Then for $t \neq 0$, $K(t) \in \mathcal{B}_2(\mathcal{H})$ and is continuous in the norm topology of $\mathcal{B}_2(\mathcal{H})$ in each $t \neq 0$, while

$$\| K(t) \|_2 = |4\pi t|^{-n/2} \|\phi\|_2 \|\psi\|_2, \quad t \neq 0.$$

Proof: It remains to establish the continuity in cases (b) and (c). We do so for case (c), the other case goes similarly. It follows from the uniform boundedness of $\| K(t) \|_4$ on each interval disjunct form zero and the fact that $K(t)$ is continuous in the strong operator topology [part (a) of the theorem] that $K(t)$ is continuous in the weak topology on $\mathcal{B}_4$. Now for $t_n - t_0 \neq 0$ we have weak-$\mathcal{B}_4$- $\lim_{n\to\infty} K(t_n) = K(t_0)$ and $\lim_{t_n \to t_0} \| K(t_n) \|_4 = \| K(t_0) \|_4$. Since $\mathcal{B}_4$ is uniformly convex (see Ref. 7), it follows (see Ref. 5 or Ref. 6) that $K(t_n)$ converges to $K(t_0)$ in the norm topology of $\mathcal{B}_4$. Consequently, $K(t)$ is continuous in t_0 with respect to the norm topology of $\mathcal{B}_4$. ∎

4. PROPERTIES OF $\widetilde{K}(z)$

If, in part(a) of Theorem 3.2, $\phi, \psi \in L_{p_1} \cap L_{p_2}$, $2 \leqslant p_1 < p_2 \leqslant \infty$, then

$$\int_0^\infty dt \, |K(t)|^r = \left(\int_0^1 + \int_1^\infty\right) dt \, |K(t)|^r < \infty \quad \text{if } p_1/n < r < p_2/n.$$

Since $K(t)$ is strongly continuous and consequently strongly measurable, the situation where $r = 1$ leads to the Bochner integrability of $K(t)f$, $f \in \mathcal{H}$. This case was considered by Kato.[2] In view of part (b) of Theorem 3.2 we can make stronger statements if in addition $\phi, \psi \in L_p$, $2 \leqslant p \leqslant 4$, since then $K(t) \in \mathcal{B}_4$.

Theorem 4.1: (a) Let $\phi, \psi \in L_{p_1} \cap L_{p_2}$, $2 \leqslant p_1 < n < p_2 \leqslant \infty$. Then for every $f \in \mathcal{H}$ $\exp(izt)K(t)f$, $0 \leqslant \arg z \leqslant \pi$ and $\exp(-izt)K(-t)f$, $\pi < \arg z < 2\pi$ are Bochner integrable over $(0, \infty)$. The Bochner integral

$$\widetilde{K}(z)f = \begin{cases} \int_0^\infty dt \exp(izt)K(t)f, & 0 \leqslant \arg z \leqslant \pi, \\ -\int_0^\infty dt \exp(-izt)K(-t), & \pi < \arg z < 2\pi, \end{cases} \tag{4.1}$$

defines an element $\widetilde{K}(z) \in \mathcal{B}(\mathcal{H})$ with the properties:

1. $|\widetilde{K}(z)|$ is uniformly bounded in z;

2. $\widetilde{K}(z)$ is analytic in the open upper and lower half plane with respect to the uniform topology on $\mathcal{B}(\mathcal{H})$.

3. $\lim_{|\mathrm{Re} z| \to \infty} \widetilde{K}(z)f = 0, \ \forall f \in \mathcal{H}$.

(b) Let ϕ, ψ as in part (a) and let $n = 3$. Then $\exp(izt)K(t)$, $0 \leqslant \arg z \leqslant \pi$, and $\exp(-izt)K(-t)$, $\pi \leqslant \arg z \leqslant 2\pi$ are Bochner integrable on $\mathcal{B}_4$ over $(0, \infty)$ and the Bochner integral

$$\widetilde{K}(z) = \begin{cases} \int_0^\infty dt \exp(izt)K(t), & 0 \leqslant \arg z \leqslant \pi, \\ -\int_0^\infty dt \exp(-izt)K(-t), & \pi < \arg z < 2\pi, \end{cases} \tag{4.2}$$

defines an element $\widetilde{K}(z) \in \mathcal{B}_4$ with the properties:

1. $\| \widetilde{K}(z) \|_4$ is uniformly bounded in z;

2. $\widetilde{K}(z)$ is analytic in the open upper half plane with respect to the norm topology on $\mathcal{B}_4$;

3. $\lim_{|\mathrm{Re} z| \to \infty} \| \widetilde{K}(z) \|_4 = 0$.

(c) Let ϕ, ψ as in part (a) and let, moreover, $p_1 \leqslant 4$. Then $\exp(izt)K(t)$, $0 \leqslant \arg z \leqslant \pi$ and $\exp(-izt)K(-t)$, $\pi < \arg z < 2\pi$ are Bochner integrable on $\mathcal{B}_\infty$ over $(0, \infty)$ with respect to the uniform topology and (4.2) defines a compact operator $\widetilde{K}(z)$ with the properties (1)—(3) above with the $\mathcal{B}_4$-norm replaced by the operator (supremum) norm.

Proof: Consider case (a) Property 1 will be evident, whereas property 3 is clear from Proposition 2.1. Since for $f \in \mathcal{H}$ the operator $\widetilde{K}'(z)$

$$\widetilde{K}'(z)f = \begin{cases} i\int_0^\infty dt \, t \exp(izt)K(t)f, & \mathrm{Im} z > 0, \\ i\int_0^\infty dt \, t \exp(-izt)K(-t)f, & \mathrm{Im} z < 0 \end{cases} \tag{4.3}$$

is well-defined, the analyticity in the strong operator topology follows by showing that $\lim_{z \to z_0} |(z - z_0)^{-1}[\widetilde{K}(z)f - \widetilde{K}(z_0)f] - \widetilde{K}'(z)f| = 0$, which is a routine matter. But then this result also holds with respect to the uniform topology on $\mathcal{B}(\mathcal{H})$ (Ref. 4, Sec. 3.10).

The proof of part (b) goes similarly, As to part (c), since $p_1 \leqslant 4$ we know that $K(t) \in \mathcal{B}_4$ (and hence $\in \mathcal{B}_\infty$) and is continuous in the $\mathcal{B}_4$-topology. Since the operator norm is majorized by the $\mathcal{B}_4$-norm it follows that $K(t)$ is continuous in the uniform topology on $\mathcal{B}_\infty$ and the rest of the proof will be evident. ∎

Remark: The theorem does not apply if $n = 1, 2$ because of the conflicting requirements $2 \leqslant p_1$ and $p_1 < n$.

Under the conditions of part (b) of Theorem 4.1 we have for real ω (χ_A is the characteristic function of the set A):

$$\widetilde{K}(\omega) = \int_{-\infty}^\infty dt \exp(i\omega t)\chi_{[0,\infty]}(t) \cdot K(t), \tag{4.4}$$

and we can interprete the thus defined Fourier transform as a bounded linear transformation from $L_1(\mathbf{R}, \mathcal{B}_4)$ into $L_\infty(\mathbf{R}, \mathcal{B}_4)$. Now if there is an r, $1 \leqslant r \leqslant 2$, such that $p_1/n < r < p_2/n$, then $\chi_{[0\infty]}(t)K(t) \in L_r(\mathbf{R}, \mathcal{B}_4)$, and if $\mathcal{B}_4$ were a Hilbert space, then Corollary 2.1 states that $K(\omega) \in L_s(\mathbf{R}, \mathcal{B}_4)$, $r^{-1} + s^{-1} = 1$. However, $\mathcal{B}_4$ is not a Hilbert space, and we have to follow a more roundabout way to arrive at the above conclusion. (We do not know whether Proposition 2.2 is valid for the general Banach space case.)

Lemma 4.1: Let $1 \leqslant r \leqslant 2$ and let $T(t) \in L_r(\mathbf{R}, \mathcal{B}_4)$. Then

$$S(u) = (T^* * T)(u) = \int dt T^*(t)T(t+u) \tag{4.5}$$

exists as an element of $L_s(\mathbf{R}, \mathcal{B}_2)$, $s^{-1} = 2r^{-1} - 1$, and $\|S\|_s \leqslant \|T\|_r^2$.

Proof: Since $T(t)$ exists for almost every t as an element of $\mathcal{B}_4$, the same is true for $T^*(t)$ and the latter is measurable with respect to the norm topology of $\mathcal{B}_4$ along with $T(t)$. It follows that the function $T^*(t)T(t+u)$ of t and u exists almost everywhere and is measurable with respect to the norm topology of $\mathcal{B}_2$ (the product of two elements of $\mathcal{B}_4$ defines an element of $\mathcal{B}_2$).

Let $\{T_n(t)\} \subset L_r(\mathcal{B}_4)$ be a sequence of simple functions converging towards $T(t)$ in the norm topology of $L_r(\mathcal{B}_4)$. We write

$$T_n(t)=\sum_i \alpha_i T_i \chi_{E_i}(t),$$

where $\alpha_i \in \mathbb{C}$, $T_i \in \mathcal{B}_4$ with $\|T_i\|_4=1$ and the E_i's are a family of disjunct Borel sets with finite total measure.

If we consider a second simple function $T_{n'}(t)$ of the sequence, the corresponding sets E'_i will differ from the E_i. For fixed n, n' we, nevertheless, can find a new collection $\{F_j\}$ of disjunct Borel sets such that each E_i and E_i' can be written as a finite union of F_j's. Thus we can write

$$T_n(t)=\sum_i \alpha_i T_i \chi_{F_i}(t), \quad T_{n'}(t)=\sum_i \alpha_i' T_i' \chi_{F_i}(t),$$

where $\alpha_i, \alpha_i' \in \mathbb{C}$, $T_i, T_i' \in \mathcal{B}_4$, $\|T_i\|_4=\|T'_i\|_4=1$, and we have

$$\|T_n\|_r=\left[\sum_i |\alpha_i|^r \mu(F_i)\right]^{1/r},$$

$$\|T_n-T_{n'}\|_r=\left[\sum_i \|\alpha_i T_i-\alpha_i' T_i'\|_4^r \, \mu(F_i)\right]^{1/r}.$$

We define

$$S_n(u)=T_n^* * T_n(u)=\int dt T_n^*(t) T_n(t+u).$$

$S_n(u)$ obviously exists as an element of $\mathcal{B}_2$ since it consists of a sum of products of elements of $\mathcal{B}_4$ and convolutions of characteristic functions. Then [$s^{-1}=2r^{-1}-1$ and $\|\cdot\|_s$ refers to the norm in $L_s(\mathbf{R},\mathcal{B}_2)$]

$$\begin{aligned}\|S_n-S_{n'}\|_s&=\|T_n^* * T_n-T_{n'}^* * T_{n'}\|_s\\ &\leqslant \|T_n^* *(T_n-T_{n'})\|_s+\|(T_n^*-T_{n'}^*)T_{n'}\|_s.\end{aligned}$$

Now:

$$\begin{aligned}&\|T_n^* *(T_n-T_{n'})\|_s\\ &=[\int du \|\sum_{ij} \alpha_i T_i^*(\alpha_j T_j-\alpha_j' T_j')(\chi_{F_i} * \chi_{F_j})(u)\|_2^s]^{1/s}\\ &\leqslant\left[\int du\left\{\sum_{ij}|\alpha_i| \, \|\alpha_j T_j-\alpha_j' T_j'\|_4(\chi_{F_i} * \chi_{F_j})(u)\right\}^s\right]^{1/s}\\ &=\|\int du\left\{\left(\sum_i|\alpha_i|\chi_{F_i}\right) * \left(\|\sum_j \alpha_j T_j-\alpha_j' T_j'\|_4 \chi_{F_j}\right)(u)\right\}^s\|^{1/s}\\ &=\|\left(\sum_i|\alpha_i|\chi_{F_i}\right) * \sum_j \|\alpha_j T_j-\alpha_j' T_j'\|_4 \chi_{F_j}\|_s\\ &\leqslant\|\sum_i|\alpha_i|\chi_{F_i}\|_r\|\sum_j \|\alpha_j T_j-\alpha_j' T_j'\|_4 \chi_{F_j}\|_r\\ &=\|T_n\|_r\|T_n-T_n'\|_r,\end{aligned}$$

and the other term in (4.14) is estimated in the same way. Hence

$$\|s_n-S_{n'}\|_s \leqslant\{\|T_n\|_r+\|T_{n'}\|_r\}\|T_n-T_n'\|_r,$$

i.e., $\{S_n(u)\}$ is a Cauchy sequence in $L_s(\mathcal{B}_2)$ and it follows that its limit $S(u)$ exists as an element of $L_s(\mathcal{B}_2)$. An estimate, similar to the one above yields $\|S_n\|_s \leqslant\|T_n\|_r^2$, so that $\|S\|_s \leqslant\|T\|_r^2$. ■

Theorem 4.3: Let $1 \leqslant r \leqslant 4/3$. If $T(t) \in L_r(\mathcal{B}_4)$, then $\tilde{T}(\omega)=\int dt \exp(i\omega t) T(t)$, $\omega \in \mathbf{R}$, exists as an element of $L_u(\mathcal{B}_4)$, $r^{-1}+u^{-1}=1$, and $\|\tilde{T}\|_u \leqslant C\|T\|_r$, where $C>0$ only depends on r.

Proof: Let $\{T_n(t)\}$ be as in the preceding proof. Then

$$\tilde{T}_n(\omega)=\sum_i \alpha_i T_i \int dt \exp(i\omega t)\chi_{F_i}(t)$$

is well defined, and we have

$$\begin{aligned}&\|\tilde{T}_n-\tilde{T}_{n'}\|_u^u\\ &=\int d\omega \|\tilde{T}_n(\omega)-\tilde{T}_{n'}(\omega)\|_4^u\\ &=\int d\omega \|[\{\tilde{T}_n^*(\omega)-\tilde{T}_{n'}^*(\omega)\}\{\tilde{T}_n(\omega)-\tilde{T}_{n'}(\omega)\}]^{1/2}\|_4^u\\ &=\int d\omega\|\{\tilde{T}_n^*(\omega)-\tilde{T}_{n'}^*(\omega)\}\{\tilde{T}_n(\omega)-\tilde{T}_{n'}(\omega)\}\|_2^{u/2}.\end{aligned}$$

Now

$$\begin{aligned}\tilde{M}_{nn'}(\omega)&=\{\tilde{T}_n^*(\omega)-\tilde{T}_{n'}^*(\omega)\}\{\tilde{T}_n(\omega)-\tilde{T}_{n'}(\omega)\}\\ &=\int du \exp(i\omega u)(T_n^*-T_{n'}^*) *(T_n-T_{n'})(u)\\ &=\int du \exp(i\omega u) M_{nn'}(u).\end{aligned}$$

It follows from the preceding lemma with T replaced by $T_n-T_{n'}$ and S by $M_{nn'}$ that $M_{nn'}(u) \in L_s(\mathbf{R},\mathcal{B}_2)$, $s^{-1}=2r^{-1}-1$, and $\|M_{nn'}\|_s \leqslant\|T_n-T_{n'}\|_r^2$. Since, for $1 \leqslant r \leqslant 4/3$, s ranges between 1 and 2, we can apply Corollary 2.1, $\mathcal{B}_2$ being a Hilbert space. Thus we conclude that $\tilde{M}_{nn'}(\omega) \in L_v(\mathbf{R},\mathcal{B}_2)$, $s^{-1}+v^{-1}=1$ and $\|M_{nn'}\|_v \leqslant C^2\|M_{nn'}\|_s$, where $C>0$ depends on v but not on n, n'. Hence $\|\tilde{M}_{nn'}\|_v \leqslant C^2\|T_n-T_{n'}\|_r^2$, $v^{-1}=2(1-r^{-1})$, and taking $u=2v$, so that $r^{-1}+u^{-1}=1$, we have

$$\|\tilde{T}_n-\tilde{T}_{n'}\|_u^u=\|\tilde{M}_{nn'}\|_{u/2}^{u/2} \leqslant[C^2\|T_n-T_{n'}\|_r^2]^{u/2}$$

or

$$\|\tilde{T}_n-\tilde{T}_{n'}\|_u \leqslant C\|T_n-T_{n'}\|_r,$$

i.e., $\{\tilde{T}_n(\omega)\}$ is a Cauchy sequence in $L_u(\mathcal{B}_4)$ and consequently converges to a limit $\tilde{T}(\omega) \in L_u(\mathcal{B}_4)$. An estimate along the lines, outlined above, shows that $\|\tilde{T}_n\|_u \leqslant C\|T_n\|_r$ and hence $\|\tilde{T}\|_u \leqslant C\|T\|_r$. ■

Corollary 4.2: If $\chi_{[0,\infty]}(t) K(t) \in L_r(\mathbf{R},\mathcal{B}_4)$ for some r with $1 \leqslant r \leqslant 4/3$, then (4.12) defines an element $\tilde{K}(\omega) \in L_s(\mathbf{R},\mathcal{B}_4)$, $r^{-1}+s^{-1}=1$.

5. HIGH ENERGY BEHAVIOR OF CROSS SECTIONS

We consider the case of potential scattering in three dimensions. Thus $H=\mathbf{p}^2+V(\mathbf{x})$ is the full Hamiltonian acting in $\mathcal{H}=L^2(\mathbf{R}^3)$. We suppose that $V \in L_1(\mathbf{R}^3) \cap L_{3/2}(\mathbf{R}^3)$ and we define $V^{1/2}$ through $|V^{1/2}(\mathbf{x})|=|V(\mathbf{x})|^{1/2}$ and $\arg V^{1/2}(\mathbf{x})=\frac{1}{2}\arg V(\mathbf{x})$. Then $V^{1/2} \in L_2 \cap L_3$ and $\tilde{K}(\omega)$ is now as before with $\phi=\psi=V^{1/2}$. The scattering amplitude can be written as ($\mathbf{k}_1$ initial, $\mathbf{k}_2$ final momentum)

$$f(\mathbf{k}_1, \mathbf{k}_2)=f_B(\mathbf{k}_1, \mathbf{k}_2)+\Phi(\mathbf{k}_1, \mathbf{k}_2), \quad \mathbf{k}_1^2=\mathbf{k}_2^2=\omega \geqslant 0, \qquad (5.1)$$

where the Born term is given by

$$f_B(\mathbf{k}_1, \mathbf{k}_2)=-2\pi^2 \int d\mathbf{x} \exp[i(\mathbf{k}_1-\mathbf{k}_2) \cdot \mathbf{x}] V(\mathbf{x}) \qquad (5.2)$$

and

$$\begin{aligned}\Phi(\mathbf{k}_1, \mathbf{k}_2)=&-(4\pi)^{-1}\\ &\times(\tilde{K}(\omega)[i-\tilde{K}(\omega)]^{-1} \exp(i\mathbf{k}_1 \cdot \mathbf{x}) V^{1/2}, \exp(i\mathbf{k}_2 \cdot \mathbf{x}) V^{1/2}).\end{aligned}$$

(5.3)

Here $(\cdot, \cdot)$ denotes the inner product in $\mathcal{H}$ and $\exp(i\mathbf{k}_j \cdot \mathbf{x})$ can be interpreted as a unitary multiplication operator. The above representation exists for sufficiently large ω since $\|\tilde{K}(\omega)\|_4$ and hence $|\tilde{K}(\omega)|$ tends to zero for large ω. For further details see, for instance, Refs. 1 and 8. In fact there exists an ω_0 such that

$$|\Phi(\mathbf{k}_1, \mathbf{k}_2)| \leq (4\pi)^{-1} \|\tilde{K}(\omega)\|_4 |[i - \tilde{K}(\omega)]^{-1}| \|V\|_1$$

$$< (C/4\pi) \|\tilde{K}(\omega)\|_4 \tag{5.4}$$

for $\omega > \omega_0$, C being a positive constant.

(5.4) reflects the well-known fact that $f(\mathbf{k}_1, \mathbf{k}_2)$ tends to the Born amplitude for large ω. However, if in addition $V \in L_p$, $\frac{3}{2} \leq p \leq 2$, more can be said. Consider the total cross section $\sigma_{\text{tot}}(\omega)$. Since, according to the optical theorem, $\sigma_{\text{tot}}(\omega) = (4\pi/\omega^{1/2}) \operatorname{Im}[f(\mathbf{k}, \mathbf{k})]$ and since $f_B(\mathbf{k}, \mathbf{k})$ is real, we have for $\omega > \omega_0$

$$\omega^{1/2}\sigma_{\text{tot}}(\omega) < C \cdot \|\tilde{K}(\omega)\|_4. \tag{5.5}$$

Now we apply the results obtained in Sec. 4, in particular Corollary 4.2. Thus we see that, for V as above, $\tilde{K}(\omega) \in L_q(\mathcal{B}_4)$ with $4 \leq 2p/(2p - 3) < q \leq \infty$. Thus if $p = \frac{3}{2}$, $\tilde{K}(\omega) \in L_\infty(\mathcal{B}_4)$, but if $p = 2$, then $\tilde{K}(\omega) \in L_{4+\delta}(\mathcal{B}_4)$ for any $\delta > 0$. For finite q we then have

$$\int_{\omega_0}^{\infty} d\omega\, \omega^{q/2}[\sigma_{\text{tot}}(\omega)]^q < C^q \|\tilde{K}\|_q^q < \infty. \tag{5.6}$$

Suppose that we know from other sources that $\sigma_{\text{tot}}(\omega)$ behaves like $\omega^{-\alpha}$ for large ω. Then it follows from (5.6) that we must have $\alpha > \frac{1}{2} + 1/q$. For V continuous outside the origin the above condition on V regulates its behavior in the origin. Thus we find a connection between the former and the high energy behavior of the total cross section. This fits in with the intuitive idea (at least for repulsive V) that the higher the energy the more the shape of V close to the origin becomes important in a scattering process.

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[1] B. Simon, *Quantum Mechanic for Hamiltonians Defined as Quadratic Forms* (Princeton U. P., Princeton, N.J., 1971).
[2] T. Kato, Math. Ann. **162**, 258 (1966).
[3] R.S. Phillips, Amer. J. Math. 65, 108 (1943).
[4] E. Hille and R.S. Phillips, *Functional Analysis and Semi-groups* (Amer. Math. Soc., Providence, R.I., 1957).
[5] K. Yosida, *Functional Analysis* (Springer, Berlin-Heidelberg-New York, 1966).
[6] N. Dunford and J.T. Schwartz, *Linear Operators. I, II* (Wiley-Interscience, New York-London-Sydney-Toronto, 1957, 1963).
[7] C.A. McCarthy, C_p, Israel J. Math. 5, 249 (1967).
[8] M. Scadron, S. Weinberg, and J. Wright, Phys. Rev. 135, B202 (1964).

Wigner coefficients for the theory of five-dimensional quasispin*

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We present some Gaunt-type formulas and several classes of multiplicity-free Wigner coefficients for the noncanonical reduction $O(5)\supset SU(2)\times U(1)$.

1. INTRODUCTION

The five-dimensional quasispin formalism[1–7] has been developed for some time in nuclear theory in connection with the study of the nucleon pairing in shells. The theory exploits the group O(5), and the problem of constructing the canonical basis and evaluating the matrix elements of operators has been studied in the mathematically canonical reduction $O(5)\supset O(4)$.[1,3–5,7] Although this reduction presents no multiplicity problem, the states of this basis have no definite isospin. For physical applications more important is the noncanonical reduction $O(5)\supset SU(2)\times U(1)$, in which SU(2) is the isospin group, and the eigenvalue of the U(1) generator specifies the number of nucleons in a shell. In practical applications of a group, its Wigner coefficients often play an important role for coupling states and tensors and, in connection with the Wigner-Eckart theorem, for calculating matrix elements of physical quantities. The physically important projected states in the noncanonical reduction are not orthogonal in general, but may be expanded in terms of orthogonal states for which the Wigner coefficient can be evaluated easily. However it is an obvious advantage that they be available directly in the basis of physical interest. Hecht[6] and Hemenger[2,8] have given a large number of coupling coefficients in the reduction $O(5)\supset SU(2)\times U(1)$, concentrating their attention on the O(5) representation most needed for nuclear applications. In each of their formulas one of the six representation labels is arbitrary, while the other five have low fixed values.

Recently the general O(5) Wigner coefficient was evaluated in the canonical $SU(2)\times SU(2)$ basis by expanding the O(5) van der Waerden invariant[9]; in the present paper special cases of the same van der Waerden invariant are used to derive O(5) Wigner coefficients in the $SU(2)\times U(1)$ basis for six distinct classes of coupling which involve no internal or external multiplicity. Noncanonical bases, corresponding to the reduction $O(5)\supset SU(2)\times U(1)$, has been studied by several authors[10-12]; throughout the course of the work we use the polynomial basis states given by Ahmed and Sharp.[11] In Sec. 2 we derive certain Gaunt coefficients. They arise when a product of two states in the same variables is expanded in O(5) states. Using the results obtained in Sec. 2, in Sec. 3 we evaluate Wigner coefficients for the reduction $O(5)\supset SU(2)\times U(1)$ for the following O(5) couplings:

(i) $(p_10;\, p_20;\, p_30)$, (ii) $(0q_1;\, 0q_2;\, 0q_3)$,

(iii) $(1q_1;\, 0q_2;\, 1q_1-q_2)$, (iv) $(1q_1;\, 1q_2;\, 0q_1-q_2)$,

(v) $(1q_1;\, 0q_2;\, 1q_1-q_2-1)$, (vi) $(1q_1;\, 1q_2;\, 0q_1-q_2-1)$.

2. GAUNT COEFFICIENTS

In expanding the O(5) van der Waerden invariant[13] for the evaluation of Wigner coefficients it is necessary to combine two O(5) states in the same variables arising from different factors of the invariant into a sum of states in those variables; the Gaunt coefficients are defined as the coefficients in the sum. We now evaluate those Gaunt coefficients which will be needed in the next section. The Gaunt coefficient

$$\left\{\begin{matrix} p_10 & p_20 \\ V_1U_1 & V_2U_2 \end{matrix}\,\middle|\,\begin{matrix} p & 0 \\ V & U \end{matrix}\right\}$$

is defined by

$$\left|\begin{matrix} p_10 \\ V_1U_1M_1 \end{matrix}\right\rangle\left|\begin{matrix} p_20 \\ V_2U_2M_2 \end{matrix}\right\rangle=\sum_U\left|\begin{matrix} p\ 0 \\ V\ U\ M \end{matrix}\right\rangle\left\{\begin{matrix} p_10 & p_20 \\ V_1U_1 & V_2U_2 \end{matrix}\,\middle|\,\begin{matrix} p & 0 \\ V & U \end{matrix}\right\}\left\langle\begin{matrix} U_1U_2 \\ M_1M_2 \end{matrix}\,\middle|\,\begin{matrix} U \\ M \end{matrix}\right\rangle, \tag{1}$$

where $p=p_1+p_2$, $V=V_1+V_2$, $M=M_1+M_2$; the last factor in Eq. (1) is an SU(2) Clebsch–Gordan coefficient. The states are given by Eq. (2) of Ref. 11.

The Gaunt coefficient is easily shown to be

$$\left\{\begin{matrix} p_10 & p_2\,0 \\ V_1U_1 & V_2U_2 \end{matrix}\,\middle|\,\begin{matrix} p & 0 \\ V & U \end{matrix}\right\}=\left(\frac{(\frac{1}{2}p+V+1)!\,(\frac{1}{2}p-V+1)!\,(2U_1+1)(2U_2+1)}{(\frac{1}{2}p_1+V_1)!\,(\frac{1}{2}p_1-V_1)!\,(\frac{1}{2}p_2+V_2)!\,(\frac{1}{2}p_2-V_2)!}\right)^{1/2}$$
$$\times\left\{\begin{matrix} \frac{1}{4}p_1+\frac{1}{2}V_1 & \frac{1}{4}p_2+\frac{1}{2}V_2 & \frac{1}{4}p+\frac{1}{2}V \\ \frac{1}{4}p_1-\frac{1}{2}V_1 & \frac{1}{4}p_2-\frac{1}{2}V_2 & \frac{1}{4}p-\frac{1}{2}V \\ U_1 & U_2 & U \end{matrix}\right\}. \tag{2}$$

The last factor in Eq. (2) is a doubly stretched $9-j$ symbol[14] and contains one sum. The $(0q)$ state, Eq. (3) of Ref. 11, may be written

$$\left|\begin{matrix} 0 & q & \\ V & U & U \end{matrix}\right\rangle = N_{VU}\eta^U \xi^{(q-V-U)/2}\theta^{(q+V-U)/2} + \text{unwanted}, \tag{3a}$$

where

$$N_{VU} = \{U!\,(q+U+V+1)!!\,(q+U-V+1)!!\,[\tfrac{1}{2}(q-U+V)]!\,[\tfrac{1}{2}(q-U-V)]!\}^{-1/2}\times[(2U+1)!!\,(2q+1)!!]^{1/2}, \tag{3b}$$

and "unwanted" refers to states belonging to irreducible representations (IR's) lower than $(0q)$. The normalization (3b) is verified by taking the scalar product of (3a) with Eq. (3) of Ref. 11.

The Gaunt coefficient

$$\left\{\begin{matrix} 0q_1 & ; & 0q_2 \\ V_1U_1 & & V_2U_2 \end{matrix}\left|\begin{matrix} 0 & q \\ V & U \end{matrix}\right.\right\}$$

is defined by

$$\left|\begin{matrix} 0q_1 \\ V_1U_1M_1 \end{matrix}\right\rangle \left|\begin{matrix} 0q_2 \\ V_2U_2M_2 \end{matrix}\right\rangle = \sum_{qU} \left|\begin{matrix} 0q \\ VUM \end{matrix}\right\rangle \left\{\begin{matrix} 0q_1 & ; & 0q_2 \\ V_1U_1 & & V_2U_2 \end{matrix}\left|\begin{matrix} 0 & q \\ V & U \end{matrix}\right.\right\} \left\langle\begin{matrix} U_1U_2 \\ M_1M_2 \end{matrix}\left|\begin{matrix} U \\ M \end{matrix}\right.\right\rangle, \tag{4}$$

where $V = V_1 + V_2$, $M = M_1 + M_2$. For the stretched case $q = q_1 + q_2$ (the only case we need), it turns out to be

$$\begin{aligned} \left\{\begin{matrix} 0q_1 & ; & 0q_2 \\ V_1U_1 & & V_2U_2 \end{matrix}\left|\begin{matrix} 0 & q \\ V & U \end{matrix}\right.\right\} &= (-1)^{(U_1+U_2-U)/2}\left(\frac{2^{U_1+U_2-U}(q+U+V+1)!!}{(2q+1)!!\,(q_1+U_1+V_1+1)!!}\right)^{1/2} \\ &\times\left(\frac{(q+U-V+1)!!\,[\frac{1}{2}(q-U+V)]!\,[\frac{1}{2}(q-U-V)]!(2q_1+1)!!\,(2q_2+1)!!}{(q_2+U_2+V_2+1)!!\,(q_1+U_1-V_1+1)!!\,(q_2+U_2-V_2+1)!!\,[\frac{1}{2}(q_1-U_1+V_1)]!}\right)^{1/2} \\ &\times\left(\frac{(2U_1+1)(2U_2+1)(U_1+U_2-U-1)!!\,(U+U_1-U_2-1)!!\,(U+U_2-U_1-1)!!}{[\frac{1}{2}(q_2-U_2+V_2)]!\,[\frac{1}{2}(q_1-U_1-V_1)]!\,[\frac{1}{2}(q_2-U_2-V_2)]!\,[\frac{1}{2}(U_1+U_2-U)]!}\right)^{1/2} \\ &\times\{[\tfrac{1}{2}(U+U_1-U_2)]!\,[\tfrac{1}{2}(U+U_2-U_1)]!\,(U_1+U_2+U+1)!\}^{-1/2}. \end{aligned} \tag{5}$$

Eq. (5) is deduced by putting $M_1 = U_1$, $M_2 = -U_2$ in Eq. (4) and taking the scalar product with $\left|{}^{0}_{VU}\;{}^{q}_{U_1-U_2}\right\rangle$; use Eq. (3) for the states on the right-hand side of the scalar product ($\eta \to \zeta$ for $M = -U$), and Eq. (3) of Ref. 11 with the replacement Eq. (4) of Ref. 11 for the state on the left.

Finally we need the Gaunt coefficients of $1q$ states in the product of a (10) state and a $(0q)$ state; they are just reduced Clebsch–Gordan coefficients and are found by putting $p=1$ in Eq. (10) of Ref. 11 and normalizing

$$\left\{\begin{matrix} 1 & 0 & ; & 0 & q \\ \pm'\frac{1}{2} & \frac{1}{2} & & V & U \end{matrix}\left|\begin{matrix} 1 & q \\ V\pm'\frac{1}{2} & U\pm\frac{1}{2} \end{matrix}\right.\right\} = \left(\frac{q\pm(U+\frac{1}{2})\pm' V+\frac{5}{2}}{2q+3}\right)^{1/2}. \tag{6}$$

The primed and unprimed ± signs in (6) are to be chosen independently of each other.

3. WIGNER COEFFICIENTS

A. Reduced Wigner coefficients of the form

$$\begin{pmatrix} p_10 & ; & p_20 & ; & p_30 \\ V_1U_1 & & V_2U_2 & & V_3U_3 \end{pmatrix}$$

are found by expanding the normalized van der Waerden invariant

$$\begin{aligned} S_1 &= \sqrt{6}[a_1!\,a_2!\,a_3!\,(a_1+a_2+a_3+3)!\,]^{-1/2}A_1^{a_1}A_2^{a_2}A_3^{a_3} \\ &= \sum_{VUM}\left|\begin{matrix} p_10 \\ V_1U_1M_1 \end{matrix}\right\rangle_1 \left|\begin{matrix} p_20 \\ V_2U_2M_2 \end{matrix}\right\rangle_2 \left|\begin{matrix} p_30 \\ V_3U_3M_3 \end{matrix}\right\rangle_3 \\ &\times\begin{pmatrix} U_1U_2U_3 \\ M_1M_2M_3 \end{pmatrix}\begin{pmatrix} p_10 & ; & p_20 & ; & p_30 \\ V_1U_1 & & V_2U_2 & & V_3U_3 \end{pmatrix}. \end{aligned} \tag{7a}$$

Here $a_i = \frac{1}{2}(p_j + p_k - p_i)$ and, from Ref. 9,

$$A_i = \alpha_j\beta_k - \beta_j\alpha_k + \gamma_j\delta_k - \delta_j\gamma_k. \tag{7b}$$

ijk are a cyclic permutation of 123: The expansion may be achieved by first substituting

$$A_i^{a_i} = a_i!\sum_{W_iT_iN_i}\left|\begin{matrix} a_i0 \\ W_iT_iN_i \end{matrix}\right\rangle_j \left|\begin{matrix} a_i0 \\ -W_iT_i-N_i \end{matrix}\right\rangle_k (-1)^{a_i/2-N_i}, \tag{8}$$

and then combining the two factors in each of the 1, 2, 3 variables with the help of Eq. (1). The final result is

$$\begin{aligned} \begin{pmatrix} p_10 & ; & p_20 & ; & p_30 \\ V_1U_1 & & V_2U_2 & & V_3U_3 \end{pmatrix} &= \left(\frac{6a_1!\,a_2!\,a_3!\,(2U_1+1)(2U_2+1)(2U_3+1)}{(a_1+a_2+a_3+3)!}\right)^{1/2} \\ &\times\sum_{WT_1T_2T_3}(-1)^{(a_1+a_2+a_3)/2+T_1+T_2+T_3}\begin{Bmatrix} U_1U_2U_3 \\ T_1T_2T_3 \end{Bmatrix} \\ &\times\left\{\begin{matrix} a_3 & 0 & ; & a_2 & 0 \\ W-V_2 & T_3 & & -W-V_3 & T_2 \end{matrix}\left|\begin{matrix} p_10 \\ V_1U_1 \end{matrix}\right.\right\} \end{aligned}$$

$$\times\left\{\begin{array}{cc@{;}cc|cc} a_1 & 0 & a_3 & 0 & p_2 & 0 \\ W & T_1 & V_2 - W & T_3 & V_2 & U_2 \end{array}\right\}$$

$$\times\left\{\begin{array}{cc@{;}cc|cc} a_2 & 0 & a_1 & 0 & p_3 & 0 \\ W + V_3 & T_2 & -W & T_1 & V_3 & U_3 \end{array}\right\}. \tag{9}$$

The right-hand side of Eq. (9) contains eight sums. In Appendix B an alternative treatment is given, leading to a formula with just six sums.

In the stretched case $p_3 = p_1 + p_2$, Eq. (9) simplifies enormously:

$$\begin{pmatrix} p_1 & 0 ; & p_2 & 0 ; & p_1 + p_2 & 0 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix} = (-1)^{(p_1+p_2)/2-U_3}\left(\frac{6p_1!\,p_2!\,(2U_3+1)}{(p_1+p_2+3)!}\right)^{1/2}$$

$$\times\left\{\begin{array}{cc@{;}cc|cc} p_1 & 0 & p_2 & 0 & p_1 + p_2 & 0 \\ -V_1 & U_1 & -V_2 & U_2 & V_3 & U_3 \end{array}\right\}. \tag{10}$$

B. The reduced Wigner coefficient

$$\begin{pmatrix} 0 & q_1 ; & 0 & q_2 ; & 0 & q_3 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$

is found by making an expansion similar to (7a) of the van der Waerden invariant

$$S_{II} = N_{II} P B_1^{b_1} B_2^{b_2} B_3^{b_3} \tag{11a}$$

where, from Ref. 9.

$$b_i = \tfrac{1}{2}(q_j + q_k - q_i), \tag{11b}$$

$$B_i = \lambda_j \lambda_k - \eta_j \zeta_k - \zeta_j \eta_k - \theta_j \xi_k - \xi_j \theta_k. \tag{11c}$$

(η of Ref. 9 is the negative of our η). The projection operator P is an instruction to retain only the part which is stretched in all IR labels (in accordance with 11b); the normalization constant is

$$N_{II} = \left(\frac{6(2b_1+2b_2+1)!!\,(2b_2+2b_3+1)!!\,(2b_3+2b_1+1)!!}{b_1!\,b_2!\,b_3!\,(2b_1+1)!!\,(2b_2+1)!!\,(2b_3+1)!!}\right)^{1/2}$$

$$\times[(b_1+b_2+b_3+2)!\,(2b_1+2b_2+2b_3+3)!!]^{-1/2} \tag{11d}$$

The expansion of S_{II} is achieved by substituting

$$PB_i^{b_i} = b_i! \sum_{W_i T_i N_i} \left|\begin{matrix} 0 & b_i \\ W_i T_i N_i \end{matrix}\right\rangle_j \left|\begin{matrix} 0 & b_i & \\ -W_i & T_i & -N_i \end{matrix}\right\rangle_k (-1)^{W_i - N_i} \tag{12}$$

and combining the states with the help of Eq. (5). The result is

$$\begin{pmatrix} 0 & q_1 ; & 0 & q_2 ; & 0 & q_3 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$

$$= N_{II} b_1!\,b_2!\,b_3!\,[(2U_1+1)(2U_2+1)(2U_3+1)]^{1/2}$$

$$\times(-1)^{(q_1+q_2+q_3)/2} \sum_{WT_1T_2T_3} \begin{Bmatrix} U_1 & U_2 & U_3 \\ T_1 & T_2 & T_3 \end{Bmatrix}$$

$$\times\left\{\begin{array}{cc@{;}cc|cc} 0 & b_3 & 0 & b_2 & 0 & q_1 \\ W - V_2 & T_3 & -W - V_3 & T_2 & V_1 & U_1 \end{array}\right\}$$

$$\times\left\{\begin{array}{cc@{;}cc|cc} 0 & b_1 & 0 & b_3 & 0 & q_2 \\ WT_1 & & V_2 - WT_3 & & V_2 & U_2 \end{array}\right\}\left\{\begin{array}{cc@{;}cc|cc} 0 & b_2 & 0 & b_1 & 0 & q_3 \\ W + V_3 & T_2 & -W & T_1 & V_3 & U_3 \end{array}\right\}. \tag{13}$$

The right-hand side of (13) contains five sums. The stretched case $q_3 = q_1 + q_2$ involves no sums, i.e.,

$$\begin{pmatrix} 0 & q_1 ; & 0 & q_2 ; & 0 & q_1 + q_2 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$

$$= (-1)^{q_1+q_2}\left(\frac{6q_1!\,q_2!\,(2U_3+1)}{(q_1+q_2+2)!\,(2q_1+2q_2+3)}\right)^{1/2}$$

$$\times\left(\begin{array}{cc@{;}cc|cc} 0 & q_1 & 0 & q_2 & 0 & q_1 + q_2 \\ -V_1 & U_1 & -V_2 & U_2 & V_3 & U_3 \end{array}\right). \tag{14}$$

C. The Wigner coefficient

$$\begin{pmatrix} 1 & q_1 ; & 0 & q_2 ; & 1 & q_1 + q_2 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$

is found by expanding the invariant

$$S_{III} = \sqrt{3}[2q_1!\,q_2!\,(q_1+q_2+3)!]^{-1/2} PB_2^{q_1} B_1^{q_2} A_2. \tag{15}$$

$PB_2^{q_1} B_1^{q_2}$ is expanded with the help of (14), A_2 with the help of (8), and the factors are combined with the help of (6). The result is

$$\begin{pmatrix} 1 & q_1 ; & 0 & q_2 ; & 1 & q_1 + q_2 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$

$$= (-1)^{U_3-1/2}\left(\frac{3(2U_1+1)(2U_3+1)}{2q_1!\,q_2!\,(q_1+q_2+3)!}\right)^{1/2}$$

$$\times\sum_{W}(-1)^{V_3-W}(2T_3+1)^{1/2}\begin{Bmatrix} T_1 & U_1 & \frac{1}{2} \\ U_3 & T_3 & U_2 \end{Bmatrix}$$

$$\times\left\{\begin{array}{cc@{;}cc|cc} 0 & q_1 & 0 & q_2 & 0 & q_1 + q_2 \\ -V_1 - W & T_1 & -V_2 & U_2 & V_3 - W & T_3 \end{array}\right\}$$

$$\times\left\{\begin{array}{cc@{;}cc|cc} 1 & 0 & 0 & q_1 & 1 & q_1 \\ -W & \frac{1}{2} & W + V_1 & T_1 & V_1 & U_1 \end{array}\right\}$$

$$\times\left\{\begin{array}{cc@{;}cc|cc} 1 & 0 & 0 & q_1 + q_2 & 1 & q_1 + q_2 \\ W & \frac{1}{2} & V_3 - W & T_3 & V_3 & U_3 \end{array}\right\}. \tag{16}$$

Here $T_1 = U_1 \pm \frac{1}{2}$, whichever has the same parity as $q_1 - V_1 - W$, and $T_3 = U_3 \pm \frac{1}{2}$, whichever has the same parity as $q_1 + q_2 - V_3 + W$. The only sum in (16) is the trivial one over W which takes the two values $\pm\frac{1}{2}$.

D. The coefficient

$$\begin{pmatrix} 1 & q_1 ; & 1 & q_2 ; & 0 & q_1 + q_2 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$

is found by expanding

$$S_{IV} = \sqrt{3}[2q_1!\,q_2!\,(q_1+q_2+2)!\,(2q_1+2q_2+3)]^{-1/2} PB_2^{q_1} B_1^{q_2} A_3. \tag{17}$$

The result is

$$\begin{pmatrix} 1 & q_1 ; & 1 & q_2 ; & 0 & q_1+q_2 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix} = (-1)^{q_1+q_2+U_1-1/2}$$

$$\times\left(\frac{3q_1!\,q_2!\,(2U_1+1)(2U_2+1)(2U_3+1)}{2(q_1+q_2+2)!\,(2q_1+2q_2+3)}\right)^{1/2}$$

$$\times\sum_W(-1)^{T_1}\left\{\begin{matrix} T_2 & T_1 & U_3 \\ U_1 & U_2 & \frac{1}{2}\end{matrix}\right\}$$

$$\times\left\{\begin{array}{cccc|cc} 0 & q_1 ; & 0 & q_2 & 0 & q_1+q_2 \\ W-V_1 & T_1 & -W-V_2 & T_2 & V_3 & U_3 \end{array}\right\}$$

$$\times\left\{\begin{array}{cccc|cc} 1 & 0 ; & 0 & q_2 & 1 & q_2 \\ -W & \frac{1}{2} & W+V_2 & T_2 & V_2 & U_2 \end{array}\right\}\left\{\begin{array}{cccc|cc} 1 & 0 ; & 0 & q_1 & 1 & q_1 \\ W & \frac{1}{2} & V_1-W & T_1 & V_1 & U_1 \end{array}\right\}.$$

Here $T_1=U_1\pm\frac{1}{2}$, whichever has the same parity as q_1-W+V_1, and $T_2=U_2\pm\frac{1}{2}$, whichever has the same parity as q_2+V_2+W. The only sum in (18) is over W which takes the values $\pm\frac{1}{2}$.

E. The coefficient

$$\begin{pmatrix} 1 & q_1 ; & 0 & q_2 ; & 1 & q_1+q_2-1 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$

is found in the expansion of

$$S_V=\sqrt{3}[2q_1!\,(q_2-1)!\,(q_1+q_2+2)!$$
$$\times(2q_2+3)]^{-1/2}PB_1^{q_2-1}B_2^{q_1}C_2. \tag{19}$$

C_2 is the elementary scalar

$$C_2=\lambda_2(\alpha_3\beta_1-\beta_3\alpha_1+\delta_3\gamma_1-\gamma_3\delta_1)+\sqrt{2}\eta_2(\beta_3\delta_1-\delta_3\beta_1)$$
$$+\sqrt{2}\theta_2(\beta_3\gamma_1-\gamma_3\beta_1)+\sqrt{2}\xi_2(\alpha_3\delta_1-\delta_3\alpha_1)+$$
$$+\sqrt{2}\zeta_2(\gamma_3\alpha_1-\alpha_3\gamma_1)$$
$$=4\sqrt{5}\sum_{V_1V_2M_1M_2}\left|\begin{matrix} 1 & 0 & \\ V_1 & \frac{1}{2} & M_1\end{matrix}\right\rangle_1\left|\begin{matrix} 0 & 1 & \\ V_2 & S & M_2\end{matrix}\right\rangle_2\left|\begin{matrix} 1 & 0 & \\ V_3 & \frac{1}{2} & M_3\end{matrix}\right\rangle_3$$
$$\times\begin{pmatrix} \frac{1}{2} & S & \frac{1}{2} \\ M_1 & M_2 & M_3\end{pmatrix}\begin{pmatrix} 1 & 0 ; & 0 & 1 ; & 1 & 0 \\ V_1 & \frac{1}{2} & V_2 & S & V_3 & \frac{1}{2}\end{pmatrix}, \tag{20}$$

where $S=1-|V_2|$, and the reduced Wigner coefficients have the values

$$\begin{pmatrix} 1 & 0 ; & 0 & 1 ; & 1 & 0 \\ \pm\frac{1}{2} & \frac{1}{2} & \mp 1 & 0 & \pm\frac{1}{2} & \frac{1}{2}\end{pmatrix}=\pm\frac{\sqrt{5}}{5}\quad\begin{pmatrix} 1 & 0 ; & 0 & 1 ; & 1 & 0 \\ \pm\frac{1}{2} & \frac{1}{2} & 0 & 1 & \mp\frac{1}{2} & \frac{1}{2}\end{pmatrix}=\mp\frac{\sqrt{30}}{10}. \tag{21}$$

Combining the factors in (19) with the help of the Gaunt coefficients in Eqs. (5) and (6) leads to the desired result, i.e.,

$$\begin{pmatrix} 1 & q_1 ; & 0 & q_2 ; & 1 & q_1+q_2-1 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$
$$=\left(\frac{120q_1!\,(q_2-1)!\,(2U_1+1)(2U_2+1)(2U_3+1)}{(q_1+q_2+2)!\,(2q_3+3)}\right)^{1/2}$$
$$\times(-1)^{q_1+q_2-1}\sum_{YZT_2}(2T_3+1)^{1/2}$$
$$\times\left\{\begin{array}{cccc|cc} 0 & q_1 ; & 0 & q_2-1 & 0 & q_1+q_2-1 \\ Y-V_1 & T_1 & -Y-Z-V_2 & T_2 & V_3-Z & T_3 \end{array}\right\}$$
$$\times\left\{\begin{array}{cccc|cc} 1 & 0 ; & 0 & q_1 & 1 & q_1 \\ Y & \frac{1}{2} & V_1-Y & T_1 & V_1 & U_1 \end{array}\right\}$$
$$\times\left\{\begin{array}{cccc|cc} 0 & 1 ; & 0 & q_2-1 & 0 & q_2 \\ -Y-Z & S & Y+Z+V_2 & T_2 & V_2 & U_2 \end{array}\right\}$$
$$\times\left\{\begin{array}{cccc|cc} 1 & 0 ; & 0 & q_1+q_2-1 & 1 & q_1+q_2-1 \\ Z & \frac{1}{2} & V_3-Z & T_3 & V_3 & T_3 \end{array}\right\}$$
$$\times\left\{\begin{matrix} 1 & 0 ; & 0 & 1 ; & 1 & 0 \\ Y & \frac{1}{2} & -Y-Z & S & Z & \frac{1}{2} \end{matrix}\right\}$$
$$\times\left\{\begin{matrix} T_1 & T_2 & T_3 \\ \frac{1}{2} & S & \frac{1}{2} \\ U_1 & U_2 & U_3 \end{matrix}\right\}, \tag{22}$$

In the sum in (22) the dummies Y and Z take independently the values $\pm\frac{1}{2}$. When $Y=Z$, $S=0$ and $T_2=U_2$; when $Y=-Z$, $S=1$ and T_2 takes the values $U_2\pm 1$. Also $T_1=U_1\pm\frac{1}{2}$, whichever has the parity of q_1-V_1+Y, and $T_3=U_3\pm\frac{1}{2}$, whichever has the parity of $q_1+q_2-V_3+Z+1$.

F. Finally the coefficient

$$\begin{pmatrix} 1 & q_1 ; & 1 & q_2 ; & 0 & q_1+q_2+1 \\ V_1 & U_1 & V_2 & U_2 & V_3 & U_3 \end{pmatrix}$$

is found by expanding the invariant

$$S_{VI}=\sqrt{3}[2q_1!\,q_2!\,(q_1+q_2+3)!\,(2q_1+2q_2+5)]^{-1/2}PB_1^{q_2}B_2^{q_1}C_3. \tag{23}$$

C_3 is just the invariant Eq. (20) with the states relabelled 1 → 2 → 3 → 1. The result is

$$\begin{pmatrix} 1 & q_1 ; & 1 & q_2 & 0 & q_1+q_2+1 \\ V_1 & U_1 & V_2 & U_2 ; & V_3 & U_3 \end{pmatrix}=$$
$$=\left(\frac{120q_1!\,q_2!\,(2U_1+1)(2U_2+1)(2U_3+1)}{(q_1+q_2+3)!\,(2q_1+2q_2+5)}\right)^{1/2}$$
$$\times(-1)^{q_1+q_2}\sum_{YZT_3}(2T_3+1)^{1/2}$$
$$\times\left\{\begin{array}{cccc|cc} 0 & q_1 ; & 0 & q_2 & 0 & q_1+q_2 \\ Y-V_1 & T_1 & Z-V_2 & T_2 & Y+Z+V_3 & T_3 \end{array}\right\}$$
$$\times\left\{\begin{array}{cccc|cc} 1 & 0 ; & 0 & q_1 & 1 & q_1 \\ Y & \frac{1}{2} & V_1-Y & T_1 & V_1 & U_1 \end{array}\right\}\left\{\begin{array}{cccc|cc} 1 & 0 ; & 0 & q_2 & 1 & q_2 \\ Z & \frac{1}{2} & V_2-Z & T_2 & V_2 & U_2 \end{array}\right\}$$
$$\times\left\{\begin{array}{cccc|cc} 0 & 1 ; & 0 & q_1+q_2 & & q_1+q_2+1 \\ -Y-Z & S & Y+Z+V_3 & T_3 & V_3 & U_3 \end{array}\right\}$$
$$\times\left\{\begin{matrix} 1 & 0 ; & 0 & 1 ; & 1 & 0 \\ Z & \frac{1}{2} & -Y-Z & S & Y & \frac{1}{2} \end{matrix}\right\}\left\{\begin{matrix} T_1 & T_2 & T_3 \\ \frac{1}{2} & \frac{1}{2} & S \\ U_1 & U_2 & U_3 \end{matrix}\right\}. \tag{24}$$

In Eq. (24) Y and Z independently take the values $\pm\frac{1}{2}$. When $Y=Z$, $S=0$ and $T_3=U_3$; when $Y=-Z$, $S=1$ and T_3 takes the values $U_3\pm 1$. Also $T_1=U_1\pm\frac{1}{2}$, whichever has the parity of q_1-V_1+Y, and $T_2=U_2\pm\frac{1}{2}$, whichever has the parity of q_2-V_2+Z.

The internal sums in Eqs. (16), (18), (22), and (24) are trivial in the sense that they contain at most six terms. They could be done by hand in each case but this would entail a proliferation of formulas, for the details depend on the relative parities of the labels.

The classes of the O(5)⊃SU(2)×U(1) Wigner coefficients we have evaluated do not exhaust all multiplicity-free cases; other examples are the O(5) couplings $(n+m\ 0;\ n+m\ 0;\ 0\ n)$, $(n+m\ 1;\ n+m\ 0;\ 1\ n)$, $(0\ n+m;\ 0\ n+m;\ 2n\ 0)$, $(1\ n+m;\ 1\ n+m;\ 2n\ 0)$, $(1\ n+m;\ 1\ n+m;\ 2n+1\ 0)$, $(0\ n+m;\ 1\ n+m;\ 2n+1\ 0)$. The classes we have calculated include all those involving only trivial internal summations.

4. CONCLUSION

The method of van der Waerden invariants is a powerful technique for calculating coupling coefficients of low order compact groups in any basis. We are planning to evaluate the general O(5)⊃SU(2)×U(1) Wigner coefficient; the relatively simple coefficients found in this paper will be needed in expressing the general formula.

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APPENDIX A

The O(5)⊃SU(2)×U(1) Clebsch–Gordan coefficient may be defined by

$$\left|\begin{matrix} p_3 & q_3 \\ V_3\ U_3 & M_3\end{matrix}\right\rangle_{12}=\sum_{VUM}\left|\begin{matrix} p_1 & q_1 \\ V_1\ U_1 & M_1\end{matrix}\right\rangle_1\left|\begin{matrix} p_2 & q_2 \\ V_2\ U_2 & M_2\end{matrix}\right\rangle_2 \times\left\langle\begin{matrix} U_1 & U_2 \\ M_1 & M_2\end{matrix}\middle|\begin{matrix} U \\ M\end{matrix}\right\rangle\left\langle\begin{matrix} p_1\ q_1 ; p_2\ q_2 \\ V_1\ U_1 ; V_2\ U_2\end{matrix}\middle|\begin{matrix} p_3\ q_3 \\ V_3\ U_3\end{matrix}\right\rangle \tag{25}$$

The state on the left is a composite state formed from products of the states labeled 1 and 2.

$$\left\langle\begin{matrix} p_1\ q_1 ; p_2\ q_2 \\ V_1\ U_1\ V_2\ U_2\end{matrix}\middle|\begin{matrix} p_3\ q_3 \\ V_3\ U_3\end{matrix}\right\rangle$$

is the reduced Clebsch–Gordan coefficient which we wish to relate to the reduced Wigner coefficient. All states are normalized and we suppose the IR's present no internal labeling problem, i.e., $p=0$ or 1 or else $q=0$.

The normalized van der Waerden invariant may be expanded in two ways:

$$S=\sum_{VUM}\left|\begin{matrix} p_1 & q_1 \\ V_1\ U_1 & M_1\end{matrix}\right\rangle_1\left|\begin{matrix} p_2 & q_2 \\ V_2\ U_2 & M_2\end{matrix}\right\rangle_2\left|\begin{matrix} p_3 & q_3 \\ V_3\ U_3 & M_3\end{matrix}\right\rangle_3 \times\begin{pmatrix} U_1 & U_2 & U_3 \\ M_1 & M_2 & M_3\end{pmatrix}\begin{pmatrix} p_1\ q_1 ; p_2\ q_2 ; p_3\ q_3 \\ V_1\ U_1\ V_2\ U_2\ V_3\ U_3\end{pmatrix}$$

$$=\epsilon\sum_{VUM}\left|\begin{matrix} p_3 & q_3 \\ V_3\ U_3 & M_3\end{matrix}\right\rangle_3\left|\begin{matrix} p_3 & q_3 \\ V_3\ U_3 & M_3\end{matrix}\right\rangle^*_{12} D_3^{-1/2}, \tag{26}$$

where

$$D_3=\tfrac{1}{6}(p_3+1)(q_3+1)(p_3+q_3+2)(p_3+2q_3+3), \tag{27}$$

and

$$\left|\begin{matrix} p_3 & q_3 \\ V_3\ U_3 & M_3\end{matrix}\right\rangle^*=\left|\begin{matrix} p_3 & & q_3 \\ -V_3 & U_3 & -M_3\end{matrix}\right\rangle(-1)^{\Phi_3-M_3}, \tag{28}$$

is the state conjugate to

$$\left|\begin{matrix} p_3 & q_3 \\ V_3\ U_3 & M_3\end{matrix}\right\rangle.$$

The phase ϕ_3 is q_3+U_3 for $p_3=0,1$ and $\frac{1}{2}p_3$ for $q_3=0$; ϵ is a phase factor which depends in an arbitrary way on the IR labels. Substituting from (28), (25) in (26) and equating coefficients yields the desired result;

$$\left\langle\begin{matrix} p_1\ q_1 ; p_2\ q_2 \\ V_1\ U_1\ V_2\ U_2\end{matrix}\middle|\begin{matrix} p_3\ \ q_3 \\ -V_3\ U_3\end{matrix}\right\rangle=\begin{pmatrix} p_1\ q_1 ; p_2\ q_2 ; p_3\ q_3 \\ V_1\ U_1\ V_2\ U_2\ V_3\ U_3\end{pmatrix}$$

$$\times D_3^{1/2}(2U_3+1)^{-1/2}(-1)^{U_2-U_1+\phi_3}\epsilon. \tag{29}$$

The phase factor ϵ may be defined as unity or may be chosen to make a particular Clebsch–Gordan coefficient positive, say the one with $V_3=\frac{1}{2}p_3+q_3$, $U_3=\frac{1}{2}p_3$, $V_1=\frac{1}{2}p_1+q_1$, $U_1=\frac{1}{2}p_1$, $V_2=V_3-V_1$, $U_2=p_2+q_2-V_2$.

APPENDIX B

An alternative derivation of the reduced Wigner coefficient

$$\begin{pmatrix} p_1\ 0 ; p_2\ 0 ; p_3\ 0 \\ V_1\ U_1\ V_2\ U_2\ V_3\ U_3\end{pmatrix}$$

yields a formula somewhat simpler than Eq. (9) (six sums instead of eight).

Projecting the van der Waerden invariant S_I, Eq. (7), onto a product of one-particle states gives

$$\begin{pmatrix} p_1\ 0 ; p_2\ 0 ; p_3\ 0 \\ V_1\ U_1\ V_2\ U_2\ V_3\ U_3\end{pmatrix}=(-1)^{U_1+U_2+U_3}[(2U_1+1)\,(2U_2+1)\,(2U_3+1)]^{1/2}\,\langle(U_{1a}U_{1b}U_1)(U_{2a}U_{2b}U_2)(U_{3a}U_{3b}U_3)\,|\,S_I(U_1U_2U_3)\rangle, \tag{30a}$$

where $(U_1U_2U_3)$, etc., are SU(2) van der Waerden invariants. The subscript a refers to isospin states which are Wigner monomials in the $V=\frac{1}{2}$ variables $\alpha\delta$; b denotes an isospin state in the $V=-\frac{1}{2}$ variables $\gamma\beta$. Numerically,

$$U_a=\tfrac{1}{4}p+\tfrac{1}{2}V, \quad U_b=\tfrac{1}{4}p-\tfrac{1}{2}V. \tag{30b}$$

Expanding S_1 leads to

$$\begin{aligned}\begin{pmatrix} p_10 & ; & p_20 & ; & p_30 \\ V_1\ U_1 & & V_2\ U_2 & & V_3\ U_3\end{pmatrix} &= (-1)^{U_1+U_2+U_3}[6a_1!\,a_2!\,a_3!\,(2U_1+1)\,(2U_2+1)\,(2U_3+1)]^{1/2}\\ &\times[(a_1+a_2+a_3+3)!\,]^{-1/2}\sum_x \langle(U_{1a}U_{1b}U_1)(U_{2a}U_{2b}U_2)(U_{3a}U_{3b}U_3)\,|\\ &\times|\,(\tfrac{1}{2}x)_{2a,3b}(\tfrac{1}{2}a_1-\tfrac{1}{2}x)_{2b,3a}(U_{1b}-U_{2a}+\tfrac{1}{2}x)_{3a,1b}(U_{3b}-\tfrac{1}{2}x)_{3b,1a}(U_{1a}-U_{3b}+\tfrac{1}{2}x)_{1a,2b}(U_{2a}-\tfrac{1}{2}x)_{1b,2a}\rangle[(x+1)(a_1-x+1)]^{1/2}\\ &\times[(2U_{1b}-2U_{2a}+x+1)(2U_{3b}-x+1)(2U_{1a}-2U_{3b}+x+1)(2U_{2a}-x+1)]^{1/2},\end{aligned} \tag{31a}$$

where

$$(J)_{12}\equiv\sum_M \left|\begin{matrix}J\\M\end{matrix}\right\rangle_1 \left|\begin{matrix}J\\-M\end{matrix}\right\rangle_2 (-1)^{J-M}(2J+1)^{-1/2}. \tag{31b}$$

The following evaluation of the scalar product on the right-hand side of (31a) is similar to the procedure used in Ref. 15. It may be viewed as

$$[(2U_{2a}+1)!\,]^{1/2}[(x+1)!\,(2U_{2a}-x+1)!\,]^{-1/2}$$

times the scalar product of

$$|\,U_{2a},U_2\rangle=\langle(U_{2a}U_{2b}U_2)\,|\,(\tfrac{1}{2}x,U_{2a}-\tfrac{1}{2}x,U_{2a})(U_1U_2U_3)\rangle, \tag{32a}$$

with

$$|\,A\rangle=\langle(\tfrac{1}{2}a_1-\tfrac{1}{2}x)_{2b,3a}(U_{1a}-U_{3b}+\tfrac{1}{2}x)_{1a,2b}(U_{1b}-U_{2a}+\tfrac{1}{2}x)_{3a,1b}(U_{3b}-\tfrac{1}{2}x)_{3b,1a}\,|\,(U_{1a}U_{1b}U_1)(U_{3a}U_{3b}U_3)\rangle. \tag{32b}$$

The isospins $\frac{1}{2}x$, $U_{2a}-\frac{1}{2}x$, U_{2a} on the right side of (32a) are in the variables labelled $3b$, $1b$, $2a$ respectively. $|A\rangle$ is a state in which the isospins $\frac{1}{2}x$, $U_{2a}-\frac{1}{2}x$, U_1, U_3 are coupled to give a total isospin of U_{2b}. $|\,U_{2a},U_2\rangle$ is a complete set of such states with $\frac{1}{2}x$, $U_{2a}-\frac{1}{2}x$ coupled to U_{2a} and U_1, U_3 coupled to U_2. Hence we can expand $|A\rangle$ in $|\,U_{2a},U_2\rangle$, i.e.,

$$|A\rangle=\sum_{U_{2a},U_2}|\,U_{2a},U_2\rangle\,(2U_2+1)\,(2U_{2a}+1)\,\langle U_{2a},U_2|A\rangle. \tag{33}$$

The scalar product $\langle U_{2a},U_2|A\rangle$ is found by expanding $|A\rangle$ and $|\,U_{2a},U_2\rangle$ in products of the "one-particle states," i.e.,

$$\left|\begin{matrix}\frac{1}{2}x\\M_{3b}\end{matrix}\right\rangle_{3b}\left|\begin{matrix}U_{2a}-\frac{1}{2}x\\M_{1b}\end{matrix}\right\rangle_{1b}\ \left|\begin{matrix}U_1\\M_1\end{matrix}\right\rangle_1\left|\begin{matrix}U_3\\M_3\end{matrix}\right\rangle_3\ {}_{2b}\left\langle\begin{matrix}U_{2b}\\M_{2b}\end{matrix}\right|\ ,$$

and equating coefficients. The final result is

$$\begin{aligned}\begin{pmatrix} p_10 & ; & p_20 & ; & p_30 \\ V_1\ U_1 & & V_2\ U_2 & & V_3\ U_3\end{pmatrix} &= \left(\frac{6a_1!\,a_2!\,a_3!\,(2U_1+1)(2U_2+1)(2U_3+1)}{(a_1+a_2+a_3+3)!\,(U_1+U_2+U_3)!\,(U_2+U_3-U_1)!}\right)^{1/2}\\ &\times\left(\frac{(U_2+V_2)!\,(U_2-V_2)!\,(\frac{1}{2}p_2-U_2)!\,(\frac{1}{2}p_2+U_2+1)!\,(U_1+U_3-U_2)!}{(U_1+U_2+U_3+1)!}\right)^{1/2}\\ &\times\sum_{Muvx}(-1)^{U_3+U_{1b}+U_{2a}+U_{3b}+u+v-M}\begin{pmatrix}U_{3a} & U_{3b} & U_3\\ -M-v+\frac{1}{2}x & v-\frac{1}{2}x & M\end{pmatrix}\begin{pmatrix}U_{1a} & U_{1b} & U_1\\ U_{2a}-U_2+M+u-\frac{1}{2}x & -U_{2a}-u+\frac{1}{2}x & U_2-M\end{pmatrix}\\ &\times\left(\frac{(U_{1a}-U_2+U_{2a}+M+u-\frac{1}{2}x)!}{(U_{1b}-U_{2a}-u+\frac{1}{2}x)!}\right)^{1/2}\left(\frac{(U_{1a}+U_2-U_{2a}-M-u+\frac{1}{2}x)!\,(U_{1b}+U_{2a}+u-\frac{1}{2}x)!\,(U_1+U_2-M)!}{(U_1-U_2+M)!\,(U_{3b}+v-\frac{1}{2}x)!\,(U_3-M)!}\right)^{1/2}\\ &\times[(U_{3a}-M-v+\tfrac{1}{2}x)!\,(U_{3a}+M+v-\tfrac{1}{2}x)!\,(U_{3b}-v+\tfrac{1}{2}x)!\,(U_3+M)!\,]^{1/2}\,[x!\,(2U_{2a}-x)!\\ &\times(U_{1b}-U_{2a}+u+\tfrac{1}{2}x)!\,(\tfrac{1}{2}a_1+u+v+M-x)!\,]^{-1}[(\tfrac{1}{2}a_1-u-v-M)!\,(U_{1a}-U_{2a}-U_{3b}+U_2-M-u-v+x)!\,]^{-1}\\ &\times[(U_{1a}+U_{2a}-U_2-U_{3b}+u+v+M)!\,(U_{3b}-v-\tfrac{1}{2}x)!\,]^{-1}.\end{aligned} \tag{34}$$

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[1] B.H. Flowers, Proc. R. Soc. London, A **212**, 248 (1952); A.R. Edmonds and B.H. Flowers, Proc. R. Soc. London A **214**, 515 (1952); K. Helmers, Nucl. Phys. **23**, 594 (1961); J.C. Parikh, Nucl. Phys. **63**, 214 (1965).

[2] R.P. Hemenger, 1968 Dissertation, U. of Michigan (1968); Technical Report 07591-3-T.

[3] J.N. Ginocchio, Nucl. Phys. **74**, 321 (1965).

[4] K.T. Hecht, Nucl. Phys. **63**, 177 (1965).

[5] K.T. Hecht, Phys. Rev. B **139**, 794 (1965).

[6] K.T. Hecht, Nucl. Phys. A **102**, 11 (1967).

[7] M. Ichimura, Prog. Theor. Phys. **33**, 215 (1965).

[8] R.P. Hemenger and K.T. Hecht, Nucl. Phys. A **145**, 468 (1970).

[9] M. Hongoh, R.T. Sharp, and D.E. Tilley, J. Math. Phys. **15**, 782 (1974).

[10] G.N. Afanas'ev, Izv. Akad. Nauk Kaz. SSR Ser. Fiz. Mat. **6**, 19 (1969).

[11] K. Ahamed and R.T. Sharp, J. Math. Phys. **11**, 1112 (1970).

[12] Yu.F. Smirnov and V.N. Tolstoy, Rep. Math. Phys. **4**, 97 (1973).

[13] For the O(5) van der Waerden invariant see Ref. 9 and references therein.

[14] A 9-j symbol is called stretched if one of the elements is the sum of the other elements in the same row (column). It is well-know that the general 9-j symbol contains a quadruple sum whereas the singly and doubly stretched 9-j symbol contains a double and a single sum respectively.

[15] C.K. Chew and R.T. Sharp, Nucl. Phys. B **2**, 697 (1967).

Neutron transport operators in C and L_2 spaces*

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We study the stationary neutron transport equation (in its integral form) in plane and spherical symmetry. The investigation is carried out in both L_2 and C spaces, by means of standard methods of functional analysis. The equivalence between the eigenvalue problems in the two spaces is proved, and the space C seems often to be more appropriate than L_2 for investigating the main properties of the eigenfunctions. Results of functional analysis are applied in establishing some properties of the eigenvalues and the eigenfunctions. Moreover, the continuous dependence of neutron flux on optical and spatial parameters is shown.

1. INTRODUCTION

In this paper, we are concerned with the stationary neutron transport Boltzmann equation as applied to homogeneous multiplying slabs and spheres. Whereas nearly all previous work on the subject has been performed in L_2, our work is carried out in both the Lebesgue space L_2 and the space C (with the sup norm). Our aim is to show that C is also natural space in which to study the transport operator. In particular, we investigate in detail the well-known fact that the study of a sphere can be reduced to that of a slab. By investigating directly the two original kernels for a slab and for a sphere, all relevant physical properties of the solution can be obtained in a rigorous way from the Boltzmann equation. Finally, we are able to prove that the neutron flux depends continuously on the optical and spatial parameters.

2. PRELIMINARIES

Let us consider an infinite homogeneous multiplying slab embedded in an infinite purely absorbing medium or in the vacuum, so that no neutron may enter the slab from outside. The material properties of the slab are characterized by c $(c>1)$, the average number of secondary neutrons per collision, and by Σ $(\Sigma>0)$, the total macroscopic cross section for all processes (fission, scattering, and absorption). Neutrons are supposed monoenergetic and the processes are taken to be spherically symmetric in the laboratory system.

Now, let 2α $(\alpha>0)$ be the optical thickness (Σ times the geometrical length) of the slab along the coordinate axis x; moreover, let $x=0$ be the middle plane of the slab. By making use of the optical unit α along the axis x, then the slab extends merely from $x=-1$ to $x=1$; clearly, α is also the parameter characterizing both the geometrical and material properties of the slab.

For the physical situation illustrated above and in absence of external sources, by putting $\lambda=1/c$, the stationary neutron total flux ϕ_α in the slab must satisfy the linear integral Boltzmann equation[1]

$$\lambda\phi_\alpha(x)=\int_{-1}^{1} T_\alpha(x,x')\,\phi_\alpha(x')\,dx', \tag{1}$$

where

$$T_\alpha(x,x')=\tfrac{1}{2}\alpha E(\alpha\,|x-x'|) \tag{2}$$

for any $(x,x')\in[-1,1]\times[-1,1]$ and any $\alpha>0$ and where

$$E(u)=\int_1^{+\infty} t^{-1}\exp(-tu)\,dt,\quad u>0, \tag{3}$$

is the exponential integral.[2]

If we consider now an homogeneous multiplying sphere of optical radius α $(\alpha>0)$, then the stationary neutron total flux ψ_α in the sphere must satisfy the linear integral equation (Ref. 1)

$$\lambda\psi_\alpha(x)=\tfrac{1}{2}\alpha\int_0^1[E(\alpha\,|x-x'|)-E(\alpha\,|x+x'|)](x'/x)\,\psi_\alpha(x')\,dx', \tag{4}$$

where x is the distance from the center. Since, as is easily seen,

$$\lim_{x\to 0^+}[E(\alpha\,|x-x'|)-E(\alpha\,|x+x'|)]x'/x=2\exp(-\alpha x'),$$

for any $x'\in(0,1]$, we rewrite Eq. (4) as follows:

$$\lambda\psi_\alpha(x)=\int_0^1 U_\alpha(x,x')\,\psi_\alpha(x')\,dx', \tag{5}$$

where

$$U_\alpha(x,x')=\begin{cases}\tfrac{1}{2}\alpha[E(\alpha\,|x-x'|)-E(\alpha\,|x+x'|)]x'/x, & 0<x\le 1,\ 0\le x'\le 1\\ \alpha\exp(-\alpha x'), & x=0,\ 0<x'\le 1\end{cases} \tag{6}$$

for any $\alpha>0$. We shall study Eqs. (1) and (5) by making use of the operator valued functions T_α and U_α $(\alpha>0)$, whose kernels (using the same symbol for the operator and for its kernel) are respectively $T_\alpha(x,x')$ and $U_\alpha(x,x')$.

We now observe that if we substitute $\psi_1(x)=x\psi_\alpha(x)$ into Eq. (5) and extend the definition of ψ_1 by $\psi_1(x)=x\psi_\alpha(-x)$, we then obtain the integral equation governing the neutron distribution $\psi_1(x)$ in a slab of thickness $2\alpha/\Sigma$. For this reason, the study of homogeneous spheres with isotropic scattering is usually included in that of a slab whose half-thickness is equal to the radius of the sphere.

3. SOME PROPERTIES OF T_α AND U_α

We establish here some properties of T_α and U_α which are true for any $\alpha > 0$. The first step is to choose the spaces in which the operators T_α and U_α act.

By taking into account (2), it is easily seen that

$$\int_{-1}^{1} |T_\alpha(x,x')|^2\,dx' \tag{7}$$

is a continuous function of $x \in [-1,1]$ and that

$$\int_{-1}^{1} |T_\alpha(y,x') - T_\alpha(x,x')|^2\,dx' \to 0 \quad \text{as } |y-x| \to 0. \tag{8}$$

From (8) it follows at once that T_α can act on the whole of the space $C[-1,1]$; on the other hand, both (7) and (8) imply that T_α will be compact as an operator acting in $C[-1,1]$.[3] Moreover, (7) implies also that $T_\alpha(x,x')$ is a Fredholm kernel (that is, square integrable on $[-1,1]\times[-1,1]$) and hence, as is well known, T_α can act also on the whole of the space $L_2[-1,1]$ and it will be compact in this space.

By recalling the definition of U_α, it is possible to prove, by tedious calculations, that conditions analogous to (7) and (8) are also true for the kernel $U_\alpha(x,x')$. Consequently, U_α can now be considered as an operator acting in both the spaces $C[0,1]$ and $L_2[0,1]$ and which is also compact in both these spaces.

Here $C[a,b]$ $(a<b)$ is the space of the real-valued functions defined and continuous on $[a,b]$ with the usual sup norm, and $L_2[a,b]$ is the Hilbert space of the real-valued functions defined and square integrable (in the Lebesgue sense) over $[a,b]$ with the usual inner product $(f,g) = \int_a^b f(x)g(x)\,dx$, $f,g \in L_2[a,b]$ and the L_2-norm $\|f\| = (f,f)^{1/2}$.

Let now T_α act in $L_2[-1,1]$ (we shall consider U_α later). Since the kernel T_α (x,x') is real and symmetric, the operator T_α is symmetric; moreover, as is well known,[4] T_α is also positive definite. It follows that T_α has a denumerable infinite set of positive eigenvalues forming a sequence

$$\lambda_1(\alpha) \geq \lambda_2(\alpha) \geq \cdots \geq \lambda_n(\alpha) \geq \cdots$$

converging to zero (but zero is not an eigenvalue) and each eigenvalue is of finite multiplicity (Ref. 3). The first eigenvalue is given by the formula

$$\lambda_1(\alpha) = \max_{\|f\|=1} (T_\alpha f, f), \quad f \in L_2[-1,1]. \tag{9}$$

At this point, we observe that T_α, as an operator acting in $C[-1,1]$, has the same eigenvalues and eigenfunctions as an operator acting in $L_2[-1,1]$. Indeed, the eigenfunctions of T_α as an operator in $L_2[-1,1]$ must be continuous since T_α maps $L_2[-1,1]$ into its subspace of bounded functions and this subspace into that of continuous functions.[5] The vice-versa is obvious. Analogous considerations are available for U_α.

Since the kernel $T_\alpha(x,x')$ is also even, see (2), the eigenfunctions of T_α must have definite parity. Let now H_e and H_o be the closed subspaces of $L_2[-1,1]$ having as elements the functions which are respectively even and odd (almost everywhere). Moreover, let S_α be the linear integral operator acting in H_e whose kernel is

$$S_\alpha(x,x') = [T_\alpha(x,x') + T_\alpha(x,-x')]/2$$

for any $(x,x') \in [-1,1]\times[-1,1]$, and let A_α be the linear integral operator acting in H_0 whose kernel is

$$A_\alpha(x,x') = [T_\alpha(x,x') - T_\alpha(x,-x')]/2 \tag{10}$$

for any $(x,x') \in [-1,1]\times[-1,1]$. As T_α, the operators S_α and A_α are compact, symmetric, positive definite; unlike T_α, it is of no interest that S_α and A_α can act in other spaces that are not H_e and H_o respectively.

We remark that the eigenvalue problem of T_α in $L_2[-1,1]$ is equivalent to the two eigenvalue problems of S_α in H_e and of A_α in H_0.

Now, we establish the following theorem.

Theorem 1: (i) The operators A_α and U_α acting in $H_0 \subset L_2[-1,1]$ and in $C[0,1]$ or $L_2[0,1]$, respectively, have the same eigenvalues. (ii) The first eigenvalue of U_α is the second of T_α. (iii) The first two eigenvalues of T_α are simple.

Proof: (i) Let $\lambda(\alpha)$ be an eigenvalue of A_α corresponding to the eigenfunction ϕ_α, that is

$$\lambda(\alpha)\,\phi_\alpha(x) = \int_{-1}^{1} A_\alpha(x,x')\,\phi_\alpha(x')\,dx'. \tag{11}$$

In the Appendix we show that the odd continuous function ϕ_α can be written as

$$\phi_\alpha(x) = x\tilde{\psi}_\alpha(x), \quad x \in [-1,1], \tag{12}$$

where $\tilde{\psi}_\alpha$ is an even continuous function. Let ψ_α be the restriction of $\tilde{\psi}_\alpha$ to $[0,1]$; then, by inserting (12) into (11) and by taking into account definition (10), it follows that

$$\lambda(\alpha)x\psi_\alpha(x) = \int_0^1 [T_\alpha(x,x') - T_\alpha(x,-x')]\,x'\psi_\alpha(x')\,dx' \tag{13}$$

and, hence, by substituting exponential integrals and by recalling the definition of the kernel U_α, we get Eq. (5). Hence, $\lambda(\alpha)$ is an eigenvalue of U_α. The converse is true; indeed, let $\lambda(\alpha)$ be an eigenvalue of U_α as acting in $L_2[0,1]$ corresponding to the eigenfunction ψ_α. It follows from definitions (6) and (2) that Eq. (13) is satisfied. If $\tilde{\psi}_\alpha$ is the even extension of ψ_α to $[-1,1]$, then ϕ_α defined in (12) satisfies Eq. (11) and hence $\lambda(\alpha)$ is an eigenvalue of A_α as acting in H_o.

(ii) Because U_α and A_α have the same eigenvalues, we refer to Ref. 6 where the proof that the first eigenvalue of A_α is the second one of T_α is given in the more general case of systems with reflectors.

(iii) See again Ref. 6.

Finally, we add the following remark. Since $\lambda_1(\alpha)$ is the largest eigenvalue of S_α, an eigenfunction of T_α corresponding to it (which is even and continuous) must be either positive or negative in $[-1,1]$, see Ref. 6. Likewise, since $\lambda_2(\alpha)$ is the largest eigenvalue of A_α, an eigenfunction of T_α corresponding to it (which is odd and continuous) must be either positive or negative in $(0,1]$. Hence, from (12), (see also the Appendix), it follows that an eigenfunction of U_α corresponding to $\lambda_2(\alpha)$ (which is continuous) must be either positive or negative in $[0,1]$.

In the sequel, we also need this theorem.

Theorem 2: Let $\alpha \in (0, +\infty)$. Then

(i) as operators acting respectively in $C[-1,1]$ and $C[0,1]$, T_α and U_α depend continuously on α, in the uniform topology;

(ii) moreover, T_α depends continuously on α also as an operator acting in $L_2[-1,1]$;

(iii) $T_\beta - T_\alpha$ is a positive definite operator in $L_2[-1,1]$ if $\beta > \alpha$.

Proof: (i) Let us consider the operator T_α. If we show that

$$M_{\alpha\beta} = \sup_{x\in[-1,1]} \int_{-1}^{1} |T_\beta(x,x') - T_\alpha(x,x')|\,dx' \to 0 \text{ as } \beta\to\alpha, \tag{14}$$

then clearly T_α depends continuously on α as an operator acting in $C[-1,1]$. It is sufficient to prove (14).

The exponential integral is a strictly decreasing function in $(0, +\infty)$ and

$$\int_{-1}^{1} T_\alpha(x,x')\,dx' < \int_{-\infty}^{+\infty} T_\alpha(x,x')\,dx' = 1$$

for any $x \in [-1,1]$ and any $\alpha > 0$. By taking $\beta > \alpha$ and recalling (2), we get the inequalities

$$\begin{aligned}\int_{-1}^{1} &|T_\beta(x,x') - T_\alpha(x,x')|\,dx' \\ &\leq (1-\alpha/\beta)\int_{-1}^{1} T_\beta(x,x')\,dx' + \int_{-1}^{1}[T_\alpha(x,x') \\ &\quad - (\alpha/\beta)\,T_\beta(x,x')]\,dx' \\ &\leq 2|\beta-\alpha|/\beta,\end{aligned}$$

which are true for any $x \in [-1,1]$. This is also true for $\beta < \alpha$; therefore, (14) is proved.

Let us consider the operator U_α. By recalling the definition of the kernel of U_α and by making use of the series expansion of the exponential integral, we can see that

$$\sup_{x\in[0,1]} \int_0^1 |U_\beta(x,x') - U_\alpha(x,x')|\,dx' \to 0 \quad \text{as } \beta\to\alpha$$

so that U_α depends continuously on α as an operator acting in $C[0,1]$.

(ii) Since the kernel $T_\alpha(x,x')$ is symmetric, again from (14) we can deduce that T_α depends continuously on α also as an operator acting in $L_2[-1,1]$. Indeed, let $f \in L_2[-1,1]$, $\|f\| = 1$; we write

$$\begin{aligned}|[(T_\beta - T_\alpha)f](x)|^2 &\\ \leq [\int_{-1}^{1} &|T_\beta(x,x') - T_\alpha(x,x')|\;|f(x')|\,dx']^2 \\ \leq \int_{-1}^{1} &|T_\beta(x,x') - T_\alpha(x,x')|\,dx' \\ \times \int_{-1}^{1} &|T_\beta(x,x') - T_\alpha(x,x')|\;|f(x')|^2\,dx' \\ \leq M_{\alpha\beta} \int_{-1}^{1} &|T_\beta(x,x') - T_\alpha(x,x')|\;|f(x')|^2\,dx',\end{aligned} \tag{15}$$

where we have used the Schwarz inequality and (14). Now, by integrating (15) over $[-1,1]$, from the well-known definition of the norm of an operator and also from (14), we get that

$$\|T_\beta - T_\alpha\| \leq M_{\alpha\beta}.$$

Hence the result follows at once.

(iii) The proof of (iii), with slight modifications, is the same as that given in Ref. 4. Clearly, $T_\beta - T_\alpha$ is also a compact, symmetric operator.

We can now give a theorem that summarizes some properties of the eigenvalues of T_α.

Theorem 3: Let $\alpha \in (0, +\infty)$. Then

(i) for any $n \geq 1$ the eigenvalues $\lambda_n(\alpha)$ of T_α (and hence those of U_α) are continuous and strictly increasing functions of α;

(ii) for any $n \geq 1$ and any $\alpha > 0$ we have $0 < \lambda_n(\alpha) < 1$; moreover, $\lim_{\alpha\to 0^+} \lambda_n(\alpha) = 0$ for any $n \geq 1$;

(iii) if $n = 1, 2$ we have $\lim_{\alpha\to+\infty} \lambda_n(\alpha) = 1$.

Proof: The proof of (i) follows easily from Theorem 2, see again Ref. 4.

As far as case (ii) is concerned, since the eigenfunctions of T_α are bounded, we have

$$0 < \lambda_1(\alpha) \leq \sup_{x\in[-1,1]} \int_{-1}^{1} T_\alpha(x,x')\,dx' = \int_{-1}^{1} T_\alpha(0,x')\,dx' < 1,$$

for any $\alpha > 0$. On the other hand, from the well-known inequality

$$\lambda_1(\alpha) \leq \left(\int_{-1}^{1}\int_{-1}^{1} |T_\alpha(x,x')|^2\,dx\,dx'\right)^{1/2}$$

it follows at once that $\lambda_1(\alpha) \to 0$ as $\alpha \to 0^+$ because

$$\begin{aligned}\int_{-1}^{1}\int_{-1}^{1} |T_\alpha(x,x')|^2\,dx\,dx' &\leq \int_{-1}^{1} dx \int_{-\infty}^{+\infty} |T_\alpha(x,x')|^2\,dx' \\ &= 2\alpha\log 2,\end{aligned}$$

as is easily seen by making use of (3). The proof of (ii) is complete.

Clearly, to prove (iii), it is sufficient to consider the case $n = 2$. For this, let $f(x) = \sqrt{3/2}\,x$, $x \in [-1,1]$; then $f \in H_o$, $\|f\| = 1$. From (9) and from Theorem 1, we get

$$(A_\alpha f, f) \leq \lambda_2(\alpha) < 1, \quad \alpha > 0,$$

where we have used also (ii). Now, a simple calculation shows that

$$(A_\alpha f, f) = 1 - \tfrac{3}{4}\alpha - (\tfrac{3}{4}\alpha^2)\exp(-2\alpha) + (\tfrac{3}{8}\alpha^3)[1 - \exp(-2\alpha)],$$

and hence the result follows at once.

4. THE SOLUTION OF THE ORIGINAL PROBLEM

We are now in a position to prove some properties of the original Eqs. (1) and (5). These properties are summarized in the following theorem.

Theorem 4: (i) For any $\alpha > 0$ there is one and only one neutron flux $\phi_\alpha \in C[-1,1]$ in the slab such that $\phi_\alpha(x) > 0$ for any $x \in [-1,1]$, $\|\phi_\alpha\| = 1$, ϕ_α being also an even function in $[-1,1]$, and there is one and only one neutron flux $\psi_\alpha \in C[0,1]$ in the sphere such that $\psi_\alpha(x) > 0$ for any $x \in [0,1]$, $\|\psi_\alpha\| = 1$.

(ii) Let $c_S(\alpha)$ and $c_A(\alpha)$ be respectively the critical values in the slab (of half-thickness α) and in the sphere (of radius α), $\alpha > 0$. Then $c_S(\alpha)$ and $c_A(\alpha)$ are continuous and strictly decreasing functions in $(0, +\infty)$ and for any $\alpha > 0$ we have $c_A(\alpha) > c_S(\alpha) > 1$. Moreover,

$$\lim_{\alpha\to 0^+} c_i(\alpha) = +\infty, \quad \lim_{\alpha\to+\infty} c_i(\alpha) = 1, \quad i = A, S.$$

(iii) If $\beta \to \alpha$, then $\|\phi_\beta - \phi_\alpha\| \to 0$ and $\|\psi_\beta - \psi_\alpha\| \to 0$ so that both the neutron fluxes $\phi_\alpha(x)$ and $\psi_\alpha(x)$ are continuous functions respectively in $(0, +\infty) \times [-1, 1]$ and in $(0, +\infty) \times [0, 1]$.

Proof: Points (i) and (ii) follow at once from Theorems 1 and 3 and from the remark which follows Theorems 1.

To prove (iii), we consider only the neutron flux ϕ_α in the slab because the proof for the neutron flux ψ_α in the sphere is the same.

Let $\{\alpha_n\}$ be a sequence converging to α, and let $\{\phi_{\alpha_n}\}$ be the corresponding sequence of positive normalized eigenfunctions. Since T_α is compact as an operator acting in $C[-1, 1]$, the sequence $\{T_\alpha \phi_{\alpha_n}\}$ contains a subsequence $\{T_\alpha \phi_{\alpha_{n_k}}\}$ converging to an element of $C[-1, 1]$, which we write $\lambda_1(\alpha)\overline{\phi}$. From the equality

$$\lambda_1(\alpha)[\phi_{\alpha_{n_k}} - \overline{\phi}] = \lambda_1(\alpha)\,\lambda_1^{-1}(\alpha_{n_k})\,T_{\alpha_{n_k}}\phi_{\alpha_{n_k}} - T_\alpha \phi_{\alpha_{n_k}}$$
$$+ T_\alpha \phi_{\alpha_{n_k}} - \lambda_1(\alpha)\overline{\phi}$$

and since $\lambda_1(\alpha)$ and T_α depend continuously on α, we see that $\phi_{\alpha_{n_k}}$ goes to $\overline{\phi}$. The boundedness of T_α implies that $T_\alpha \phi_{\alpha_{n_k}} \to T_\alpha \overline{\phi}$ and so $T_\alpha \overline{\phi} = \lambda_1(\alpha)\,\overline{\phi}$. Since $\lambda_1(\alpha)$ is simple, then $\overline{\phi} = \phi_\alpha$, and $\phi_{\alpha_{n_k}} \to \phi_\alpha$. Only one limit point for $\{T_\alpha \phi_{\alpha_n}\}$ exists, it is $\lambda_1(\alpha)\,\phi_\alpha$. Hence, $T_\alpha \phi_{\alpha_n} \to \lambda_1(\alpha)\,\phi_\alpha$ and

$$T_\beta \phi_\beta \to \lambda_1(\alpha)\phi_\alpha \quad \text{as } \beta \to \alpha.$$

Thus, the theorem is proved.

We finally observe that all the statements of the theorem have an obvious physical meaning. For example, we have $c_A(\alpha) > c_S(\alpha)$ because the loss of neutrons by leakage is smaller in the slab than in the sphere. Also the fact that the neutron distributions are continuous functions of (α, x) has an interesting physical meaning, that is, for small variations of Σ the neutron distributions vary uniformly in all the domain of the spatial coordinates.

APPENDIX

In Sec. 3 we need the following result. If ϕ_α is an odd continuous eigenfunction, defined by Eq. (11), then

$$\phi_\alpha(x) = x f_\alpha(x), \quad x \in [-1, 1]$$

where $f_\alpha(x)$ is an even continuous function.

We begin by recalling that the kernel $A_\alpha(x, x')$ is odd as function of x'. If ϕ_α satisfies Eq. (11), then its restriction to $[0, 1]$, $\tilde{\phi}_\alpha$, satisfies

$$\lambda(\alpha)\tilde{\phi}_\alpha(x) = \tfrac{1}{2}\alpha \int_0^1 [E(\alpha|x - x'|)$$
$$- E(\alpha|x + x'|)]\,\tilde{\phi}_\alpha(x')\,dx'. \tag{16}$$

A simple computation shows that

$$\lim_{x \to 0^+} [\tilde{\phi}_\alpha(x)/x^p] = 0, \quad 0 < p < 1.$$

Hence, we can write $\tilde{\phi}_\alpha(x) = x^p g_\alpha(x)$, $x \in [0, 1]$, where g_α is a continuous function on $[0, 1]$ [here, we put $g_\alpha(0) = 0$ for continuity].

Now, by introducing this factorization in the rhs of (16), we can prove that $\lim_{x \to 0^+}[\tilde{\phi}_\alpha(x)/x]$ does exist and it is finite. Actually,

$$\lim_{x \to 0^+} \frac{\alpha}{2} \int_0^1 [E(\alpha|x - x'|) - E(\alpha|x + x'|)]\,\frac{x'^p}{n}\,g_\alpha(x')\,dx'$$
$$= \alpha \int_0^1 \frac{\exp(-\alpha x')}{x'^{1-p}}\,g_\alpha(x')\,dx'.$$

Indeed,

$$\left|\frac{\alpha}{2} \int_0^1 \left([E(\alpha|x - x'|) - E(\alpha|x + x'|)]\,\frac{x'^p}{x} - \frac{2\exp(-\alpha x')}{x'^{1-p}} \right)\right.$$
$$\left. \times g_\alpha(x')\,dx' \right|$$
$$\leq \frac{M\alpha}{2} \int_0^1 \left| [E(\alpha|x - x'|) - E(\alpha|x + x'|)]\,\frac{x'}{x}\right.$$
$$\left. - 2\exp(-\alpha x') \right| x'^{p-1}\,dx'$$

because $|g_\alpha(x')| \leq M$. If $\frac{1}{2} < p < 1$, by Schwarz inequality, this is bounded by

$$\frac{M\alpha}{2p - 1} \int_0^1 \left| [E(\alpha|x - x'|) - E(\alpha|x + x'|)]\,\frac{x'}{x}\right.$$
$$\left. - 2\exp(-\alpha x') \right|^2 dx'. \tag{17}$$

We can say that (17) approaches zero if we prove that

$$\lim_{x \to 0^+} \int_0^1 |[E(\alpha x') - E(\alpha|x + x'|)]x'/x$$
$$- \exp(-\alpha x')|^2\,dx' = 0 \tag{18}$$

and

$$\lim_{x \to 0^+} \int_0^1 |[E(\alpha|x - x'|) - E(\alpha x')]x'/x$$
$$- \exp(-\alpha x')|^2\,dx' = 0. \tag{19}$$

The limit (18) follows from the fact that $(x'/x)[E(\alpha x') - E(\alpha|x + x'|)]$ is dominated by $\exp(-\alpha x')$ for $x \in (0, 1]$ and $x' \in [0, 1]$. The integral in (19) can be split in two integrals over $[0, x]$ and $[x, 1]$. Then, by some tedious manipulations, we obtain (19).

By taking into account that $\lim_{x \to 0^+}[\tilde{\phi}_\alpha(x)/x]$ exists and is finite, we can write

$$\tilde{\phi}_\alpha(x) = x f_\alpha(x), \quad x \in [0, 1],$$

where f_α is a continuous function on $[0, 1]$.

Finally, if we put $f_\alpha(-x) = f_\alpha(x)$, we then extend $\tilde{\phi}_\alpha$ to $[-1, 1]$, obtaining an odd function $\phi_\alpha = x f_\alpha$ that satisfies Eq. (11).

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[1] See, for example, B. Davison, *Neutron Transport Theory* (Clarendon, Oxford, 1958).

[2] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965), p. 228.

[3] A. Taylor, *Functional Analysis* (Wiley, New York, 1958), p. 276.

[4] G.M. Wing, *An Introduction to Transport Theory* (Wiley, New York, 1962), Chap. 8.

[5] G. Busoni and L. Mangiarotti, Meccanica 6, 211 (1973).

[6] G. Busoni, G. Frosali, and L. Mangiarotti, J. Math. Anal. Appl. 52, 220 (1975).

Null geodesic deviation. II. The Schwarzschild metric

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The equation of geodesic deviation is solved in the Schwarzschild geometry in a covariant manner. The solution is exact for null geodesics, and is given as an integral equation otherwise. The solution is then used to evaluate second derivatives of the world function and derivatives of the parallel propagator, which need to be known in order to find the Green's function for wave equations. The method of null geodesic limits is used to calculate higher order derivatives, and the results are applied to the scalar Green's function in the Schwarzschild geometry.

I. INTRODUCTION

In a previous paper,[1] designated I in the following, a new method of solution of the equation of geodesic deviation was outlined for space–times in which the Riemann tensor could be expressed in terms of simple tensors of lower rank. The specific example of I was any conformally flat space–time. The solution was used to evaluate covariant derivatives of two-point geometrical quantities, following Synge,[2] and the results were applied to find the Green's function for the scalar wave equation. A computational method, called null geodesic limits in analogy with coincidence limits of Synge[2] and DeWitt,[3] was developed, which proved more useful than brute force application of the solutions.

In this paper we treat the same topics for the Schwarzschild geometry, in which the Riemann tensor has a simple decomposition in terms of a tensor field of lower rank. In Sec. II we write down the equation of geodesic deviation and find its solution in a covariant manner. The solution is exact for null geodesics and gives an iterative series in the nonnull case. In Sec. III the solution is used to evaluate second derivatives of the world function and derivatives of the parallel propagator. In Sec. IV the technique of null geodesic limits is applied to finding higher order derivatives, and then used to evaluate the d'Alembertian of $\Delta^{1/2}$. In Sec. V this last calculation is applied to the scalar Green's function as an illustration, and the weak field limit of the solution is exhibited.

II. GEODESIC DEVIATION

The Schwarzschild metric, in standard coordinates, is given by[4]

$$ds^2 = (1 - 2m/r)\, dt^2 - (1 - 2m/r)^{-1}\, dr^2 - r^2\, d\Omega^2. \tag{2.1}$$

The Riemann tensor, computed from (2.1) can be expressed in the form

$$R^{\mu\nu}{}_{\alpha\beta} = \phi[\delta^\mu_\alpha \delta^\nu_\beta - \delta^\mu_\beta \delta^\nu_\alpha + 3(p^\mu_\alpha p^\nu_\beta - p^\mu_\beta p^\nu_\alpha)], \tag{2.2}$$

where, in the coordinate system defined by (2.1),

$$\phi = -m/2r^3 \tag{2.3}$$

and

$$p^0_0 = p^1_1 = -p^2_2 = -p^3_3 = 1. \tag{2.4}$$

Although (2.2) was obtained only in one coordinate system, we can define (2.2) to be valid in any other coordinate system if we define ϕ to be a scalar and p^ν_μ to be a tensor.

As an aside remark, we note that the assignment of the tensor transformation properties to (2.3) and (2.4) is not without some physical justification. First, ϕ depends only on r, which is determined by the surface area ($4\pi r^2$) of a sphere of symmetry in any coordinate system, and thus a scalar. Second, the relations (2.4) can be deduced from the spherically symmetric solutions of the tensor algebraic equations

$$p^\alpha_\mu p^\nu_\alpha = \delta^\nu_\mu, \quad p^\alpha_\alpha = 0, \quad p^0_0 > 0. \tag{2.5}$$

These equations remind one of the algebraic equations encountered in the geometrization of the electromagnetic field following Rainich,[5] Misner, and Wheeler.[6] In fact if we consider the Reissner–Nordström solution with a small charge ϵ, and compute the energy momentum tensor $T^{\mu\nu}$ of the electromagnetic field,[7] then p^ν_μ is given as

$$p^\nu_\mu = \lim_{\epsilon \to 0} 2T^\nu_\mu/(T_{\alpha\beta}T^{\alpha\beta})^{1/2}, \tag{2.6}$$

where in the limit $\epsilon \to 0$, the Reissner–Nordström solution becomes the Schwarzschild solution. Thus the physical interpretation of p^ν_μ is that of a normalized energy-momentum tensor of a "ghost" electromagnetic field arising from an infinitesimal charge added to the Schwarzschild geometry.

Following the notation of I the equation of geodesic deviation for the Riemann tensor (2.2) is

$$\frac{\delta^2 V^\mu}{\delta u^2} + \phi(V^\mu U_\alpha U^\alpha - U^\mu U_\alpha V^\alpha) + 3\phi(\tilde{V}^\mu \tilde{U}_\alpha U^\alpha - \tilde{U}^\mu \tilde{U}_\alpha V^\alpha) = 0, \tag{2.7}$$

where V^μ is the deviation vector, U^μ is the tangent vector, and where we have defined the operation $\tilde{A}^\mu$ on a vector A^μ by

$$\tilde{A}^\mu = p^\mu_\alpha A^\alpha. \tag{2.8}$$

This operation has the properties that $\tilde{\tilde{A}}^\mu = A^\mu$, $\tilde{A}_\alpha \tilde{A}^\alpha = A_\alpha A^\alpha$, and $\tilde{A}_\alpha B^\alpha = A_\alpha \tilde{B}^\alpha$. As in I we wish to solve (2.7) for $V^\mu(u)$ for end values $V^\mu(u_1) = 0$ and $V^\mu(u_2) = V^{\mu_2}$, an arbitrary deviation vector. In the first term of the first bracket in (2.7) the factor $U_\alpha U^\alpha$ vanishes if the fiducial geodesic is null, and that term can be treated as a small perturbation if the fiducial geodesic is nearly null. In the second term of the first bracket $U_\alpha V^\alpha$ is known, as in I, by the integral of (2.7),

$$U_\alpha V^\alpha = [(u - u_1)/(u_2 - u_1)]\, U_{\alpha_2} V^{\alpha_2}. \tag{2.9}$$

The covariant derivatives of $p_{\mu\nu}$ can be evaluated in the coordinate system (2.1), although the final expressions are valid generally. First we define the scalar ψ in the coordinate system (2.1) by $\psi = \ln r$ so that $\phi = -(m/2)\exp(-3\psi)$. Then the covariant derivative of $p_{\mu\nu}$ is found to be

$$p_{\mu\nu;\lambda} = \psi_{;\mu}(g_{\nu\lambda} - p_{\nu\lambda}) + \psi_{;\nu}(g_{\mu\lambda} - p_{\mu\lambda}). \qquad (2.10)$$

This operation introduces a new vector, $\psi_{;\mu}$, which has the property that $\tilde{\psi}_{;\mu} = \psi_{;\mu}$. The covariant derivative of $\psi_{;\mu}$ is similarly found to be

$$\psi_{;\mu;\nu} = -\psi_{;\mu}\psi_{;\nu} - Mg_{\mu\nu} - Np_{\mu\nu}, \qquad (2.11)$$

where

$$M = -(m/2)\exp(-3\psi) + \tfrac{1}{2}\exp(-2\psi),$$

$$N = (3m/2)\exp(-3\psi) - \tfrac{1}{2}\exp(-2\psi).$$

Note that (2.10) and (2.11) are sufficient to evaluate any higher covariant derivatives of $p_{\mu\nu}$ or $\psi_{;\mu}$ that are desired without introducing new vectors or tensors. This follows from the fact that

$$M_{;\lambda} = -\tfrac{1}{2}\psi_{;\lambda}(3M - N), \quad N_{;\lambda} = -\tfrac{1}{2}\psi_{;\lambda}(3M + 7N). \qquad (2.12)$$

The closure property, illustrated by (2.10), (2.11), and (2.12) is needed in order to establish a trial solution of (2.7) with scalar coefficients.

Two integrals along the geodesic can be found directly from (2.10) and (2.11). If we multiply (2.10) by $U^\mu U^\nu U^\lambda$, we find that

$$(\tilde{U}_\alpha - U_\alpha)\,U^\alpha = 2h^2\exp(-2\psi), \qquad (2.13)$$

where h is a constant. In standard notation $h = r^2(d\phi/du)$ when $\theta = \pi/2$, so that (2.13) is equivalent to the angular momentum integral of motion. Also multiplying (2.11) by $U^\mu U^\nu$ leads to

$$\tfrac{1}{2}(\tilde{U}_\alpha + U_\alpha)\,U^\alpha[1 - 2m\exp(-\psi)] + \exp(2\psi)(\delta\psi/\delta u)^2 = K^2, \qquad (2.14)$$

where K is a constant [equal to $(1 - 2m/r)(dt/du)$ in standard notation] and where $\delta\psi/\delta u = \psi_{;\lambda}U^\lambda$. (2.14) is thus equivalent to the energy integral of motion.

The trial solution of (2.7) can now be written as

$$V^\mu = Ag^\mu{}_{\alpha_2}V^{\alpha_2} + BU^\mu + Cp^\mu_\alpha g^\alpha{}_{\beta_2}V^{\beta_2} + D\tilde{U}^\mu + E\psi^{;\mu}, \qquad (2.15)$$

where A, B, C, D, and E are scalar functions of u along the geodesic. The boundary conditions are $A_1 = B_1 = C_1 = D_1 = E_1 = 0$, $A_2 = 1$, $B_2 = C_2 = D_2 = E_2 = 0$, where $A_1 = A(u_1)$, etc. An algebraic relation among the scalar coefficients follows directly from (2.9):

$$[A - (u - u_1)/(u_2 - u_1)]\,U_{\alpha_2}V^{\alpha_2} + BU_\alpha U^\alpha + C\tilde{U}_\alpha g^\alpha{}_{\beta_2}V^{\beta_2} + D\tilde{U}_\alpha U^\alpha + E\,\delta\psi/\delta u = 0. \qquad (2.16)$$

Substitution of (2.15) in (2.7), using (2.10) and (2.11), leads to five coupled ordinary differential equations for the scalar coefficients, found by requiring that coefficients of like vectors in (2.7) separately vanish. From the coefficients of the first and third vectors on the right side of (2.15) we find respectively the differential equations

$$A'' + \phi U_\alpha U^\alpha A + 3\phi\tilde{U}_\alpha U^\alpha C = 0, \qquad (2.17)$$

$$C'' + \phi U_\alpha U^\alpha C + 3\phi\tilde{U}_\alpha U^\alpha A = 0, \qquad (2.18)$$

where prime denotes differentiation with respect to u. These equations are decoupled by defining $g(u) = A + C$ and $h(u) = A - C$, so that g and h satisfy

$$g'' + [\phi(U_\alpha U^\alpha + 3\tilde{U}_\alpha U^\alpha)]g = 0, \qquad (2.19)$$

$$h'' + [\phi(U_\alpha U^\alpha - 3\tilde{U}_\alpha U^\alpha)]h = 0, \qquad (2.20)$$

subject to the boundary conditions $g_1 = h_1 = 0$, $g_2 = h_2 = 1$. (2.19) and (2.20) are of the form of a Schrödinger's equation, and the bracket terms may be identified with effective potentials. A major distinction is, however, that the boundary conditions are inhomogeneous. Note that from (2.13) each bracket is a known function of ψ, so that if one gives $\psi(u)$ [or $r(u)$] for the fiducial geodesic, then the solutions of (2.19) and (2.20) can be explicitly found by numerical integration or other techniques. For the case of null fiducial geodesics the brackets in (2.19) and (2.20) are proportional to $\exp(-5\psi)$ (or $1/r^5$). For null fiducial geodesics the bracket in (2.19) is always negative, and that of (2.20) is always positive. Therefore the solution for $g(u)$, subject to the boundary conditions, is always well behaved; however there could exist end points such that $h(u)$ is zero at both end points so that $h(u)$ could not then be scaled to the value 1 at $u = u_2$. Note, however, that there is no singular behavior to either $g(u)$ or $h(u)$ as r approaches $2m$.

For the case of null fiducial geodesics, we can find one explicit solution of (2.19), namely

$$g_0(u) = \frac{1}{2}\frac{\delta}{\delta u}\exp(2\psi) = [K^2\exp(2\psi) - h^2 + 2mh^2\exp(-\psi)]^{1/2}. \qquad (2.21)$$

The other independent solution is then

$$g_0(u)\int^u \frac{du}{g_0^2(u)}, \qquad (2.22)$$

which can be expressed explicitly in terms of a derivative of an elliptic integral of the first kind with respect to the parameter K^2/h^2. The desired solution is then the linear combination of (2.21) and (2.22) that satisfies $g_1 = 0$ and $g_2 = 1$:

$$g(u) = \frac{g_0(u)}{g_0(u_2)}\int_{u_1}^{u}\frac{du}{g_0^2(u)} \quad \int_{u_1}^{u_2}\frac{du}{g_0^2(u)}. \qquad (2.23)$$

If $g_0(u) = 0$ between u_1 and u_2, then one has to consider $g(u)$ in the two segments (u_1, u_0) and (u_0, u_2) separately. A formal solution to (2.20) can be obtained by consideration of elliptic functions of a complex argument. However in practice it would probably be simpler to numerically integrate both (2.19) and (2.20) in order to find $g(u)$ and $h(u)$.

From (2.17)–(2.20) we have explicit solutions for the scalar coefficients A and C, and these terms may be treated as known quantities in the remaining three differential equations. The decoupling of the differential equations resulting from the coefficients of the second, fourth, and fifth vectors of (2.15) in (2.7) gives rise to the differential equation for E,

$$E'' + 3\phi\tilde{U}_\alpha U^\alpha E = \times 2[1/(u_2 - u_1) - A' - C']\,U_{\alpha_2}V^{\alpha_2} + O(U_\alpha U^\alpha), \qquad (2.24)$$

which (with the boundary conditions $E_1 = E_2 = 0$) determines E. Then D is determined, to order $(U_\alpha U^\alpha)^0$, from (2.16), which automatically satisfies the boundary conditions $D_1 = D_2 = 0$. Finally B is found to satisfy the differential equation

$$\begin{aligned} B'' = &- D'' - (4\phi E)' + \phi(A + C)[U_{\alpha_2} V^{\alpha_2} \\ &+ 3\tilde{U}_\alpha g^\alpha{}_{\beta_2} V^{\beta_2}] + O(U_\alpha U^\alpha), \end{aligned} \tag{2.25}$$

where the right-side is known from the above and the boundary conditions are $B_1 = B_2 = 0$.

If $U_\alpha U^\alpha = 0$, the homogeneous equation for E in (2.24) is the same as that for $g(u)$ in (2.19). Therefore, the two independent solutions of the homogeneous equation for E are $g(u)$ and $g(u) \int^u du/g^2$. We then generate the complete solution to (2.24),

$$E(u) = G(u)\, U_{\alpha_2} V^{\alpha_2} + O(U_\alpha U^\alpha), \tag{2.26}$$

where

$$\begin{aligned} G(u) = g(u)[&(u_2 - u) \\ &- 2/(u_2 - u_1) \textstyle\int_u^{u_2} (du'/g^2) \int_{u_1}^{u'} du''\, g]. \end{aligned} \tag{2.27}$$

Equation (2.25) can also be integrated, since the right-hand side is known. In order to avoid having an integral with the parallel propagator in the integrand, we first let

$$\begin{aligned} B(u) = &- D(u) + H(u)\, U_{\alpha_2} V^{\alpha_2} + J(u) + K(u) \\ &- (u - u_1)/(u_2 - u_1)[J(u_2) + K(u_2)], \end{aligned} \tag{2.28}$$

where

$$J(u) = -2\psi_{;\alpha} g^\alpha{}_{\nu_2} V^{\nu_2} \textstyle\int_{u_1}^u g\, du, \tag{2.29}$$

$$K(u) = (\tilde{U}_\alpha g^\alpha{}_{\nu_2} V^{\nu_2}/\tilde{U}_\beta U^\beta)[-g(u) + 2\psi_{;\gamma} U^\gamma \textstyle\int_{u_1}^u g\, du], \tag{2.30}$$

and where $H(u)$ then satisfies the differential equation

$$H'' - [(2\psi_{;\alpha} U^\alpha/\tilde{U}_\beta U^\beta) - 2\phi \textstyle\int_{u_1}^u g\, du]' + (4\phi G)' = \phi g. \tag{2.31}$$

Then $H(u)$ is determined to be

$$H(u) = L(u) - (u - u_1)/(u_2 - u_1)\, L(u_2), \tag{2.32}$$

where

$$\begin{aligned} L(u) = (1/\tilde{U}_\alpha U^\alpha) - \textstyle\int_{u_1}^u &(4\phi G + 2\phi \textstyle\int_{u_1}^{u'} g du'' \\ &- \textstyle\int_{u_1}^{u'} \phi g\, du'')\, du'. \end{aligned} \tag{2.33}$$

It is convenient, as in I, to have the deviation vector at u expressed explicitly in terms of the arbitrary endpoint deviation V^{ν_2}. Define the two-point tensor $S^\mu{}_{\nu_2}$ by

$$V^\mu(u) = S^\mu{}_{\nu_2} V^{\nu_2}. \tag{2.34}$$

Then $S^\mu{}_{\nu_2}$ has the explicit form

$$\begin{aligned} S^\mu{}_{\nu_2} = &\tfrac{1}{2}(g + h)\, g^\mu{}_{\nu_2} + \tfrac{1}{2}(g - h)\, p^\mu{}_\alpha g^\alpha{}_{\nu_2} + G\psi^{;\mu} U_{\nu_2} \\ &+ \frac{1}{\tilde{U}_\alpha U^\alpha} \left(\frac{u - u_1}{u_2 - u_1} - \tfrac{1}{2}(g + h) - G\psi_{;\beta} U^\beta \right) (\tilde{U}^\mu - U^\mu)\, U_{\nu_2} \\ &+ \frac{1}{2\tilde{U}_\alpha U^\alpha} (h - g)(\tilde{U}^\mu - U^\mu)\, \tilde{U}_\beta g^\beta{}_{\nu_2} \\ &+ HU^\mu U_{\nu_2} - 2 \left(\int_{u_1}^u g\, du \right) U^\mu \psi_{;\alpha} g^\alpha{}_{\nu_2} \\ &+ \frac{1}{\tilde{U}_\alpha U^\alpha} \left(-g + 2\psi_{;\beta} U^\beta \int_{u_1}^u g\, du \right) U^\mu \tilde{U}_\gamma g^\gamma{}_{\nu_2} \\ &+ 2 \frac{u - u_1}{u_2 - u_1} \left(\int_{u_1}^{u_2} g\, du \right) U^\mu \psi_{;\nu_2} \\ &- \frac{u - u_1}{u_2 - u_1} \left(\frac{1}{\tilde{U}_{\alpha_2} U^{\alpha_2}} \right) \left(-1 + 2\psi_{;\beta_2} U^{\beta_2} \int_{u_1}^{u_2} g\, du \right) U^\mu \tilde{U}_{\nu_2} \\ &+ O(U_\alpha U^\alpha). \end{aligned} \tag{2.35}$$

One can verify that $U_\mu S^\mu{}_{\nu_2} = (u - u_1)/(u_2 - u_1)\, U_{\nu_2}$, as is required from (2.9).

III. GEOMETRICAL RELATIONS

In this section we compute the second derivatives of the world function, derivatives of the parallel propagator, and evaluate the two-point scalar $\Delta^{1/2}$ for two space—time points in the Schwarzschild geometry which are separated by a null geodesic. Our calculations follow the formalism of Synge[2] and DeWitt[3] as outlined in I.

Let Ω be the world-function (or geodesic interval). Then

$$\Omega_{;\mu_1} = -(u_2 - u_1)\, U_{\mu_1} \quad \text{and} \quad \Omega_{;\mu_2} = (u_2 - u_1)\, U_{\mu_2}.$$

The second derivatives are found by varying these relations with respect to the end point x_2 and using the expression for the deviation vector V^μ. From (I.3.3) and (I.3.4) we have generally that

$$\Omega_{;\mu_1;\nu_2} = -(u_2 - u_1) \left[\frac{\delta}{\delta u} S_{\mu\nu_2} \right]_{u=u_1}, \tag{3.1}$$

$$\Omega_{;\mu_2;\nu_2} = (u_2 - u_1) \left[\frac{\delta}{\delta u} S_{\mu\nu_2} \right]_{u=u_2}. \tag{3.2}$$

Taking the derivatives of $S_{\mu\nu_2}$ gives for (3.1),

$$\begin{aligned} \Omega_{;\mu_1;\nu_2} = -(u_2 - u_1) \Big\{ &\tfrac{1}{2}(g'_1 + h'_1)\, g_{\mu_1\nu_2} + \tfrac{1}{2}(g'_1 - h'_1)\, p_{\mu_1\alpha_1} g^{\alpha_1}{}_{\nu_2} \\ &+ G'_1 \psi_{;\mu_1} U_{\nu_2} + \frac{1}{\tilde{U}_{\alpha_1} U^{\alpha_1}} \left[\frac{1}{u_2 - u_1} - \tfrac{1}{2}(g'_1 + h'_1) \right. \\ &\left. - G'_1 \psi_{;\beta_1} U^{\beta_1} \right] (\tilde{U}_{\mu_1} - U_{\mu_1})\, U_{\nu_2} \\ &+ \frac{1}{2\tilde{U}_{\alpha_1} U^{\alpha_1}} (h'_1 - g'_1)(\tilde{U}_{\mu_1} - U_{\mu_1})\, \tilde{U}_{\beta_1} g^{\beta_1}{}_{\nu_2} \\ &+ H'_1 U_{\mu_1} U_{\nu_2} - \frac{g'_1}{\tilde{U}_{\alpha_1} U^{\alpha_1}} U_{\mu_1} \tilde{U}_{\beta_1} g^{\beta_1}{}_{\nu_2} \\ &+ \frac{2}{u_2 - u_1} \left[\int_{u_1}^{u_2} g\, du \right] U_{\mu_1} \psi_{;\nu_2} \\ &+ \frac{1}{u_2 - u_1} \frac{1}{\tilde{U}_{\alpha_2} U^{\alpha_2}} \left[1 - 2\psi_{;\beta_2} U^{\beta_2} \int_{u_1}^{u_2} g\, du \right] U_{\mu_1} \tilde{U}_{\nu_2} \\ &+ O(U_\alpha U^\alpha). \end{aligned} \tag{3.3}$$

It can be verified that $U^{\mu_1} \Omega_{;\mu_1;\nu_2} = -U_{\nu_2}$ and $\Omega_{;\mu_1;\nu_2} U^{\nu_2} = -U_{\mu_1}$ as is required from differentiating the identity $\Omega_{;\mu} \Omega^{;\mu} = 2\Omega$. For (3.2) we find

$$\begin{aligned}\Omega_{;\mu_2;\nu_2} = (u_2-u_1)\Big\{ & \tfrac{1}{2}(g_2'+h_2')\,g_{\mu_2\nu_2} + \tfrac{1}{2}(g_2'-h_2')\,p_{\mu_2\nu_2} \\ & + (\psi_{;\mu_2}U_{\nu_2} + U_{\mu_2}\psi_{;\nu_2})\left[-1 + \frac{2}{u_2-u_1}\int_{u_1}^{u_2} g\,du\right] \\ & + \frac{\tilde{U}_{\mu_2}U_{\nu_2} + U_{\mu_2}\tilde{U}_{\nu_2}}{\tilde{U}_{\alpha_2}U^{\alpha}}\left[\frac{1}{u_2-u_1} - \tfrac{1}{2}(g_2'+h_2')\right. \\ & \left. + \psi_{;\beta_2}U^{\beta_2}\left(1 - \frac{2}{u_2-u_1}\int_{u_1}^{u_2} g\,du\right)\right] \\ & + \frac{1}{2}\,\frac{\tilde{U}_{\mu_2}\tilde{U}_{\nu_2}}{\tilde{U}_{\alpha_2}U^{\alpha_2}}(h_2'-g_2') + \frac{U_{\mu_2}U_{\nu_2}}{\tilde{U}_{\alpha_2}U^{\alpha_2}}\left[-\frac{1}{u_2-u_1}\right. \\ & + \tfrac{1}{2}(g_2'+h_2') - 2\psi_{;\beta_2}U^{\beta_2} + H_2'\tilde{U}_{\alpha_2}U^{\alpha_2} \\ & + 2\Big(M\tilde{U}_{\alpha_2}U^{\alpha_2} + (\psi_{;\alpha_2}U^{\alpha_2})^2 \\ & \left. + \frac{\psi_{;\alpha_2}U^{\alpha_2}}{u_2-u_1}\Big)\int_{u_1}^{u_2} g\,du\right]\Big\} + O(U_\alpha U^\alpha). \end{aligned} \tag{3.4}$$

Again we can show explicitly that $U^{\mu_2}\Omega_{;\mu_2;\nu_2} = U_{\nu_2}$. The contraction of (3.4) results in a simple expression

$$\Omega_{;\mu_2}{}^{;\mu_2} = (u_2-u_1)(g_2'+h_2') + 2 + O(U_\alpha U^\alpha). \tag{3.5}$$

The differential equation for $\Delta^{1/2}$, defined in I.4.5, is then

$$\frac{d}{du_2}\ln(\Delta^{1/2}) = (1/u_2-u_1) - \tfrac{1}{2}(g_2'+h_2') + O(U_\alpha U^\alpha) \tag{3.6}$$

which has the solution (normalized to $\Delta^{1/2}=1$ when P_1 and P_2 coincide)

$$\Delta^{1/2} = (u_2-u_1)[g_1'h_1']^{1/2} + O(U_\alpha U^\alpha), \tag{3.7}$$

where care has to be taken in solving (3.6) to distinguish between derivatives with respect to u_2 and derivatives with respect to u keeping u_2 fixed. As noted before, g_1' is always finite. However if the points P_1 and P_2 are situated such that h_1' is infinite, then $\Delta^{1/2}$ will become infinite. For a fixed P_1 the locus of such points P_2 defines a caustic surface.

The derivatives of the parallel propagator, expressed in terms of $S^{\mu}{}_{\nu_2}$, is

$$g_{\mu_1\nu_2;\lambda_2} = \textstyle\int_{u_1}^{u_2} g_{\mu_1\alpha}g_{\nu_2\beta}R^{\alpha\beta}{}_{\gamma\delta}S^{\gamma}{}_{\lambda_2}U^{\delta}\,du. \tag{3.8}$$

Using (2.2) and (2.35) results in the explicit expression

$$\begin{aligned} g_{\mu_1\nu_2;\lambda_2} = {} & \tfrac{1}{2}g_{\mu_1\lambda_2}\int_{u_1}^{u_2}\phi[(g+h)\,U_{\nu_2} + 3(g-h)\,g_{\nu_2\alpha}\tilde{U}^{\alpha}]\,du \\ & + \tfrac{1}{2}U_{\nu_2}\int_{u_1}^{u_2}\phi(g-h)\left[g_{\mu_1\alpha}p^{\alpha\sigma}g_{\sigma\lambda_2}\right. \\ & \left. + \frac{2}{\tilde{U}_\alpha U^\alpha}\,g_{\mu_1\beta}\tilde{U}^{\beta}g_{\lambda_2\sigma}\tilde{U}^{\sigma}\right]du \\ & + \frac{3}{2}\int_{u_1}^{u_2}\phi(g+h)\Big(g_{\mu_1\alpha}p^{\alpha\sigma}g_{\sigma\lambda_2} \\ & - \frac{2}{3}\,\frac{U_{\mu_1}U_{\lambda_2}}{\tilde{U}_\alpha U^\alpha}\Big)\,g_{\nu_2\beta}\tilde{U}^{\beta}\,du \\ & + U_{\lambda_2}\int_{u_1}^{u_2}\phi\Big\{3G(g_{\mu_1\alpha}\psi^{;\alpha}g_{\nu_2\beta}\tilde{U}^{\beta}) \\ & + U_{\nu_2}\left[G\left(g_{\mu_1\alpha}\psi^{;\alpha} + 2\,\frac{\psi_{;\beta}U^{\beta}}{\tilde{U}_\alpha U^\alpha}\,g_{\mu_1\gamma}\tilde{U}^{\gamma}\right)\right. \\ & \left. - \frac{2}{\tilde{U}_\alpha U^\alpha}\left(\frac{u-u_1}{u_2-u_1}\right)g_{\nu_2\gamma}\tilde{U}^{\gamma}\right]\Big\}\,du - (\mu_1\leftrightarrow\nu_2) \\ & + O(U_\alpha U^\alpha). \end{aligned} \tag{3.9}$$

From (3.9) it follows that $g_{\mu_1\nu_2;\lambda_2}U^{\lambda_2}=0$ and $g_{\sigma_2}{}^{\mu_1}g_{\mu_1\nu_2;\lambda_2} = -g_{\sigma_2\mu_1;\lambda_2}g^{\mu_1}{}_{\nu_2}$ as expected. The contraction of (3.9), which appears in the integral equation for the Green's function for a vector wave equation, is

$$\begin{aligned} g_{\mu_1\nu_2}{}^{;\nu_2} = U_{\mu_1} & \int_{u_1}^{u_2}\phi\left[2\left(\frac{u-u_1}{u_2-u_1}\right) - (g+h)\right]du \\ & - 3\int_{u_1}^{u_2}\phi(g-h)\,g_{\mu_1\alpha}\tilde{U}^{\alpha} \\ & - 3\int_{u_1}^{u_2}\phi\,G[\psi_{;\alpha}U^{\alpha}(U_{\mu_1} + g_{\mu_1\beta}\tilde{U}^{\beta}) \\ & - U_\alpha\tilde{U}^{\alpha}g_{\mu_1\beta}\psi^{;\beta}]\,du + O(U_\alpha U^\alpha). \end{aligned} \tag{3.10}$$

In a series expansion in powers of the Riemann tensor, (3.9) is of first order in the Riemann tensor, whereas (3.10) is seen to be of second order.

IV. NULL GEODESIC LIMITS

As noted in I further derivatives of (3.3), (3.4), (3.7), and (3.8) require a knowledge of the terms of order $U_\alpha U^\alpha$, which have been ignored thus far. The methods of null geodesic limits allows us to compute these derivatives more easily than brute force calculations. We illustrate this for the computation of the third derivatives of Ω and for the evaluation of $(\Delta^{1/2})_{;\lambda}{}^{;\lambda}$, which has to be known in order to define the scalar Green's function in the Schwarzschild geometry.

We first write $\Omega_{;\mu;\nu}$ in the form

$$Q_{;\mu;\nu} = ag_{\mu\nu} + bp_{\mu\nu} + c_\mu\Omega_{;\nu} + c_\nu\Omega_{;\mu} + \exp(\tilde{\Omega}_{;\mu}\tilde{\Omega}_{;\nu} + f_{\mu\nu}\Omega), \tag{4.1}$$

where a, b, c_μ, and e can be read off from (3.4) by comparison. $f_{\mu\nu}$ is not defined by (3.9); however we assume that $f_{\mu\nu}$ is that quantity which makes (4.1) valid both for null and nonnull geodesics. There is an arbitrariness in the definition of the coefficients in (4.1). In particular we produce the same $\Omega_{;\mu;\nu}$ under the "gauge" transformation

$$\begin{aligned} & f_{\mu\nu}\to f'_{\mu\nu} = f_{\mu\nu} + \alpha g_{\mu\nu} + \beta p_{\mu\nu} + \gamma_\mu\Omega_{;\nu} + \gamma_\nu\Omega_{;\mu} + \delta\tilde{\Omega}_{;\mu}\tilde{\Omega}_{;\nu} \\ & a\to a' = a - \alpha\Omega, \quad b\to b' = b - \beta\Omega, \\ & c_\mu\to c'_\mu = c_\mu - \gamma_\mu\Omega, \quad e\to e' = e - \delta\Omega. \end{aligned} \tag{4.2}$$

A "gauge" will be chosen that results in the simplest relations.

The identity $\Omega^{;\nu}\Omega_{;\mu;\nu} = \Omega_{;\mu}$ leads to constraint equations on (4.1):

$$c_\nu\Omega^{;\nu} + (a-1) = m\Omega, \tag{4.3}$$

$$b + e\Omega_{;\alpha}\tilde{\Omega}^{;\alpha} = n\Omega, \tag{4.4}$$

and

$$2c_\mu + f_{\mu\alpha}\Omega^{;\alpha} + m\Omega_{;\mu} + n\tilde{\Omega}_{;\mu} = 0, \tag{4.5}$$

where we have used $\Omega^{;\alpha}\Omega_{;\alpha} = 2\Omega$ and where m and n are undetermined by the constraint condition. In the geodesic limit (NGL) the right-sides of (4.3) and (4.4) vanish. Using (4.3) and (4.4), the trace of (4.1) becomes

$$\Omega_{;\alpha}{}^{;\alpha}=2(a+1)+\Omega\,[\,f_{\alpha}{}^{\alpha}+2e+2m] \qquad (4.6)$$

which agrees with (3.5) in the NGL.

If we differentiate the identiy $\Omega_{;\mu}=\Omega_{;\mu;\alpha}\Omega^{;\alpha}$, we find

$$\Omega_{;\mu;\nu}=\Omega_{;\mu;\nu;\alpha}\Omega^{;\alpha}+R_{\sigma\mu\alpha\nu}\Omega^{;\sigma}\Omega^{;\alpha}+\Omega_{;\mu;\alpha}\Omega^{;\alpha}{}_{;\nu}. \qquad (4.7)$$

On the left-side we can substitute (4.1) directly. On the right-side the first term can be evaluated directly from (4.1), and, in the NGL, $f_{\mu\nu}$ does not appear. In the second term on the right we use (2.2), and in the third term on the right we use (4.1) twice. After substitution the resulting expressions are reduced to linear combinations of the tensors $g_{\mu\nu}$ and $p_{\mu\nu}$ and tensors proportional to $\Omega_{;\mu}$ and $\tilde{\Omega}_{;\mu}$. Equating coefficients of like tensors results in a series of differential equations for the functions a, b, c_{μ}, and e along the geodesic. From the coefficient of $g_{\mu\nu}$ we find

$$a_{;\alpha}\Omega^{;\alpha}+a^2-b^2-a=0, \qquad \text{(NGL)} \quad (4.8)$$

and from the coefficient of $p_{\mu\nu}$

$$b_{;\alpha}\Omega^{;\alpha}+2ab-b+3\phi\Omega_{;\alpha}\tilde{\Omega}^{;\alpha}=0, \qquad \text{(NGL)} \quad (4.9)$$

where $a_{;\alpha}\Omega^{;\alpha}=da(u)/d\ln(u-u_1)$, etc. Taking the sum and difference of (4.8) and (4.9) leads to the uncoupled equations for $(a+b)$ and $(a-b)$,

$$(a+b)_{;\alpha}\Omega^{;\alpha}=(a+b)-(a+b)^2-3\phi\Omega_{;\alpha}\tilde{\Omega}^{;\alpha}, \qquad \text{(NGL)}(4.10)$$

$$(a-b)_{;\alpha}\Omega^{;\alpha}=(a-b)-(a-b)^2+3\phi\Omega_{;\alpha}\tilde{\Omega}^{;\alpha}. \qquad \text{(NGL)} \quad (4.11)$$

In terms of (3.4), $(a+b)=(u_2-u_1)\,g_2'$ and $(a-b)=(u_2-u_1)\,h_2'$ where a and b are evaluated at the end point u_2. It can then be shown that (4.10) and (4.11) are satisfied by the normalized g and h which are solutions of (2.19) and (2.20).

From the coefficient of $\Omega_{;\nu}$ in (4.7) we find the differential equation for c_{μ},

$$c_{\mu;\alpha}\Omega^{;\alpha}=-c_{\mu}(1+a)-b(\tilde{c}_{\mu}+\psi_{;\mu})+\tfrac{1}{2}\Omega_{;\mu}(\phi-c_{\alpha}c^{\alpha})$$
$$-e\tilde{\Omega}_{;\mu}(b+\tilde{\Omega}_{;\alpha}c^{\alpha}+\psi_{;\beta}\Omega^{;\beta}), \qquad \text{(NGL)} \quad (4.12)$$

and from the coefficient of $\tilde{\Omega}_{;\nu}$ in (4.7) we find the differential equation for e,

$$e_{;\alpha}\Omega^{;\alpha}=e(2\psi_{;\alpha}\Omega^{;\alpha}-2a-1)+3\phi, \qquad \text{(NGL)} \quad (4.13)$$

which is consistent with the condition (4.4). Further, the equation for the vector function c_{μ} can be reduced to a series of scalar functions by letting

$$c_{\mu}=p\psi_{;\mu}+s\Omega_{;\mu}+t\tilde{\Omega}_{;\mu}, \qquad \text{(NGL)} \quad (4.14)$$

which when substituted in (4.12) yields

$$p_{;\alpha}\Omega^{;\alpha}+p(1+a+b)=1-a-b, \qquad \text{(NGL)} \quad (4.15)$$

$$s_{;\alpha}\Omega^{;\alpha}+3s=Mp-\tfrac{1}{2}p^2\psi_{;\alpha}\psi^{;\alpha} \qquad \text{(NGL)} \quad (4.16)$$
$$-(p+1)\,t\psi_{;\alpha}\Omega^{;\alpha}-tb+\tfrac{1}{2}\phi,$$

$$t_{;\alpha}\Omega^{;\alpha}+t(2+a+b-\psi_{;\alpha}\Omega^{;\alpha})$$
$$=Np-e(1+b-a+\psi_{;\alpha}\Omega^{;\alpha}), \qquad \text{(NGL)} \quad (4.17)$$

where

$$c_{\alpha}c^{\alpha}=p^2\psi_{;\alpha}\psi^{;\alpha}+2p(s+t)\,\psi_{;\alpha}\Omega^{;\alpha}+2st\,\Omega_{;\alpha}\tilde{\Omega}^{;\alpha}, \qquad \text{(NGL)}$$

$$c_{\alpha}\tilde{\Omega}^{;\alpha}=\tilde{c}_{\alpha}\Omega^{;\alpha}=p\psi_{;\alpha}\Omega^{;\alpha}+s\Omega_{;\alpha}\tilde{\Omega}^{;\alpha}, \qquad \text{(NGL)}$$

and one integral of (4.15) and (4.17) is known:

$$\Omega^{\alpha}c_{\alpha}=1-a=p\psi_{;\alpha}\Omega^{;\alpha}+t\,\Omega_{;\alpha}\tilde{\Omega}^{;\alpha}. \qquad \text{(NGL)}$$

A more detailed set of relations can be found from the equality

$$\Omega_{;\mu;\nu;\lambda}-\Omega_{;\mu;\lambda;\nu}-R^{\sigma}_{\mu\nu\lambda}\,\Omega_{;\sigma}=0, \qquad (4.18)$$

where the third derivatives of Ω, found from (4.1), involve $f_{\mu\nu}$ and thus a knowledge of (4.1) off the null geodesic. We therefore substitute (4.1) and (2.2) into (4.18), and, after differentiations are carried out, we take the NGL. As before this leads to a series of equalities of coefficients of various tensor terms. In deriving the information extracted from these equalities, one must introduce new undetermined functions,- since, for example, a term in (4.18) of the form $g_{\mu\nu}\Omega_{;\lambda}$ could appear both as a coefficient of $g_{\mu\nu}$ and of $\Omega_{;\lambda}$. In the following these unknown functions appear on the right-sides of the equations. We shall find many can be eliminated by a judicious choice or gauge, using (4.2). In order below, the equations follow from the coefficients in (4.18) of $g_{\mu\nu}$ (or $g_{\mu\lambda}$),

$p_{\mu\nu}$ (or $p_{\mu\lambda}$), $\Omega_{;\mu}, \Omega_{;\nu}$ (or $\Omega_{;\lambda}$), $\tilde{\Omega}_{;\mu}$ and $\tilde{\Omega}_{;\nu}$ (or $\tilde{\Omega}_{;\lambda}$):

$$a_{;\lambda}-b\psi_{;\lambda}-ac_{\lambda}-e\tilde{\Omega}_{;\lambda}(b+\psi_{;\alpha}\Omega^{;\alpha})+\phi\Omega_{;\lambda}=q\Omega_{;\lambda}+r\tilde{\Omega}_{;\lambda}, \qquad (4.19)$$

$$b_{;\lambda}+b\psi_{;\lambda}-bc_{\lambda}-e\tilde{\Omega}_{;\lambda}(a-\psi_{;\alpha}\Omega^{;\alpha})+3\phi\tilde{\Omega}_{;\lambda}=v\Omega_{;\lambda}+w\tilde{\Omega}_{;\lambda}, \qquad (4.20)$$

$$c_{\nu;\lambda}-c_{\lambda;\nu}=\Omega_{;\nu}F_{\lambda}-\Omega_{;\lambda}F_{\nu}+\tilde{\Omega}_{;\nu}G_{\lambda}-\tilde{\Omega}_{;\lambda}G_{\nu}, \qquad (4.21)$$

$$c_{\mu;\lambda}-c_{\mu}c_{\lambda}-e\tilde{\Omega}_{;\lambda}(\psi_{;\mu}+\tilde{c}_{\mu}-e\tilde{\Omega}_{;\mu})-e\Omega_{;\mu}(\psi_{;\lambda}+\tilde{c}_{\lambda})-f_{\mu\lambda}$$
$$=qg_{\mu\nu}+vp_{\mu\lambda}-\Omega_{;\mu}F_{\lambda}+H_{\mu}\Omega_{;\lambda}+J_{\mu}\tilde{\Omega}_{;\lambda}+\tilde{\Omega}_{;\mu}K_{\lambda}, \qquad (4.22)$$

$$\tilde{\Omega}_{;\nu}[e_{;\lambda}+e(c_{\lambda}+\psi_{;\lambda})]-\tilde{\Omega}_{;\lambda}[e_{;\nu}+e(c_{\nu}+\psi_{;\nu})]$$
$$=\Omega_{;\lambda}K_{\nu}-\Omega_{;\nu}K_{\lambda}+L_{\lambda}\tilde{\Omega}_{;\nu}-L_{\nu}\tilde{\Omega}_{;\lambda}, \qquad (4.23)$$

$$0=+rg_{\mu\lambda}+wp_{\mu\lambda}-\Omega_{;\mu}G_{\lambda}+J_{\mu}\Omega_{;\lambda}-\tilde{\Omega}_{;\mu}L_{\lambda}+M_{\mu}\Omega_{;\lambda}. \qquad \text{(NGL)}$$

Because of the antisymmetry of (4.18) in ν and λ, F_{λ} is only defined up to terms parallel to $\Omega_{;\lambda}$ and G_{λ}, L_{λ} and M_{λ} are defined only up to terms parallel to $\tilde{\Omega}_{;\lambda}$. Further, consistency of (4.21) and (4.22) places further restrictions.

If we successively multiply (4.24) by $g^{\mu\lambda}$, $\Omega^{;\mu}\tilde{\Omega}^{;\lambda}$, and $\tilde{\Omega}^{;\mu}\Omega^{;\lambda}$, the three resulting equations imply that $r=0$. Similarly if we successively multiply (4.24) by $p^{\mu\lambda}, \Omega^{;\mu}\Omega^{;\lambda}$, and $\tilde{\Omega}^{;\mu}\tilde{\Omega}^{;\lambda}$, the three resulting equations imply that $w=0$. Returning then to (4.24), and multiplying successively by $\Omega^{;\mu}$, $\Omega^{;\lambda}$, $\tilde{\Omega}^{;\mu}$, and $\tilde{\Omega}^{;\lambda}$, one can then show that G_{λ}, J_{λ}, L_{λ}, and M_{λ} are linear combinations of $\Omega_{;\lambda}$ and $\tilde{\Omega}_{;\lambda}$, with scalar coefficients. Moreover there are only four independent coefficients, so that we can unite

$$G_{\lambda}=f_1\Omega_{;\lambda}+f_2\tilde{\Omega}_{;\lambda},\quad L_{\lambda}=f_3\Omega_{;\lambda}+f_4\tilde{\Omega}_{;\lambda},$$
$$J_{\lambda}=f_1\Omega_{;\lambda}+f_3\tilde{\Omega}_{;\lambda},\quad M_{\lambda}=f_2\Omega_{;\lambda}+f_4\tilde{\Omega}_{;\lambda}, \qquad \text{(NGL)} \quad (4.25)$$

where f_1, f_2, f_3, and f_4 are functions which are not determined by (4.24), and f_2 and f_4 are undetermined by (4.18) in the NGL. If we multiply (4.19) and (4.20) by $\Omega^{;\lambda}$, setting $r=w=0$ as determined above, we reproduce (4.8) and (4.9). If we multiply (4.22) by $\Omega^{;\lambda}$ we obtain (4.12) only if the chosen functions obey the consistency conditions

$$m-q+F_\lambda\Omega^{;\lambda}-f_1\Omega_{;\alpha}\tilde{\Omega}^{;\alpha}=\tfrac{1}{2}(c_\alpha c^\alpha-\phi), \qquad \text{(NGL)} \quad (4.26)$$

$$n-v-K_\lambda\Omega^{;\lambda}-f_3\Omega_{;\alpha}\tilde{\Omega}^{;\alpha}=2e(b+\tilde{c}_\alpha\Omega^{;\alpha}+\psi_{;\alpha}\Omega^{;\alpha}). \qquad \text{(NGL)} \quad (4.27)$$

We now make use of the "gauge" transformations (4.2) in order to eliminate some of our undetermined functions. In particular if we choose

$$\alpha=-q, \quad \beta=-v, \quad \gamma_\mu=F_\mu-f_1\tilde{\Omega}_{;\mu}, \qquad (4.28)$$

then in the new gauge the right sides of (4.19), (4.20), and (4.21) vanish. In particular this last equation shows in this gauge

$$c_{\mu;\nu}=c_{\nu;\mu}. \qquad \text{(NGL)} \quad (4.29)$$

(4.22) is then consistent with (4.29) only if the further restriction holds that

$$\Omega_{;\alpha}(F^\alpha+H^\alpha)=\tilde{\Omega}_{;\alpha}(J^\alpha-K^\alpha). \qquad (4.30)$$

With (4.30) and the gauge choice (4.28), the right side of (4.22) becomes just a linear combination of $\Omega_{;\mu}\Omega_{;\lambda}$ and $\tilde{\Omega}_{;\mu}\tilde{\Omega}_{;\lambda}$ with scalar coefficients. We can then take the trace of (4.22), which yields

$$c_\alpha{}^{;\alpha}-c_\alpha c^\alpha-2e[\psi\,{}_\alpha\Omega\,{}^\alpha+(1-a)]-f_\alpha{}^\alpha=0. \qquad \text{(NGL)} \quad (4.31)$$

This last expression is particularly important for the evaluation of $(\Delta^{1/2})_{;\lambda}{}^{;\lambda}$.

The differential equation for $\Delta^{1/2}$ is

$$(\ln\Delta^{1/2})_{;\alpha}\Omega^{;\alpha}=\tfrac{1}{2}(4-\Omega_{;\alpha}{}^{;\alpha}). \qquad (4.32)$$

In the NGL (4.32) becomes

$$(\ln\Delta^{1/2})_{;\alpha}\Omega^{;\alpha}=1-a. \qquad \text{(NGL)} \quad (4.33)$$

If we differentiate (4.32) and take the NGL we obtain the differential equation for $(\ln\Delta^{1/2})_{;\mu}$:

$$(\ln\Delta^{1/2})_{;\mu;\alpha}\Omega^{;\alpha}=-(\ln\Delta^{1/2})_{;\alpha}\Omega^{;\alpha}{}_{;\mu}-\tfrac{1}{2}\Omega_{;\alpha}{}^{;\alpha}{}_{;\mu}. \qquad (4.34)$$

We substitute $\Omega^{;\alpha}{}_{;\mu}$ from (4.1), setting $\Omega=0$. We find the last term from (4.6), setting $\Omega=0$ after the derivative is taken. This yields the differential equation in the NGL:

$$\begin{aligned}(\ln\Delta^{1/2})_{;\mu;\alpha}\Omega^{;\alpha}&+a(\ln\Delta^{1/2})_{;\mu}+bp_\mu{}^\alpha(\ln\Delta^{1/2})_{;\alpha}\\&+c^\alpha(\ln\Delta^{1/2})_{;\alpha}\Omega_{;\mu}+c_\mu(1-a)+e\tilde{\Omega}_{;\mu}\tilde{\Omega}^{;\alpha}(\ln\Delta^{1/2})_{;\alpha}+a_{;\mu}\\&+\tfrac{1}{2}\Omega_{;\mu}(f_\alpha{}^\alpha+2e+2m)=0.\end{aligned} \qquad \text{(NGL)} \quad (4.35)$$

The solution to (4.35) is

$$(\ln\Delta^{1/2})_{;\mu}=c_\mu+\zeta\Omega_{;\mu}+\pi_\mu\Omega, \qquad (4.36)$$

where ζ satisfies the differential equation

$$\zeta_{;\alpha}\Omega^{;\alpha}+2\zeta-\tfrac{1}{2}\phi+\tfrac{1}{2}c_\alpha c^\alpha+\tfrac{1}{2}f_\alpha{}^\alpha+e+m=0, \qquad \text{(NGL)} \quad (4.37)$$

and π_μ is undetermined by (4.35). If we differentiate (4.3) and use (4.12) and (4.29) we find that in the chosen gauge

$$m=\tfrac{1}{2}c_\alpha c^\alpha-\tfrac{1}{2}\phi, \qquad \text{(NGL)} \quad (4.38)$$

so that m can be eliminated from (4.37). If we differentiate (4.36) and require that the expression be symmetric, then

$$\pi_\mu=\zeta_{;\mu}+\epsilon\,\Omega_{;\mu}, \qquad \text{(NGL)} \quad (4.39)$$

where ϵ is undetermined. However, $\Omega^{;\mu}\pi_\mu=\Omega^{;\mu}\zeta_{;\mu}$ is determined by (4.37) and (4.38). Therefore, we can take the divergence of (4.36).

$$(\ln\Delta^{1/2})_{;\mu}{}^{;\mu}=c_\mu{}^{;\mu}-2c_\alpha c^\alpha-2e+2\phi-f_\alpha{}^\alpha+2\zeta(a-1). \qquad \text{(NGL)} \quad (4.40)$$

We then use (4.31), (4.36), and (4.40) to find

$$(\Delta^{1/2})_{;\alpha}{}^{;\alpha}=2\Delta^{1/2}[e(\psi_{;\alpha}\Omega^{;\alpha}-a)+\phi]. \qquad \text{(NGL)} \quad (4.41)$$

In terms of the parameters of Sec. III, (4.41) can be expressed as

$$\begin{aligned}(\Delta^{1/2})_{;\alpha_2}{}^{;\alpha_2}=(u_2-u_1)(g_1'h_1')^{1/2}\{&(h_2'-g_2')/\tilde{U}_{\alpha_2}U^{\alpha_2}[\psi_{;\beta_2}U^{\beta_2}\\&-\tfrac{1}{2}(g_2'+h_2')]-m/r_2^3\}.\end{aligned} \qquad \text{(NGL)} \quad (4.42)$$

V. GREEN'S FUNCTION AND DISCUSSION

As shown in I the Green's function for the scalar wave equation can be written in the integral form

$$\begin{aligned}\psi(x,z)=\Delta^{1/2}/4\pi\,\delta_R(\Omega(x,z))&\\-(1/4\pi)\int[\Delta^{1/2}(x',z)]_{;\alpha'}{}^{;\alpha'}\,&\delta_R(\Omega(x',z))\,\psi(x,x')\\\times\sqrt{-g'}\,d^4x'&\end{aligned} \qquad (5.1)$$

where δ_R indicates that only the retarded root of $\Omega=0$ contributes, and where there is an implied sum over multiple null geodesics. It can be seen from (4.41) or (4.42) that the last term in (5.1) vanishes in flat space–time, so that in a curved space–time (5.1) represents an iterative expansion in powers of the Riemann tensor. However the scattering term in (5.1) is known exactly through (4.41), so one does not have to perform an expansion also on that term, as would be the case in a general space–time.

It is somewhat instructive to examine (5.1) in a weak-field limit, in order to gain some feeling as to the effects of the scattered contributions. To first order in the mass m, g and h can be written as

$$g=(u-u_1)/(u_2-u_1)-\chi, \qquad (5.2)$$

$$h=(u-u_1)/(u_2-u_1)+\chi, \qquad (5.3)$$

where χ is a function, linear in m, which satisfies

$$\chi''=-(3mh^2/r^5)(u-u_1)/(u_2-u_1), \qquad (5.4)$$

subject to the boundary conditions $\chi_1=\chi_2=0$. In the integration of (5.4) we make use of approximate radial equation

$$\left(\frac{dr}{du}\right)^2=1-(h^2/r^2)(1-2m/r)\approx 1-h^2/r^2, \qquad (5.5)$$

where u is normalized such that $|dr/du|\to 1$ for large

r, and where the additional term that is ignored contributes to χ in order m^2. The minimum in r along the null geodesic joining u_1 and u_2, has the value r_0 $(=h)$ and occurs at $u=u_0$. The relation between r and u is, from (5.5),

$$|u-u_0|=(r^2-r_0^2)^{1/2}. \tag{5.6}$$

The solution of (5.4) is then

$$\chi=m/(u_2-u_1)\{(u-u_1)(1/r-1/r_2) \\ +2(u_0-u_1)/r_0^2[(r_1-r)-(u-u_1)/(u_2-u_1)(r_1-r_2)]\}. \tag{5.7}$$

From (5.2), (5.3), and (3.7) it can be seen that there is no contribution to $\Delta^{1/2}$ which is linear in m, so that $\Delta^{1/2}=1$. However if we evaluate g_1' separately we find that the assumption of small χ breaks down if the null geodesic between u_1 and u_2 passes sufficiently close to m. Specifically if $r_1 \gg r_0$ and $r_2 \gg r_0$, then g_1' becomes

$$g_1'=1/(r_1+r_2)[1-(4m/r_0^2)\,r_1r_2/(r_1+r_2)]. \tag{5.8}$$

Noting that the deflection angle θ, to order m, is $4m/r_0$, we can apply (5.8) only in a region for which $\theta_a \ll (1/r_1+1/r_2)$. This means simply that (5.8) cannot be applied to null geodesics which are deflected in passing m such that P_1 and P_2 lie on a straight line through the origin. Moreover, in the computation of $\Delta^{1/2}$, there will be corrections linear in m whenever the second term in (5.8) is of order $(m/r_0)^{1/2}$. This means that generally one must perform a calculation beyond the linear approximation to treat those null geodesics emanating from P_1 in a solid angle of order m/r_1 directed towards m. Thus the linear calculation does not treat focusing of the null geodesics or those which undergo large deflections or wrap-arounds. Although the latter geodesics will be found at points other than the backward direction, their amplitude (i.e., $\Delta^{1/2}$) will be insignificant in the linear approximation.

In the linear approximation we can rewrite (4.36) in terms of χ_2' so that the resulting expression can be used in the Green's function (5.1):

$$(\Delta^{1/2})_{;\alpha_2}{}^{;\alpha_2}=\frac{\chi_2' r_2^2}{r_0^2}\left[\frac{1}{r_2}\left(\frac{dr}{du}\right)_2-\frac{1}{u_2-u_1}\right]-\frac{m}{r_2^3}, \tag{5.9}$$

where χ_2' is, from (5.7),

$$\chi_2'=-\frac{m}{u_2-u_1}\left\{\left(\frac{dr}{du}\right)_2\left[\frac{u_2-u_1}{r_2^2}+\frac{2(u_0-u_1)}{r_0^2}\right] \\ +\frac{2(u_0-u_1)}{r_0^2}\left(\frac{r_1-r_2}{u_2-u_1}\right)\right\}. \tag{5.10}$$

It is not obvious from (5.9) and (5.10) where the dominant region of scattering is located and what effect this scattering will have on the Green's function (5.1). Let us consider the case in which the scattering point $\mathbf{r}$ is situated such that $r \ll r_1$. Let ρ and z be polar coordinates with axis the straight line from r_1 through the origin, with positive z being on the opposite side of the origin from r_1. Then (5.9) and (5.10) give the scattering

$$\Delta^{1/2}{}_{;\alpha}{}^{;\alpha}=-m\left[\frac{z^2}{\rho^2 r^3}+\frac{2z}{\rho^4}\left(1+\frac{z}{r}\right)+\frac{1}{r^3}\right]. \tag{5.11}$$

Note that for $z=0$, (5.11) becomes $-m/r^3$, which is of order the nonzero components of the Riemann tensor at r; For $z<0$, $|z| \gg \rho$, (5.11) becomes approximately $-m/(4rz^2)$, which is again of order the components of the Riemann tensor, and which approaches 0 as $|z|$ is increased towards r_1. For $z>0$, $|z| \gg \rho$, (5.11) approaches $-m(4z/\rho^4+(1/4r)\,z^2]$, which grows as z increases. This growth continues until the assumption $|z| \ll r_1$ breaks down. In fact if $|z| \gg r_1 \gg \rho$, (5.9) and (5.10) imply that $\Delta^{1/2}{}_{;\alpha}{}^{;\alpha} \rightarrow -4mr_1^3/\rho^4 z^2$, which decays to 0 for large z.

The dominant effect of the scattering (5.11) is a decrease in the amplitude of the signal being propagated from r_1 to r. Again with $r \ll r_1$, the incident signal is

$$\psi^{(0)}=(1/4\pi r_1)\exp[i\omega(r_1+z)], \tag{5.12}$$

where a Fourier time transform has been taken, and terms of order m in the incident signal are ignored since the scattering is of order m. If we consider the wave

$$\psi^{(1)}=-\frac{m}{4\pi r_1}\exp[i\omega(r_1+z)]\frac{1}{r}\frac{(r+z)}{(r-z)}, \tag{5.13}$$

we find that

$$(\nabla^2+\omega^2)\psi^{(1)}=(1/4\pi r_1)\exp[i\omega(r_1+z)]\Delta^{1/2}{}_{;\alpha}{}^{;\alpha} \\ +(2i\omega/r)(2-z/r)\psi^{(1)}, \tag{5.14}$$

so that $\psi^{(1)}$, added to the first term of (5.1), accommodates all of the scattering effects in the zero frequency limit. The correction, arising from the last term of (5.14), is an effective scattering which is localized near the line $\rho=0$, $z>0$. Part of this scattering generates a further correction to ψ with phase $\exp(i\omega z)$. The remainder generates a scattering which propagates radially outward from the line $\rho=0$, $z>0$, with a phase which indicates propagation to some point z on the line, and then propagation from that point to the observer's position. This scattered component is in agreement with that found for the scalar wave equation in a weak field approximation by a different technique,[8] in which it was assumed that there was a spherical body of mass m at the origin.

The application of (5.1) is not restricted to weak field calculations, of course. On the other hand, it appears that a simple analytic solution is not possible for the Green's function, since (5.1) indicates an iterative solution. The use of (5.1) in, say, radiation problems would therefore indicate that numerical methods would have to be employed. The method derived in this paper does allow an exact calculation of the scattering term, which otherwise would have to be found by a further approximation scheme. Moreover the results for geodesic deviation away from null geodesics has many possible applications aside from the Green's function calculation.

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[1] P.C. Peters, J. Math. Phys. 16, 1780 (1975).

[2] J.L. Synge, *Relativity: The General Theory* (North-Holland, Amsterdam, 1960), Chap. II.

[3] B.S. DeWitt, in *Relativity, Groups and Topology*, edited by C. DeWitt and B. DeWitt (Gordon and Breach, New York, 1964).

[4] In the following we set $c=G=1$.

[5] G.Y. Rainich, Trans. Am. Math. Soc. 27, 106 (1925).

[6] C.W. Misner and J.A. Wheeler, Am. Phys. (N.Y.) 2, 525 (1957).

[7] For example, see R. Adler, M. Bazin, and M. Schiffer, *Introduction to General Relativity* (McGraw-Hill, New York, 1975), Chap. 13.

[8] P.C. Peters, Phys. Rev. 146, 938 (1966).

Determination of unitary, analytic representations of the conformal group in 2+1 dimensions using the operator formalism of the Gel'fand–Naimark Z basis

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Operator formalism of the Gel'fand–Naimark Z basis is used to determine the unitary, analytic representations of the conformal group in two space dimensions and one time dimension [SO(3,2)]. For this purpose an operator Z, which is an operator valued function of the generators, is formed. Common eigenstates, labeled by d, s, and Z of three commuting operators Z, I_1, I_2, are taken as the basis states of the representation space. Two series of the representations $d=\sigma$ and $d=-1/2+id_1$ are obtained for $S=0$. An invariant scalar product is obtained in the space of homogenous functions $f(Z)$.

I. INTRODUCTION

The operator treatment of the Gel'fand—Naimark Z basis was first used for the groups $\mathrm{SL}(2,c)$, $\mathrm{SL}(2,R)$, and SO(2,2).[1,2] The formalism can be outlined as follows.

Let $\Lambda=\left(\begin{smallmatrix}a & b\\ c & d\end{smallmatrix}\right)$ be an element of the finite-dimensional representation of a noncompact group G, and U be any unitary representation of the same group. If an operator Z which is a function of the generators J_{ab} of U can be found with the transformation law

$$UZU^{-1}=Z'=(aZ+b)(cZ+d)^{-1}, \tag{1}$$

then the eigenstates of the operator Z, which are labeled by the eigenvalue Z, can be considered as the basis states of the representation space.

To obtain such an operator Z, let Ω be a matrix satisfying the equation

$$U\Omega U^{-1}=\Lambda^{-1}\Omega\Lambda, \tag{2}$$

and ψ be the diagonalizing matrix satisfying

$$\Omega\psi=\psi\omega, \tag{3}$$

where ω is a diagonal matrix and

$$\psi=\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}.$$

Let us define the operator Z as

$$Z=\psi_1\psi_2^{-1}. \tag{4}$$

A transformation law for Z can be obtained using Eqs. (2) and (3). Indeed

$$U\Omega U^{-1}U\psi U^{-1}=U\psi\omega U^{-1}. \tag{5}$$

Since ω commutes with U^{-1}, the above equation becomes

$$U\Omega U^{-1}U\psi U^{-1}=U\psi U^{-1}\omega; \tag{6}$$

but

$$\Lambda^{-1}\Omega\Lambda\, U\psi U^{-1}=U\psi U^{-1}\omega \tag{7}$$

or

$$\Omega(\Lambda\, U\psi U^{-1})=(\Lambda\, U\psi U^{-1})\omega. \tag{8}$$

This shows that $\Lambda U\psi U^{-1}$ is equal to ψ up to a diagonal matrix $\lambda(\Lambda)$, i.e.,

$$\Lambda\, U\psi U^{-1}=\psi\lambda(\Lambda),\quad U\psi U^{-1}=\Lambda^{-1}\psi\lambda(\Lambda), \tag{9}$$

or

$$U\psi_1U^{-1}=(a\psi_1+b\psi_2)\lambda(\Lambda),\quad U\psi_2U^{-1}=(c\psi_1+d\psi_2)\lambda(\Lambda). \tag{10}$$

So the transformation law for the operator Z becomes

$$UZU^{-1}=(aZ+b)\ (cZ+d)^{-1}. \tag{11}$$

II. A REVIEW OF SO(3,2)

In this paper SO(3,2) will be treated as the conformal group in $2+1$ dimensions. The conformal group in $2+1$ dimensions consists of Lorentz transformations J^{ij}, SO(2,1) subgroups, two space and one time translation p^k, dilatation D, and special conformal transformations C^k $(i, J, k=0,1,3)$. Commutation relations of these generators are given as:

$$[J^{kl},\ P^m]=i(g^{km}P^l-g^{lm}P^k),\quad [J^{kl},\ C^m]=i(g^{km}C^l-g^{lm}C^k),$$

$$[C^k,\ C^l]=[P^k,\ P^l]=0,\quad [D,\ P^k]=iP^k, \tag{12}$$

$$[D,\ C^k]=iC^k,\quad [C^k,\ P^l]=(i/2)(g^{kl}D+J^{kl}).$$

Here $g^{00}=-1$, $g''=g^{33}=1$ are the elements of the metric matrix and k,l,m run through 0, 1, 3. SO(3,2) has two Casimir operators, namely

$$I_1=J^{ab}J_{ab},\quad I_2=\tfrac{1}{64}\omega^a\omega_a, \tag{13}$$

where

$$\omega_a=\epsilon_{abcde}J^{bc}J^{de},$$

and ϵ_{abcde} is the Levi-Civita symbol in five dimensions.

III. CONSTRUCTION OF THE OPERATOR Z

To construct the operator Z let us consider the 4×4 real representation Λ of SO(3,2) with infinitesimal generators γ_{ab} and a unitary representation U with infinitesimal generators J_{ab}. If the invariant operator Ω is defined as

$$\Omega=2i\gamma_{ab}J^{ab}, \tag{14}$$

then it satisfies the condition

$$U\Omega U^{-1}=\Lambda^{-1}\Omega\Lambda.$$

Let us consider the generators γ_{AB} of the 4×4 representation of O(5) in order to determine γ_{ab};

$$\gamma_{AB}=(1/4i)[\gamma_a,\gamma_b],\quad A,B=0,1,3,5,6,$$

where

$$\gamma_1=I\otimes\sigma_3,\quad \gamma_0=\rho_3\otimes\sigma_2,\quad \gamma_6=\rho_1\otimes\sigma_2,$$
$$\gamma_5=\rho_2\otimes\sigma_2,\quad \gamma_3=-I\otimes\sigma_1. \tag{15}$$

Here σ_1, σ_2, σ_3, ρ_1, ρ_2, ρ_3 are the usual Pauli spin matrices, I is the 2×2 identity matrix, and ⊗ means the direct product.

Letting $\gamma_0\to-i\gamma_0$, $\gamma_6\to-i\gamma_6$, and indicating $\rho_a\otimes\sigma_b$ as $\rho_a\sigma_b$, one obtains the generators of the 4×4 representation of SO(3, 2) as

$$\gamma_{56}=-(i/2)\rho_3I,\quad \gamma_{30}=-(i/2)\rho_3\sigma_3,\quad \gamma_{10}=-(i/2)\rho_3\sigma_1,$$
$$\gamma_{31}=\tfrac{1}{2}I\sigma_2,\quad \gamma_{60}=-(i/2)\rho_2I,\quad \gamma_{50}=-(i/2)\rho_1I,$$
$$\gamma_{63}=-(i/2)\rho_1\sigma_3,\quad \gamma_{61}=-(i/2)\rho_1\sigma_1,\quad \gamma_{53}=\tfrac{1}{2}\rho_2\sigma_3,$$
$$\gamma_{51}=\tfrac{1}{2}\rho_2\sigma_1. \tag{16}$$

Using the metric $g_{00}=g_{66}=-1$, $g_{11}=g_{33}=g_{55}=+1$, we find that

$$\Omega=2i\gamma_{ab}J^{ab}$$
$$=\begin{pmatrix} D+\sigma_3K_3+\sigma_1K_1+i\sigma_2J_2 & C^0-\sigma_3C^3-\sigma_1C^1 \\ P^0+\sigma_3P^3+\sigma_1P^1 & -D-\sigma_3K_3-\sigma_1K_1+i\sigma_2J_2 \end{pmatrix}, \tag{17}$$

where $K_3\equiv J_{30}$, $K_1\equiv J_{10}$, and $J_2\equiv J_{31}$ are the generators of the SO(2, 1) subgroup. Defining the quaternions

$P=P^0+\sigma_3P^3+\sigma_1P^1$ (2×2 real symetric matrix),
$Z=Z^0+\sigma_3Z^3+\sigma_1Z^1$ (2×2 real symetric matrix),
$C=C^0+\sigma_3C^3+\sigma_1C^1$ (2×2 real symetric matrix),
$J=\sigma_3K^3+\sigma_1K^1-i\sigma_2J_2$ (2×2 real traceless matrix), (18)

the operator Ω can be written as

$$\Omega=\begin{pmatrix} D+J^T & \overline{C} \\ P & -D-J \end{pmatrix}. \tag{19}$$

Here $\overline{C}$ represents the quaternion conjugate of the matrix C, and is defined as

$$\overline{C}=\sigma_2C^T\sigma_2=C^0-\sigma_3C^3-\sigma_1C^1. \tag{20}$$

Now, let us diagonalize the matrix Ω by the matrix $\psi=\binom{\psi_1}{\psi_2}$, i.e.,

$$\Omega\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=i\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}\omega, \tag{21}$$

where ψ_1, ψ_2 are 2×2 matrices with operator elements and ω is a 4×4 diagonal matrix. Defining the operator $\overline{Z}$, the quaternion conjugate of Z, as

$$\overline{Z}=\psi_1\psi_2^{-1} \tag{22}$$

and using Eq. (19), we obtain

$$\begin{pmatrix} D+J^T & \overline{C} \\ P & -D-J \end{pmatrix}\begin{pmatrix}\overline{Z}\psi_2\\ \psi_2\end{pmatrix}=i\begin{pmatrix}\overline{Z}\psi_2\\ \psi_2\end{pmatrix}\begin{pmatrix}\omega_1 & 0\\ 0 & \omega_1\end{pmatrix}, \tag{23}$$

and

$$(D+J^T)\overline{Z}\psi_2+\overline{C}\psi_2=i\overline{Z}\psi_2\omega_1, \tag{24}$$
$$P\overline{Z}\psi_2-(D+J)\psi_2=i\psi_2\omega_1. \tag{25}$$

Since Ω is an invariant operator, its eigenvalues can be written in terms of the eigenvalues d and s of two Casimir operators of SO(3, 2). In fact we will determine two Casimir operators in terms of d and s in the following section. Here d is the eigenvalue of the dilatation operator D, and $s(s+1)$ is the eigenvalue of the Casimir operator ${K_1}^2+{K_3}^2-{J_2}^2$ of the SO(2, 1) subgroup.

Writing $i\psi_2\omega\psi_2^{-1}$ as the sum of a diagonal matrix $-id$ and a traceless matrix $-\Omega'$, where Ω', invariant of the SO(2, 1) subgroup[3] is given as

$$\Omega'=\sigma_1S_1+\sigma_3S_3-i\sigma_2S_2 \tag{26}$$

[S_1, S_2, S_3 are the generators of the SO(2, 1) subgroup.] We obtain

$$\overline{Z}=P^{-1}(D-id+J-\Omega'), \tag{27}$$
$$\overline{C}=-\overline{Z}P\overline{Z}-2id\overline{Z}-\overline{Z}\Omega'-\Omega'^T\overline{Z}. \tag{28}$$

The scalar part of $P\overline{Z}$ gives the dilatation generator D. In fact the scalar part of $P\overline{Z}=\frac{1}{2}\,\mathrm{Tr}(P\overline{Z})=D-id=-P_iZ^i$, so

$$D=-P_iZ^i+id. \tag{29}$$

Therefore we obtained the generators C and D in terms of P, Z and Ω'.

IV. DETERMINATION OF THE CASIMIR OPERATORS I_1, I_2 IN TERMS OF COMPLEX NUMBERS d AND S

The invariant operator Ω satisfies the following equations:

$$\Omega^2=-I_1+3i\Omega+A,\quad \Omega^4=I_1^2-9\Omega^2+A^2-6iI_1\Omega+2I_1A+3i[\Omega,A]_+, \tag{30}$$

where

$$A=[\gamma_{56},\ \gamma_{30}]_+J_{56}J_{30}+[\gamma_{56},\ \gamma_{10}]_+J_{56}J_{10}+[\gamma_{56},\ \gamma_{31}]_+J_{56}J_{31}+[\gamma_{50},\ \gamma_{63}]_+J_{50}J_{63}+[\gamma_{30},\ \gamma_{61}]_+J_{30}J_{61}-[\gamma_{30},\ \gamma_{51}]_+$$
$$\times J_{30}J_{51}-[\gamma_{10},\ \gamma_{53}]_+J_{10}J_{53}+[\gamma_{31},\ \gamma_{60}]_+J_{31}J_{60}-[\gamma_{31},\ \gamma_{50}]_+J_{31}J_{50}+[\gamma_{60},\ \gamma_{53}]_+J_{60}J_{53}+[\gamma_{60},\ \gamma_{51}]_+$$
$$\times J_{60}J_{51}+[\gamma_{10},\ \gamma_{63}]_+J_{10}J_{53}+[\gamma_{60},\ \gamma_{61}]_+J_{60}J_{61}-[\gamma_{63},\ \gamma_{51}]_+J_{63}J_{51}-[\gamma_{61},\ \gamma_{53}]_+J_{61}J_{53},$$

and $[\gamma_{ab}, \gamma_{cd}]_+$ shows the anticommutator of γ_{ab} and γ_{cd}. Using

$$\mathrm{Tr}\,\Omega = \mathrm{Tr}A = 0, \quad \mathrm{Tr}\Omega^2 = -2I_1, \quad \mathrm{Tr}A^2 = \tfrac{1}{2}I_2, \quad \mathrm{Tr}(I_1\Omega) = \mathrm{Tr}(I_1A) = \mathrm{Tr}[\Omega, A]_+ = 0, \tag{31}$$

we obtain

$$I_1 = -\tfrac{1}{2}\,\mathrm{Tr}\Omega^2, \quad I_2 = 2\,\mathrm{Tr}\Omega^4 - 4I_1^2 - 36I_1. \tag{32}$$

So, we should determine the diagonal form ω of the operator Ω to determine I_1, and I_2. Since the diagonal form of Ω' is given as[3]

$$\Omega'\begin{pmatrix} \eta_1 \\ \\ \eta_2 \end{pmatrix} = i\begin{pmatrix} S & 0 & \\ & & \\ 0 & -S & -1 \end{pmatrix}, \tag{33}$$

the diagonal form of Ω can be written as

$$i\omega = \begin{pmatrix} -d+S & 0 \\ & \\ 0 & -d-S-1 \end{pmatrix}. \tag{34}$$

In this paper we will consider the case $S=0$. Hence

$$i\omega = \begin{pmatrix} -d & 0 \\ & \\ 0 & -d-1 \end{pmatrix}. \tag{35}$$

Using the fact that Casimir operators I_1 and I_2 should be real numbers for unitary representations, we obtain the following conditions for $S=0$:

(a) $d=\sigma$, (b) $d=-\frac{1}{2}+id_1$, where σ and d_1 are real numbers. (36)

V. CONSTRUCTION OF THE REPRESENTATION SPACE

Let us define the common eigenstates of three commuting operators I_1, I_2, and $\overline{Z}$, as the ket $|d,Z\rangle$.

Under a unitary representation U, the ket transforms as

$$U|d,Z\rangle = \mu(Z,\Lambda)\,|\,d,Z'\rangle, \tag{37}$$

where $\mu(Z,\Lambda)$ is a multiplier to be determined and $Z' = (AZ+B)(CZ+D)^{-1}$. Let us first determine the infinitesimal generators C^0, C^1, C^3, J_{10}, J_{31}, J_{30} in terms of canonically conjugate operators Z^0, Z^1, Z^3 and P^0, P^1, P^3. Equation (28) can be written as

$$\overline{C} = -\overline{Z}P\overline{Z} - 2id\overline{Z}, \tag{38}$$

for $S=0$. Using the quaternion forms of P, and $\overline{Z}$, operators C^0, C^1, C^3 can be obtained as follows:

$$\begin{aligned} C^0 &= 2Z^0(Z_kP^k) - P^0(Z_kZ^k) - 2idZ^0, \\ C^1 &= 2Z^1(Z_kP^k) - P^1(Z_kZ^k) - 2idZ^1, \\ C^3 &= 2Z^3(Z_kP^k) - P^3(Z_kZ^k) - 2idZ^3 \quad (k=0,1,3). \end{aligned} \tag{39}$$

Besides,

$$\begin{aligned} J_{10} &= Z_1P_0 - Z_0P_1 = -Z_1P^0 - Z_0P^1, \\ J_{31} &= Z_3P_1 - Z_1P_3 = Z_3P^1 - Z_1P^3, \\ J_{30} &= Z_3P^0 - Z_0P_3 = -Z_3P^0 - Z_0P^3. \end{aligned} \tag{40}$$

Here the metric matrix with elements $g_{00}=-1$, $g_{11}=g_{33}=1$ is used for lowering and raising the indices. The unitary representation U of SO(3, 2) can be written in infinitesimal form as

$$\begin{aligned} U_{\mathrm{inf}} = 1 + i(&\alpha_0P^0 + \alpha_1P^1 + \alpha_3P^3 + \beta_0C^0 \\ &+ \beta_1C^1 + \beta_3C^3 + \gamma_1J_{10}\,\gamma_2J_{31}\,i\gamma_3J_{30} + \delta D), \end{aligned} \tag{41}$$

where all α's, β's, γ's, and δ are real infinitesimal parameters. Since $\overline{Z}$ and P are canonically conjugate operators, we can take

$$P^0 = -i\frac{\partial}{\partial Z_0}, \quad P^1 = -i\frac{\partial}{\partial Z_1}, \quad P^3 = -i\frac{\partial}{\partial Z_3}. \tag{42}$$

Hence,

$$\begin{aligned} U_{\mathrm{inf}} = 1 &+ \lambda_0\frac{\partial}{\partial Z_0} + \lambda_1\frac{\partial}{\partial Z_1} + \lambda_3\frac{\partial}{\partial Z_3} \\ &+ 2d(\beta_1Z_1 + \beta_3Z_3 - \beta_0Z_0) - \delta, \end{aligned} \tag{43}$$

where

$$\begin{aligned} \lambda_0 &= \alpha_0 - \beta_0(Z_0^2 + Z_1^2 + Z_3^2) + 2Z_0Z_3\beta_3 \\ &\quad + 2Z_1Z_0\beta_1 - \gamma_1Z_1 - \gamma_3Z_3 - \delta Z_0, \\ \lambda_1 &= \alpha_1 + \beta_1(Z_1^2 - Z_3^2 + Z_0^2) - 2Z_0Z_1\beta_0 \\ &\quad + 2Z_3Z_1\beta_3 - Z_0\gamma_1 + Z_3\gamma_2 - \delta Z_1, \\ \lambda_3 &= \alpha_3 + \beta_3(Z_3^2 - Z_1^2 + Z_0^2) + 2Z_1Z_3\beta_1 \\ &\quad - 2Z_0Z_3\beta_0 - \gamma_2Z_1 - \gamma_3Z_0 - \delta Z_3. \end{aligned} \tag{44}$$

Ignoring the second-order infinitesimal parameters, U_{inf} can be written as

$$\begin{aligned} U_{\mathrm{inf}} = &\left(1 + \lambda_0\frac{\partial}{\partial Z_0} + \lambda_1\frac{\partial}{\partial Z_1} + \lambda_3\frac{\partial}{\partial Z_3}\right) \\ &\times\{1 + d[2(\beta_1Z_1 + \beta_3Z_3 - \beta_0Z_0) - \delta]\}. \end{aligned} \tag{45}$$

Hence the transformation law for the covariant basis

$|d,Z\rangle$ is

$$U_{\rm inf}|d,Z_0,Z_1,Z_3\rangle \qquad (46)$$
$$=\{1+[\delta-2(\beta_1Z_1+\beta_3Z_3-\beta_0Z_0)]\}^{-d}|d,Z_0',Z_1',Z_3'\rangle,$$

where

$$Z_0'=Z_0+\lambda_0,\quad Z_1'=Z_1+\lambda_1,\quad Z_3'=Z_3+\lambda_3.$$

Now let us consider the infinitesimal form of the 4×4 real representation Λ^{-1}, of SO(3, 2), i.e.,

$$\Lambda_{\rm inf}^{-1}=1-i\alpha_0P^0-i\alpha_1P^1-i\alpha_3P^3-i\beta_0C^0$$
$$-i\beta_3C^3-i\gamma_1J_{10}-i\gamma_2J_{31}-i\gamma_3J_{30}-i\delta D, \qquad (47)$$

where

$$P^0=\tfrac{1}{2}(J_{05}+J_{06}),\quad P^1=\tfrac{1}{2}(J_{15}+J_{16}),$$
$$P^3=\tfrac{1}{2}(J_{35}+J_{36}),\quad C^0=\tfrac{1}{2}(J_{05}-J_{06}),\quad C^1=\tfrac{1}{2}(J_{15}-J_{16}),$$
$$C^3=\tfrac{1}{2}(J_{35}-J_{36}),\quad D=J_{56}, \qquad (48)$$

J_{ab} $(a,b=0,1,3,5,6)$ are given in Eq. (16). Hence $\Lambda_{\rm inf}^{-1}$ is found in 2×2 form as

$$\Lambda_{\rm inf}^{-1}=\begin{pmatrix}A_{\rm inf} & B_{\rm inf}\\ C_{\rm inf} & D_{\rm inf}\end{pmatrix}, \qquad (49)$$

where

$$A_{\rm inf}=I-\tfrac{1}{2}[\gamma_1\sigma_1+\gamma_2i\sigma_2+\gamma_3\sigma_3+\delta I],$$
$$B_{\rm inf}=\alpha_0I+\alpha_1\sigma_1+\alpha_3\sigma_3,\quad C_{\rm inf}=\beta_0I-\beta_1\sigma_1-\beta_3\sigma_3,$$
$$D_{\rm inf}=I+[\tfrac{1}{2}\gamma_1\sigma_1+\gamma_2i\sigma_2+\gamma_3\sigma_3+\delta I], \qquad (50)$$

satisfying

$$A_{\rm inf}D_{\rm inf}-B_{\rm inf}C_{\rm inf}=I. \qquad (51)$$

Using these equations and doing necessary calculations, the multiplier in Eq. (46) turns out to be $\det(C_{\rm inf}Z+D_{\rm inf})$. Hence the transformation law is

$$U|d,Z\rangle=[\det(CZ+D)]^{-d}|d,Z'\rangle, \qquad (52)$$

where

$$Z'=(AZ+B)\,(CZ+D)^{-1}. \qquad (53)$$

Using the transformation law for the covariant kets we can determine the transformation law for the function $f(Z)$. Indeed,

$$U|F\rangle=\int f(Z)\,U|Z\rangle\,|dZ|, \qquad (54)$$

where

$$|dZ|=\prod_{i=0,1,3}({\rm Re}dZi)\,({\rm Im}dZi).$$

Hence

$$U|F\rangle=\int f(Z)(\det CZ+D)^{-d}|Z'\rangle\,|dZ|. \qquad (55)$$

Considering Eqs. (44) and noting

$$|dZ|=|\det CZ+D|^6\,|dZ'|,\quad Z=(D'Z'-B')(-CZ'+A)^{-1},$$

where

$$\Lambda=\begin{pmatrix}D' & -B'\\ -C' & A'\end{pmatrix} \qquad (56)$$

such that

$$\Lambda^{-1}\Lambda=\begin{pmatrix}A & B\\ C & D\end{pmatrix}\begin{pmatrix}D' & -B'\\ -C' & A'\end{pmatrix}=\begin{pmatrix}{\rm I} & 0\\ 0 & {\rm I}\end{pmatrix}, \qquad (57)$$

Eq. (55) becomes

$$U|F\rangle=\int f(D'Z'-B')(-C'Z'+A)^{-1}$$
$$\times[\det|(-C'Z'+A')]^{d-6}\,|Z'\rangle\,|dZ'|. \qquad (58)$$

Hence the transformation law for the operator valued functions $f(Z)$ turns out to be

$$f'(Z)=[\det(-C'Z+A')]^{d-6}f(D'Z-B')\,(-C'Z+A'). \qquad (59)$$

If the kets transform with Λ matrices instead of Λ^{-1} matrices, then the transformation law for $f(Z)$ becomes,

$$f'(Z)=[\det(CZ+D)]^{d-6}f(AZ+B)\,(CZ+D)^{-1}. \qquad (60)$$

This transformation shows that d must be an integer for analytic representations.

The homogeneous functions of degree n (n real) have the same transformation law as the function $f(Z)$. Indeed, consider the homogeneous functions $M(\psi_1,\psi_2)$ of two operators ψ_1 and ψ_2. Under the group SL(2,R), ψ_1 and ψ_2 transform like

$$\psi_1'=L\psi_1,\quad\text{and}\quad\psi_2'=L\psi_2, \qquad (61)$$

where 2×2 real matrices L are the elements of SL(2,R). Choosing $M(\psi_1,\psi_2)$ to be

$$M(\psi_1\overline{\psi}_1,\ \psi_2\overline{\psi}_2,\ \psi_1\overline{\psi}_2,\ \psi_2\overline{\psi}_1), \qquad (62)$$

we satisfy the condition

$$M(\psi_1',\psi_2')=M(L\psi_1,L\psi_2)=LM(\psi_1,\psi_2)L^{-1}. \qquad (63)$$

Since $M(\psi_1,\psi_2)$ is a homogeneous function of degree n it fulfills the condition

$$M(\lambda^2\psi_1\overline{\psi}_1,\ \lambda^2\psi_2\overline{\psi}_2,\ \lambda_1^2\psi_1\overline{\psi}_2,\ \lambda^2\psi_2\overline{\psi}_1)$$
$$=\lambda^{2n}M(\psi_1\overline{\psi}_1,\ \psi_2\overline{\psi}_2,\ \psi_1\overline{\psi}_2,\ \psi_2\overline{\psi}_1), \qquad (64)$$

where n is a real number. Letting

$$\lambda^2=(\det\psi_2)^{-1}=\psi_2^{-1}\overline{\psi}_2^{-1} \qquad (65)$$

and noting $\overline{Z}=\psi_1\psi_2^{-1}$, we obtain

$$M(\psi_1\psi_1,\ \psi_2\psi_2,\ \psi_1\psi_2,\ \psi_2\psi_1)=(\det\psi_2)^nM(Z_0,\ Z_1,\ Z_3). \qquad (66)$$

By using the transformation law for ψ_2, the transformation law for $M(Z_0,\ Z_1,\ Z_3)$ is obtained as

$$M'(Z_0,\ Z_1,\ Z_3)=[\det(-C'Z+A')]^nM(Z_0',\ Z_1',\ Z_3'). \qquad (67)$$

Hence the functions $f(Z)$ and $M(Z)$ have the same transformation law provided d is a real number.

Now we can define the norm (and the scalar product), in the space of homogeneous functions $f(Z)$, as[4]

$$\|F\|^2 = C \int \ |f(Z)|^2 \ (\det \mathrm{Im}\overline{Z})^{d-3} |dZ|, \tag{68}$$

where $\mathrm{Im}\overline{Z} = (1/2i)(\overline{Z} - \overline{Z}^+)$.

The transformation law for the operator $\det \mathrm{Im}\overline{Z}$ can be obtained by using the transformation law for the operator Z. Indeed,

$$\det \mathrm{Im}\overline{Z}' = \det(CZ + D)^+ \det(CZ + D) \det \mathrm{Im}\overline{Z}. \tag{69}$$

Using the transformation laws

$$f'(Z) = [\det(CZ + D)]^{d-6} f(Z'),$$

$$|dZ| = [\det(CZ + D)^+(CZ + D)]^3 \ |dZ'|,$$

the invariance of the norm can easily be shown. Besides, the norm is positive definite if the operator $\det \mathrm{Im}\overline{Z}$ is positive definite. Using Eq. (27) we obtain

$$\overline{Z} - \overline{Z}^+ = [P^{-1}, D] - iP^{-1}(d + d^*) + [P^{-1}, J], \tag{70}$$

besides,

$$[P^{-1}, D] = -iP^{-1}, \tag{71}$$

$$[P^{-1}, J] = 2iP^{-1}. \tag{72}$$

Hence the imaginary part of $\overline{Z}$ turns out to be

$$\mathrm{Im}\overline{Z} = \tfrac{1}{2}(1 - \rho)P^{-1}, \tag{73}$$

where $\rho = d + d^*$. Since P is Hermitian for unitary representations, $\mathrm{Im}\overline{Z}$ is also Hermitian. Therefore, the space of all measurable homogeneous functions $f(Z)$ satisfying the condition

$$\int_{\det \mathrm{Im}\overline{Z} > 0} \quad |f(Z)|^2 (\det \mathrm{Im}\overline{Z}) \overset{d-3}{|dZ|} < \infty \tag{74}$$

forms the representation space for the unitary analytic representations of the conformal group in $2+1$ dimensions, for d an integer.

VI. CONCLUSION

We determined the unitary, analytic representations of SO(3, 2) for $s = 0$ using an algebraic method developed by F. Gürsey. We study SO(3, 2) only to apply the method to SO(3, 2) as an extension of the previous works.[1-3] Since SO(3, 2) is a noncompact semisimple Lie group it has a principal and supplementary series of representations. In this paper we obtained that for $s = 0$, principal series is labeled by a real number σ and supplementary series is labeled by a complex number $d = -\frac{1}{2} + id_1$. These results are in agreement with the previous works on SO(3, 2).[5,6] The unitary representations of SO(3, 2) for $s \neq 0$ will be studied later.

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[1] I. Bars and F. Gürsey, J. Math. Phys. **13**, 131 (1972).
[2] F. Gürsey and S. Orfanidis, Phys. Rev. D **7**, 2414 (1973).
[3] F. Gürsey, Lecture notes, M.E.T.U. 1973 (unpublished).
[4] W. Rühl, Commun. Math. Phys. **27**, 53 (1972).
[5] R. Raizka, N. Limić, and J. Niederle, J. Math. Phys. **7**, 2026 (1966).
[6] L. Castell, J. Math. Phys. **11**, 1669 (1970).

Padé approximant bounds for the difference of two series of Stieltjes

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Over the complex plane cut along the negative real axis let $f(z)$ be an analytic function of the form $f(z)=\int_0^\infty d\phi(u)/(1+uz)$, where $\phi(u)$ is of bounded variation on $0\leq u<\infty$. Suppose that the first $(N+1)$ moments defined by $f_n=\int_0^\infty u^n d\phi(u)$, $n=0,1,\ldots,N$, exist and are known. Suppose further that $d\phi(u)$ undergoes at most p sign changes, where $0\leq p\leq N$, as u goes from zero to infinity, the locations of an associated set of points $u=u_l$, $l=1,2,\ldots,p$, being known. Then, by means of a simple modification to the customary Padé approximant method, best possible upper and lower bounds can be imposed on $f(x)$ for all $0<x<\infty$. Similarly, for given z in the cut complex plane, a best possible inclusion region can be imposed upon $f(z)$. Finally it is shown that a best possible inclusion region can be imposed upon $f(z)$ when the constraint that the set of points $u=u_l$, $l=1,2,\ldots,p$, is known is either relaxed or disposed of altogether.

1. INTRODUCTION

Over the complex plane cut along the negative real axis, hereafter referred to as the cut complex plane, let $f(z)$ be an analytic function of the form

$$f(z)=\int_0^\infty d\phi(u)/(1+uz), \tag{1.1}$$

where $\phi(u)$ is of bounded variation on $0\leqslant u<\infty$. Suppose that the first $(N+1)$ moments

$$f_n=\int_0^\infty u^n d\phi(u), \quad n=0,1,\ldots,N, \tag{1.2}$$

exist and are known. That is, we know that as z approaches zero through points in the cut complex plane $f(z)$ behaves like

$$f(z)\sim f_0-f_1z+\cdots+(-1)^N f_N z^N + \text{terms of higher order with unknown or divergent coefficients.} \tag{1.3}$$

We suppose further that $d\phi(u)$ is known to undergo at most p changes of sign, where $0\leqslant p\leqslant N$, as u progresses from zero to infinity, the locations of an associated set of points $u=u_l$, $l=1,2,\ldots,p$, being known. By this we mean the assumption that we know a set of points

$$0+\leqslant u_1<u_2<\cdots<u_p<\infty \tag{1.4}$$

such that

$\phi(u)$ is monotone nondecreasing (nonincreasing) on $0\leqslant u<u_1$

$\phi(u)$ is monotone nonincreasing (nondecreasing) on $u_1<u<u_2$

. . . .

$\phi(u)$ is monotone nonincreasing (nondecreasing) on $u_p<u<\infty$ (p odd)

$\phi(u)$ is monotone nondecreasing (nonincreasing) on $u_p<u<\infty$ (p even). (1.5)

We do not assume that we know which of the two possibilities, either "nondecreasing" or "nonincreasing," pertains to a given interval: We assume only that there is an interchange between the possibilities as u goes from one interval to the next. The case $u_1=0+$ refers to the eventuality that $\phi(u)$ has a "jump" in one direction *at* $u=0$ and then proceeds off in the opposite direction for $u>0$.

Given the above information about $f(z)$, we ask[1] what are the best possible upper and lower bounds which can be imposed on $f(x)$ for all $0<x<\infty$. The requisite bounds are obtained in Sec. 2 by means of a simple modification to the customary Padé approximant method for imposing bounds on functions which are representable by series of Stieltjes.[2] In Sec. 3 the bounds obtained in Sec. 2 are shown to be best possible on the basis of the given information. Further, it is shown how a best possible inclusion region can be imposed on $f(z)$ for given z lying anywhere in the cut complex plane.

In Sec. 4 we describe briefly how best possible bounds on $f(x)$ for all $0<x<\infty$ [more generally, a best possible inclusion region for $f(z)$] can be imposed when the constraint that the locations of the points $u=u_l$, $l=1,2,\ldots,p$, be known is relaxed or disposed of altogether. The feasibility of the procedure is demonstrated with a simple example.

The motivation and justification for the present paper is this: Functions of the form (1.1) occur frequently in problems in theoretical physics, and a means for imposing best possible bounds on such functions, on the basis of as little as possible given information, is much needed. This is borne out by the numerous powerful applications of such bounds which have been effected in the case where $d\phi(u)$ is known to have *no* sign changes in $0\leqslant u<\infty$.[3-5]

2. COMPLEMENTARY BOUNDS FOR $f(x)$, $0<x<\infty$

We consider the effect of the following sequence of successive transformations on $f(z)$: Let

$$f_0(z)=f(z), \tag{2.1}$$

and define

$$f_k(z)=[(1+u_kz)f_{k-1}(z)-f_{k-1}(0)]/z,$$

$$k = 1, 2, \ldots, p. \tag{2.2}$$

We have at the first step

$$f_1(z) = (1/z)[(1 + u_1 z)\int_0^\infty d\phi(u)/(1 + uz) - \int_0^\infty d\phi(u)]. \tag{2.3}$$

Now since $d\phi(u)$ is of bounded variation on $0 \leqslant u < \infty$, that is

$$\int_0^\infty |d\phi(u)| < \infty, \tag{2.4}$$

it follows that for any z in the cut complex plane both of the integrals in (2.3) are absolutely convergent. Hence we may combine the two integrals, yielding

$$f_1(z) = \int_0^\infty d\phi_1(u)/(1 + uz), \tag{2.5}$$

where

$$\phi_1(u) = \int_0^u (u_1 - u)\, d\phi(u). \tag{2.6}$$

We now establish the following: $\phi_1(u)$ in (2.5) is such that (i) it is of bounded variation in $0 \leqslant u < \infty$, (ii) $d\phi_1(u)$ undergoes at most $(p-1)$ sign changes as u progresses from zero to infinity, the locations of these sign changes being associated with the points $u = u_l$, $l = 2, 3, \ldots, p$, and (iii) the first N moments

$$f_j^{(1)} = \int_0^\infty u^j\, d\phi_1(u), \quad j = 0, 1, \ldots, N-1, \tag{2.7}$$

exist and can be determined.

To establish (i), we simply observe that

$$\begin{aligned}\int_0^\infty |d\phi_1(u)| &= \int_0^\infty |u_1 - u|\, |d\phi(u)| \\ &\leqslant u_1 \int_0^\infty |d\phi(u)| + \int_0^\infty u\, |d\phi(u)| \\ &= u_1 \int_0^\infty |d\phi(u)| + \left| \int_0^\infty u\, d\phi(u) - \int_0^{u_p} u\, d\phi(u) \right| \\ &\quad + \int_0^{u_p} u\, |d\phi(u)| \\ &\leqslant u_1 \int_0^\infty |d\phi(u)| + |f_1| + 2u_p \int_0^\infty |d\phi(u)| < \infty.\end{aligned} \tag{2.8}$$

The assertion (ii) is immediate from

$$d\phi_1(u) = (u_1 - u)\, d\phi(u), \tag{2.9}$$

together with the original assumption (1.5) on $\phi(u)$. Finally, we have

$$f_j^{(1)} = \int_0^\infty u^j\, d\phi_1(u) = u_1 f_j - f_{j+1}, \quad j = 0, 1, \ldots, N-1, \tag{2.10}$$

which establishes (iii).

The following theorem now follows at once by induction through the sequence of transformations (2.2).

Theorem I: We can write

$$f_k(z) = \int_0^\infty d\phi_k(u)/(1 + uz), \quad k = 1, 2, \ldots, p, \tag{2.11}$$

where

$$\phi_k(u) = \int_0^u (u_k - u)(u_{k-1} - u) \cdots (u_1 - u)\, d\phi(u), \tag{2.12}$$

and $\phi_k(u)$ is such that (i) it is of bounded variation on $0 \leqslant u < \infty$, (ii) $d\phi_k(u)$ undergoes at most $(p-k)$ sign changes as u progresses from zero to infinity, the locations of these sign changes being associated with the points $u = u_l$, $l = (k+1), \ldots, p$, and (iii) the first $(N+1) - k$ moments

$$f_j^{(k)} = \int_0 u^j\, d\phi_k(u) = \sum_{i=0}^{k} f_{i+j} a_i^{(k)}, \quad j = 0, 1, \ldots, N-k, \tag{2.13}$$

exist and can be determined. In (2.13) we have $a_i^{(k)}$ which is the coefficient of u^i occurring in the polynomial $(u_k - u)(u_{k-1} - u) \cdots (u_1 - u)$.

In particular, $f_p(z)$ is either a series of Stieltjes or the negative of a series of Stieltjes.[2] That is,

$$f_p(z) = \int_0^\infty d\phi_p(u)/(1 + uz),$$

where $\phi_p(u)$ is a bounded function on $0 \leqslant u < \infty$, either monotone nondecreasing or monotone nonincreasing over this interval. Here we allow the possibility that $\phi_p(u)$ attains only finitely many different values on $0 \leqslant u < \infty$. When we wish to underline a case where

$$\phi_p(u) \text{ attains infinitely many different values on } 0 \leqslant u < \infty, \tag{2.14}$$

we will say $f_p(z)$ is a *strict* series of Stieltjes.

Let us now restrict attention to the case $z = x > 0$. Then the set of moments (2.13) with $k = p$ constitutes exactly enough information about $f_p(x)$ for the construction of the complementary pair of Padé approximants,[6]

$$\tilde{f}_p(x) = [\mathrm{Int}\{(N-p)/2\}/\mathrm{Int}\,[(N-p+1)/2\}]_{f_p(x)} \tag{2.15}$$

and

$$\tilde{f}_p^c(x) = \begin{cases} [\mathrm{Int}\{(N-p-1)/2\}/\mathrm{Int}\{(N-p)/2\}]_{f_p(x)} \\ 0 \quad \text{if } N = p. \end{cases} \tag{2.16}$$

Here we use the notation

$$\mathrm{Int}\{r\} = \text{integer part of the nonnegative real number } r, \tag{2.17}$$

and we write $[m/n]_{h(x)}$ to denote the $[n, m]$ Padé approximant to the function $h(x)$. The pair of approximants $\tilde{f}_p(x)$ and $\tilde{f}_p^c(x)$ impose complementary upper and lower bounds on $f_p(x)$ for all $x > 0$[2,6]; that is, either

$$\tilde{f}_p^c(x) \leqslant f_p(x) \leqslant \tilde{f}_p(x) \quad \text{for all } 0 < x < \infty, \tag{2.18}$$

or else

$$\tilde{f}_p(x) \leqslant f_p(x) \leqslant \tilde{f}_p^c(x) \quad \text{for all } 0 < x < \infty. \tag{2.19}$$

Furthermore, the pair of bounds obtained in this way are the best possible upper and lower bounds which can be imposed upon $f_p(x)$ for all $0 < x < \infty$, on the basis of the moments $f_0^{(p)}, f_1^{(p)}, \ldots, f_{N-p}^{(p)}$. We note that the existence of the two approximants (2.15) and (2.16) is assured.[2,7]

The inverse of the sequence of transformations (2.2) is, for $z = x > 0$,

$$f_{k-1}(x) = [x\, f_k(x) + f_0^{(k-1)}]/(1 + u_k x), \quad k = p, p-1, \ldots, 1, \tag{2.20}$$

$$f(x) = f_0(x). \tag{2.21}$$

Let us write $\tilde{f}_p^{(c)}(x)$ to denote the pair of approximants $\tilde{f}_p(x)$ and $\tilde{f}_p^c(x)$. Then on replacing $f_p(x)$ by $\tilde{f}_p^{(c)}(x)$ in the first step in the sequence of inverse transformations (2.20), we obtain a sequence of pairs of approximants $\tilde{f}_{p-1}^{(c)}(x)$, $\tilde{f}_{p-2}^{(c)}(x), \ldots, \tilde{f}_1^{(c)}(x)$, and $\tilde{f}_0^{(c)}(x)=\tilde{f}^{(c)}(x)$, corresponding respectively to the functions $f_{p-1}(x), f_{p-2}(x), \ldots, f_1(x)$, and $f_0(x)=f(x)$. These approximants are given by

$$\tilde{f}_{k-1}^{(c)}(x)=[x\,\tilde{f}_k^{(c)}(x)+f_0^{(k-1)}]/(1+u_kx),$$

$$k=p,\ p-1,\ldots,1, \qquad (2.22)$$

$$\tilde{f}^{(c)}(x)=\tilde{f}_0^{(c)}(x). \qquad (2.23)$$

Now, since the pair of approximants $\tilde{f}_p^{(c)}(x)$ impose complementary upper and lower bounds on $f_p(x)$ for all $0<x<\infty$, it follows by comparison of (2.22) with (2.20) when $k=p$ that the pair of approximants $\tilde{f}_{p-1}^{(c)}(x)$ impose complementary upper and lower bounds on $f_{p-1}(x)$ for all $0<x<\infty$. Hence, proceeding inductively through the cases $k=p-1,\ p-2,\ldots,1$ we deduce that *the pair of approximants* $\tilde{f}^{(c)}(x)$ *impose complementary upper and lower bounds on* $f(x)$ *for all* $0<x<\infty$. That is, we must have either

$$\tilde{f}^c(x)\leqslant f(x)\leqslant\tilde{f}(x)\quad\text{for all } 0<x<\infty, \qquad (2.24)$$

or else

$$\tilde{f}(x)\leqslant f(x)\leqslant\tilde{f}^c(x)\quad\text{for all } 0<x<\infty. \qquad (2.25)$$

Let us examine these two approximants $\tilde{f}(x)$ and $\tilde{f}^c(x)$. Firstly, there is no doubt concerning their existence: No snags can occur in the constructive procedure given above, wherein we start with $\tilde{f}_p(x)$ and $\tilde{f}_p^c(x)$, both of which are guaranteed to exist. Secondly, let us write

$$\tilde{f}_p(x)=A(x)/B(x) \qquad (2.26)$$

and

$$\tilde{f}_p^c(x)=A^c(x)/B^c(x), \qquad (2.27)$$

where

$$B(0)=B^c(0)=1. \qquad (2.28)$$

Where $A(x)$ is a polynomial of degree at most $\mathrm{Int}\{(N-p)/2\}$, $B(x)$ is a polynomial of degree at most $\mathrm{Int}\{(N-p+1)/2\}$, $A^c(x)$ is a polynomial of degree at most $\mathrm{Int}\{(N-p-1)/2\}$ $(N\neq p)$ or else identically zero $(N=p)$, and $B^c(x)$ is a polynomial of degree at most $\mathrm{Int}\{(N-p)/2\}$. Then it follows from (2.22) that

$$\tilde{f}(x)=D(x)/(1+u_1x)(1+u_2x)\circ\circ\circ(1+u_px)B(x) \qquad (2.29)$$

and

$$\tilde{f}^c(x)=D^c(x)/(1+u_1x)(1+u_2x)\circ\circ\circ(1+u_px)B^c(x), \qquad (2.30)$$

where $D(x)$ is a polynomial of degree at most $\mathrm{Int}\{(N+p)/2\}$ and $D^c(x)$ is a polynomial of degree at most $\mathrm{Int}\{(N+p-1)/2\}$. Thirdly, we observe that from (2.20) and (2.22) we have

$$\begin{aligned} f_{k-1}(x)-\tilde{f}_{k-1}^{(c)}(x)&=x[f_k(x)-\tilde{f}_k^{(c)}(x)]/(1+u_kx)\\ &=x^{p-k+1}[f_p(x)-\tilde{f}_p^{(c)}(x)]/(1+u_kx)\\ &\quad\times(1+u_{k+1}x)\circ\circ\circ(1+u_px),\\ &\quad k=p,\ p-1,\ldots,1. \end{aligned} \qquad (2.31)$$

Now, by the very definition of the pair of Padé approximants $\tilde{f}_p^{(c)}(x)$, we have[2]

$$f_p(x)-\tilde{f}_p(x)\sim O(x^{N-p+1})\quad\text{as } x\to 0+, \qquad (2.32)$$

and

$$f_p(x)-\tilde{f}_p^c(x)=O(x^{N-p})\quad\text{as } x\to 0+. \qquad (2.33)$$

Substituting the latter two relations into (2.31) when $k=1$, we derive

$$f(x)-\tilde{f}(x)=f_0(x)-\tilde{f}_0(x)\sim O(x^{N+1})\quad\text{as } x\to 0+, \qquad (2.34)$$

and

$$f(x)-\tilde{f}^c(x)=f_0(x)-\tilde{f}_0^c(x)\sim O(x^N)\quad\text{as } x\to 0+. \qquad (2.35)$$

The above three observations taken together yield a succinct characterization for the two approximants $\tilde{f}(x)$ and $\tilde{f}^c(x)$. The requirements (2.28) and (2.34) are sufficient on their own to define uniquely the polynomials $B(x)$ and $D(x)$ in (2.29). The existence of the polynomials is assured. Similarly, the requirements (2.28) and (2.33) are sufficient on their own to define uniquely the two polynomials $B^c(x)$ and $D^c(x)$ in (2.30). Hence the approximants $\tilde{f}(x)$ and $\tilde{f}^c(x)$ are determined in a similar way to Padé approximants: The unknown coefficients in the polynomials $B(x)$, $D(x)$, $B^c(x)$, and $D^c(x)$ are fixed by the equations

$$B(x)(1+u_1x)(1+u_2x)\circ\circ\circ(1+u_px)f(x)-D(x)\sim O(x^{N+1})$$

$$\text{as } x\to 0+, \qquad (2.36)$$

and

$$B^c(x)(1+u_1x)(1+u_2x)\circ\circ\circ(1+u_px)f(x)-D^c(x)\sim O(x^N). \qquad (2.37)$$

Once obtained, the approximants impose complementary upper and lower bounds on $f(x)$ for all $0<x<\infty$; that is, we have either (2.24) or (2.25). It can be shown that $\tilde{f}(x)$ imposes an upper or lower bound according as $f_0^{(p)}(-1)^{N-p}$ is negative or positive, respectively, and we note that $\tilde{f}^c(x)$ is precisely the "$f(x)$" which one would construct if N was replaced by $N-1$. However, in practice, one needs only to construct the approximants and then see which one is the larger at some chosen point $x_0>0$. In the next section we prove, among other things, that the bounds imposed by the pair $\tilde{f}^{(c)}(x)$ are best possible on the basis of the given information.

3. BEST POSSIBLE BOUNDS AND INCLUSION REGIONS

In order to establish that the bounds obtained in Sec. 2 are best possible, and in order to secure a best possible inclusion region for $f(z)$ at given z in the cut complex plane, we need the following results.

For any $k\in\{0,1,\ldots,p\}$, let $\Phi_k(u)$ be a cumulative distribution function which has the same properties as $\phi_k(u)$ in Sec. 2 $[\phi_0(u)=\phi(u)]$; that is, $\Phi_k(u)$ is such that (i) it is of bounded variation on $0\leqslant u<\infty$, (ii) $d\Phi_k(u)$ undergoes at most $p-k$ sign changes as u progresses from zero to infinity, the locations of these sign changes being associated with the points $u=u_l$, $l=(k+1),(k+2),\ldots,p$, and (iii) the first $(N+1)-k$ moments are

$$\int_0^\infty u^j\,d\Phi_k(u)=f_j^{(k)}\quad\left(=\int_0^\infty u^j\,d\phi_k(u)\right),$$

$$j=0,1,\ldots,N-k. \qquad (3.1)$$

We note that from (2.12) $\phi_k(u)$ has the property

$$d\phi_k(u_s) \text{ for } s=1,2,\ldots,k. \tag{3.2}$$

Correspondingly, we here impose the stipulation

$$\text{(iv)}\ \ d\Phi_k(u)=0 \ \text{ for } u\in I_1\cup I_2\cup\cdots\cup I_k, \tag{3.3}$$

where I_l is some small open interval such that $u_l\in I_l$, $l=1,2,\ldots,p$.

Theorem II: Let any $\Phi_{k+1}(u)$ be given for some $k\in\{0,1,\ldots,(p-1)\}$, and set

$$F_{k+1}(z)=\int_0^\infty d\Phi_{k+1}(u)/(1+uz). \tag{3.4}$$

Then there exists some $\Phi_k(u)$ such that the function

$$F_k(z)=\int_0^\infty d\Phi_k(u)/(1+uz) \tag{3.5}$$

has the property

$$F_k(z)=[f_0^{(k)}+zF_{k+1}(z)]/(1+u_{k+1}z). \tag{3.6}$$

This theorem is essentially the converse of Theorem I.

Proof: We set

$$\Phi_k(u)=\int_0^u d\Phi_{k+1}(u)/(u_{k+1}-u)+[f_0^{(k)}-\int_0^\infty d\Phi_{k+1}(u)/(u_{k+1}-u)]$$
$$\times\int_0^u \delta(u_{k+1}-u)\,du \tag{3.7}$$

and demonstrate that this function has properties (i), (ii), (iii), and (iv), above, starting from the assumption that $\Phi_{k+1}(u)$ has these same properties when k is replaced by $k+1$. In (3.7) $\delta(\nu)$ denotes the delta function of variable ν.

Since $\Phi_{k+1}(u)$ is of bounded variation on $0\le u<\infty$, and since $d\Phi_{k+1}(u)=0$ for all $u\in I_{k+1}$, it follows that the function

$$\int_0^u d\Phi_{k+1}(u)/(u_{k+1}-u) \tag{3.8}$$

is also of bounded variation on $0\le u<\infty$. In particular, the total variation in the second quantity on the right-hand side of (3.7) is

$$f_0^{(k)}-\int_0^\infty d\Phi_{k+1}(u)/(u_{k+1}-u), \tag{3.9}$$

and this is necessarily finite. Hence $\Phi_k(u)$ is of bounded variation on $0\le u<\infty$, which demonstrates (i). For all $u\ne u_k$ we have

$$d\Phi_k(u)=d\Phi_{k+1}(u)/(u_{k+1}-u). \tag{3.10}$$

Recalling the sign change property of $d\Phi_{k+1}(u)$, it now follows that $\Phi_k(u)$ has property (ii). Further, since

$$d\Phi_{k+1}(u)=0 \ \text{ for all } u\in I_1\cup I_2\cup\cdots\cup I_{k+1}, \tag{3.11}$$

it follows *a fortiori* via (3.10) that $\Phi_k(u)$ has property (iv). Finally, we have

$$\int_0^\infty u^j d\Phi_k(u)=\int_0^\infty u^j d\Phi_{k+1}(u)/(u_{k+1}-u)$$
$$-[\int_0^\infty d\Phi_{k+1}(u)/(u_{k+1}-u)-f_0^{(k)}]u_{k+1}^j$$
$$=f_0^{(k)}u_{k+1}^j-\int_0^\infty[(u_{k+1}^j-u^j)/(u_{k+1}-u)]\,d\Phi_{k+1}(u) \tag{3.12}$$

so that (3.1) is true when $j=0$. For $j=1,2,\ldots,N-k$, we can write (3.12) as

$$\int_0^\infty u^j\, d\Phi_k(u)=f_0^{(k)}u_{k+1}^j-\int_0^\infty(u_{k+1}^{j-1}+u_{k+1}^{j-2}u+\cdots+u^{j-1})d\Phi_{k+1}(u)$$
$$=f_0^{(k)}u_{k+1}^j-(u_{k+1}^{j-1}f_0^{(k+1)}+u_{k+1}^{j-2}f_1^{(k+1)}+\cdots+f_{j-1}^{(k+1)})$$
$$=f_j^{(k)}, \tag{3.13}$$

where we have made use of (2.13) in the last simplifying step. Hence $\Phi_k(u)$ has property (iii). This completes the proof of Theorem II.

Now let any $\Phi_p(z)$ be given, and define

$$F_p(z)=\int_0^\infty d\Phi_p(u)/(1+uz). \tag{3.14}$$

Then it follows by induction through the cases $k=p-1$, $p-2,\ldots,0$ in Theorem II, that there exists a $\Phi_0(u)$ such that the function

$$F(z)=F_0(z)=\int_0^\infty d\Phi_0(u)/(1+uz) \tag{3.15}$$

is related to $F_p(z)$ via the expression.

$$F(z)=\left[\frac{f_0+z\left[\dfrac{f_0^{(1)}+z\left[\dfrac{f_0^{(2)}+z\left[\dfrac{f_0^{(3)}+\cdots+z\left[\dfrac{f_0^{(p-1)}+zF_p(z)}{(1+u_pz)}\right]}{(1+u_4z)}\right]}{(1+u_3z)}\right]}{(1+u_2z)}\right]}{(1+u_1z)}\right]. \tag{3.16}$$

Let us write the relationship between $F_p(z)$ and $F(z)$ expressed in (3.16) as

$$F(z)=T(F_p(z)). \tag{3.17}$$

Then we observe that

$$f(z)=T(f_p(z)), \tag{3.18}$$

and

$$\tilde{f}_p^{(c)}(z)=T(\tilde{f}_p^{(c)}(z)), \tag{3.19}$$

as can be seen from the inverse transformations (2.20) and (2.22). For any z in the cut complex plane, and any complex number $g(z)$, it is easy to see that the complex number $T(g(z))$ is uniquely defined.

We now observe that the function $F(z)$ has all of the properties which were originally ascribed to $f(z)$ in Sec. 1. Hence, given any $F_p(z)$, the resulting $F(z)$ given by (3.17) is indistinguishable from $f(z)$ on the basis of the given information. For given z in the cut complex plane let $\mathcal{F}_p(z)$ denote the set of values $F_p(z)$ obtained as $\Phi_p(u)$ ranges through all possibilities, the open $I_1, I_2, \ldots, I_p$ being allowed to become arbitrarily small; and let $\overline{\mathcal{F}}_p(z)$ denote the closure of $\mathcal{F}_p(z)$. Then since the value of $F(z)$ is continuously related to the value of $F_p(z)$, we have that *$f(z)$ may lie arbitrarily close to $T(g(z))$ for any given $g(z) \in \overline{\mathcal{F}}_p(z)$, on the basis of the given information.*

Next, we make use of the following theorem.

Theorem III: $f_p(z) \in \overline{\mathcal{F}}_p(z)$ for given z in the cut complex plane.

Proof: Let any $f_p(z)$ and $\epsilon > 0$ be given. Then

$$f_p(z) = \int_0^\infty d\phi_p(u)/(1+uz), \tag{3.20}$$

where $\phi_p(u)$ has the properties (i), (ii), and (iii), given above for $\Phi_p(u)$, and satisfies (3.2) with $k=p$. Let J_l denote a small open interval such that $u_l \in J_l$ for $l = 1, 2, \ldots, p$, and such that $\phi_p(u)$ does not have a jump associated with the end points of any of the intervals. Define a distribution function $\Phi_p(u)$ on $0 \leqslant u < \infty$ by

$$d\tilde{\Phi}_p(u) = \begin{cases} d\phi_p(u) & u \notin J_1 \cup J_2 \cup \cdots \cup J_p, \\ 0 & u \in J_1 \cup J_2 \cup \cdots \cup J_p. \end{cases} \tag{3.21}$$

Then

$$f_p(z) = \int_0^\infty d\tilde{\Phi}_p(u)/(1+uz) + \sum_{l=1}^{p} f_p^l(z), \tag{3.22}$$

where

$$f_p^l(z) = \int_{J_l} d\phi_p(u)/(1+uz). \tag{3.23}$$

If $\phi_p(u)$ attains only finitely many different values on J_l, then $f_p^l(z)$ can be expressed in the form

$$f_p^l(z) = \sum_{m=1}^{M_l} \frac{v_m^l}{(1+E_m^l z)}, \tag{3.24}$$

where M_l is a finite integer, $v_m^l > 0$, $E_m^l \in J_l$, and $E_m^l \neq u_l$ for $m = 1, 2, \ldots, M_l$. The latter statement is true because of (3.2) with $k=p$.

If $\phi_p(u)$ attains infinitely many different values on J_l, then $f_p^l(z)$ is a strict series of Stieltjes with finite radius of convergence. But then, from the theory of Padé approximants to such functions[2] we know that we can find an integer Q_l such that for all $n > Q_l$ we have

$$\left| f_p^l(z) - [n-1/n]_{f_p^l(z)} \right| < \epsilon/p. \tag{3.25}$$

Because the poles of $[n-1/n]_{f_p^l(z)}$ are all located in J_l, and because of the strict interlacing property of the pole locations of successive approximants,[2] we can in particular choose $n = M_l > Q_l$ such that none of the poles of $[M_l - 1/M_l]_{f_p^l(z)}$ coincide with the point $z = -1/u_l$. We can also insist that Q_l be large enough so that

$$f_p^l(z) - [M_l - 1/M_l]_{f_p^l(z)} = O(x^{N-p+1}). \tag{3.26}$$

Hence we can write

$$[M_l - 1/M_l] = \sum_{m=1}^{M_l} \frac{v_m^l}{(1+E_m^l z)}, \tag{3.27}$$

where the v_m^l's and E_m^l's have precisely the properties given below (3.24) and where we have again invoked the theory of Padé approximants for series of Stieltjes.

It now follows that, regardless of whether or not $\phi_p(u)$ has infinitely many different values on J_l, each l, we have

$$\left| f_p(z) - \tilde{\tilde{f}}_p(z) \right| < \epsilon, \tag{3.28}$$

where

$$\tilde{\tilde{f}}_p(z) = \int_0^\infty \frac{d\tilde{\Phi}_p(u)}{(1+uz)} + \sum_{l=1}^{p} \left(\sum_{m=1}^{M_l} \frac{v_m^l}{(1+E_m^l z)} \right), \tag{3.29}$$

the v_m^l's and E_m^l's having the properties given below (3.24) and where

$$f_p(z) - \tilde{\tilde{f}}_p(z) = O(z^{N-p+1}). \tag{3.30}$$

But (3.29) can be rewritten

$$\tilde{\tilde{f}}_p(z) = \int_0^\infty d\tilde{\tilde{\Phi}}_p(u)/(1+uz), \tag{3.31}$$

where

$$d\tilde{\tilde{\Phi}}_p(u) = \begin{cases} d\tilde{\Phi}_p(u), & u \notin J_1 \cup J_2 \cup \cdots \cup J_p \\ \sum_{l=1}^{p} \left(\sum_{m=1}^{M_l} v_m^l \, \delta(u - E_m^l) \right), & u \in J_1 \cup J_2 \cup \cdots \cup J_p. \end{cases} \tag{3.32}$$

In particular, $\tilde{\tilde{\Phi}}_p(u)$ clearly has properties (i), (ii), and (iii). Moreover, since none of the points E_m^l coincide with any of the points u_l, $l = 1, 2, \ldots, p$, it follows that there exist open intervals $\tilde{\tilde{I}}_l$ such that $u_l \in \tilde{\tilde{I}}$, $l = 1, 2, \ldots, p$, and such that

$$d\tilde{\tilde{\Phi}}_p(u) = 0, \quad u \in \tilde{\tilde{I}}_1 \cup \tilde{\tilde{I}}_2 \cup \cdots \cup \tilde{\tilde{I}}_p. \tag{3.33}$$

Hence $\tilde{\tilde{\Phi}}_p(u)$ has property (iv). Hence $\tilde{\tilde{f}}_p(z) \in \mathcal{F}_p(z)$. Hence, since $\epsilon > 0$ can be made arbitrarily small in (3.28), it follows that $f_p(z) \in \overline{\mathcal{F}}_p(z)$, which completes the proof.

By putting together the above theorem, the italicized remark immediately preceding it, and (3.18), it follows that the best possible inclusion region which can be imposed upon $f(z)$ on the basis of the given information is precisely the image under T of $\overline{\mathcal{F}}_p(z)$, for any given z in the cut complex plane.

Now let $\overline{\not{f}}_p(z)$ denote the set of values $f_p(z)$ obtained as $\phi_p(u)$ ranges through all possibilities, and let $\overline{\not{f}}_p(z)$ denote its closure, for given z in the cut complex plane.

Corollary to Theorem III: $\overline{\not{f}}_p(z) \equiv \overline{\mathcal{F}}_p(z)$, for given z in the cut complex plane.

Proof: Given any $F_p(z) \in \mathcal{F}_p(z)$, we have at once that $F_p(z) \in \not{f}_p(z)$ since any $\Phi_p(u)$ is a possible $\phi_p(u)$. Hence $\mathcal{F}_p(z) \subset \not{f}_p(z)$, and so $\overline{\mathcal{F}}_p(z) \subset \overline{\not{f}}_p(z)$. But by Theorem III, any $f_p(z) \in \overline{\not{f}}_p(z)$ also belongs to $\overline{\mathcal{F}}_p(z)$. Hence $\not{f}_p(z) \subset \overline{\mathcal{F}}_p(z)$, and so $\overline{\not{f}}_p(z) \subset \overline{\mathcal{F}}_p(z)$, which completes the proof.

We now have that the best possible inclusion region which can be imposed upon $f(z)$ on the basis of the given information is precisely the image under T of $\not{f}_p(z)$, for given z in the cut complex plane.

But if we now allow

$$d\phi_p(u_s) \neq 0, \quad s = 1, 2, \ldots, p, \tag{3.34}$$

which clearly makes no difference to the set $\overline{\not{f}}_p(z)$, then we see that $\not{f}_p(z)$ is precisely the lens-shaped inclusion region, described by Baker,[5,7] which corresponds to the information that $f(z)$ is a series of Stieltjes (or else the negative of one) which behaves like

$$f_p(z) \sim f_0^{(p)} - zf_1^{(p)} + \cdots + (-1)^{N-p} z^{N-p} f_{N-p}^{(p)} + \begin{array}{l}\text{terms of higher order with unknown}\\ \text{or divergent coefficients}\end{array} \qquad (3.35)$$

as z approaches zero through points in the cut complex plane. Hence $\bar{\not{f}}_p(z)$ can in principle be determined exactly. A corresponding best possible inclusion region for $f(z)$ can then be obtained by applying T to $\bar{\not{f}}_p(z)$. The resulting inclusion region has a lens-shaped character.

In particular, it follows from the work of Baker[7] that for $0 < x < \infty$, $\bar{\not{f}}_p(x)$ contains the points $\tilde{f}_p^{(c)}(x)$. Hence, using (3.19), it follows that the bounds of Sec. 2 are best possible on the basis of the given information.

4. BEST POSSIBLE BOUNDS WHEN THE POINTS $\{u_l\}_{l=1}^{p}$ ARE UNKNOWN

Here we describe how best possible bounds on $f(x)$ [or an inclusion region for $f(z)$] may be imposed when $f(z)$ is given as in Sec. 1, but the locations of a set of points $\{u_l\}_{l=1}^{p}$ associated with the at most p sign changes of $d\phi(u)$ are unknown. Having described the method in principle, we demonstrate its feasibility with a simple example.

Whatever the locations of the associated points $\{u_l\}_{l=1}^{p}$ are, we may assume that

$$0+ \leq u_1 \leq u_2 \leq \cdots \leq u_p \leq \infty. \qquad (4.1)$$

If we now follow the sequence of transformations in Sec. 2, with the slightly weaker assumption (4.1) replacing (1.4), we still find that the resulting $f_p(z)$ must be either a series of Stieltjes or the negative of one. Let

$$D^{(p)}(m,n) = \begin{vmatrix} f_m^{(p)} & f_{m+1}^{(p)} & \cdots & f_{m+n}^{(p)} \\ f_{m+1}^{(p)} & f_{m+2}^{(p)} & \cdots & f_{m+n+1}^{(p)} \\ \vdots & \vdots & & \vdots \\ f_{m+n}^{(p)} & f_{m+n+1}^{(p)} & \cdots & f_{m+2n}^{(p)} \end{vmatrix}, \qquad (4.2)$$

for $m, n = 0, 1, 2, \cdots$. Then $f_p(z)$ is indistinguishable from a series of Stieltjes on the basis of the given information if and only if[2]

$$D^{(p)}(m,n) \geq 0 \quad \text{for all } (m,n) \in S, \qquad (4.3)$$

where S is the set of all pairs (m,n) such that the corresponding determinant $D^{(p)}(m,n)$ only involves moments taken from the set $\{f_j^{(p)}\}_{j=0}^{N-p}$. If we now substitute for the $f_j^{(p)}$'s from (2.13) into (4.3), we obtain a set of necessary and sufficient conditions to be satisfied by $\{u_l\}_{l=1}^{p}$ if $f_p(z)$ is to be indistinguishable from a series of Stieltjes on the basis of the given information. Similarly, $f_p(z)$ is indistinguishable from the negative of a series of Stieltjes on the basis of the given information if and only if

$$(-1)^{n+1} D^{(p)}(m,n) \geq 0 \quad \text{for all } (m,n) \in S. \qquad (4.4)$$

Let U^+ denote the set of choices for $\{u_l\}_{l=1}^{p}$ such that (4.1) and (4.3) are satisfied, and let U^- denote the set of choices for $\{u_l\}_{l=1}^{p}$ such that (4.1) and (4.4) are satisfied. Assume for the sake of brevity that $N-p$ is odd. Then if $f_p(z)$ is to be a series of Stieltjes, it follows from the above and from the theory of Secs. 2 and 3, that the best possible bounds which can be imposed on $f(x)$ for given $0 < x < \infty$ are

$$\inf_{\{u_l\}_{l=1}^{p} \in U^+} \tilde{f}^c(x) \leq f(x) \leq \sup_{\{u_l\}_{l=1}^{p} \in U^+} \tilde{f}(x). \qquad (4.5)$$

Similarly, if $f_p(z)$ is to be the negative of a series of Stieltjes, then the best possible bounds which can be imposed on $f(x)$ for $0 < x < \infty$ are

$$\inf_{\{u_l\}_{l=1}^{p} \in U^-} \tilde{f}(x) \leq f(x) \leq \sup_{\{u_l\}_{l=1}^{p} \in U^-} \tilde{\bar{f}}(x). \qquad (4.6)$$

Since we do not know *a priori* whether $f_p(z)$ is a series of Stieltjes or the negative of one, the maximum of the upper bounds in (4.5) and (4.6) is the best possible upper bound which can be imposed on $f(x)$ for given $0 < x < \infty$. Similarly, the best possible lower bound is the minimum of the lower bounds in (4.5) and (4.6). Likewise, best possible upper and lower bounds can be obtained when $N-p$ is even.

If one is given, for example, the additional information that $\phi(u)$ is monotone nondecreasing on $0 \leq u \leq u_1$, then, of course we know that $f_p(z)$ is necessarily a series of Stieltjes. Then in case $N-p$ is even we have at once that the best possible bounds for given $0 < x < \infty$ are (4.5). Again, it may turn out that one of the U^+ or U^- is empty, in which case the best bounds will derive from a search over U^- or U^+, respectively.

More generally a best possible inclusion region can be imposed upon $f(z)$ for given z in the cut complex plane. This inclusion region will be the union of all inclusion regions obtained as the set $\{u_l\}_{l=1}^{p}$ ranges through all possibilities in both U^+ and U^-.

We demonstrate the feasibility of the above method with a very simple example. Suppose we are given that

$$f(z) = \int_0^\infty d\phi(u)/(1+uz), \qquad (4.7)$$

where $d\phi(u)$ has at most *one* sign change on $0 \leq u < \infty$, and that

$$f_0 = 2, \quad f_1 = 2, \quad f_2 = 0. \qquad (4.8)$$

Then what are the best possible upper and lower bounds which can be imposed on $f(x)$ for given $0 < x < \infty$? Suppose that the sign change of $d\phi(u)$ is associated with the point u_1 such that

$$0 \leq u_1 \leq \infty. \qquad (4.9)$$

Then we have

$$f_0^{(1)} = 2(u_1 - 1), \quad f_1^{(1)} = 2u_1. \qquad (4.10)$$

Consequently, the set U^- is empty and

$$U^+ = \{u_1 \mid 1 \leq u_1 \leq \infty\} \qquad (4.11)$$

whence the best possible bounds which can be imposed on $f(x)$ for given $0 < x < \infty$ are

$$\inf_{u_1 \in U^+} \frac{4(u_1-1) + (4u_1^2 - 4u_1 + 4)x}{(1+u_1x)(2(u_1-1) + 2u_1x)} \leq f(x) \leq \sup_{u_1 \in U^+} \frac{2 + 2(u_1-1)x}{(1+u_1x)}. \qquad (4.12)$$

In particular, at $x=1$, the best possible bounds which can be imposed on the function on the basis of the given information are

$$\tfrac{8}{9} \leq f(1) \leq 2. \tag{4.13}$$

We note that on the basis of the given information $f(z)$ *could* have been the function

$$f(z)=1/(1+z)+2/(1+2z)-1/(1+3z). \tag{4.14}$$

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[1] In a previous paper [M. F. Barnsley, J. Math. Phys. 16, 918 (1975)] a related problem was considered. Namely, given that $f(z)$ has the form (1.1), and given that the $[N-1/N]$ and $[N/N]$ Padé approximants to $f(z)$ can be constructed, what is the nature of correction terms to the Padé approximants such that bounds on $f(x)$, $0<x<\infty$, are obtained?

[2] G. A. Baker Jr., Advan. Theor. Phys. 1, 1 (1965).

[3] G. A. Baker Jr., in *The Padé Approximant in Theoretical Physics*, edited by G. A. Baker and J. L. Gammel (Academic, New York and London, 1970).

[4] *Padé Approximants and Their Applications*, edited by P. R. Graves-Morris (Academic, New York and London, 1973).

[5] G. A. Baker Jr., *Essentials of Padé Approximants* (Academic, New York, San Francisco, and London, 1975).

[6] M. F. Barnsley, J. Math. Phys. 14, 299 (1973).

[7] G. A. Baker Jr., J. Math. Phys. 10, 814 (1968).

On path integral solutions of the Schrödinger equation, without limiting procedure*

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Techniques for integration in function spaces which are not necessarily vector spaces are presented in the light of DeWitt-Morette's recent redefinition of path integrals, which does not involve the usual limiting process, and is therefore free from the ambiguities inherent in this approach. General translated Gaussian measures defined by their Fourier transforms are introduced on various path spaces and used to derive generalized moments formulas, and what is essentially the Feynman–Kac formula for the expression of solutions of the Schrödinger equation as functional integrals.

I. INTRODUCTION

Recently, C. DeWitt-Morette[1,2] introduced a new approach to the Feynman path integral formulation of quantum mechanics. Its strength lies in the fact that it does not rest on the usual limiting process, which involves the division of the time interval into a very large number of very small subintervals. By a generalization of the work of the Bourbaki group[3] on Gaussian promeasures for integration on infinite-dimensional Hausdorff locally convex topological vector spaces, what plays the role of a measure[4] in path space is defined by its Fourier transform, which is a simple closed form expression, usually the exponential of a quadratic form defined on the dual of the path space for physical applications. This enables one to reduce many path integrals of interest in physics to ordinary integrals by use of linear mappings into $\mathbb{R}^n$. For example, one has the formula,[2]

$$\int_{\mathcal{C}} F(\langle\mu_1,q\rangle, \cdots, \langle\mu_n,q\rangle)\, dw_C(q)$$
$$= (2\pi)^{-n/2}\, (\det \mathcal{W})^{-1/2} \int_{\mathbb{R}^n} F(u_1, \ldots, u_n)$$
$$\times \exp[-(1/2)(\mathcal{W}^{-1})^{ij} u_i u_j]\, du_1 \cdots du_n, \qquad (1)$$

where

(a) $\mathcal{C}$ is a vector space of paths (functions) $q: t \mapsto q(t)$ on the time interval $T \equiv [t_a, t_b]$.

(b) the μ_i's are bounded measures on T, i.e., elements of the dual $\mathcal{M}$ of $\mathcal{C}$. $\langle\mu,q\rangle \equiv \int_T q(t)\, d\mu(t)$ if μ is induced by a function f, $[d\mu(t) \equiv f(t)\, dt]$, and $\langle\mu,q\rangle \equiv q(t)$ if $\mu = \delta_t$, the "delta function" measure at t.

(c) w_C is the Gaussian measure on $\mathcal{C}$, of covariance the kernel $C(t,t')$, whose Fourier transform (defined on $\mathcal{M}$) is

$$\mathcal{F}w_C(\mu) = \exp[-\tfrac{1}{2} \int_T \int_T C(t,t')\, d\mu(t)\, d\mu(t')]$$
$$\equiv \exp[-\tfrac{1}{2} W_C(\mu)]. \qquad (2)$$

(d) $$\mathcal{W}_{ij} \equiv W_C(\mu_i, \mu_j) \equiv \int_T \int_T C(t,t')\, d\mu_i(t)\, d\mu_j(t'). \qquad (3)$$

(e) The Einstein summation convention over repeated indices is used throughout this paper.

C is real for the Wiener integral and imaginary for the Feynman integral.

For simplicity, the same symbol is used for the bilinear form $W_C(\mu, \nu)$ on $\mathcal{M}$ and its corresponding quadratic form $W_C(\mu)$. In other words, $W_C(\mu,\mu) \equiv W_C(\mu)$.

If the μ's are δ's, then,

$$W_C(\delta_t, \delta_{t'}) \equiv C(t,t'), \quad W_C(\mu, \delta_t) \equiv \int_T C(t,t')\, d\mu(t'). \qquad (4)$$

In this paper, we further exploit this formalism and, among other general formulas, present a proof of what is essentially the well-known Feynman–Kac formula for the expression of solutions of the Schrödinger equation as functional integrals.

II. INTEGRATION OVER SUBSETS OF VECTOR SPACES

An example of a vector space of paths on the time interval T is

$$\mathcal{C}_- \equiv \{q \text{ on } T \,|\, q(t_a) = 0,\ q(t_b) \text{ undetermined}\}. \qquad (5)$$

Let w_C be a Gaussian measure on $\mathcal{C}_-$. If we now fix the second endpoint $[q(t_b) = q_b$, where q_b is constant], the resulting subspace $\mathcal{C}_{0b}$ is no longer a closed vector space. Can we still define a measure on it and apply the theory? The answer is yes, and the procedure is described below.

More generally, suppose we want to integrate a functional $\varphi[q]$, only over those paths in $\mathcal{C}_-$ satisfying $\langle\mu_i, q\rangle = b_i$ for n given measures μ_i and real numbers b_i. Define $\mathcal{C}_{n\mu} \subset \mathcal{C}_-$ as follows:

$$\mathcal{C}_{n\mu} \equiv \{q \in \mathcal{C}_- \,|\, \langle\mu_i, q\rangle = b_i, \quad i = 1, \ldots, n, \quad \mu_i \in \mathcal{M}, \quad b_i \in \mathbb{R}\}. \qquad (6)$$

The integration over $\mathcal{C}_{n\mu}$ can be reduced to an integration over $\mathcal{C}_-$ if in the integrand we insert *characteristic functions* χ which vanish when $q \notin \mathcal{C}_{n\mu}$. Indeed, if we define

$$\chi(x) = \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{if } x \neq 0 \end{cases},$$

then,

$$\int_{\mathcal{C}_{n\mu}} \varphi[q]\, dw^{n\mu}(q) = [N(b_i, \mu_i)]^{-1} \int_{\mathcal{C}_-} \varphi[q]\, dw_C(q)$$
$$\times \chi(\langle\mu_1, q\rangle - b_1) \cdots \chi(\langle\mu_n, q\rangle - b_n), \qquad (7)$$

where:

(a) $w^{n\mu}$ is a Gaussian measure on $\mathcal{C}_{n\mu}$, induced by w_C (this is proved below for $n=1$). Its covariance is, by definition,

$$C_{n\mu}(t,t') \equiv \int_{\mathcal{C}_{n\mu}} [q(t)-\overline{q}(t)][q(t')-\overline{q}(t')]\,dw^{n\mu}(q), \tag{8}$$

where the integration is performed as indicated above. The average path $\overline{q}(t)$ is defined by

$$\overline{q}(t) \equiv \int_{\mathcal{C}_{n\mu}} q(t)\,dw^{n\mu}(q). \tag{9}$$

(b) N is a *normalization factor*, insuring that

$$\int_{\mathcal{C}_{n\mu}} dw^{n\mu}(q) = 1.$$

It is obvious that

$$N(b_i,\mu_i) = \int_{\mathcal{C}_-} \chi(\langle\mu_1,q\rangle - b_1)\cdots\chi(\langle\mu_n,q\rangle - b_n)\,dw_C(q). \tag{10}$$

To evaluate N, we map $\mathcal{C}_-$ into $\mathbb{R}^n$ by $q \mapsto u_i \equiv \langle\mu_i,q\rangle$, and use (1). The characteristic function maps into a δ function and we get

$$N = \frac{(\det\mathcal{W})^{-1/2}}{(\sqrt{2\pi})^n}\int_{\mathbb{R}^n} \delta(u_1-b_1)\cdots\delta(u_n-b_n)$$
$$\times \exp(-\tfrac{1}{2}\mathcal{W}^{-1}_{ij}u_iu_j)\,du_1\cdots du_n$$
$$= \frac{(\det\mathcal{W})^{-1/2}}{(\sqrt{2\pi})^n}\exp(-\tfrac{1}{2}\mathcal{W}^{-1}_{ij}b_ib_j), \tag{11}$$

where

$$\mathcal{W} \equiv \begin{pmatrix} W_C(\mu_1,\mu_n) & \cdots & W_C(\mu_1,\mu_n) \\ \vdots & & \vdots \\ W_C(\mu_n,\mu_1) & \cdots & W_C(\mu_n,\mu_n) \end{pmatrix}. \tag{12}$$

Note: If the b_i's are allowed to vary, then if we integrate over them, after having performed the functional integral of $\varphi[q]$ over $\mathcal{C}_{n\mu}$, we should recover the functional integral of $\varphi[q]$ over all of $\mathcal{C}_-$. From (7) it is clear that

$$\int_{\mathbb{R}^n} db_1\cdots db_n N(b_i,\mu_i)\int_{\mathcal{C}_{n\mu}}\varphi[q]\,dw^{n\mu}(q)$$
$$= \int_{\mathcal{C}_-}\varphi[q]\,dw_C(q). \tag{13}$$

This provides an easy verification of certain formulas, and is, in fact, a generalization of the method of "reservation of variables" (see Appendix A).

Theorem:

$$I(\varphi) \equiv \int_{\mathcal{C}_{n\mu}}\varphi(\langle\nu,q\rangle)\,dw^{n\mu}(q)$$
$$= \exp\Bigl(\tfrac{1}{2}\sum_{i,j=1}^{n} b_ib_j(\mathcal{W}^{-1}_{ij} - \overline{\mathcal{W}}^{-1}_{ij})\Bigr)\Bigl(\frac{\det\mathcal{W}}{2\pi\det\overline{\mathcal{W}}}\Bigr)^{1/2}$$
$$\times\int_{\mathbb{R}}\varphi(u)\exp\Bigl(\frac{-\det\mathcal{W}}{2\det\overline{\mathcal{W}}}u^2 - u\sum_{i=1}^{n} b_i\overline{\mathcal{W}}^{-1}_{i,n+1}\Bigr)du, \tag{14}$$

where $\mathcal{W}$ is defined in (12) and

$$\overline{\mathcal{W}} \equiv \begin{pmatrix} W_C(\mu_1\mu_1) & \cdots & W_C(\mu_1,\mu_n) & W_C(\mu_1,\nu) \\ \vdots & & \vdots & \vdots \\ W_C(\mu_n,\mu_1) & \cdots & W_C(\mu_n,\mu_n) & W_C(\mu_n,\nu) \\ W_C(\nu,\mu_1) & \cdots & W_C(\nu,\mu_n) & W_C(\nu,\nu) \end{pmatrix}. \tag{15}$$

Proof: (7) gives

$$I(\varphi) = N^{-1}\int_{\mathcal{C}_-}\chi(\langle\mu_1,q\rangle - b_1)\cdots\chi(\langle\mu_n,q\rangle - b_n)$$
$$\times\varphi(\langle\nu,q\rangle)\,dw_C(q). \tag{16}$$

If we map $\mathcal{C}_-$ into $\mathbb{R}^{n+1}$ by $q\mapsto\{u_i = \langle\mu_i,q\rangle$ for $i=1,2,\ldots,n;\ u_{n+1} = \langle\nu,q\rangle\}$, we get

$$I(\varphi) = N^{-1}\int_{\mathbb{R}^{n+1}}\frac{(\det\overline{\mathcal{W}})^{-1/2}}{(\sqrt{2\pi})^{n+1}}\delta(u_1-b_1)\cdots\delta(u_n-b_n)$$
$$\times\varphi(u_{n+1})\,du_1\cdots du_{n+1}\exp\Bigl[-\tfrac{1}{2}\sum_{i,j=1}^{n}\overline{\mathcal{W}}^{-1}_{ij}u_iu_j$$
$$-\tfrac{1}{2}\overline{\mathcal{W}}^{-1}_{n+1,n+1}u_{n+1}^2 - \sum_{i=1}^{n}\overline{\mathcal{W}}^{-1}_{i,n+1}u_iu_{n+1}\Bigr]$$
$$= \Bigl(\frac{\det\mathcal{W}}{2\pi\det\overline{\mathcal{W}}}\Bigr)^{1/2}\exp\Bigl[\sum_{i,j=1}^{n}\tfrac{1}{2}b_ib_j(\mathcal{W}^{-1}_{ij} - \overline{\mathcal{W}}^{-1}_{ij})\Bigr]$$
$$\times\int_{\mathbb{R}}\varphi(u_{n+1})\exp\Bigl[-\tfrac{1}{2}\overline{\mathcal{W}}^{-1}_{n+1,n+1}u_{n+1}^2$$
$$-u_{n+1}\sum_{i=1}^{n}\overline{\mathcal{W}}^{-1}_{i,n+1}b_i\Bigr]du_{n+1} \tag{17}$$

The result follows from the fact that

$$\overline{\mathcal{W}}^{-1}_{n+1,n+1} = \det\mathcal{W}/\det\overline{\mathcal{W}}. \tag{18}$$

Corollary:

$$I_{mn} \equiv \int_{\mathcal{C}_{n\mu}}\langle\nu,q\rangle^m\,dw^{n\mu}(q)$$
$$= \Bigl(\frac{-\det\overline{\mathcal{W}}}{2\det\mathcal{W}}\Bigr)^{m/2} H_m\Bigl(-\sum_{i=1}^{n} b_i\overline{\mathcal{W}}^{-1}_{n+1,i}\Bigl(\frac{-\det\overline{\mathcal{W}}}{2\det\mathcal{W}}\Bigr)^{1/2}\Bigr)$$
$$\times\exp\Bigl[\sum_{i,j=1}^{n}\frac{1}{2}b_ib_j(\mathcal{W}^{-1}_{ij} - \overline{\mathcal{W}}^{-1}_{ij})$$
$$+\frac{1}{2}\frac{\det\overline{\mathcal{W}}}{\det\mathcal{W}}\Bigl(\sum_{i=1}^{n} b_i\overline{\mathcal{W}}^{-1}_{n+1,i}\Bigr)^2\Bigr], \tag{19}$$

where H_m is the Hermite polynomial of order m.

Proof: Use the formula,

$$\int_{\mathbb{R}} x^m\exp(ax^2+bx)\,dx = (-1)^m\,2^{-m}a^{-m/2}H_m(b/2\sqrt{a})$$
$$\times(-\pi/a)^{1/2}\exp(-b^2/4a), \quad [\mathrm{Re}(a)\leqslant 0], \tag{20}$$

derived from $\int_{\mathbb{R}}\exp(ax^2+bx)\,dx = (-\pi/a)^{1/2}\exp(-b^2/4a)$, by differentiating with respect to b m times.

Application: Average and covariance in $\mathcal{C}_\mu$ $(n = 1)$

(a) *Average in* $\mathcal{C}_{n\mu}$: For $m=1$ $[H_1(x) = 2x]$, and $\nu = \delta_t$ we get,

$$\bar{q}(t) \equiv \int_{\mathcal{C}_{n\mu}} q(t)\, dw^{n\mu}(q) = \frac{-\det\bar{\mathcal{W}}}{\det\mathcal{W}} \left(\sum_{i=1}^{n} b_i \bar{\mathcal{W}}^{-1}_{n+1,i}\right)$$

$$\times \exp\left[\tfrac{1}{2} \sum_{i,j=1}^{n} b_i b_j (\mathcal{W}^{-1}_{ij} - \bar{\mathcal{W}}^{-1}_{ij})\right.$$

$$\left. + \frac{1}{2} \frac{\det\bar{\mathcal{W}}}{\det\mathcal{W}} \left(\sum_{i=1}^{n} b_i\, \bar{\mathcal{W}}^{-1}_{n+1,i}\right)^2 \right]. \tag{21}$$

If $b_i = 0$, $\bar{q}(t) = 0$, the average path is zero in all subspaces of $\mathcal{C}_-$ of finite codimension. For $n = 1$,

$$\mathcal{C}_\mu \equiv \{q \in \mathcal{C}_- | \langle \mu, q\rangle = b\}, \quad \mathcal{W} = [W_C(\mu)],$$

$$\bar{\mathcal{W}} = \begin{pmatrix} W_C(\mu) & W_C(\mu,\nu) \\ W_C(\mu,\nu) & W_C(\nu) \end{pmatrix},$$

$$\bar{\mathcal{W}}^{-1} = \frac{1}{\det\bar{\mathcal{W}}} \begin{pmatrix} W_C(\nu) & -W_C(\mu,\nu) \\ -W_C(\mu,\nu) & W_C(\mu) \end{pmatrix}, \tag{22}$$

and the integral is simply

$$I_{m1} \equiv \int_{\mathcal{C}_\mu} \langle \nu, q\rangle^m dw^\mu(q) = \left(\frac{-\det\bar{\mathcal{W}}}{2W_C(\mu)}\right)^{m/2}$$

$$\times H_m\left(bW_C(\mu,\nu)\left(\frac{-1}{2W_C(\mu)\det\bar{\mathcal{W}}}\right)^{1/2}\right) \tag{23}$$

where $\det\bar{\mathcal{W}} = W_C(\mu)\, W_C(\nu) - W_C^2(\mu,\nu)$.

It is interesting to check this formula by use of (13), i.e., verify that

$$\int_{\mathbf{R}} db\, \frac{\exp[-b^2/2W_C(\mu)]}{\sqrt{2\pi W_C(\mu)}} \int_{\mathcal{C}_\mu} \langle \nu, q\rangle^m dw^\mu(q)$$

$$= \int_{\mathcal{C}_-} \langle \nu, q\rangle^m dw_C(q). \tag{24}$$

The right-hand side is equal to 0 if m is odd, and equal to $(2n)![W_C(\nu)]^n/2^n n!$, if $m = 2n$ [use (1) for the proof]. To evaluate the left hand side, use the following result (Abramowitz and Stegun,[5] p. 786, with $t = au$):

$$\int_{\mathbf{R}} \exp(-a^2u^2) H_n(axu)\, du$$

$$= \begin{cases} \dfrac{\sqrt{\pi}}{a} \dfrac{(2m)!}{m!} (x^2 - 1)^m, & \text{for } n = 2m, \\ 0, & \text{for } n \text{ odd.} \end{cases} \tag{25}$$

It turns out to be equal to the right-hand side.

(b) Average in $\mathcal{C}_\mu$: Let $m = 1$, $\nu = \delta_t$ in the above to get

$$\bar{q}(t) = bW_C\ (\mu, \delta_t)/W_C(\mu). \tag{26}$$

(c) Average in $\mathcal{C}_{\delta_{t_0}}$ *(the space of paths in* $\mathcal{C}_-$*, with specified value at* $t = t_0$*)*: If $\mu = \delta_{t_0}$, $b = q_0$, then

$$\bar{q}(t) = q_0\, C(t, t_0)/C(t_0, t_0). \tag{27}$$

General condition on $C(t, t')$

Since we would like for the "average path" to be in the space, i.e., $\bar{q} \in \mathcal{C}_-$, we have the requirement $\bar{q}(t_a) = 0$. Since t_0 in (27) is arbitrary, this forces the important general condition

$$C(t_a, t') = 0, \tag{28}$$

for all legitimate covariances in $\mathcal{C}_-$.

(d) *Average in* $\mathcal{C}_{0b}$: Let $t_0 = t_b$. Then $\mathcal{C}_{\delta_{t_0}} \equiv \mathcal{C}_{0b}$ and

$$\bar{q}(t) = q_b\, C(t_b, t)/C(t_b, t_b). \tag{29}$$

(e) *Covariance in* $\mathcal{C}_\mu$:

$$C_\mu(t, t') = C(t, t') - \frac{W_C(\mu, \delta_t)\, W_C(\mu, \delta_{t'})}{W_C(\mu)}, \tag{30}$$

satisfies the same boundary conditions as the paths, i.e.,

$$C_\mu(t_a, t') = 0; \quad \langle \mu_t, C_\mu\rangle \equiv \int_T C_\mu(t, t')\, d\mu(t) = 0. \tag{31}$$

Proof: We will need the following:

(i) (23) with $m = 2$ [*note*: $H_2(x) = 4x^2 - 2$]:

$$\int_{\mathcal{C}_\mu} \langle \nu, q\rangle^2\, dw^\mu(q) = \frac{\det\bar{\mathcal{W}}}{W_C(\mu)} \left(\frac{b^2 W_C^2(\mu,\nu)}{W_C(\mu)\det\bar{\mathcal{W}}} + 1\right)$$

$$= W_C(\nu) - \frac{W_C^2(\mu,\nu)}{W_C(\mu)} + \frac{b^2 W_C^2(\mu,\nu)}{W_C^2(\mu)}. \tag{32}$$

(ii) $W_C(\delta_t + \delta_{t'}) = W_C(\delta_t) + W_C(\delta_{t'}) + 2W_C(\delta_t, \delta_{t'})$. (33)

(iii) $W_C^2(\mu, \delta_t + \delta_{t'}) = [W_C(\mu, \delta_t) + W_C(\mu, \delta_{t'})]^2$

$$= W_C^2(\mu, \delta_t) + W_C^2(\mu, \delta_{t'}) + 2W_C(\mu, \delta_t)\, W_C(\mu, \delta_{t'}). \tag{34}$$

We have

$$C_\mu(t, t')$$

$$\equiv \int_{\mathcal{C}_\mu} \langle \delta_t, q - \bar{q}\rangle \langle \delta_{t'}, q - \bar{q}\rangle\, dw^\mu(q)$$

$$= \int_{\mathcal{C}_\mu} \langle \delta_t, q\rangle \langle \delta_{t'}, q\rangle\, dw^\mu(q) - \bar{q}(t)\, \bar{q}(t')$$

$$= \tfrac{1}{2} \int_{\mathcal{C}_\mu} [\langle \delta_t + \delta_{t'}, q\rangle^2 - \langle \delta_t, q\rangle^2 - \langle \delta_{t'}, q\rangle^2]\, dw^\mu(q)$$

$$- b^2 W_C(\mu, \delta_t)\, W_C(\mu, \delta_{t'})/W_C^2(\mu)$$

$$= \tfrac{1}{2} \left[W_C(\delta_t + \delta_{t'}) - \frac{W_C^2(\mu, \delta_t + \delta_{t'})}{W_C(\mu)} + \frac{b^2 W_C^2(\mu, \delta_t + \delta_{t'})}{W_C^2(\mu)}\right.$$

$$- W_C(\delta_t) + \frac{W_C^2(\mu, \delta_t)}{W_C(\mu)} - \frac{b^2 W_C^2(\mu, \delta_t)}{W_C^2(\mu)} - W_C(\delta_{t'})$$

$$\left. + \frac{W_C^2(\mu, \delta_{t'})}{W_C(\mu)} - \frac{b^2 W_C^2(\mu, \delta_{t'})}{W_C^2(\mu)}\right] - \frac{b^2 W_C(\mu, \delta_t)\, W_C(\mu, \delta_{t'})}{W_C^2(\mu)}$$

$$= W_C(\delta_t, \delta_{t'}) - \frac{W_C(\mu, \delta_t)\, W_C(\mu, \delta_{t'})}{W_C(\mu)}. \tag{35}$$

QED

Also,

$$\int_T C_\mu(t,t')\,d\mu(t)$$

$$= \int_T C(t,t')\,d\mu(t) - \frac{W_C(\mu,\delta_{t'})}{W_C(\mu)} \int_T \left[\int_T C(t,s)\,d\mu(s)\right]$$

$$\times d\mu(t) \equiv 0, \tag{36}$$

by definition of W_C. **QED**

It is most remarkable that the covariance C_μ does not depend on b. However, the *measure* w^μ does depend on b through the average path [see (g) below].

(f) *Covariance in* $\mathcal{C}_{0b}$: We have:

$$C_{0b}(t,t') = C(t,t') - \frac{C(t_b,t)\,C(t_b,t')}{C(t_b,t_b)}. \tag{37}$$

C_{0b} vanishes at both endpoints; $C_{0b}(t_a,t') = C_{0b}(t_b,t') = 0$. Since it is independent of q_b, it is also the covariance in $\mathcal{C}_{00}$, the space of paths vanishing at both endpoints. Often, if $C(t,t')$ is a Green function of some operator, then so is $C_{0b}(t,t')$. This is not true in general for $C_\mu(t,t')$.

(g) *Fourier transform of* w^μ*—Translated Gaussians*:

The Fourier transform of the measure w^μ is

$$(\mathcal{F}w^\mu)(\nu) = \exp[-i\langle\nu,\bar{q}\rangle - \tfrac{1}{2}W_{C_\mu}(\nu)]. \tag{38}$$

Because of the factor involving the average path $\bar{q}$, w^μ is said to be a *translated* Gaussian measure.

Proof: A remarkable property of the Fourier transform of a measure w on $\mathcal{C}$ is that it can be written

$$(\mathcal{F}w)(\mu) = \int_{\mathcal{C}} \exp(-i\langle\mu,q\rangle)\,dw(q), \tag{39}$$

which is readily recognized as a generalization to infinite-dimensional spaces of the familiar formula for the Fourier transform of a measure in $\mathbb{R}^n$ [try, for example, (1) with $n=1$, $F(x) = \exp(-ix)$]. This follows from the definition of the Fourier transform in infinite-dimensional space as found in Bourbaki.[3]

From this and (14), we get

$$(\mathcal{F}w^{n\mu})(\nu) = \int_{\mathcal{C}_{n\mu}} \exp[-i\langle\nu,q\rangle]\,dw^{n\mu}(q)$$

$$= \exp\left\{\frac{1}{2}\left[\sum_{i,j=1}^{n} b_i b_j(\mathcal{W}^{-1}_{ij} - \overline{\mathcal{W}}^{-1}_{ij})\right.\right.$$

$$\left.\left. + \frac{\det\overline{\mathcal{W}}}{\det\mathcal{W}}\left(i + \sum_{i=1}^{n} b_i\overline{\mathcal{W}}^{-1}_{i,n+1}\right)^2\right]\right\}. \tag{40}$$

For $n=1$, we use (22), which yields

$$\sum_{i,j=1}^{n} b_i b_j(\mathcal{W}^{-1}_{ij} - \overline{\mathcal{W}}^{-1}_{ij})$$

$$= b^2\left(\frac{1}{W_C(\mu)} - \frac{W_C(\nu)}{\det\overline{\mathcal{W}}}\right) = \frac{-b^2W_C^2(\mu,\nu)}{W_C(\mu)\det\overline{\mathcal{W}}}, \tag{41}$$

$$\sum_{i=1}^{n} b_i\overline{\mathcal{W}}^{-1}_{i,n+1} = b\overline{\mathcal{W}}^{-1}_{12} = -\frac{b\,W_C(\mu,\nu)}{\det\overline{\mathcal{W}}}. \tag{42}$$

The Fourier transform is,

$$(\mathcal{F}w^\mu)(\nu) = \exp\left\{\frac{1}{2}\left[\frac{-b^2W_C^2(\mu,\nu)}{W_C(\mu)\det\overline{\mathcal{W}}} + \frac{\det\overline{\mathcal{W}}}{W_C(\mu)}\right.\right.$$

$$\left.\left.\times\left(i - b\,\frac{W_C(\mu,\nu)}{\det\overline{\mathcal{W}}}\right)^2\right]\right\}$$

$$= \exp\left[-\frac{1}{2}W_C(\nu) + \frac{1}{2}\,\frac{W_C^2(\mu,\nu)}{W_C(\mu)} - \frac{ibW_C(\mu,\nu)}{W_C(\mu)}\right]. \tag{43}$$

From the expression for the average path given in (26), we have,

$$\langle\nu,\bar{q}\rangle = \frac{b}{W_C(\mu)}\int_T d\nu(t)\int_T C(t,t')\,d\mu(t')$$

$$= bW_C(\mu,\nu)/W_C(\mu). \tag{44}$$

From the expression of the covariance C_μ given in (30), we have,

$$W_{C_\mu}(\nu) = \int_{T^2} C(t,t') - \frac{W_C(\mu,\delta_t)\,W_C(\mu,\delta_{t'})}{W_C(\mu)}\;d\nu(t)\,d\nu(t')$$

$$= W_C(\nu) - \frac{W_C^2(\mu,\nu)}{W_C(\mu)} = \frac{\det\overline{\mathcal{W}}}{\det\mathcal{W}}. \tag{45}$$

Substituting (44) and (45) into (43) yields the desired result.

(h) *Indefinite functional integrals*: We can define an "indefinite" integral of a functional $F[q]$ with respect to a Gaussian measure w_C on some space of paths $\mathcal{C}$, by functionally integrating over all paths q such that $q(t) \geqslant q_0(t)$ for all t, where q_0 is a fixed path in $\mathcal{C}$. One way to define it would be

$$G[q_0] \equiv \int_{t_a}^{t_b} dt \int_{\mathcal{C}} F[q]\,Y(\langle\delta_t,q\rangle - q_0(t))\,dw_C(q), \tag{46}$$

where $Y(t)$ is the Heaviside step function, equal to 0 for $t<0$ and to 1 otherwise. For example, if $\mathcal{C} = \mathcal{C}_-$, $F[q]=1$, then,

$$G[q_0] = \int_{t_a}^{t_b} \frac{dt}{\sqrt{2\pi iC(t,t)}}\int_{q_0(t)}^{\infty} \exp[iu^2/2C(t,t)]\,du, \tag{47}$$

where (1) has been used $[u = q(t)]$. Finally,

$$G[q_0] = \frac{1}{2}\int_{t_a}^{t_b} dt\;\mathrm{erfc}\left(\frac{q_0(t)}{\sqrt{2iC(t,t)}}\right). \tag{48}$$

Remark: In general, we see that a measure w on an infinite-dimensional Hausdorff locally convex topological vector space E, enables one to integrate over a subset A of E, even if this subset is *not* a vector space, by

$$\int_A F[q]\,dw|_A(q) \equiv \int_E \chi_A[q]\,F[q]\,dw(q)$$

$$\times\left(\int_E \chi_A[q]\,dw(q)\right)^{-1}, \tag{49}$$

where $\chi_A[q]=1$ if $q\in A$ and is 0 otherwise. This is how we integrated over $\mathcal{C}_{n\mu}$. As we will see in the next section, we can define a measure on "translated subsets," such as $\mathcal{C}_{ab}$. The latter results from adding a nonzero constant to each path in a subset of $\mathcal{C}_-$ (and hence, is not itself a subset of $\mathcal{C}_-$).

We now slightly change our notation; since we are primarily concerned with the Feynman integral, the covariances will be purely imaginary. However, we will now write them as "C" rather than "iC" so as to explicitly display the "i" in the formulas.

III. INTEGRATION OVER THE SPACE OF PATHS WITH BOTH ENDPOINTS FIXED

Consider first the case of a free particle of mass M. The covariance on $\mathcal{C}_-$ that will give us the correct physical results is,[3,1]

$$C_-(t,t') = (\hbar/M)\ \inf(t-t_a,\ t'-t_a), \tag{50}$$

where "inf" denotes the smaller of the two arguments.

From it, one can use (37) to build the covariance on $\mathcal{C}_{0b}$. The result is,

$$C_{0b}(t,t') = \frac{\hbar(t-t_a)(t_b-t')}{M(t_b-t_a)}\,Y(t'-t)\ + t \sim t', \tag{51}$$

where $F(t,t') + t\sim t' \equiv F(t,t') + F(t',t)$. Both C_- and C_{0b} are Green functions of the small disturbance operator for the free particle, $-d^2/dt^2$. For simplicity, the subscript "C_-" will be denoted by "$-$". Thus, $w_{C_-} \equiv w_-$. The average path in $\mathcal{C}_{0b}$, as given by (29), is $q_b(t-t_a)/(t_b-t_a)$. It is interesting to note that $\lim_{t_b\to\infty} C_{0b}(t,t') = C_-(t,t')$.

Now let us define integration over the space of paths where both endpoints are fixed and not necessarily zero. The path space

$$\mathcal{C}_{ab} \equiv \{q \text{ on } T\,|\,q(t_a)=q_a,\quad q(t_b)=q_b\}$$

is obtained by translation by a constant amount q_a from the path space

$$\mathcal{C}_{0,b-a} = \{q \text{ on } T\,|\,q(t_a)=0,\quad q(t_b)=q_b-q_a\},$$

on which we have the Gaussian measure $w_{0,b-a}$, induced by w_- on $\mathcal{C}_-$ (see Sec. II). One can naturally define a measure w_{ab} on $\mathcal{C}_{ab}$ by,

$$\int_{\mathcal{C}_{ab}} F[q]\,dw_{ab}(q) \equiv \int_{\mathcal{C}_{0,b-a}} F[x+q_a]\,dw_{0,b-a}(x). \tag{52}$$

This is possible since the system is translationally invariant (the associated Lagrangian, $L=\frac{1}{2}M\dot{q}^2$, does not depend explicitly on position). As for the Fourier transform of w_{ab}, since [see (38)]

$$(\mathcal{F}w_{0,b-a})(\mu) = \exp[-i\langle\mu,\bar{q}_{0,b-a}\rangle - (i/2)\,W_{ab}(\mu)] \tag{53}$$

(where $\bar{q}_{0,b-a}(t) = (q_b-q_a)(t-t_a)/(t_b-t_a)$ is the average path in $\mathcal{C}_{0,b-a}$), then, by setting $F[q]=\exp(-i\langle\mu,q\rangle)$ in (52), we get,

$$(\mathcal{F}w_{ab})(\mu) = \exp[-i\langle\mu,\bar{q}\rangle - (i/2)\,W_{ab}(\mu)], \tag{54}$$

where

$$\bar{q}(t) = \bar{q}_{0,b-a}(t) + q_a = \frac{q_a(t_b-t)+q_b(t-t_a)}{t_b-t_a} \tag{55}$$

is the average path in $\mathcal{C}_{ab}$ with respect to w_{ab}. By use of the characteristic function, we can rewrite (52) as,

$$\int_{\mathcal{C}_{ab}} F[q]\,dw_{ab}(q) = \int_{\mathcal{C}_-} \chi[\langle\delta_{t_b},y\rangle - (q_b-q_a)]\ \times F[y+q_a]\,\frac{dw_-(y)}{K_0(B,A)}, \tag{56}$$

where

$$K_0(B,A) \equiv \int_{\mathcal{C}_-} \chi[\langle\delta_{t_b},y\rangle - (q_b-q_a)]\,dw_-(y) \tag{57}$$

is the free particle propagator,[6] easily obtained by use of (1) with $n=1$, $F=\delta$:

$$K_0(B,A) = \sqrt{M/2\pi i\hbar(t_b-t_a)}\ \ Y(t_b-t_a)\ \times\exp[iM(q_b-q_a)^2/2\hbar(t_b-t_a)]. \tag{58}$$

Let us mention that in the case where the covariances are real, the functional integral over $\mathcal{C}_{ab}$ with covariance (51) is equivalent to what is called the "conditional Wiener integral" in the literature [the "regular" Wiener integral being over $\mathcal{C}_-$ with covariance (50)].

This reduction to an integral over $\mathcal{C}_-$ may, in some instances, make calculations easier.[7] However, it is quite possible to integrate directly over $\mathcal{C}_{ab}$, since w_{ab} is a well-defined translated Gaussian. This is illustrated below.

Cylindrical functionals on $\mathcal{C}_{ab}$

We seek an analog of (1) for translated Gaussian measures. It is found that, for an *arbitrary* Gaussian measure w_{ab} on $\mathcal{C}_{ab}$, with covariance $C(t,t')$,

$$\int_{\mathcal{C}_{ab}} F(\langle\mu_1,q\rangle,\ldots,\langle\mu_n,q\rangle)\,dw_{ab}(q) = \frac{(\det\mathcal{W})^{-1/2}}{(\sqrt{2\pi i}\,)^n}\int_{\mathbb{R}^n} F(u_1,\ldots,u_n) \times\exp[(i/2)(\mathcal{W}^{-1})^{ij}(u_i-a_i)(u_j-a_j)]\,du_1\cdots du_n, \tag{59}$$

where

$$\text{(a) } (\mathcal{F}w_{ab})(\mu) \equiv \exp[-i\langle\mu,\bar{q}\rangle - (i/2)W(\mu)],$$

$$\text{(b) } a_i \equiv \langle\mu_i,\bar{q}\rangle, \tag{60}$$

$$\text{(c) } \mathcal{W}_{ij} \equiv W(\mu_i,\mu_j) = \int_T\int_T C(t,t')\,d\mu_i(t)\,d\mu_j(t').$$

Proof: The proof parallels that of (1), as found in the second reference,[2] the only difference being, that now the average path is nonzero. We treat the general case first. Let w be a measure on a path space $\mathcal{C}$, and consider the linear continuous mapping P_n:

$$P_n: \mathcal{C} \to \mathbb{R}^n \text{ by } q \mapsto u, \text{ where } u_i \equiv \langle\mu_i,q\rangle.$$

Under this mapping, we have,

$$\int_{\mathcal{C}} F(\langle\mu_1,q\rangle,\ldots,\langle\mu_n,q\rangle)\,dw(q) = \int_{\mathbb{R}^n} F(u_1,\ldots,u_n)\,(dw)_{P_n}(u), \tag{61}$$

where w_{P_n} is the image of w under P_n. This image is a measure in $\mathbb{R}^n$. By theorem,[3] $(\mathcal{F}w)_{P_n}(\xi) = \mathcal{F}w[\tilde{P}_n(\xi)]$, where $\xi\in\mathbb{R}^n$ and $\tilde{P}_n$, is the transpose mapping from $\mathbb{R}^n$ to $\mathcal{M}$. We have,

$$\langle\tilde{P}_n(\xi),\,q\rangle \equiv \langle\xi,\ P_n(q)\rangle = \langle\xi,u\rangle = \xi^i u_i = \xi^i\langle\mu_i,q\rangle = \langle\xi^i\mu_i,q\rangle, \tag{62}$$

and hence $\tilde{P}_n(\xi) = \xi^i\mu_i$. Therefore,

$$(dw)_{P_n}(u) = \mathcal{F}_\xi^{-1}[\mathcal{F}w(\xi^i\mu_i)]$$
$$= \frac{du_1 \cdots du_n}{(2\pi)^n}\int_{\mathbf{R}^n} \exp(i\xi^j u_j)$$
$$\times(\mathcal{F}w)(\xi^i\mu_i)\,d\xi^1 \cdots d\xi^n, \qquad (63)$$

when the integral exists. This can be substituted in (61) in order to convert the path integral over $\mathcal{C}$ to an ordinary integral over $\mathbb{R}^n$. Since w is usually defined by its Fourier transform $\mathcal{F}w(\mu)$, which is given explicitly, the right-hand side of (63) can, at least in principle, be written in closed form.

Such is the case when $\mathcal{C} = \mathcal{C}_{ab}$ and $w = w_{ab}$, as defined in (60a). By use of the well-known formula[8]

$$\int_{\mathbf{R}^n} \varphi(b^i u_i)\exp(-\tfrac{1}{2}A^{ij}u_i u_j)\,du_1 \cdots du_n$$
$$= \frac{(\sqrt{2\pi})^{n-1}}{|c|\sqrt{\det A}}\int_{\mathbf{R}} \varphi(u)\exp\left(-\frac{u^2}{2c^2}\right)du, \qquad (64)$$

where $c^2 \equiv b^i b^j (A^{-1})_{ij}$, we obtain the result, for $\varphi(u) = \exp(iu)$. We emphasize that w_{ab} in (59) is an arbitrary Gaussian measure on $\mathcal{C}_{ab}$, which means that we have complete freedom in choosing the covariance C (which must vanish at t_a and t_b) and the average path $\bar{q}$ [which must be in $\mathcal{C}_{ab}$, i.e., such that $\bar{q}(t_a) = q_a$, $\bar{q}(t_b) = q_b$].

Generalized moments formula

It is often useful to know the various moments (e.g., of position at different times) with respect to a translated Gaussian measure. It is found that

$$\int_{\mathcal{C}_{ab}} \langle\mu_1, q\rangle \cdots \langle\mu_n, q\rangle\, dw_{ab}(q)$$
$$= i^n \mathcal{H}_n(-ia_1/2, \ldots, -ia_n/2), \qquad (65)$$

where w_{ab}, a_i and $\mathcal{W}_{ij}$ are defined in (60), $\mathcal{H}_n$ is the generalized Hermite polynomial[9] of order n, and matrix $C_{ij} = (i/2)\mathcal{W}_{ij}$, defined by:

$$\mathcal{H}_n(C_{i1}x^i, \ldots, C_{in}x^i) \equiv (-1)^n \exp(C_{ij}x^i x^j)$$
$$\times \frac{\partial^n}{\partial x^1 \cdots \partial x^n}\exp(-C_{ij}x^i x^j), \qquad (66)$$

which is a generalization to n dimensions of the Rodriguez formula for ordinary Hermite polynomials. One can show[9] that $\mathcal{H}_n$ indeed depends on $x^1, \ldots, x^n$, only through the combinations $C_{ij}x^i = X_j$. Their explicit expression is found to be,[9]

$$\mathcal{H}_n(X_i) \equiv \mathcal{H}_n(X_1, \ldots, X_n)$$
$$= \sum_{k=0}^{\leq n} (-1)^{k/2}\, 2^{n-(k/2)} {\sum}' X_{i_1}X_{i_2} \cdots X_{i_{n-k}}$$
$$\times C_{i_{n-k+1}i_{n-k+2}}\ C_{i_{n-1}i_n}, \qquad (67)$$

where the first summation symbol denotes the sum over all *even* k from $k=0$ to the largest even number smaller than or equal to n; and the second summation denotes the sum over all different combinations of different indices i_i, where $\{i_1, i_2, \ldots, i_n\} = \{1, 2, \ldots, n\}$; that is, all i_i are different, and if $f(i_1, i_2) = f(i_2, i_1)$, we count it only once in the sum. There are $(2m-1)(2m-3)\cdots 5.3$ different terms in such a sum for $n = 2m$. The first few are:

$$\mathcal{H}_1(X_1) = 2X_1,$$
$$\mathcal{H}_2(X_1, X_2) = 4X_1X_2 - 2C_{12}, \qquad (68)$$
$$\mathcal{H}_3(X_1, X_2, X_3) = 8X_1X_2X_3 - 4C_{12}X_3 - 4C_{23}X_1 - 4C_{31}X_2.$$

For example, the first few moments are:

$$\int_{\mathcal{C}_{ab}} \langle\mu, q\rangle\, dw_{ab}(q) = \langle\mu, \bar{q}\rangle, \qquad (69a)$$

$$\int_{\mathcal{C}_{ab}} \langle\mu, q\rangle\langle\nu, q\rangle\, dw_{ab}(q) = \langle\mu, \bar{q}\rangle\langle\nu, \bar{q}\rangle + iW(\mu, \nu), \qquad (69b)$$

$$\int_{\mathcal{C}_{ab}} \langle\mu, q\rangle\langle\nu, q\rangle\langle\sigma, q\rangle\, dw_{ab}(q)$$
$$= \langle\mu, \bar{q}\rangle\langle\nu, \bar{q}\rangle\langle\sigma, \bar{q}\rangle + i\langle\sigma, \bar{q}\rangle W(\mu, \nu)$$
$$+ i\langle\nu, \bar{q}\rangle W(\sigma, \mu) + i\langle\mu, \bar{q}\rangle W(\nu, \sigma), \qquad (69c)$$

$$\int_{\mathcal{C}_{ab}} \langle\mu_1, q\rangle\langle\mu_2, q\rangle\langle\mu_3, q\rangle\langle\mu_4, q\rangle\, dw_{ab}(q)$$
$$= a_1a_2a_3a_4 + i\mathcal{W}_{14}a_2a_3 + i\mathcal{W}_{24}a_1a_3 + i\mathcal{W}_{34}a_1a_2$$
$$+ i\mathcal{W}_{12}a_3a_4 + i\mathcal{W}_{23}a_1a_4 + i\mathcal{W}_{31}a_2a_4 - \mathcal{W}_{12}\mathcal{W}_{34}$$
$$- \mathcal{W}_{23}\mathcal{W}_{14} - \mathcal{W}_{31}\mathcal{W}_{24}.$$

Proof:

$$J \equiv \int_{\mathcal{C}_{ab}} \exp(i\lambda^i\langle\mu_i, q\rangle)\, dw_{ab}(q) = (\mathcal{F}w_{ab})(-\lambda^i\mu_i)$$
$$= \exp[-i\langle -\lambda^i\mu_i, \bar{q}\rangle - (i/2)W(-\lambda^i\mu_i)]$$
$$= \exp[i\lambda^i a_i - (i/2)\lambda^i\lambda^j\mathcal{W}_{ij}].$$

$$\left.\frac{\partial^n J}{\partial\lambda^1 \cdots \partial\lambda^n}\right|_{\lambda=0} = i^n\int_{\mathcal{C}_{ab}} \langle\mu_1, q\rangle \cdots \langle\mu_n, q\rangle\, dw_{ab}(q)$$
$$= \left(\frac{\partial^n}{\partial\lambda^1 \cdots \partial\lambda^n}\exp\left[i\lambda^i a_i - \frac{i}{2}\lambda^i\lambda^j\mathcal{W}_{ij}\right]\right)_{\lambda=0}$$
$$= \exp\left(\frac{i}{2}(\mathcal{W}^{-1})^{ij}a_i a_j\right)$$
$$\times\left[\frac{\partial^n}{\partial\lambda^1 \cdots \partial\lambda^n}\exp\left(-\frac{i}{2}[\lambda^i - (\mathcal{W}^{-1})^{il}a_l]\right.\right.$$
$$\left.\left.\times[\lambda^j - (\mathcal{W}^{-1})^{js}a_s]\mathcal{W}^{ij}\right)\right]_{\lambda=0}$$

$$\equiv (-1)^n\exp[\tfrac{1}{2}i(\mathcal{W}^{-1})^{ij}a_i a_j]$$
$$\times\Big\{\exp\{-\tfrac{1}{2}i[\lambda^i - (\mathcal{W}^{-1})^{il}a_l]$$
$$\times[\lambda^j - (\mathcal{W}^{-1})^{js}a_s]\mathcal{W}_{ij}\}$$
$$\times\mathcal{H}_n\Big[\sum_j \tfrac{1}{2}i\,\mathcal{W}_{ij}(\lambda^j - (\mathcal{W}^{-1})^{jl}a_l)\Big]\Big\}_{\lambda=0}, \qquad (70)$$

where we have used definition (66). The result readily follows.

If $\mu_i=\delta_{t_i}$, then $\langle\mu_i,q\rangle=q(t_i)$, $a_i=\overline{q}(t_i)$, $\mathcal{W}_{ij}=C(t_i,t_j)$, and we get the ordinary moments formula for position at different times (yielding, for example, the various Feynman diagrams in quantum electrodynamics). On the vector spaces $\mathcal{C}=\mathcal{C}_-$ or $\mathcal{C}=\mathcal{C}_{00}$, the average path is zero, and, by using the fact that

$$\mathcal{H}_n(0,\ldots,0) = \begin{cases} 0, & \text{if } n \text{ is odd,} \\ (-1)^{n/2}\,2^{n/2}\sum{}' \, C_{i_1i_2}C_{i_3i_4}\cdots C_{i_{n-1}i_n}, & \text{if } n \text{ is even,} \end{cases} \tag{71}$$

we get the well-known formula,

$$\int_{\mathcal{C}} q(t_1)q(t_2)\cdots q(t_n)\,dw_C(q) = \begin{cases} 0, & \text{if } n \text{ is odd,} \\ \sum{}' \, C(t_{i_1},t_{i_2})\cdots C(t_{i_{2m-1}},t_{i_{2m}}), & \text{if } n=2m. \end{cases} \tag{72}$$

IV. THE SCHRÖDINGER EQUATION AND PATH INTEGRALS IN THE NEW FORMULATION: THE FEYNMAN-KAC FORMULA

Our aim in this section is to show that the propagator *in path integral form*, using the new definition, satisfies the Schrödinger equation. This proof will involve no series expansions, questionable limiting procedures, or handwaving arguments about a "midpoint rule."[10]

Consider a particle of mass M in one-dimension in a velocity-independent potential $V(q,t)$, such that,

$$\int_{\mathbb{R}} V(q,t)\exp(aq^2)\,dq<\infty, \text{ for } \operatorname{Re}(a)\leqslant 0. \tag{73}$$

The measure w_{ab} absorbs the free particle (kinetic energy) part of the action functional $S[q]\equiv\int_T[(M/2)\dot{q}^2(t) - V(q(t),t)]\,dt$. We are therefore led to write the following theorem (in complete form, including relevant definitions):

Theorem: The propagator $K_V(B,A)$, or probability amplitude that the particle at (q_a,t_a) will arrive at (q_b,t_b), can be written in path-integral form as follows:

$$K_V(B,A)=K_0(B,A)\int_{\mathcal{C}_{ab}}\exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b}V(q(t),t)\,dt\right] \times dw_{ab}(q), \tag{74}$$

where K_0 is the free particle propagator (58) and w_{ab} is the induced (translated) Gaussian measure on $\mathcal{C}_{ab}$ defined as follows:

$$\mathcal{F}w_{ab}(\mu) \equiv \exp\left(-i\int_{t_a}^{t_b}\overline{q}(t)\,d\mu(t)-(i/2)\int_{t_a}^{t_b}\int_{t_a}^{t_b}C_{ab}(t,t') \times d\mu(t)\,d\mu(t')\right), \tag{75}$$

where the average path $\overline{q}$ on $\mathcal{C}_{ab}$ (with respect to w_{ab}) is

$$\overline{q}(t)\equiv\int_{\mathcal{C}_{ab}}q(t)\,dw_{ab}(q)=\frac{q_b(t-t_a)+q_a(t_b-t)}{t_b-t_a}, \tag{76}$$

and the kernel $C_{ab}(t,t')$ is the Green function of the small disturbance operator for the free particle (i.e., $-Md^2/dt^2$) vanishing at $t=t_a$ and $t=t_b$:

$$C_{ab}(t,t')=\frac{\hbar(t-t_a)(t_b-t')}{M(t_b-t_a)}\,Y(t'-t)+t\sim t'. \tag{77}$$

K_V can be shown, from its path integral form (74), to satisfy the Schrödinger equation at B, i.e.,

$$-i\hbar\frac{\partial K_V}{\partial t_b}+V(q_b,t_b)K_V-\frac{\hbar^2}{2M}\frac{\partial^2K_V}{\partial q_b^2} =-i\hbar\,\delta(q_b-q_a)\,\delta(t_b-t_a), \tag{78}$$

and its complex conjugate at A. (74) is the well-known *Feynman–Kac formula*[11] in disguise. The proof presented here through Fourier transforms is very different from Kac's proof, where he used the usual time-slicing definition of Wiener measure. Our proof does not seem to require his assumption that the potential is bounded.[12]

Proof: The normalization factor in (74) is equal to the free particle propagator because when $V=0$, we want $K_V=K_0$, and also so that when $t_b\to t_a$, $K_V\to\delta(q_b-q_a)$; a condition that K_0 satisfies. We now show directly that (74) satisfies the Schrödinger equation (78).

Let us write $K_V=K_0J$, where J is the path integral. As we take derivatives of (74), we must remember: (a) that the measure w_{ab} itself depends on t_b and q_b through $\overline{q}$ and C_{ab}, (b) that we consider only the *explicit* dependence on t_b and q_b. For example, we have $(\partial/\partial t_b)\int_{t_a}^{t_b}V[q(t),t]\,dt=V(q_b,t_b)$, even though there is an implicit dependence on t_b in $V[q(t),t]$, since all paths q are such that $q(t_b)=q_b$.

For Lagrangians of the type considered here, ordinary differentiation commutes with path integration in our expressions. Thus, we have,

$$\begin{aligned} -i\hbar\frac{\partial K_V}{\partial t_b}&+V(q_b,t_b)K_V-\frac{\hbar^2}{2M}\frac{\partial^2K_V}{\partial q_b^2} \\ &=-i\hbar\frac{\partial K_0}{\partial t_b}J-i\hbar K_0\left[-\frac{i}{\hbar}V(q_b,t_b)\right]J+V(q_b,t_b) \\ &\quad\times K_0J-i\hbar K_0\int_{\mathcal{C}_{ab}}\exp\left(-\frac{i}{\hbar}\int_{t_a}^{t_b}V[q(t),t]\,dt\right) \\ &\quad\times\frac{\partial}{\partial t_b}dw_{ab}(q)-\frac{\hbar^2}{2M}\frac{\partial^2K_0}{\partial q_b^2}J-\frac{\hbar^2}{M}\frac{\partial K_0}{\partial q_b} \\ &\quad\times\int_{\mathcal{C}_{ab}}\exp\left(-\frac{i}{\hbar}\int_{t_a}^{t_b}V[q(t),t]\,dt\right)\frac{\partial}{\partial q_b}dw_{ab}(q) \\ &\quad-\frac{\hbar^2}{2M}K_0\times\int_{\mathcal{C}_{ab}}\exp\left(-\frac{i}{\hbar}\int_{t_a}^{t_b}V[q(t),t]\,dt\right) \\ &\quad\times\frac{\partial^2}{\partial q_b^2}dw_{ab}(q). \end{aligned} \tag{79}$$

The terms proportional to $V(q_b, t_b)$ on the right hand side cancel, and since K_0 is itself a Green function, we have:

$$\left(-i\hbar\frac{\partial K_0}{\partial t_b}-\frac{\hbar^2}{2M}\frac{\partial^2 K_0}{\partial q_b^2}\right)J=-i\hbar\,\delta(q_b-q_a)\,\delta(t_b-t_a)J$$
$$=-i\hbar\delta(q_b-q_a)\,\delta(t_b-t_a). \tag{80}$$

Further, from (58) we have

$$\frac{\partial K_0}{\partial q_b}=\frac{iM(q_b-q_a)}{\hbar(t_b-t_a)}.$$

Therefore, what remains to be shown is that

$$\int_{C_{ab}}\exp\left(-\frac{i}{\hbar}\int_{t_a}^{t_b}V[q(t),t]\,dt\right)$$
$$\times\left(-i\hbar\frac{\partial}{\partial t_b}-i\hbar\,\frac{q_b-q_a}{t_b-t_a}\frac{\partial}{\partial q_b}-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial q_b^2}\right)dw_{ab}(q)=0. \tag{81}$$

Before we can proceed, we must define what we mean by an operator $\mathbf{D}_{q_b}$ or $\mathbf{D}_{t_b}$ acting on the measure w_{ab}. It is natural to do this through Fourier transforms. We have the property

$$\mathcal{F}w_{ab}(\mu)=\int_{C_{ab}}dw_{ab}(q)\exp\{-i\int_{t_a}^{t_b}q(t)\,d\mu(t)\}. \tag{82}$$

This enables us to define $\mathbf{D}_{q_b}w_{ab}$ by

$$[\mathcal{F}(\mathbf{D}_{q_b}w_{ab})](\mu)\equiv\mathbf{D}_{q_b}(\mathcal{F}w_{ab})(\mu), \tag{83}$$

since the integrand in (82) does not contain q_b explicitly (it is assumed that $\mathbf{D}_{q_b}$ is linear). This integrand does contain t_b, however, so for $\mathbf{D}_{t_b}$ we must look further. We will need the following derivatives:

$$\frac{\partial}{\partial t_b}C_{ab}(t,t')$$
$$=\frac{\hbar(t-t_a)(t'-t_a)}{M(t_b-t_a)^2}\quad\text{(note that it is } C^\infty \text{ in } t \text{ and } t')$$

$$\frac{\partial}{\partial q_b}C_{ab}(t,t')=0,\quad\frac{\partial}{\partial t_b}\bar{q}(t)=\frac{-(t-t_a)(q_b-q_a)}{(t_b-t_a)^2},$$

$$\frac{\partial}{\partial q_b}\bar{q}(t)=\frac{t-t_a}{t_b-t_a},$$

$$\frac{\partial}{\partial t_b}\int_{t_a}^{t_b}\int_{t_a}^{t_b}C_{ab}(t,t')\,d\mu(t)\,d\mu(t')$$
$$=\int_{t_a}^{t_b}\int_{t_a}^{t_b}\left[\frac{\partial}{\partial t_b}C_{ab}(t,t')\right]d\mu(t)\,d\mu(t'). \tag{84}$$

In the last formula, we used Leibnitz's formula for differentiating an integral, i.e.,

$$\frac{d}{dx}\int_{\alpha(x)}^{\beta(x)}f(x,t)\,dt$$
$$=\int_{\alpha(x)}^{\beta(x)}\frac{\partial f(x,t)}{\partial x}\,dt+f[x,\beta(x)]\,\beta'(x)-f[x,\alpha(x)]\,\alpha'(x). \tag{85}$$

In our case, the integrated terms vanish on account of $C_{ab}(t_b,t)=0$, $C_{ab}(t',t_b)=0$.

We now want to define $\partial w_{ab}/\partial t_b$. The easiest is to differentiate the two equivalent expressions of the Fourier transform of w_{ab} with respect to t_b. Using (82) and (75), we have:

$$0=\frac{\partial}{\partial t_b}\left[\int_{C_{ab}}\exp\left(-i\int_{t_a}^{t_b}q(t)\,d\mu(t)\right)dw_{ab}(q)\right.$$
$$-\exp\left(-i\int_{t_a}^{t_b}\bar{q}(t)\,d\mu(t)\right.$$
$$\left.\left.-\frac{i}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b}C_{ab}(t,t')\,d\mu(t)\,d\mu(t')\right)\right]$$
$$=\left[\int_{C_{ab}}\exp(-i\langle\mu,q\rangle)\frac{\partial}{\partial t_b}dw_{ab}(q)\right] \tag{86}$$
$$-i\left[\frac{\partial}{\partial t_b}\int_{t_a}^{t_b}q(t)\,d\mu(t)\right]\mathcal{F}w_{ab}(\mu)$$
$$-\left(-i\frac{\partial}{\partial t_b}\int_{t_a}^{t_b}\bar{q}(t)\,d\mu(t)-\frac{i}{2}\int_{t_a}^{t_b}\int_{t_a}^{t_b}\frac{\partial C_{ab}(t,t')}{\partial t_b}\right.$$
$$\left.\times d\mu(t)\,d\mu(t')\right)\mathcal{F}w_{ab}(\mu).$$

Note that we have taken $(\partial/\partial t_b)\int_{t_a}^{t_b}q(t)\,d\mu(t)$, outside the path integral because it does *not* depend on the path q. It depends only on the intergrand at t_b, and $q(t_b)=q_b$ is constant. Using formulas (84), we have

$$\frac{\partial}{\partial t_b}\int_{t_a}^{t_b}[q(t)-\bar{q}(t)]\,d\mu(t)=-\int_{t_a}^{t_b}\frac{\partial\bar{q}(t)}{\partial t_b}\,d\mu(t)$$
$$=\frac{(q_b-q_a)}{(t_b-t_a)^2}\int_{t_a}^{t_b}(t-t_a)\,d\mu(t). \tag{87}$$

Finally,

$$\mathcal{F}\left(\frac{\partial}{\partial t_b}w_{ab}\right)(\mu)=\left(\frac{i(q_b-q_a)}{(t_b-t_a)^2}S(\mu)-\frac{i\hbar}{2M(t_b-t_a)^2}S^2(\mu)\right)$$
$$\times\mathcal{F}w_{ab}(\mu), \tag{88}$$

where

$$S(\mu)\equiv\int_{t_a}^{t_b}(t-t_a)\,d\mu(t). \tag{89}$$

In the general case, if μ is a regular measure $[d\mu(t)=\mathring{\mu}(t)\,dt$, where $\mathring{\mu}$ is an integrable function$]$, then,

$$\mathcal{F}\left(\frac{\partial w_{ab}}{\partial t_b}\right)(\mu)=\left(\frac{\partial}{\partial t_b}-iq_b\mathring{\mu}(t_b)\right)\mathcal{F}w_{ab}(\mu). \tag{90}$$

Taking (83) and (88) into account, we conclude, with the aid of formulas (84), that

$$\mathcal{F}\left[\left(-i\hbar\frac{\partial}{\partial t_b}-\frac{i\hbar(q_b-q_a)}{t-t_a}\frac{\partial}{\partial q_b}-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial q_b^2}\right)w_{ab}\right](\mu)=0. \tag{91}$$

Assuming that the only measure with a vanishing Fourier transform is the zero measure, we conclude that (81) is satisfied and that (74) does indeed satisfy Schrödinger's equation. Alternatively, this proof can be regarded as a derivation of Schrödinger's equation from the path integral in a manner not involving a limiting process.

(91) can be regarded in a sense as a *"differential equation"* for the measure w_{ab}. A curious fact is that for $q_a = q_b$ (e.g., on the vector space $\mathcal{C}_{00}$), the measure itself "satisfies" the Schrödinger equation for the free particle!

By expanding the exponential in (74), one obtains a perturbation expansion where each term can be reduced to an ordinary definite integral of V by using (59). The time integral can be evaluated in closed form, even in three dimensions.[7] If the potential $V(q)$ is a polynomial in q, the generalized moments formula can immediately be applied to calculate all the terms explicitly. An example, the propagator for a particle in a constant force field, is worked out in Appendix B.

One is not restricted to the "free particle" measure w_{ab} used in this paper. It is usually more fruitful to absorb the quadratic portion of the potential (or, more generally, of the action functional expanded about a classical path) into the measure, which yields a new Gaussian measure whose elements are closely related to the equation for small disturbances of the system. This results in much improved series expansions for the propagator (e.g., WKB expansions). This technique will be presented in a subsequent paper.

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It is a pleasure to thank Professor C. DeWitt-Morette for many informal and enlightening discussions on her new approach to path integrals.

APPENDIX A: METHOD OF RESERVATION OF VARIABLES

The method described in Section II for integration over subsets of $\mathcal{C}_-$ is essentially what was called the method of "reservation of variables" by Siegel and Burke.[13] It was used by Feynman and Hibbs[14] to calculate partition functions in statistical mechanics. They assigned the average $\langle q(t)\rangle$ of the path q the fixed value b,

$$\langle \mu, q\rangle \equiv \frac{1}{T}\int_T q(t)\,dt = b,$$

then, after performing the path integrals, integrated over all possible values of b. This reads, in our notation [see (13)],

$$\int_{\mathcal{C}_-} F[q]\,dw_-(q)$$

$$= \int_{\mathbf{R}} db\ \frac{\exp[ib^2/2W_-(\mu)]}{\sqrt{2\pi i\, W_-(\mu)}} \int F[q]\,dw_\mu(q).$$

The Fourier transform of w_μ is given by (38). The path integral expression (74) of the propagator, together with (56) gives:

$$K_V = K_0 \int_{\mathbf{R}} db\ \exp[ib^2/2W_-(\mu)]\,[2\pi i W_-(\mu)]^{-1/2}$$
$$\times \int_{\mathcal{C}_\mu} \chi\{\langle \delta_{t_b}, q\rangle - (q_b - q_a)\}$$
$$\times \exp(-i \int_T V[q(t) + q_a]\,dt)\,dw_\mu(q).$$

If we expand the potential around b,

$$V[q(t)+q_a]$$
$$= V(b) + [q(t) + q_a - b]\,V'(b) + \tfrac{1}{2}[q(t) + q_a - b]^2\,V''(b) + \cdots$$

and integrate over T, the second term is just the constant $q_a T V'(b)$. This is why we chose this particular μ. We are now left with:

$$K_V = K_0\ \exp\{-iT[V(b) + q_a V'(b)]\}$$
$$\times \int_{\mathbf{R}} db\ \frac{\exp[ib^2/2W_-(\mu)]}{\sqrt{2\pi i\, W_-(\mu)}} \int_{\mathcal{C}_\mu} \chi[\langle \delta_{t_b}, q\rangle - (q_b - q_a)]$$
$$\times dw_\mu(q)\, \exp\Big(-i \sum_{n=2}^{\infty} \frac{V^{(n)}(b)}{n\,!}$$
$$\times \int_T\ [q(t) + q_a - b]^n\ dt\Big).$$

This is best suited for polynomial potentials, for which the series over n terminates. One can then expand the exponential in the path integral, and, by using the moments formula, obtain a *nonperturbative* series expansion.

APPENDIX B; PARTICLE IN A CONSTANT FORCE FIELD

As an illustration of (74), we can compute the propagator for a particle of mass M in a constant force field, with potential

$$V(q) = -fq,$$

f being a constant. It is:

$$K(B,A) = K_0(B,A) \int_{\mathcal{C}_{ab}} \exp(if \int_T q(t)\,dt)\,dw_{ab}(q)$$
$$= K_0[2\pi i W_{ab}\quad(\lambda)]^{-1/2} \int_{\mathbf{R}} du$$
$$\times \exp[ifu/\hbar + i(u-a)^2/2W_{ab}(\lambda)]$$
$$= K_0 \exp[(-i/2\hbar^2)W_{ab}(\lambda)f^2 + (i/\hbar)\,af],$$

where λ is the Lebesgue measure, $[d\lambda(t) = dt]$,

$$a = \langle \lambda, \bar{q}\rangle = \int_T \bar{q}(t)\,dt = \tfrac{1}{2}(q_a + q_b)(t_b - t_a),$$

$W_{ab}(\lambda)$ is the variance associated with the covariance C_{ab} in (77), and K_0 is the free propagator (58). The result is,

$$K(B,A) = \sqrt{M/2\pi i\hbar T}\ \exp(iS_c/\hbar),$$

where S_c is the classical action,[15]

$$S_c = \frac{M(q_b - q_a)^2}{2T} + \frac{fT(q_b + q_a)}{2} - \frac{f^2T^3}{24M}\quad .$$

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†Address as of August 1, 1975.

[1] C. DeWitt-Morette, Comm. Math. Phys. **28**, 47 (1972).

[2] C. DeWitt-Morette, Comm. Math. Phys. **37**, 63 (1974).

[3] N. Bourbaki, *Eléments de Mathématiques* (Hermann, Paris, 1969), Vol. XXXV, Box VI, Chap. IX.

[4] The theory of promeasures does not apply to the Feynman integral, since the imaginary Gaussian measures on $\mathbb{R}^n$, building blocks of the promeasure, are not bounded. Nevertheless, generalization of promeasures in the case of unbounded measures on $\mathbb{R}^n$ can be made, provided one works with their Fourier transforms. C. DeWitt-Morette calls the resulting objects "pseudomeasures." For simplicity, we will call them "measures," as they will be formally used as such. It is hoped that current research on the mathematical theory of functional integration will soon build a firm basis for this formalism.

[5] *Handbook of Mathematical Functions*, Milton Abramowitz, and Irene A. Stegun, eds. (Dover, New York, 1965).

[6] We follow the custom of defining the propagators to be zero for $t_b < t_a$, thereby turning them into Green functions. Indeed $[(-\hbar^2/2M)\partial^2/\partial q_b^2 - i\hbar\partial/\partial t_b]K_0(B,A) = -i\hbar\delta(q_b - q_a)\delta(t_b - t_a)$.

[7] See, for example, the treatment of the perturbation expansion in Maurice M. Mizrahi, "An Investigation of the Feynman Path Integral Formulation of Quantum Mechanics," Ph.D. dissertation, The University of Texas at Austin, 1975, Chap. 3, Sec. VI.

[8] This formula can, incidentally, be proved by using (1). The path integral $\int_C F[b^i\langle\mu_i, q\rangle]dw_C(q)$ can be converted either into an integral over $\mathbb{R}$ by the mapping $\{P_1 : \mathcal{C} \to \mathbb{R}$ by $q \mapsto u = \langle b^i\mu_i, q\rangle\}$ or into an integral over $\mathbb{R}^n$ by the mapping $\{P_n : \mathcal{C} \to \mathbb{R}^n$ by $q \mapsto u_i = \langle\mu_i, q\rangle\}$. Equating the two resulting integrals over $\mathbb{R}$ and $\mathbb{R}^n$, and using the fact that $W_C(b^i\mu_i) = \mathcal{W}_{ij}b^ib^j$, yields the result, for $A \equiv \mathcal{W}^{-1}$.

[9] Maurice M. Mizrahi, J. Comput. Appl. Math. **1**, 3,4 (1975).

[10] In the usual time-slicing procedure, it is found that for consistency with the Schrödinger equation one must always evaluate position-dependent terms at the midpoint $(1/2)(q_{j+1} + q_j)$ rather than at the subdivision point q_j, or anywhere else. This rule remains true even for arbitrary Hamiltonians, as can be shown from a peculiar relationship between Weyl transforms and path integrals (see Maurice M. Mizrahi (J. Math. Phys. **16**, 2201 (1975). When one does away with the limiting process, this rule naturally disappears also.

[11] See Kac's mathematical proof (for the case of the heat equation) in the *Proceed. Sec. Berkeley Symp. Math. Stat. Prob.*, University of California Press, 1951; also *Probability and Related Topics in the Physical Sciences* (Interscience, New York, 1959), Chap. VI.

[12] I. M. Koval'chik ("The Wiener Integral," Russian Math. Survey [trans. of Usepkhi Matematicheshikh Nauk (YMH **18**, p. 109 (1963)] remarks that the restriction $0 \leq V(x) \leq M$ in Kac's proof "can be dispensed with, since it is relevant only to the method of proof, and the results remain valid when $V(x)$ is unbounded above," and refers the reader to Rosenblatt [Trans. Amer. Math. Soc. **71**, 120 (1951)]. The lower bound on V seems to remain, but our proof does not call for it.

[13] Siegel, Armand, and Terence Burke, J. Math. Phys. 13, 1681 (1972), with erratum in **14**, 2018 (1973).

[14] Feynman and Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965), p. 279.

[15] Note, incidentally, that the expression of this propagator in Feynman and Hibbs, p. 64, is incorrect.

Geometrical optics in general relativity: A study of the higher order corrections

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The higher order corrections to geometrical optics are studied in general relativity for an electromagnetic test wave. An explicit expression is found for the average energy–momentum tensor which takes into account the first-order corrections. Finally the first-order corrections to the well-known area-intensity law of geometrical optics are derived.

1. INTRODUCTION

The aim of this paper is to display some effect of the space–time curvature upon the propagation of a high-frequency electromagnetic test wave.

It is a well-known result[1,2] that, in the geometrical optics approximation, an electromagnetic wave possesses an average energy–momentum tensor of the form of a null fluid (the averaging is over many periods of the wave). Such a form for the energy–momentum tensor means that, in this approximation, we deal with a directed flow of radiation, i. e., the wave carries energy only along the propagation vector. This property is of constant use in relativistic astrophysics (e. g., when dealing with radiation emitted near a black hole) or in cosmology (e. g., when dealing with radiation propagating over cosmological distances).

It is therefore of some interest to investigate the deviations occurring when one considers the first-order corrections to geometrical optics.

The geometrical optics field is usually defined as the first term in an appropriate expansion of the electromagnetic field in inverse powers of the frequency. In this paper we shall investigate[3] the nature of the first-order corrections to the geometrical optics field.

In Sec. 2 we set up the basic techniques for geometrical optics in general relativity. The main ideas are essentially due to Ehlers.[1] However our treatment differs from Ehlers' in the following points: (i) we adopt the Newman–Penrose[4] formalism, which enables us to write explicitly the equations satisfied by all the higher order corrections to the geometrical optics field, and (ii) we check the consistency of the set of recursive equations we have obtained.

In Sec. 3 we investigate the structure of the energy–momentum tensor when the first-order corrections are taken into account. The latter corrections cause the energy momentum tensor to differ from that of a directed flow of radiation. In particular we find that there is diffusion of the wave. This can be interpreted physically as arising in part from the continuous back-scattering of the wave off the space–time curvature.

In Sec. 4 we consider the corrections induced in the well-known area-intensity law of geometrical optics. An explicit formula is derived for the deviations from this law, which could be of importance for cosmology and relativistic astrophysics.

Finally in Sec. 5 we discuss in detail a simple example and conclusions are drawn.

Notation: Latin indices $a, b, \cdots$, generally run over the four space-time coordinates labels $0, 1, 2, 3$.

Capital Latin indices $A, B, A', B', \cdots$, indicate spinor indices and run over $0, 0', 1, 1'$.

The metric signature is taken to be -2.

Units are such that the velocity of light c and the gravitational constant G are equal to 1, $c = G = 1$.

Symmetrization of indices is indicated by ( ), antisymmetrization by [ ]. Ordinary derivatives are indicated by ∂_a or a comma, covariant derivatives by ∇_a or a semicolon. $\langle\ \rangle$ denotes averaging with respect to a statistical ensemble.

2. GENERAL FORMALISM

In this section we shall employ the notation of Newman and Penrose.[4]

In the spinor formalism the Maxwell equations in vacuo are[5]

$$\nabla^{AA'}\phi_{AB} = 0, \tag{1}$$

where ϕ_{AB} is the spinor equivalent of the Maxwell bivector G_{ab}.[1]

In this formalism Ehlers' ansatz[1] reads

$$\phi_{AB} = \exp[i\omega S(x)]\sum_{n=0}^{\infty}\omega^{-n}\overset{(n)}{K}_{AB}(x) + \exp[-i\omega S(x)]\sum_{n=0}^{\infty}\omega^{-n}\overset{(n)}{L}_{AB}(x), \tag{2}$$

where the expansion in (2) is interpreted as an asymptotic series in ω^{-1}.[6] ω is a large parameter to be interpreted as the frequency of the wave. The phase $S(x)$ is a scalar function of the space–time point x. $\overset{(n)}{K}_{AB}(x)$ and $\overset{(n)}{L}_{AB}(x)$ are symmetric spinor fields in space–time. Inserting (2) into (1) we obtain

$$(\nabla^{AA'}S)\overset{(0)}{K}_{AB} = 0, \quad (\nabla^{AA'}S)\overset{(0)}{L}_{AB} = 0, \tag{3}$$

$$\nabla^{AA'}\overset{(n)}{K}_{AB} + i(\nabla^{AA'}S)\overset{(n+1)}{K}_{AB} = 0, \tag{4a}$$

$$\nabla^{AA'}\overset{(n)}{L}_{AB} - i(\nabla^{AA'}S)\overset{(n+1)}{L}_{AB} = 0. \tag{4b}$$

Let us write $l_a = \nabla_a S$ and define the rays as those curves $x^a = x^a(r)$ having l^a as tangent vector,

$$\frac{dx^a}{dr} = l^a.$$

Then, from (3) it is shown in the usual way[1,5] that $l_a l^a = 0$ and $l_a \nabla^a l_b = 0$. Therefore the rays form a twist-free congruence of null geodesics (r being an affine parameter along such null geodesics).[1] S is therefore a null hypersurface. Let o^A be the spinor equivalent of the null vector l^a. From (3) it is easily shown that

$$\overset{(0)}{K}_{AB}\, o^A = \overset{(0)}{L}_{AB}\, o^A = 0, \qquad (5)$$

stating that the zeroth order field is a null field having the propagation vector l^a as principal null vector. This field is defined to be the geometrical optics field.[1] Now let us choose a spinor basis o^A, l^A such that

$$o_A l^A = 1,$$

which we parallelly propagate along the rays

$$D o_A = D l_A = 0,$$

where $D \equiv l^a \nabla_a$.

Then it is easily seen that one has $\epsilon = \kappa = \pi = o$, $\rho = \bar{\rho}$, and $\tau = \bar{\alpha} + \beta$, where ϵ, κ, π, ρ, τ, α, β are spin-coefficients defined in the paper by Newman and Penrose.[4]

Now we project the spinor fields $\overset{(n)}{K}_{AB}$ and $\overset{(n)}{L}_{AB}$ into the spinor basis o_A, l_A. Let us write, for $n \geqslant 0$,

$$\overset{(n)}{K}_{AB} = \overset{(n)}{A}{}^{+} o_A o_B + \overset{(n)}{B}{}^{+} o_A l_B + \overset{(n)}{B}{}^{+} l_A o_B + \overset{(n)}{C}{}^{+} l_A l_B,$$

$$\overset{(n)}{L}_{AB} = \overset{(n)}{A}{}^{-} o_A o_B + \overset{(n)}{B}{}^{-} o_A l_B + \overset{(n)}{B}{}^{-} l_A o_B + \overset{(n)}{C}{}^{-} l_A l_B.$$

Then it is easily seen that (4) yields the following sets of recursive equations:

$$-D\overset{(n)}{B}{}^{+} - \bar{\delta}\overset{(n)}{C}{}^{+} + 2\rho\overset{(n)}{B}{}^{+} + 2\alpha\overset{(n)}{C}{}^{+} = 0, \qquad (6a)$$

$$D\overset{(n)}{A}{}^{+} - \rho\overset{(n)}{A}{}^{+} + \bar{\delta}\overset{(n)}{B}{}^{+} + \lambda\overset{(n)}{C}{}^{+} = 0, \qquad (6b)$$

$$-i\overset{(n+1)}{C}{}^{+} + \sigma\overset{(n)}{A}{}^{+} - \delta\overset{(n)}{B}{}^{+}$$
$$- \Delta\overset{(n)}{C}{}^{+} + 2\tau\overset{(n)}{B}{}^{+} + (2\gamma - \mu)\overset{(n)}{C}{}^{+} = 0, \qquad (6c)$$

$$i\overset{(n+1)}{B}{}^{+} + \delta\overset{(n)}{A}{}^{+} + (-\tau + 2\beta)\overset{(n)}{A}{}^{+}$$
$$+ \Delta\overset{(n)}{B}{}^{+} + 2\mu\overset{(n)}{B}{}^{+} + \nu\overset{(n)}{C}{}^{+} = 0, \qquad (6d)$$

$$-D\overset{(n)}{B}{}^{-} - \bar{\delta}\overset{(n)}{C}{}^{-} + 2\rho\overset{(n)}{B}{}^{-} + 2\alpha\overset{(n)}{C}{}^{-} = 0, \qquad (7a)$$

$$D\overset{(n)}{A}{}^{-} - \rho\overset{(n)}{A}{}^{-} + \bar{\delta}\overset{(n)}{B}{}^{-} + \lambda\overset{(n)}{C}{}^{-} = 0, \qquad (7b)$$

$$i\overset{(n+1)}{C}{}^{-} + \sigma\overset{(n)}{A}{}^{-} - \delta\overset{(n)}{B}{}^{-} - \Delta\overset{(n)}{C}{}^{-} + 2\tau\overset{(n)}{B}{}^{-} + (2\gamma - \mu)\overset{(n)}{C}{}^{-} = 0, \qquad (7c)$$

$$-i\overset{(n+1)}{B}{}^{-} + \delta\overset{(n)}{A}{}^{-} + (-\tau + 2\beta)\overset{(n)}{A}{}^{-} + \Delta\overset{(n)}{B}{}^{-} + 2\mu\overset{(n)}{B}{}^{-} + \nu\overset{(n)}{C}{}^{-} = 0, \qquad (7d)$$

where the symbols D, δ, $\bar{\delta}$, Δ and the spin coefficients ρ, α, λ, τ, γ, σ, μ, ν, β have the meaning employed in the paper by Newman and Penrose.[4]

The terms containing $\overset{(n)}{K}_{AB}$ represent a right-handed polarized wave, whereas the terms containing $\overset{(n)}{L}_{AB}$ represent a left-handed polarized wave. From Eqs. (6) and (7) we see that all the states of polarization decouple to all orders. Therefore, hereafter we shall consider only the set of Eqs. (6), dropping the upper plus$^{(+)}$ wherever unnecessary.

Now we ask ourselves how the arbritrariness in the choice of the spinor basis is reflected in the quantities $\overset{(n)}{A}$, $\overset{(n)}{B}$, $\overset{(n)}{C}$. It is easily seen that the basis o^A, l^A is fixed up to the transformation

$$o^A \rightarrow \exp(iM)\, o^A,$$
$$l^A \rightarrow \exp(-iM) l^A + N o^A, \qquad (8)$$

where M is a scalar real field and N a complex scalar field such that $DM = DN = 0$ (in order to preserve $Do^A = Dl^A = 0$). It is apparent that under the transformation (8) the quantities $\overset{(n)}{A}$, $\overset{(n)}{B}$, $\overset{(n)}{C}$ change according to

$$\overset{(n)}{A} \rightarrow \exp(-2iM)\overset{(n)}{A} - 2\exp(-iM)N\overset{(n)}{B} + N^2\overset{(n)}{C},$$

$$\overset{(n)}{B} \rightarrow \exp(-iM)\overset{(n)}{B} - N\overset{(n)}{C},$$

$$\overset{(n)}{C} \rightarrow \exp(2iM)\overset{(n)}{C}. \qquad (9)$$

The solution (2), together with Eqs. (6) and (7), enables us to solve the initial value problem for the Eqs. (1).[1,7] Let $\mathcal{H}$ be a hypersurface which does not contain the rays. We give $\overset{(n)}{A}$ on the hypersurface $\mathcal{H}$. From Eq. (3) it is apparent that $\overset{(0)}{B} = \overset{(0)}{C} = 0$. Hence Eq. (6b) together with the condition $\overset{(0)}{B} = \overset{(0)}{C} = 0$, yields $A^{(0)}$ everywhere in a normal neighborhood D of the initial hypersurface. Then (6c) and (6d) give $\overset{(1)}{B}$ and $\overset{(1)}{C}$ everywhere in D. By iteration we obtain $\overset{(n)}{A}$, $\overset{(n)}{B}$, $\overset{(n)}{C}$ everywhere in D. Now the question arises whether the values for $\overset{(n)}{A}$, $\overset{(n)}{B}$, $\overset{(n)}{C}$ obtained in such a way do in fact satisfy Eq. (6a). It has been proved by Ehlers[1] that if the series (2), as well as its derivatives, converge uniformly in D, then Eq. (6a) is automatically satisfied. It is well-known[8] that even when it is not convergent the series (2) provides a good approximation to the Maxwell fields in the case in which it converges asymptotically. It is then of some interest, in the latter case, to enquire under which conditions the set of Eqs. (6) is self-consistent.

In Appendix A we prove the following theorem.

Theorem: For a general background Lorentz metric the equations of system (6) are consistent.

Having set up a self-consistent approximation scheme for geometrical optics, in the next section we turn to some questions of physical interpretation.

3. THE AVERAGED ENERGY-MOMENTUM TENSOR

In this section we investigate the energy—momentum tensor of the electromagnetic field up to the first-order corrections to the geometrical optics field. In terms of the complex self-dual Maxwell divector G_{ab}, the energy—momentum tensor of the electromagnetic field reads

$$T_a{}^b = \tfrac{1}{4}(G_{am}\bar{G}^{bm} + \bar{G}_{am}G^{bm}). \qquad (10)$$

The spinor equivalent of $T_a{}^b$ is

$$T_{AA'}{}^{BB'} = -\tfrac{1}{2}\phi_A{}^B \bar{\phi}_{A'}{}^{B'}. \qquad (11)$$

Now let us write

$$\phi_A{}^B = \exp(i\omega S)K_A{}^B + \exp(-i\omega S)L_A{}^B, \qquad (12)$$

where

$$K_A{}^B=\sum_{n=0}^{\infty}\omega^{-n}\overset{(n)}{K}_{AB},\quad L_A{}^B=\sum_{n=0}^{\infty}\omega^{-n}\overset{(n)}{L}_{AB}. \tag{13}$$

Also, let us put

$$\Theta_{AA'}{}^{BB'}=K_A{}^B\overline{K}_{A'}{}^{B'}+L_A{}^B\overline{L}_{A'}{}^{B'}, \tag{14}$$

$$\Xi_{AA'}{}^{BB'}=\exp(2i\omega S)K_A{}^B\overline{L}_{A'}{}^{B'}+\exp(-2i\omega S)L_A{}^B\overline{K}_{A'}{}^{B'}. \tag{15}$$

Then we can write

$$T_{AA'}{}^{BB'}=-\tfrac{1}{2}[\Theta_{AA'}{}^{BB'}+\Xi_{AA'}{}^{BB'}]. \tag{16}$$

Next we average out to zero the rapidly oscillating terms of the kind $\exp(\pm 2i\omega S)F$. This averaging is to be interpreted as an "ensemble" averaging: That is, at each space—time point we average over many realizations of the radiation field. Via a suitable ergodic hypothesis it should correspond physically to averaging over a time which is long compared to the period of the wave, but much shorter than the characteristic time of change of the gravitational field.

By averaging $\Xi_{AA'}{}^{BB'}$ we obtain

$$\langle\Xi_{AA'}{}^{BB'}\rangle=0,$$

hence

$$\langle T_{AA'}{}^{BB'}\rangle=-\tfrac{1}{2}\langle\Theta_{AA'}{}^{BB'}\rangle. \tag{17}$$

Next let us consider the conservation equations,

$$\nabla^{AA'}T_{AA'}{}^{BB'}=-\tfrac{1}{2}[\nabla^{AA'}\Theta_{AA'}{}^{BB'}+\nabla^{AA'}\Xi_{AA'}{}^{BB'}]=0. \tag{18}$$

By averaging (18), since $\langle\nabla^{AA'}\Xi_{AA'}{}^{BB'}\rangle=0$ we obtain

$$\langle\nabla^{AA'}\Theta_{AA'}{}^{BB'}\rangle=0. \tag{19}$$

Since the averaging we consider commutes with space—time differentiation, we can write

$$\nabla^{AA'}\langle T_{AA'}{}^{BB'}\rangle=0. \tag{20}$$

We have therefore constructed a conserved averaged energy—momentum tensor for the radiation field defined by Eq. (2).

From (20) it is apparent that the tensor $\langle T_{AA'}{}^{BB'}\rangle$ is conserved to all orders in $1/\omega$. We have then to check the consistency of the conservation equations with our approximation scheme. In Appendix *B* we prove that Eqs. (19) or (20) are satisfied to all orders in $1/\omega$ as a consequence of the recursive set of Eqs. (3) and (4).

An inspection of Eq. (14) shows that to all orders in $1/\omega$, in the averaged energy—momentum tensor, left-handed and right-handed polarizations decouple. Therefore, in the following, we shall consider only one kind of polarization. The zeroth-order averaged energy—momentum tensor is given by

$$\langle\overset{(0)}{T}_{AA'}{}^{BB'}\rangle=-\tfrac{1}{2}\langle\overset{(0)}{K}{}_A^B\ \overset{\overline{(0)}}{K}_{A'}{}^{B'}\rangle. \tag{21}$$

From Eqs. (6) we have $\overset{(0)}{K}_{AB}=\overset{(0)}{A}o_Ao_B$, and $D\overset{(0)}{A}-\rho\overset{(0)}{A}=0$. Hence it is easily shown that

$$D\langle\overset{(0)}{T}_{AA'}{}^{BB'}\rangle=2\rho\langle\overset{(0)}{T}_{AA'}{}^{BB'}\rangle. \tag{22}$$

Now let us look at $\langle\overset{(1)}{T}_{AA'}{}^{BB'}\rangle$. We have

$$\langle\overset{(1)}{T}_{AA'}{}^{BB'}\rangle=-\tfrac{1}{2}\langle\overset{(0)}{K}_A{}^B\overset{\overline{(1)}}{K}_{A'}{}^{B'}+\overset{(1)}{K}_A{}^B\overset{\overline{(0)}}{K}_{A'}{}^{B'}\rangle. \tag{23}$$

Now we project $\langle\overset{(1)}{T}_{AA'}{}^{BB'}\rangle$ onto the spinor basis o^A, l^A.[4,5] From the symmetry of $\langle\overset{(1)}{T}_{ab}\rangle$, the vanishing of its trace, and the relation

$$\langle\overset{(1)}{T}_{ab}\rangle l^b=0, \tag{24}$$

which is easily verified from representation (23), we deduce that $\langle\overset{(1)}{T}_{ab}\rangle$ has only five independent real components. Similarly we find that $\langle\overset{(1)}{T}_{AA'}{}^{BB'}\rangle$ has only three independent components in the spinor basis $\{o^A, l^A\}$: Two of them are complex and the other is real. These are given by

$$H=\langle\overset{(1)}{T}_{ABA'B'}\rangle o^Ao^B\overline{l}^{A'}\overline{l}^{B'}=-\tfrac{1}{2}\langle\overset{\overline{(0)}}{A}\overset{(1)}{C}\rangle, \tag{25a}$$

$$\Pi=\langle\overset{(1)}{T}_{ABA'B'}\rangle l^Ao^B\overline{l}^{A'}l^{B'}=\tfrac{1}{2}\langle\overset{\overline{(0)}}{A}\overset{(1)}{B}\rangle, \tag{25b}$$

$$\tfrac{1}{2}W=\langle\overset{(1)}{T}_{ABA'B'}\rangle l^Al^B\overline{l}^{A'}l^{B'}=-\tfrac{1}{2}\langle\overset{(0)}{A}\overset{\overline{(1)}}{A}+\overset{\overline{(0)}}{A}\overset{(1)}{A}\rangle, \tag{25c}$$

where $\overset{(1)}{A}$, $\overset{(1)}{B}$, and $\overset{(1)}{C}$ satisfy

$$D\overset{(1)}{A}-\rho\overset{(1)}{A}+\overline{\delta}\overset{(1)}{B}+\lambda\overset{(1)}{C}=0, \tag{26a}$$

$$i\overset{(1)}{C}=\sigma\overset{(0)}{A}, \tag{26b}$$

$$i\overset{(1)}{B}=(\tau-2\beta)\overset{(0)}{A}-\delta\overset{(0)}{A}. \tag{26c}$$

The spinor basis $\{o^A, l^A\}$ has been fixed up to transformation (8). Therefore the quantities H, Π, and W are subject to the following transformations [which can be easily derived from Eq. (9)]:

$$H\rightarrow\exp(4iM)H,\quad \Pi\rightarrow\exp(iM)\,\Pi-N\exp(2iM)H, \tag{27}$$

$$W\rightarrow W+4\exp(-iM)\overline{N}\overline{\Pi}$$
$$+4\exp(iM)N\Pi+2\overline{N}^2\exp(-2iM)+2N^2\exp(2iM)\overline{H}.$$

From Eq. (27) it is easily seen that H can be made real and Π made to vanish at a point by a suitable choice of M and N. Furthermore, since the latter quantities are constrained only to satisfy $DM=DN=0$, this can be done all over a hypersurface given by $r=\text{constant}$. Therefore the physical status of the quantities H, Π, and W requires further elucidation. In order to come to grips with the problem of physical interpretation we proceed as follows.

We introduce an observer O with normalized 4-velocity u^a, $u^au_a=1$. Then at any point P along the worldline Γ of observer O we have two given vectors, u^a and l^a. Now out of these two vectors we construct an orthonormal frame and a null frame. Let $\Omega\equiv l_au^a$, then $\omega\Omega\equiv\omega(l_au^a)$ is the frequency of the wave as measured by observer O with 4-velocity u^a.

First we define a spacelike unit vector ν_a, representing the wave's propagation vector in the 3-rest-frame of the observer. We have

$$\nu_a=(1/\Omega)l_a-\Omega u_a. \tag{28a}$$

Obviously $\nu_a\nu^a=-1$, $\nu_au^a=0$.

From the vectors l^a, u^a we also form a null vector n^a, defined by

$$n_a=u_a/\Omega-l_a/2\Omega^2. \tag{28b}$$

Obviously $n_an^a=0$, $n_al^a=1$.

Next we choose two spacelike unit vectors $\underset{(1)}{e}_a$, $\underset{(2)}{e}_a$ orthogonal both to u^a and to ν^a, i.e.,

$$\underset{(1)}{e}_a u^a = \underset{(1)}{e}_a \nu^a = \underset{(2)}{e}_a u^a = \underset{(2)}{e}_a \nu^a = 0. \tag{28c}$$

Finally we define two complex null vectors by

$$m_a = (1/\sqrt{2}\,)(\underset{(1)}{e}_a + i\,\underset{(2)}{e}_a), \quad \overline{m}_a = (1/\sqrt{2}\,)(\underset{(1)}{e}_a - i\,\underset{(2)}{e}_a). \tag{28d}$$

Then it is immediate that the vectors $u^a, \nu^a, \underset{(1)}{e}^a, \underset{(2)}{e}^a$ form an orthonormal frame attached to observer O, while $l^a, n^a, m^a, \overline{m}^a$ form a null frame at the same space–time point $P \in \Gamma$. Now we repeat this construction at each point of Γ and then we parallelly propagate the null frame so obtained along the rays, assuming that each ray cuts Γ only once. In this way we obtain a null frame l^a, n^a, m^a, m^a or equivalently a spinor basis o^A, l^A[4,5] defined at each point of the congruence and satisfying $Do^A = Dl^A = 0$. Therefore our former analysis applies, with the spin coefficients and the derivative operators appropriate to this null frame. Now, however, the arbitrariness in the definitions of o^A, and l^A is more restricted. In fact, along Γ, both u^a and l^a are given vectors, subject to no arbitrariness. Hence, along Γ, o^A and l^A are determined up to the transformation

$$o^A \rightarrow \exp(iM)o^A, \quad l^A \rightarrow \exp(-iM)l^A, \tag{29}$$

where M is an arbitrary function of $P \in \Gamma$. Since $\{o^A, l^A\}$ is defined at each point of the congruence by parallel propagation off Γ, it follows that such a spinor basis is determined up to the transformations (9), with M subject to $DM = 0$. Also it follows that H, Π and W are subject to the transformation (27) with $N = 0$, i.e.,

$$H \rightarrow \exp(4iM)H, \quad \Pi \rightarrow \exp(iM)\Pi, \quad W \rightarrow W.$$

In order to gain more insight into the physical nature of Π, H, and W we project the averaged energy–momentum tensor onto the orthonormal frame $\{u^a, \nu^a, \underset{(1)}{e}^a, \underset{(2)}{e}^a\}$. From Eq. (21) we have for the zeroth-order averaged energy–momentum tensor

$$\langle \overset{(0)}{T}_{ab} \rangle = -\tfrac{1}{2}\langle | \overset{(0)}{A} |^2 \rangle\, l_a l_b . \tag{30}$$

Given the orthonormal frame $\{u^a, \underset{(3)}{e}^a, \underset{(1)}{e}^a, \underset{(2)}{e}^a\}$ with $\underset{(3)}{e}^a = \nu^a$ and the tensor $\langle \overset{(0)}{T}_{ab} \rangle$ we can compute the energy–flow vector, the pressures, and the energy–density.[9]

The energy–density is

$$\overset{(0)}{E} = -\langle \overset{(0)}{T}_{ab} \rangle u^a u^b = \tfrac{1}{2}\langle | \overset{(0)}{A} |^2 \rangle \Omega^2$$

since the metric signature is -2.

The energy–flow vector is $\overset{(0)}{q}_{(\alpha)} = \underset{(\alpha)}{e}^a \langle \overset{(0)}{T}_{ab} \rangle u^b$, $\alpha = 1, 2, 3$ and we have $\overset{(0)}{q}_{(1)} = \overset{(0)}{q}_{(2)} = 0$, whereas

$$\underset{(3)}{\overset{(0)}{q}} = \tfrac{1}{2}\langle | \overset{(0)}{A} |^2 \rangle \Omega^2 = \overset{(0)}{E}.$$

Therefore the energy flows in the direction ν^a, which is the propagation vector of the wave in the rest frame of observer O. The pressure tensor is defined by

$$\underset{(\alpha)(\beta)}{\overset{(0)}{\Theta}} = -\underset{(\alpha)}{e}^a \langle \overset{(0)}{T}_{ab} \rangle \underset{(\beta)}{e}^b .$$

The only nonzero component of $\overset{(0)}{\theta}_{(\alpha)(\beta)}$ is

$$\underset{(3)(3)}{\overset{(0)}{\theta}} = \tfrac{1}{2}\langle | \overset{(0)}{A} |^2 \rangle \Omega^2 = \overset{(0)}{E} .$$

Therefore the pressure is exerted only in the direction of propagation, ν^a, of the wave.

Now let us consider the same quantities for $\langle \overset{(1)}{T}_{ab} \rangle$. We have

$$\begin{aligned} \overset{(1)}{E} &= -\langle \overset{(1)}{T}_{ab} \rangle u^a u^b \\ &= -\Omega^2 \langle \overset{(1)}{T}_{ab} \rangle n^a n^b = -\tfrac{1}{2}\Omega^2 W. \end{aligned} \tag{31}$$

From $\underset{(\alpha)}{\overset{(1)}{q}} = \underset{(\alpha)}{e}^a \langle \overset{(1)}{T}_{ab} \rangle u^b$ we have

$$\begin{aligned} \underset{(3)}{\overset{(1)}{q}} &= -\tfrac{1}{2}\Omega^2 W, \\ \underset{(2)}{\overset{(1)}{q}} &= (1/\sqrt{2}\, i)\Omega(\Pi - \overline{\Pi}), \\ \underset{(1)}{\overset{(1)}{q}} &= (1/\sqrt{2}\,)\Omega(\Pi + \overline{\Pi}), \end{aligned} \tag{32}$$

and from

$$\underset{(\alpha)(\beta)}{\overset{(1)}{\Theta}} = -\underset{(\alpha)}{e}^a \langle \overset{(1)}{T}_{ab} \rangle \underset{(\beta)}{e}^b$$

we obtain

$$\left.\begin{array}{lll} \underset{(1)(1)}{\overset{(1)}{\theta}} = -\tfrac{1}{2}(H + \overline{H}), & \underset{(1)(2)}{\overset{(1)}{\theta}} = -(1/2i)(H - \overline{H}), & \underset{(1)(3)}{\overset{(1)}{\theta}} = (\Omega/\sqrt{2}\,)(\Pi + \overline{\Pi}) \\ \underset{(2)(1)}{\overset{(1)}{\theta}} = \underset{(1)(2)}{\overset{(1)}{\theta}}\ , & \underset{(2)(2)}{\overset{(1)}{\theta}} = \tfrac{1}{2}(H + \overline{H}), & \underset{(2)(3)}{\overset{(1)}{\theta}} = (\Omega/i\sqrt{2}\,)(\Pi - \overline{\Pi}) \\ \underset{(3)(1)}{\overset{(1)}{\theta}} = \underset{(1)(3)}{\overset{(1)}{\theta}}\ , & \underset{(3)(2)}{\overset{(1)}{\theta}} = \underset{(2)(3)}{\overset{(1)}{\theta}}\ , & \underset{(3)(3)}{\overset{(1)}{\theta}} = -\tfrac{1}{2}\Omega^2 W \end{array}\right) \tag{33}$$

We see that the total energy–density measured by the observer is

$$E = \overset{(0)}{E} + (1/\omega)\overset{(1)}{E} = \tfrac{1}{2}\Omega^2[\langle | \overset{(0)}{A} |^2 \rangle - (1/\omega)W],$$

and the total energy–flux in the ν^a direction is

$$\underset{(3)}{q} = \tfrac{1}{2}\Omega^2[\langle | \overset{(0)}{A} |^2 \rangle - (1/\omega)W].$$

Also, the total pressure on a 2-screen orthogonal to the 3-direction is

$$\underset{(3)(3)}{\theta} = \tfrac{1}{2}\Omega^2(\langle | \overset{(0)}{A} |^2 \rangle - \tfrac{1}{2}W).$$

We see that, along the propagation direction of the wave, the energy–density, the energy–flux, and the pressure relate to each other as for the zeroth-order pure geometrical optics field.

Now if we apply transformations (29) at any point we see that we can make $\Pi=\overline{\Pi}$, by a rotation through an angle M_π of the vectors $\underset{(1)}{e}^a$, $\underset{(2)}{e}^a$ in the 2-plane orthogonal to the wave's propagation direction ν^a. Also, through a rotation of an angle $\pi/2-M_\pi$ we can make $\Pi+\overline{\Pi}=0$. Similarly we can make $H=\overline{H}$ and $H+\overline{H}=0$ through rotations of angles M_H and $\pi/2-M_H$ respectively.

Therefore it is possible at a chosen point to rotate the vectors $\underset{(1)}{e}^a$, $\underset{(2)}{e}^a$ in such way as to set alternatively

$$\underset{(1)}{\overset{(1)}{q}}=0 \text{ and } \underset{(3)(1)}{\overset{(1)}{\theta}}=0, \text{ or } \underset{(2)}{\overset{(1)}{q}}=0 \text{ and } \underset{(2)(3)}{\overset{(1)}{\theta}}=0,$$

or

$$\underset{(1)(1)}{\overset{(1)}{\theta}}=\underset{(2)(2)}{\overset{(1)}{\theta}}=0 \text{ or } \underset{(1)(2)}{\overset{(1)}{\theta}}=0.$$

They correspond to some directions in the plane along which there is no energy—flux or no pressure is exerted by the radiation field.

Since all these possibilities are mutually exclusive, it follows that, correct to the first-order, the wave has energy flows in directions orthogonal to the wave's propagation vector, as well as anisotropic stresses. We interpret this as diffusion of the wave. Such effect is potentially of astrophysical and cosmological interest. In the next section we focus on a point which is important when treating the propagation of radiation in a gravitational field, the area-intensity law.

This law is sometimes postulated *a priori* in the old treatments of geometrical optics[3]; where the existence of "rays" and the propagation of the radiation along them is not deduced from Maxwell's theory, but is assumed as a theory per se.

In modern treatments of geometrical optics[1] the area-intensity law is easily shown to be a consequence of Eq. (30) for the energy—momentum tensor $\langle\overset{(0)}{T}_{ab}\rangle$ of the zeroth-order field. In the next section we investigate the deviations from the area-intensity law caused by the inclusion of first-order terms in the energy—momentum tensor.

4. THE AREA-INTENSITY LAW

Let us recall briefly how the area-intensity law is derived for the zeroth-order geometrical optics field.[2]

We have for the zeroth-order intensity, $\overset{(0)}{I}$, as measured by an observer with 4-velocity u^a,

$$\overset{(0)}{I}=\langle\overset{(0)}{T}_{ab}\rangle u^a\nu^b,$$

and we assume that u^a is parallelly propagated along the rays

$$Du^a=0 \tag{34}$$

which, in conjunction with $Dl^a=0$, means that $\Omega=u^a l_a$ is constant along the rays, i.e., we restrict ourselves to those observers who measure the same frequency.

Equation (34) also implies

$$D\nu^a=0. \tag{35}$$

Equation (22) states

$$D\langle\overset{(0)}{T}_{ab}\rangle=2\rho\langle\overset{(0)}{T}_{ab}\rangle. \tag{36}$$

Let Σ be the area of the cross section of the bundle of rays we are considering, then[2]

$$D\Sigma=-2\rho\Sigma. \tag{37}$$

From Eqs. 34—37 we obtain

$$D(\overset{(0)}{I}\Sigma)=0, \tag{38}$$

which says that $\overset{(0)}{I}\Sigma$ is constant along the rays for all those observers who measure the same frequency of the radiation. Now let us look at the first-order corrections in $1/\omega$ to Eq. (38).

The average energy—flux correct to the first-order, is

$$I=\langle\overset{(0)}{T}_{ab}\rangle u^a\nu^b+(1/\omega)\langle\overset{(1)}{T}_{ab}\rangle u^a\nu^b. \tag{39}$$

The quantity of interest here is

$$D(I\Sigma).$$

We have

$$D(I\Sigma)=-2\rho\Sigma I+\Sigma DI. \tag{40}$$

Let us write $\overset{(1)}{I}=\langle\overset{(1)}{T}_{ab}\rangle u^a\nu^b$. Then

$$I=\overset{(0)}{I}+(1/\omega)\overset{(1)}{I},$$

$$DI=D\overset{(0)}{I}+(1/\omega)D\overset{(1)}{I}.$$

Hence

$$D(I\Sigma)=(1/\omega)\Sigma(-2\rho\overset{(1)}{I}+D\overset{(1)}{I}). \tag{41}$$

From (32) we have $\overset{(1)}{I}=\underset{(3)}{\overset{(1)}{q}}=-\frac{1}{2}\Omega^2 W$ where

$$W=-\langle\overset{(0)}{A}\overset{\overline{(1)}}{A}+\overset{\overline{(0)}}{A}\overset{(1)}{A}\rangle.$$

We can write

$$D(I\Sigma)=-(1/2\omega)\Omega^2\Sigma(-2\rho W+DW).$$

After some easy manipulations one obtains

$$\begin{aligned}D(I\Sigma)=-(\Omega^2/2\omega)\Sigma\{i[\langle\overset{(0)}{A}\overset{\overline{(0)}}{A}\rangle(2\overline{\delta}\beta-\overline{\delta}\tau-\lambda\sigma)\\+(2\beta-\tau)\langle\overset{\overline{(0)}}{A}\,\overline{\delta}\overset{(0)}{A}\rangle+\langle\overset{\overline{(0)}}{A}\,\overline{\delta}\delta\overset{(0)}{A}\rangle+\text{c.c.}\}\end{aligned} \tag{42}$$

We remark that the above expression is invariant under the allowed transformations (29).

Bearing in mind the application of this formalism to astrophysics, we find it useful to express Eq. (42) in terms of initial data on a hypersurface $\mathcal{H}$ which each ray cuts only once.

Let the hypersurface $\mathcal{H}$ be given by the equation $r=r_0=$ constant. $\overset{(0)}{A}$ satisfies the equation

$$D\overset{(0)}{A}=\partial\overset{(0)}{A}/\partial r=\rho\overset{(0)}{A}$$

the solution of which is

$$\overset{(0)}{A}=Pe^F, \quad F=\int_{r_0}^{r}\rho(v)\,dv. \tag{43}$$

P is the initial value of $\overset{(0)}{A}$ on the hypersurface $\mathcal{H}$, P is a function of three variables only, i.e., $DP = \partial P/\partial r = 0$. With the help of (43), Eq. (42) can be rewritten in the form

$$D(I\Sigma) = -(\Omega^2/2\omega)\Sigma i\langle \overset{(0)}{A}\overline{\overset{(0)}{A}}\rangle\{2\bar{\delta}\beta - \bar{\delta}\tau - 2\delta\bar{\beta} + \delta\bar{\tau} + (2\beta-\tau)\bar{\delta}F - (2\bar{\beta}-\bar{\tau})\delta F + \bar{\delta}\delta F - \delta\bar{\delta}F - \lambda\sigma + \bar{\lambda}\bar{\sigma}\} - \frac{\Omega^2}{2\omega}\Sigma i \exp(2F)\{(2\beta-\tau)\langle\bar{P}\bar{\delta}P\rangle - (2\bar{\beta}-\bar{\tau}) \times \langle P\delta\bar{P}\rangle + \langle\bar{P}\bar{\delta}\delta P\rangle + \langle\bar{P}\delta P\rangle\bar{\delta}F + \langle\bar{P}\bar{\delta}P\rangle\delta F - \langle P\delta\bar{\delta}\bar{P}\rangle - \langle P\bar{\delta}\bar{P}\rangle\delta F - \langle P\delta\bar{P}\rangle\bar{\delta}F\}. \qquad (44)$$

Now we recognize $\overset{(0)}{I} = \frac{1}{2}\Omega^2\langle\overset{(0)}{A}\overline{\overset{(0)}{A}}\rangle$. Also we have that $\overset{(0)}{I}\Sigma$ is constant along the rays. Let us write $\overset{(0)}{I}\Sigma = f$ = constant along the rays. Then, using the commutation relation

$$\bar{\delta}\delta F - \delta\bar{\delta}F = (\bar{\mu}-\mu)DF - (\bar{\alpha}-\beta)\bar{\delta}F - (\bar{\beta}-\alpha)\delta F,$$

we obtain

$$D(I\Sigma) = -(i/\omega)f\{\bar{\delta}\beta - \bar{\delta}\bar{\alpha} - \delta\bar{\beta} + \delta\alpha + (\bar{\mu}-\mu)\rho + \bar{\lambda}\bar{\sigma} - \lambda\sigma + 2(\beta-\bar{\alpha})\bar{\delta}F - 2(\bar{\beta}-\alpha)\delta F\} - \frac{\Omega^2}{2\omega}\Sigma i\exp(2F)\{(2\beta-\tau)\langle\bar{P}\bar{\delta}P\rangle - (2\bar{\beta}-\bar{\tau}) \times\langle P\delta\bar{P}\rangle + \langle\bar{P}\bar{\delta}\delta P\rangle + \langle\bar{P}\delta P\rangle\bar{\delta}F + \langle\bar{P}\bar{\delta}P\rangle\delta F - \langle P\delta\bar{\delta}\bar{P}\rangle - \langle P\bar{\delta}\bar{P}\rangle\delta F - \langle P\delta\bar{P}\rangle\bar{\delta}F\}. \qquad (45)$$

Equation (45) is the main formula of this section expressing the deviation from the area-intensity law in terms of geometrical quantities associated to the null congruence and of the initial values over the hypersurface $\mathcal{H}: r = r_0$.

We remark that the quantities $\langle P\delta\bar{P}\rangle$, $\langle P\delta\bar{\delta}\bar{P}\rangle$, convey information not only about the intensity distribution over $\mathcal{H}$ but also about the polarization and the coherence state of the radiation over $\mathcal{H}$ (since P is a complex quantity).

In astrophysical situations it is perhaps convenient to characterize the initial values of the field by means of its complex coherence[10] on $\mathcal{H}$. We define

$$\Gamma(y,y') \equiv \langle P(y)\bar{P}(y')\rangle = \bar{\Gamma}(y',y), \qquad (46)$$

where $y, y' \in \mathcal{H}$.

Then $\Gamma(y,y')$ embodies all the information contained in the intensity, polarization state, and coherence properties of the zeroth-order radiation field over $\mathcal{H}$. In terms of $\Gamma(y,y')$ it is, in principle, possible to compute the quantities $\langle P\delta\bar{P}\rangle$ and $\langle P\delta\bar{\delta}\bar{P}\rangle$. In fact, since the averaging we adopted is with respect to an "ensemble," we have that averaging commutes with the derivative operators $D, \delta, \bar{\delta}, \Delta$. It follows that

$$\langle P\delta\bar{P}\rangle = \lim_{y'\to y}\delta_{y'}\Gamma(y',y)$$

$$\langle P\delta\bar{\delta}\bar{P}\rangle = \lim_{y'\to y}\delta_{y'}\bar{\delta}_{y'}\Gamma(y',y)$$

where $\delta_{y'}\bar{\delta}_{y'}$ mean derivatives with respect to the coordinates y'.

5. A SIMPLE EXAMPLE

In this section we treat in detail a somewhat idealized but easily tractable example.

We consider radiation propagating along the radial outgoing null geodesics in the Schwarzschild metric, i.e.,

$$ds^2 = (1-2M/r)\,dt^2 - (1-2M/r)^{-1}dr^2 - r^2(d\theta^2 + \sin^2\theta\, d\phi^2). \qquad (47)$$

The phase S is then given by

$$S = t - r^*, \quad r^* = r + 2M\ln[(r/2M) - 1],$$

and r is an affine parameter along such null geodesics. At each point along a geodesic we choose the following null vectors

$$l^a = [(1-2M/r)^{-1},\ 1,\ 0,\ 0]$$
$$n^a = \tfrac{1}{2}[1,\ -(1-2M/r),\ 0,\ 0] \qquad (48)$$
$$m^a = (1/\sqrt{2})\,[0,\ 0,\ 1/r,\ i/r\sin\theta]$$

Then it is easy to see that $(l^a, n^a, m^a, \bar{m}^a)$ is a null tetrad and $Dl^a = Dn^a = Dm^a = 0$.

Therefore the analysis of Sec. 2 applies. Before undertaking such an analysis we list the spin coefficients, the derivative operators and the metric components for the tetral field (48). The nonvanishing spin coefficients are

$$\rho = -1/r, \quad \beta = -\alpha = \cot\theta/2\sqrt{2}\,r,$$
$$\gamma = M/2r^2, \quad \mu = -(1/2r)(1-2M/r). \qquad (49)$$

The explicit form for the tetrad derivative operators is

$$D \equiv l^a\partial_a = \left(1-\frac{2M}{r}\right)^{-1}\frac{\partial}{\partial t} + \frac{\partial}{\partial r} = 2\left(1-\frac{2M}{r}\right)^{-1}\frac{\partial}{\partial v}$$

$$\Delta \equiv n^a\partial_a = \frac{\partial}{\partial S} \qquad (50)$$

$$\delta \equiv m^a\partial_a = \frac{1}{\sqrt{2}\,r}\left[\frac{\partial}{\partial\theta} + \frac{i}{\sin\theta}\frac{\partial}{\partial\phi}\right]$$

where $v = t + r^*$ is the advanced time.

The only nonvanishing component of the Weyl tensor is

$$\Psi_2 = M/2r^2 \qquad (51)$$

Finally, the metric functions[4] are

$$\omega = X^i = 0, \quad U = -\tfrac{1}{2}(1-2M/r)$$
$$\xi^\theta = 1/\sqrt{2}\,r, \quad \xi^\varphi = i/\sqrt{2}r\sin\theta. \qquad (52)$$

Let the hypersurface $\mathcal{H}$ be given by $r = r_0$, $r_0 > 2M$. We have for the zeroth order term

$$D\overset{(0)}{A} + (1/r)\overset{(0)}{A} = 0. \qquad (53)$$

We assume the quantities $\overset{(n)}{A}$, $\overset{(n)}{B}$, $\overset{(n)}{C}$ to be stationary. Then the solution of (53) is

$$\overset{(0)}{A} = P(\theta, \phi)/r, \tag{54}$$

with $P(\theta, \phi)$ an arbitrary function on the sphere. For the sake of simplicity we consider the case $P = \text{constant}$. Then it is easily seen that

$$\overset{(1)}{B} = 2i\beta \overset{(0)}{A} - \delta \overset{(0)}{A} = (iP/\sqrt{2}\, r^2)\cot\theta. \tag{55}$$

$\overset{(1)}{A}$ satisfies the equation $D\overset{(1)}{A} - \rho \overset{(1)}{A} + \bar{\delta} \overset{(1)}{B} = 0$. As initial condition on $\mathcal{H}$ we choose, for $n \geqslant 1$, $\overset{(n)}{A} = 0$ for $r = r_0$. It follows that

$$\overset{(1)}{A} = -(i/2\sin^2\theta)P/r^3. \tag{56}$$

To these we add, as a consequence of $\sigma = 0$,

$$\overset{(1)}{C} = 0 \tag{57}$$

We remark that the higher-order corrections destroy the spherical symmetry of the zeroth order field. This is due to the nonexistence of monopole electromagnetic radiation.

From Eqs. (55)–(57) we see that in the first-order corrections there is no curvature-induced term. Therefore in this case the first-order corrections arise because the wave is not exactly spherical, i. e., they are "near zone effects."

In the particular example we are discussing all the higher-order corrections can be obtained in a closed form. In fact it is easy to convince oneself that $\overset{(n)}{B} = \overset{(n)}{A} = 0$, for $n \geqslant 2$. Furthermore $\overset{(n)}{C}$ is given by $i\overset{(n+1)}{C} = 1/2r + \frac{1}{2}(1 - 2M/r)\partial \overset{(n)}{C}/\partial r$ for $n \geqslant 2$, with

$$\overset{(2)}{C} = -(P/2r^3)\,1/\sin^2\theta.$$

From the above formulas one sees that the curvature induced terms start to appear in $\overset{(3)}{C}$.

Now we discuss the averaged energy–momentum tensor corrected to the first-order.

From the two null vectors l^a, n^a, one can construct the timelike unit vector

$$u^a = 1/\sqrt{2}\ (l^a + n^a), \tag{57a}$$

which corresponds to the normalization $\Omega = 1/\sqrt{2}$ in (28b). The observer having u^a as 4-velocity, sees the radiation propagating in the direction of the spacelike unit vector

$$\nu^a = (1/\sqrt{2})(l^a - n^a). \tag{57b}$$

We obtain an orthonormal tetrad defining the two vectors

$$\underset{(1)}{e^a} = (1/\sqrt{2})(m^a + m^a), \quad \underset{(2)}{e^a} = (1/\sqrt{2})(m^a - m^a).$$

Then, with respect to this orthonormal tetrad, we compute the energy–density, the energy–flows, and the pressure of the radiation field, corrected to the first-order. One has

$$H = W = 0, \quad \Pi = (i/2\sqrt{2})\cot\theta/r\,\langle|\overset{(0)}{A}|^2\rangle.$$

Hence

$$\underset{(3)}{\overset{(1)}{q}} = 0, \quad \underset{(2)}{\overset{(1)}{q}} = (1/r)\cot\theta\, f/\Omega, \quad \underset{(1)}{\overset{(1)}{q}} = 0,$$

$$\underset{(\alpha)(\beta)}{\overset{(1)}{\theta}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \dfrac{\cot\theta f}{r\Omega} \\ 0 & \dfrac{\cot\theta f}{r\Omega} & 0 \end{pmatrix}.$$

Because $\underset{(3)}{\overset{(1)}{q}} = 0$, we find $D(I\Sigma) = 0$. This can also be checked[3] by direct substitution in (45).

We conclude this example by a physical interpretation of the observer defined by (57a). It is an observer moving radially outward with the velocity $dr/ds = (1/\sqrt{2})(\frac{1}{2} + M/r)$ relative to a static observer and seeing the radiation moving radially.

The example we have discussed shows that the first-order corrections can be due to "near zone" effects. However this is not always so. In fact it is well-known that the Weyl tensor induces some shear σ in an initially shear-free congruence of null geodesics. Therefore, from (6c) we see that $\overset{(1)}{C} \neq 0$ in general; an electromagnetic wave is diffused off the space–time curvature.

In the presence of a sufficiently strong gravitational field such effects may not be negligible. In particular we have in mind the cosmic microwave background propagating in a homogeneous Bianchi universe where such effects might be of observational interest. The study of Eq. (45) in these situations is under current investigation and will be the subject of a forthcoming paper.

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APPENDIX A

In this appendix we shall prove the following theorem.

Theorem: For a general background Lorentz metric the equations of the system (6) are consistent.

Proof: We shall prove the theorem by induction. For $n = 0$, being $\overset{(0)}{B} = 0$, $\overset{(0)}{C} = 0$ it is obvious that the Eqs. (6) are consistent. Next we prove that if $\overset{(n)}{B}$, $\overset{(n)}{C}$ satisfy Eq. (6a), then $\overset{(n+1)}{B}$, $\overset{(n+1)}{C}$ obtained from the Eqs. (6b), (6c), (6d), satisfy Eq. (6a) with $n + 1$.

Let us assume then that

$$D(-i\overset{(n)}{B}) - \bar{\delta}(i\overset{(n)}{C}) + 2\rho(i\overset{(n)}{B}) + 2\alpha(i\overset{(n)}{C}) = 0.$$

We shall prove that

$$Q = D(-i\overset{(n+1)}{B}) - \bar{\delta}(i\overset{(n+1)}{C}) + 2\rho(i\overset{(n+1)}{B}) + 2\alpha(i\overset{(n+1)}{C}) = 0.$$

$$Q=D\{\Delta\overset{(n)}{B}-\tau\overset{(n)}{A}+\nu\overset{(n)}{C}+\delta\overset{(n)}{A}+2\beta\overset{(n)}{A}+2\mu\overset{(n)}{B}\}-\bar{\delta}\{-\delta\overset{(n)}{B}+\sigma\overset{(n)}{A}-\mu\overset{(n)}{C}-\Delta\overset{(n)}{C}+2\tau\overset{(n)}{B}+2\gamma\overset{(n)}{C}\}$$
$$+2\rho\{-\Delta\overset{(n)}{B}+\tau\overset{(n)}{A}-\nu\overset{(n)}{C}-\delta\overset{(n)}{A}-2\beta\overset{(n)}{A}-2\mu\overset{(n)}{B}\}+2\alpha\{-\delta\overset{(n)}{B}+\sigma\overset{(n)}{A}-\mu\overset{(n)}{C}-\Delta\overset{(n)}{C}+2\tau\overset{(n)}{B}+2\gamma\overset{(n)}{C}\}.$$

$$Q=D\Delta\overset{(n)}{B}+\bar{\delta}\Delta\overset{(n)}{C}-2\rho\Delta\overset{(n)}{B}-2\alpha\Delta\overset{(n)}{C}+X+Y+Z+T,$$

where

$$X=D[-\tau\overset{(n)}{A}+\nu\overset{(n)}{C}+\delta\overset{(n)}{A}+2\beta\overset{(n)}{A}+2\mu\overset{(n)}{B}],\quad Y=-\bar{\delta}[-\delta\overset{(n)}{B}+\sigma\overset{(n)}{A}-\mu\overset{(n)}{C}+2\tau\overset{(n)}{B}+2\gamma\overset{(n)}{C}],$$
$$Z=2\rho[+\tau\overset{(n)}{A}-\nu\overset{(n)}{C}-\delta\overset{(n)}{A}-2\beta\overset{(n)}{A}-2\mu\overset{(n)}{B}],\quad T=2\alpha[-\delta\overset{(n)}{B}+\sigma\overset{(n)}{A}-\mu\overset{(n)}{C}+2\tau\overset{(n)}{B}+2\gamma\overset{(n)}{C}].$$

By using the commutation relations [(Eq. 6.8) of Newmann—Penrose] one finds

$$Q=\Delta D\overset{(n)}{B}-(\gamma+\bar{\gamma})D\overset{(n)}{B}+\tau\bar{\delta}\overset{(n)}{B}+\bar{\tau}\delta\overset{(n)}{B}+\Delta\bar{\delta}\overset{(n)}{C}-\nu D\overset{(n)}{C}+\lambda\delta\overset{(n)}{C}+(\bar{\mu}+\gamma-\bar{\gamma})\bar{\delta}\overset{(n)}{C}-\Delta(2\rho\overset{(n)}{B})$$
$$+2\overset{(n)}{B}\Delta\rho-\Delta(2\alpha\overset{(n)}{C})+2\overset{(n)}{C}\Delta\alpha+X+Y+Z+T.$$

The induction hypothesis tells us that

$$\Delta D\overset{(n)}{B}+\Delta\bar{\delta}\overset{(n)}{C}-\Delta(2\rho\overset{(n)}{B})-\Delta(2\alpha\overset{(n)}{C})=0.$$

Hence we can write

$$Q=-(\gamma+\bar{\gamma})D\overset{(n)}{B}+\tau\bar{\delta}\overset{(n)}{B}+\bar{\tau}\delta\overset{(n)}{B}+\lambda\delta\overset{(n)}{C}+(\bar{\mu}+\gamma-\gamma)\bar{\delta}\overset{(n)}{C}+2\overset{(n)}{B}\Delta\rho+2\overset{(n)}{C}\Delta\alpha-\overset{(n)}{A}D\tau-\tau D\overset{(n)}{A}$$
$$+\overset{(n)}{C}D\nu+D\delta\overset{(n)}{A}+2\beta D\overset{(n)}{A}+2\overset{(n)}{A}D\beta+2\mu D\overset{(n)}{B}+2\overset{(n)}{B}D\mu+\bar{\delta}\delta\overset{(n)}{B}-\sigma\bar{\delta}\overset{(n)}{A}-\overset{(n)}{A}\bar{\delta}\sigma$$
$$+\mu\bar{\delta}\overset{(n)}{C}+\overset{(n)}{C}\bar{\delta}\mu-2\tau\bar{\delta}\overset{(n)}{B}-2\overset{(n)}{B}\bar{\delta}\tau-2\gamma\bar{\delta}\overset{(n)}{C}-2\overset{(n)}{C}\bar{\delta}\gamma+2\rho\tau\overset{(n)}{A}-2\rho\nu\overset{(n)}{C}-2\rho\delta\overset{(n)}{A}$$
$$+4\beta\rho\overset{(n)}{A}-4\rho\mu\overset{(n)}{B}+4\alpha\tau\overset{(n)}{B}+4\alpha\gamma\overset{(n)}{C}-2\alpha\delta\overset{(n)}{B}+2\alpha\sigma\overset{(n)}{A}-2\alpha\mu\overset{(n)}{C}.$$

Grouping together the terms we find

$$Q=(-\gamma-\bar{\gamma}+2\mu)D\overset{(n)}{B}-\tau\bar{\delta}\overset{(n)}{B}+(\bar{\tau}-2\alpha)\delta\overset{(n)}{B}+\lambda\delta\overset{(n)}{C}-(-\mu-\bar{\mu}+\gamma+\bar{\gamma})\bar{\delta}\overset{(n)}{C}+a\overset{(n)}{A}+b\overset{(n)}{B}+c\overset{(n)}{C}$$
$$-(\tau-2\beta)D\overset{(n)}{A}+D\delta\overset{(n)}{A}+\bar{\delta}\delta\overset{(n)}{B}-\sigma\bar{\delta}\overset{(n)}{A}-2\rho\delta\overset{(n)}{A},$$

where, for simplicity, we have written

$$a=-D\tau+2D\beta-\bar{\delta}\sigma+2\rho\tau-4\beta\rho+2\alpha\sigma,$$
$$b=2\Delta\rho+2D\mu-2\bar{\delta}\tau-4\rho\mu+4\alpha\tau,$$
$$c=+2\Delta\alpha+D\nu+\bar{\delta}\mu-2\bar{\delta}\gamma-2\rho\nu+4\alpha\gamma-2\alpha\mu.$$

Still using the commutation relations we find

$$Q=(-\gamma-\bar{\gamma}+\mu+\bar{\mu})D\overset{(n)}{B}-(-\bar{\mu}-\mu+\gamma+\bar{\gamma})\bar{\delta}\overset{(n)}{C}-2\bar{\alpha}\bar{\delta}\overset{(n)}{B}-2\bar{\alpha}D\overset{(n)}{A}+(a+\delta\rho)\overset{(n)}{A}+b\overset{(n)}{B}-(c-\delta\lambda)\overset{(n)}{C}.$$

From the Newman—Penrose equations (4.2a)—(4*2r) we see that

$$a+\delta\rho=+2\bar{\alpha}\rho,\quad b=2\rho(\gamma+\bar{\gamma}-\mu-\bar{\mu}),\quad c-\delta\lambda=-2\bar{\alpha}\lambda+2\bar{\gamma}\alpha+2\gamma\alpha-2\bar{\mu}\alpha-2\mu\alpha.$$

Hence it follows that

$$Q=(-\gamma-\bar{\gamma}+\mu+\bar{\mu})D\overset{(n)}{B}-(-\bar{\mu}-\mu+\gamma+\bar{\gamma})\bar{\delta}\overset{(n)}{C}-2\rho(\gamma+\bar{\gamma}-\mu-\bar{\mu})\overset{(n)}{B}-(-2\bar{\gamma}\alpha-2\gamma\alpha+2\bar{\mu}\alpha+2\mu\alpha)\overset{(n)}{C}=0.$$

Therefore the theorem is proved.

APPENDIX B

In this appendix we prove the following theorem.

Theorem: Equation (19) in the text, is a consequence of Eqs. (3) and (4) at all orders in $1/\omega$.

Proof: Let us write

$$\Theta_{AX'}{}^{BY'}=\sum_{n=0}^{\infty}\omega^{-n}\overset{(n)}{\Theta}_{AX'}{}^{BY'} \tag{B1}$$

where

$$\overset{(n)}{\Theta}_{AX'}{}^{BY'}=\sum_{r+s=n}\overset{(r)}{K}_A{}^B\overset{(s)}{\bar{K}}_{X'}{}^{Y'} \tag{B2}$$

and we consider only one state of polarization.

From Eq. (4a) in the text and its complex conjugate we obtain

$$\nabla^{AX'}\overset{(n)}{\Theta}_{AX'}{}^{BY'}=-io^A\bar{o}^{X'}\sum_{r+s=n}\overset{(n+1)}{K}_A{}^B\overset{(s)}{\bar{K}}_{X'}{}^{Y'}$$
$$+io^A\bar{o}^{X'}\sum_{r+s=n}\overset{(r)}{K}_A{}^B\overset{(s+1)}{\bar{K}}_{X'}{}^{Y'}. \tag{B3}$$

Now we have

$$\sum_{r+s=n} \overset{(r)}{K}_A{}^B \overset{(s+1)}{\bar{K}}_{X'}{}^{Y'} = \overset{(0)}{K}_A{}^B \overset{(n+1)}{\bar{K}}_{X'}{}^{Y'} + \sum_{q=1}^{n} \overset{(n+1-q)}{K}_A{}^B \overset{(q)}{\bar{K}}_{X'}{}^{Y'}, \tag{B4}$$

$$\sum_{r+s=n} \overset{(r+1)}{K}_A{}^B \overset{(\bar{s})}{K}_{X'}{}^{Y'} = \overset{(\bar{0})}{K}_{X'}{}^{Y'} \overset{(n+1)}{K}_A{}^B + \sum_{p=1}^{n} \overset{(p)}{K}_A{}^B \overset{(n+1-p)}{\bar{K}}_{X'}{}^{Y'}. \tag{B5}$$

With the help of Eq. (3) in the text, we prove that

$$\nabla^{AX'} \overset{(n)}{\Theta}_{AX'}{}^{BY'} = 0, \qquad \text{QED}$$

hence, by Eq. (B1),

$$\nabla^{AX'} \Theta_{AX'}{}^{BY'} = 0.$$

[1] J. Ehlers, Z. Naturforsch. **22a**, 1328 (1967).

[2] G. Ellis, article in *General Relativity and Cosmology* (Academic, London, 1971).

[3] R. Kantowski, article in *Cargèse Lectures on Physics* (Gordon and Breach, New York, 1972).

[4] E.T. Newman and R. Penrose, J. Math. Phys. 3, 566 (1962).

[5] F.A.E. Pirani, article in *Lectures on General Relativity* (Prentice-Hall, Englewood Cliffs, New Jersey (1964).

[6] A. Erdelyi, *Asymptotic Expansions* (Dover, New York, 1956).

[7] R. Lewis, J. Math. Mech. **1**, 593 (1958).

[8] M. Kline and I.W. Kay, *Electromagnetic Theory and Geometrical Optics* (Interscience, New York, 1965).

[9] J.L. Synge, *Relativity: The General Theory* (North-Holland, Amsterdam, 1966).

[10] M. Born and E. Wolf, *Principles of Optics* (Pergamon, London, 1959).

[11] R. Penrose, article in *General Relativity* (Clarendon, Oxford, 1972).

Further heavenly metrics and their symmetries

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New developments in a continuing investigation of complex V_4's with purely self-dual conformal curvature are presented: (1) conformal and projective extensions of spaces with $\bar{C}_{\dot{A}\dot{B}\dot{C}\dot{D}} = 0$ are discussed; (2) Killing vectors for general heavenly metrics are determined; (3) the solutions, in heavenly spaces, for (massless) $D(0,s)$ spinor fields (in particular, the Maxwell field) are found; then (4) new examples of heavenly metrics of types $G\times[-]$ and $D\times[-]$ are provided; lastly, contraction of the $D\times D$ solutions of Plebański and Demiański to type $D\times[-]$ is performed, giving a complex prototype of the Kerr–Newman solution, and all solutions of the type $N\times[-]$ are given, which contain two arbitrary functions of two variables.

1. CONFORMAL AND PROJECTIVE EXTENSIONS OF STRONG HEAVEN

This article follows the notation and terminology of Plebański,[1] hereafter referred to as I, and along with Plebański and Hacyan,[2] is the third in a series of papers dedicated to the study of the "analytic continuation" of the basic structural relations of general relativity. By way of review, we mention that the study of heavenly metrics is motivated by the desire to produce general (real) solutions of the Einstein equations on a real manifold. The complex approach to this problem has been developing for the last several years through accidental discoveries of complex coordinate transformations which permit one to proceed from one real solution to another real solution.[3] Less serendipitous approaches to an explanation for this phenomenon have arisen recently which generated some of the terminology used here.[3]

In the study of real Riemannian spaces it is useful to classify them according to the degeneracy of the eigenvectors of the conformal tensor—the usual Petrov–Penrose classification. In the complex case a generalization is easily obtained by a tensor product of two (independent) such classification schemes. (See Ref. 1 for a complete derivation.) We therefore label the conformal curvature of a complex V_4 by symbols such as $G\times G$, $D\times N$, $N\times[-]$, etc., identifying as usual $G \equiv [1-1-1-1]$, $D\equiv[2-2]$, $N\equiv[4]$, etc. This classification scheme will be used often in what follows to delineate the kind of spaces under consideration. We will first indicate the nature of some conformal and projective extensions of the notion of heavenly manifolds—those for which $\bar{C}_{\dot{A}\dot{B}\dot{C}\dot{D}}=0$, $R_{ab}=0$—which generate weak heavens—only $\bar{C}_{\dot{A}\dot{B}\dot{C}\dot{D}}=0$. Then some strong results about all possible Killing vectors and all $D(0,s)$ irreducible heavenly spinorial fields definable on a strong heaven (characterizing massless particles) will be given. Lastly some more attention will be paid to explicit constructions of heavenly manifolds.

We first consider two (complex) conformally equivalent Riemannian spaces:

$$V_4\colon\ ds^2 = 2e^1e^2 + 2e^3e^4, \quad \tilde{V}_4\colon\ ds^2 = 2\tilde{e}^1\tilde{e}^2 + 2\tilde{e}^3\tilde{e}^4 \tag{1.1}$$

$$\begin{aligned} e^a &= \phi\tilde{e}^a,\\ \phi\partial_a &= \tilde{\partial}_a, \end{aligned} \tag{1.2}$$

$$de^a = e^b \wedge \Gamma^a{}_b, \quad d\tilde{e}^a = \tilde{e}^b \wedge \tilde{\Gamma}^a{}_b. \tag{1.3}$$

One easily finds that these relations imply that

$$\tilde{\Gamma}_{ab} = \Gamma_{ab} + 2(\ln\phi)_{,[a}e_{b]}. \tag{1.4}$$

Using the Hodge duality operation[4] and the usual spinor form of the connections (see I), we may write that

$$\tilde{\Gamma}_{AB} = \Gamma_{AB} - \tfrac{1}{2}(\ln\phi)_{,a}e_bS^{ab}{}_{AB} = \Gamma_{AB} + (1/2i) * (d\ln\phi \wedge S_{AB}), \tag{1.5}$$

and a completely analogous equation with dotted indices.

If the space V_4 is a strong heaven, then there is a choice of gauge such that $\Gamma_{\mathring{A}\dot{B}}=0$. Then the conformally equivalent $\tilde{V}_4$ will be a weak heaven; i.e., the anti-self-dual parts of the conformal curvature tensor will still vanish-$\tilde{\bar{C}}_{\mathring{A}\mathring{B}\mathring{C}\mathring{D}}=0$—but $\tilde{R}_{ab}\neq 0$. In fact one finds that

$$\tilde{C}_{ABCD} = \phi^2 C_{ABCD}, \quad \tilde{\bar{C}}_{\dot{A}\dot{B}\dot{C}\dot{D}} = \phi^2\bar{C}_{\dot{A}\dot{B}\dot{C}\dot{D}}, \tag{1.6}$$

$$-\tilde{R}_{ab}/2 = \tilde{\nabla}_{(a}\tilde{B}_{b)} - \tilde{B}_a\tilde{B}_b + \tfrac{1}{2}g_{ab}(\tilde{\nabla}_c\tilde{B}^c + 2\tilde{B}_c\tilde{B}^c), \tag{1.7}$$

where $\tilde{B}_b \equiv \tilde{\nabla}_b \ln\phi$ and $\tilde{\nabla}_b$ is understood to be the covariant tetradial derivative in $\tilde{V}_4$.

It is interesting to wonder whether one can use a conformal transformation to generate a new solution of Einstein's equations in vacuum (with $\tilde{R}\equiv\tilde{R}_{ab}g^{ab}$ possibly nonzero). That is, starting with V_4 as a strong heaven, how must one choose ϕ so that, in $\tilde{V}_4$, $\tilde{R}_{ab}=\tfrac{1}{4}\tilde{R}g_{ab}\neq 0$. In the Appendix it is shown that this cannot be done. If one relaxes the above condition and allows $\tilde{R}=0$ (still requiring $\tilde{R}_{ab}=\tfrac{1}{4}\tilde{R}g_{ab}$), he gets only transformations between two (in general different) strong heavens rather than one from a strong to a weak heaven. It is further shown in the Appendix that this type of transformation can be generated by a conformal transformation only when both spaces are of type $N\times[-]$.

Experience with these conformal transformations leads one to contemplate an interesting generalization which arises when we replace "$d\ln\phi$" by a general 1-form, α. (This is, of course, similar to the standard generalization of conformal structures into projective structures in real geometry.) We are thus led to considering spaces such that, in a specific choice of tetrad gauge,

$$\Gamma_{\mathring{A}\dot{B}} = -(1/2i) * (\alpha \wedge S_{\mathring{A}\mathring{B}}). \tag{1.8}$$

We note that simple algebraic manipulations show that Eq. (1.8) is equivalent to

$$dS_{\mathring{A}\dot{B}} + 2\alpha \wedge S_{\mathring{A}\mathring{B}} = 0, \tag{1.9}$$

which is, of course, also true only in a specific gauge. It is relevant to note as well that Eq. (1.9) requires that

$$d\alpha \wedge S_{\dot A\dot B}=0, \tag{1.10}$$

which implies that the 2-form $d\alpha$ must be self-dual ($*d\alpha=d\alpha$). (These equations then coincide formally with the complex extension of the homogeneous Maxwell equations.) Notice that if $\alpha=d\ln\phi$, $d\alpha=0$ and this condition is automatically satisfied. Calculating, now, the curvature quantities, one finds, perhaps surprisingly, that

$$C_{\dot A\dot B\dot C\dot D}=0. \tag{1.11}$$

Also, straightforwardly from Eq. (1.7), one has that

$$\begin{aligned} -C_{ab}/2&=\alpha_{(a;b)}-\alpha_a\alpha_b-\tfrac{1}{4}g_{ab}g^{cd}(\alpha_{c;d}-\alpha_c\alpha_d),\\ -R/12&=\alpha_{1;2}+\alpha_{3;4}+\alpha_1\alpha_2+\alpha_3\alpha_4, \end{aligned} \tag{1.12}$$

where $C_{ab}\equiv R_{ab}-(R/4)g_{ab}$ is the traceless part of the Ricci tensor. Therefore, the condition given by Eq. (1.9) guarantees that the manifold in question is a weak heaven.

We would like now to determine the canonical form of the null tetrad applicable to this condition. We apply Frobenius' theorem in the following form: If, in a star-shaped region of M_n, there are r 1-forms ω^i ($i=1,\ldots,r\leqslant n$) functionally independent—$\Omega\equiv\omega^1\wedge\cdots\wedge\omega^r\neq 0$—and there exists a 1-form θ such that $d\Omega=\theta\wedge\Omega$, then there exist functions $f^i{}_j$, g^i ($i,j=1,\ldots,r$) such that $\omega^i=f^i{}_j dg^j$. Noting that $S^{\dot 1\dot 1}=2e^4\wedge e^1$ and $S^{\dot 2\dot 2}=2e^3\wedge e^2$, Frobenius' theorem and Eq. (1.9) allow us to infer the existence of scalar functions such that

$$\begin{aligned} &e^1=\phi^{-1}e^{\sigma}(Adp+Bdq), \quad e^2=\phi^{-1}e^{-\sigma}(Edr+Fds)\\ &-e^4=\phi^{-1}e^{\sigma}(Cdp+Ddq), \quad -e^3=\phi^{-1}e^{-\sigma}(Gdr+Hds), \end{aligned} \tag{1.13}$$

normalized so that

$$AD-BC=1, \quad EH-FG=1. \tag{1.14}$$

Of course, since $0\neq e^1\wedge e^2\wedge e^3\wedge e^4=\phi^{-4}dp\wedge dq\wedge dr\wedge ds$ we see that p,q,r,s can be used as independent coordinates. By substituting Eqs. (1.13) into $S_{\dot A\dot B}$ and utilizing Eqs. (1.9), it follows that

$$\alpha=d\ln\phi+\sigma_p dp+\sigma_q dq-\sigma_r dr-\sigma_s ds, \tag{1.15}$$

so that $d\alpha$ does not, in general, vanish. In addition, the equation for $S^{\dot 1\dot 2}$ requires the existence of functions x and y such that

$$AE+CG=e^{2\sigma}x_r, \quad AF+CH=e^{2\sigma}x_s, \tag{1.16}$$

$$BE+DG=e^{2\sigma}y_r, \quad BF+DH=e^{2\sigma}y_s, \tag{1.17}$$

and

$$(e^{4\sigma}x_r)_q=(e^{4\sigma}y_r)_p, \quad (e^{4\sigma}x_s)_q=(e^{4\sigma}y_s)_p. \tag{1.18}$$

Solving Eqs. (1.17) for E,F,G, and H and inserting into the condition (1.14) gives

$$\frac{\partial(x,y)}{\partial(r,s)}=e^{-4\sigma}, \tag{1.19}$$

which means that x and y may be used as coordinates instead of r and s. By using these new coordinates and the expressions for E,F,G and H, the tetrad may be written as

$$\begin{aligned} &e^1=\Delta^{-1}(Adp+Bdq), \quad -e^4=\Delta^{-1}(Cdp+Ddq),\\ &e^2=\Delta^{-1}[D(dx+Kdp+Ldq)-C(dy+Mdp+Ndq)],\\ &-e^3=\Delta^{-1}[-B(dx+Kdp+Ldq)+A(dy+Mdp+Ndq)], \end{aligned} \tag{1.20}$$

and

$$\alpha=d\ln\phi+\xi dp+\eta dq,$$

with

$$\begin{aligned} &\Delta=\phi e^{-\sigma}, \quad K=-x_p, \quad L=-x_q, \quad M=-y_p,\\ &N=-y_q, \quad \xi=2\sigma_p, \quad \eta=2\sigma_q, \end{aligned} \tag{1.21}$$

while the derivatives, of course, refer to x and y as functions of p,q,r, and s. It is now clear that A,B,C,D such that $AD-BC=1$ simply describe the residual freedom of the heavenly gauge group—the group which does not affect $S_{\dot A\dot B}$. So, without loss of generality, we can fix this gauge by setting

$$A=1=D, \quad B=0=C. \tag{1.22}$$

Taking, therefore,

$$\begin{aligned} &e^1=\Delta^{-1}dp, \quad -e^4=\Delta^{-1}dq,\\ &e^2=\Delta^{-1}(dx+Kdp+Ldq), \quad -e^3=\Delta^{-1}(dy+Mdp+Ndq), \end{aligned} \tag{1.23}$$

as starting conditions, one finds that Eq. (1.9) is automatically satisfied for $S^{\dot 1\dot 1}$, while $S^{\dot 1\dot 2}$ implies that

$$\alpha=d\ln\Delta+\tfrac{1}{2}(L-M)_x dq-\tfrac{1}{2}(L-M)_y dp. \tag{1.24}$$

Lastly $S^{\dot 2\dot 2}$ requires the four conditions

$$\begin{aligned} &K_{,2}-L_{,3}=0, \quad M_{,2}-N_{,3}=0\\ &K_{,4}+L_{,1}=0, \quad M_{,4}+N_{,1}=0, \end{aligned} \tag{1.25}$$

where the directional derivatives are just the ones determined by Eqs. (1.23):

$$\begin{aligned} &\partial_2=\Delta\partial_x, \quad -\partial_3=\Delta\partial_y,\\ &\partial_1=\Delta(\partial_p-K\partial_x-M\partial_y), \quad -\partial_4=\Delta(\partial_q-L\partial_x-N\partial_y). \end{aligned} \tag{1.26}$$

We now note that the space under consideration is a general V_4 satisfying Eq. (1.9); therefore, a general V_4 satisfying Eq. (1.9) is conformally equivalent to the space which arises when we set $\Delta=1$ in all the appropriate equations. Therefore, setting

$$\Delta=1, \tag{1.27}$$

we may then compute the general expressions for the connections and curvature quantities. As the calculations are simply tedious, we give only the results. It is useful to note that Eqs. (1.25) give us the existence of two functions ϕ,ψ such that

$$K=-\phi_y, \quad L=\phi_x, \quad M=\psi_y, \quad N=-\psi_x, \tag{1.28}$$

which must then obey

$$2(\partial_1\partial_2+\partial_4\partial_3)\begin{pmatrix}\phi\\ \psi\end{pmatrix}=g^{ab}\partial_a\partial_b\begin{pmatrix}\phi\\ \psi\end{pmatrix}=0. \tag{1.29}$$

It is also useful to define

$$Q\equiv\phi_x-\psi_y=L-M. \tag{1.30}$$

Then we have

$$\alpha = Q_{,3}e^1 - Q_{,2}e^4. \qquad (1.31)$$

The connections are given by

$$\begin{aligned}
&\Gamma_{41} = -\tfrac{1}{2}Q_x e^2 + \tfrac{1}{2}Q_y e^3,\\
&\Gamma_{42} = -\tfrac{1}{2}(\phi_x + \psi_y)_x e^1 - \psi_{xx}e^4,\\
&-\Gamma_{12} + \Gamma_{34} = +\tfrac{1}{2}Q_y e^1 + \tfrac{1}{2}Q_x e^4, \qquad (1.32)\\
&\Gamma_{12} + \Gamma_{34} = -\tfrac{1}{2}(3\phi_x + \psi_y)_y e^1 - \tfrac{1}{2}(\phi_x + 3\psi_y)_x e^4,\\
&\Gamma_{32} = 0, \quad \Gamma_{31} = -\phi_{yy}e^1 - \tfrac{1}{2}(\phi_x + \psi_y)_y e^4.
\end{aligned}$$

The hellish components of the conformal tensor vanish, while the heavenly ones are given by

$$\begin{aligned}
&C^{(5)} = 2\psi_{xxx}, \quad C^{(4)} = \tfrac{1}{2}(\phi_x + 3\psi_y)_{xx}, \qquad (1.33)\\
&C^{(3)} = (\phi_x + \psi_y)_{xy}, \quad C^{(2)} = \tfrac{1}{2}(3\phi_x + \psi_y)_{yy}, \quad C^{(1)} = 2\phi_{yyy}.
\end{aligned}$$

Lastly, the Ricci tensor components are given explicitly by

$$\begin{aligned}
&R_{11} = -Q_{,13} - \tfrac{1}{2}Q_{,3}Q_{,3}, \quad R_{24} = \tfrac{1}{2}Q_{,22}, \quad R_{22} = 0,\\
&R_{14} = Q_{,12} + \tfrac{1}{2}Q_{,2}Q_{,3}, \quad R_{12} = -\tfrac{1}{2}Q_{,23}, \quad R_{23} = 0, \qquad (1.34)\\
&R_{44} = Q_{,42} - \tfrac{1}{2}Q_{,2}Q_{,2}, \quad R_{13} = -\tfrac{1}{2}Q_{,33}, \quad R_{33} = 0,
\end{aligned}$$

and

$$R = 0.$$

It is worthwhile to point out that if $Q = 0$, we have a function Θ such that

$$\phi = \Theta_y, \quad \psi = \Theta_x, \quad Q = 0, \qquad (1.35)$$

and this manifold becomes identical with that of the most general strong heavens discussed in I, so that this is a direct generalization.

We now want to point out some solutions of Eqs. (1.29) first writing out those equations in full:

$$\{\phi_y\partial_x\partial_x + \psi_x\partial_y\partial_y - (\phi_x + \psi_y)\partial_x\partial_y + \partial_x\partial_p + \partial_y\partial_q\}\begin{pmatrix}\phi\\ \psi\end{pmatrix} = 0. \qquad (1.36)$$

[Again note that under the conditions of Eq. (1.35) these equations reduce to the heavenly equation discussed in I.] Reduction to one equation may be accomplished by the ansatz[5]

$$\psi = J(\phi), \qquad (1.37)$$

where J is an arbitrary, sufficiently differentiable function of one variable. Equations (1.36) become then more manageable but still not solvable in general. If we now go further to the special case $\phi_{xp} + \phi_{yq} = 0$, $J'' = 0$, the most general solution is then

$$\phi = F[x + G(kx + y)], \quad \psi = k\phi, \qquad (1.38)$$

where F and G are arbitrary, sufficiently differentiable functions of one variable and $k = J'$ is a constant.

One may now explicitly calculate the components of the curvature tensor and determine the algebraic type of the corresponding conformal tensor. For convenience we set

$$a = G'''F', \quad b = 3G''F'', \quad c = F''', \quad d = G'. \qquad (1.39)$$

The conformal invariants are then

$$\overset{2}{C} = C_{ABCD}C^{ABCD} = -bc/2, \quad \overset{3}{C} = C_{ABCD}C^{CDEF}C_{EF}{}^{AB} = -3ac^2/8. \qquad (1.40)$$

We may also look at the equation for the P-spinor itself. Taking $z = K^1/K^2$ as the ratio of the two components, we have

$$0 = 2C_{ABCD}K^AK^BK^CK^D = (K_2)^4\{C^{(5)}z^4 + 4C^{(4)}z^3 + 6C^{(3)}z^2 + 4C^{(2)}z + C^{(1)}\}. \qquad (1.41)$$

With Eqs. (1.34) and (1.38) we have, with $w = 1/z$ for convenience,

$$(z + k)\{(a + db + d^3c)(w + k)^3 + (b + 3d^2c)(w + k)^2 + 3dc(w + k) + c\} = 0. \qquad (1.42)$$

The following table shows the possible algebraic types:

$$c = F''' = 0: \begin{cases} G'' = 0, & \text{conformally flat, } [-]\times[-]-d\alpha = 0,\\ G'' \neq 0: \begin{cases} G''' = 0, & \\ G''' \neq 0: \begin{cases} F'' = 0, & III\times[-],\\ & N\times[-]-\alpha = 0 \text{ (strong heaven)},\\ F'' \neq 0, & III\times[-],\end{cases}\end{cases}\end{cases}$$

$$c = F''' \neq 0: \begin{cases} G''' = 0: \begin{cases} G'' = 0, & III\times[-],\\ G'' \neq 0, & G\times[-],\end{cases}\\ G''' \neq 0: c + (4b^3)/(27a^2) \begin{cases} = 0, & II_G\times[-],\\ \neq 0, & G\times[-].\end{cases}\end{cases}$$

Note that type $D\times[-]$ cannot be obtained from this particular class of solutions. We have used

$$d\alpha = Q_{xy}(dy\wedge dq - dx\wedge dp) + Q_{xx}\,dx\wedge dq - Q_{yy}\,dy\wedge dp, \quad Q = \phi_x - \psi_y = F'.$$

Also note that the case of type $N\times[-]$ is really just another way of writing a standard strong heaven since α vanishes.

2. CONFORMAL KILLING VECTORS IN STRONG HEAVEN

We intend to determine, as explicitly as possible, the constraints on a heavenly space imposed by the existence of Killing vectors, and vice versa. We work with the "canonical Θ-formalism" of strong heaven and take the equations as

$$E_{ab}=K_{(a;b)}-2\chi g_{ab}=0. \tag{2.1}$$

We recall, in addition, that heavenly spaces are determined by key functions Θ which satisfy the heavenly equation

$$\Theta_{xx}\Theta_{yy}-(\Theta_{xy})^2+\Theta_{xp}+\Theta_{yq}=0. \tag{2.2a}$$

The tetrad then takes the form

$$\begin{aligned}&e^1=dp, \quad -e^4=dq,\\&e^2=dx-\Theta_{yy}dp+\Theta_{xy}dq,\\&-e^3=dy+\Theta_{xy}dp-\Theta_{xx}\,dq,\\&\partial_2=\partial_x, \quad -\partial_3=\partial_y,\\&\partial_1=\partial_p+\Theta_{yy}\partial_x-\Theta_{xy}\partial_y,\\&-\partial_4=\partial_q-\Theta_{xy}\partial_x+\Theta_{xx}\partial_y.\end{aligned} \tag{2.2b}$$

For more details see Paper I. For $a,b=2,3$ in Eqs. (2.1) we find

$$\partial_x K_2=0=-\partial_y K_3, \quad \partial_x K_3=\partial_y K_2. \tag{2.3}$$

We introduce a polynomial

$$A\equiv\alpha x^3y^3/36+\beta_1x^3y^2/12+\gamma_1x^2y^3/12, \tag{2.4a}$$

with

$$A^{(1)}=A_{xy}, \quad A^{(2)}=A_{xxyy}, \tag{2.4b}$$

and

$$K_2=A_x^{(2)}=\alpha y+\beta_1, \quad K_3=A_y^{(2)}=\alpha x+\gamma_1, \tag{2.4c}$$

where α, β_1, and γ_1 are unknown functions of p and q only.

Proceeding to another triple of the equations, we find that $E_{13}=-\partial_y(K_1+\Sigma_y-A_p^{(2)})=0$, from which we have the existence of a function T such that

$$K_1+\Sigma_y=A_p^{(2)}+T, \quad T_y=0, \tag{2.5a}$$

where we use Σ as an abbreviation for

$$\Sigma=\Theta_xA_y^{(2)}+\Theta_yA_x^{(2)}-3\Theta A_{xy}^{(2)}. \tag{2.5b}$$

Likewise we have that $E_{24}=\partial_x(K_4+\Sigma_x-A_q^{(2)})=0$, from which

$$K_4+\Sigma_x=A_q^{(2)}+S, \quad S_x=0. \tag{2.5c}$$

Then we manipulate

$$E_{12}-E_{34}=\partial_x(K_1+\Sigma_y+A_{yyq}^{(1)})+\partial_y(K_4+\Sigma_x+A_{xxp}^{(1)})=0. \tag{2.6}$$

Inserting the results from Eqs. (2.5) into this equation, we have

$$\begin{aligned}&\partial_x(T+2A_{yyq}^{(1)})+\partial_y(S+2A_{xxp}^{(1)})=0,\\&\partial_y(T+2A_{yyq}^{(1)})=0=\partial_x(S+2A_{xxp}^{(1)}).\end{aligned} \tag{2.7}$$

This triple of equations now has exactly the same format as Eqs. (2.3) which resulted from the first triple of Killing equations. Their solution therefore is given by a new polynomial

$$B\equiv\lambda x^2y^2/2+\beta_2x^2y/2+\gamma_2xy^2/2, \quad B^{(1)}\equiv B_{xy}, \tag{2.8}$$

and the equations

$$T+2A_{yyq}^{(1)}=B_y^{(1)}, \quad S+2A_{xxp}^{(1)}=-B_x^{(1)},$$

where, of course, λ, β_2, and γ_2 are new unknown functions of p and q only. We may conveniently insert this information into Eqs. (2.5), for K_1 and K_4, by introducing the auxiliary functions

$$\begin{aligned}&\Omega_1=\Sigma-A_{xp}^{(1)}+2A_{yq}^{(1)}-B^{(1)},\\&\Omega_2=\Sigma+2A_{xp}^{(1)}-A_{yq}^{(1)}, \quad W\equiv\Omega_2-\Omega_1.\end{aligned} \tag{2.9}$$

(We note that W is simply a third order polynomial in x and y.) We have then that

$$K_1=\partial_3\Omega_1, \quad K_4=-\partial_2\Omega_2, \tag{2.10}$$

which is a form suitable for use in the next triple of equations. Using the values of the commutators $[\partial_a,\partial_b]$ and a procedure very similar to that used for the previous triple, we find that

$$\begin{aligned}&\partial_1\Omega_1+\Theta_{yy}W_x-\Theta_yW_{xy}+\Theta W_{xyy}=M,\\&\partial_4\Omega_2+\Theta_{xx}W_y-\Theta_xW_{xy}+\Theta W_{xxy}=N.\end{aligned} \tag{2.11a}$$

where, again, we find three simple equations in the same format:

$$\begin{aligned}&\partial_x(M-A_{yyyqq}+2B_{yyq})+\partial_y(N+3A_{xxxpp}+2B_{xxp})=0,\\&\partial_y(M-3A_{yyyqq}+2B_{yyq})=0=\partial_x(N+3A_{xxxpp}+2B_{xxp}).\end{aligned} \tag{2.11b}$$

We may therefore introduce a third polynomial

$$C\equiv3\xi xy+\beta_3x+\gamma_3y, \tag{2.12a}$$

with ξ, β_3, and γ_3 unknown functions of p and q only and write, as before,

$$M-3A_{yyyqq}+2B_{yyq}=C_y, \quad N+3A_{xxxpp}+2B_{xxp}=-C_x. \tag{2.12b}$$

Inserting Eqs. (2.12b) into Eqs. (2.10), we determine the consistency requirements on our unknown functions, which, after considerable rearrangement of terms, become simply

$$\begin{aligned}&\partial_x(\Xi+V-D+2\alpha\Lambda)=-4\Theta\alpha_p,\\&\partial_y(\Xi+V+D+2\alpha\Lambda)=+4\Theta\alpha_q,\end{aligned} \tag{2.13}$$

where V and D are just polynomials in x and y given by

$$\begin{aligned}&V\equiv A_{ppxx}-A_{qqyy}+(B_{xp}+B_{yq})/2,\\&D\equiv2(A_{ppxx}-A_{pqxy}+A_{qqyy})+3(B_{xp}-B_{yq})/2+C,\end{aligned} \tag{2.14}$$

while Ξ and A carry all the Θ dependence. The quantity Ξ is just the Θ-dependent part derived in a straightforward way:

$$\begin{aligned}\Xi \equiv{}& \Theta_p A_x^{(2)} - \Theta_q A_y^{(2)} + \Theta_x(A_{xyp}^{(1)} - 2A_{yyq}^{(1)} + B_y^{(1)})\\ &+\Theta_y(2A_{xxp}^{(1)} - A_{xyq}^{(1)} + B_x^{(1)})\\ &+\Theta(4A_{yq}^{(2)} - 4A_{xp}^{(2)} - 3B_{xy}^{(1)}).\end{aligned} \tag{2.15}$$

However, Λ is an implicit function of Θ defined by

$$\Lambda_x = \Theta_q - \Theta_{,4}, \quad \Lambda_y = -\Theta_p - \Theta_{,1}, \tag{2.16a}$$

whose existence is assured because Eq. (2.2a) can simply be rewritten as

$$\partial_x(\Theta_p + \Theta_{,1}) + \partial_y(\Theta_q - \Theta_{,4}) = 0. \tag{2.16b}$$

In principal these equations now determine all conformal Killing vectors. However, $E_{12} + E_{34}$ could still tell us something if we knew more about the function χ. The heavenly nature of the space in question makes the constraint relations between Θ and χ especially strong. To see this, we look at the formal integrability conditions for Eqs. (2.1)[6]:

$$\pounds_K \Gamma_{abc} \equiv K_{a;cb} + R^d{}_{bac} K_d = (-g_{cb}\chi_{,a} + g_{ac}\chi_{,b} + g_{ab}\chi_{,c}) \tag{2.17}$$

and

$$\pounds_K R_{abcd} = g_{ca}\chi_{;bd} - g_{cb}\chi_{;ad} - g_{da}\chi_{;bc} + g_{db}\chi_{;ac}. \tag{2.18}$$

By remembering that, in heaven, R_{ab}, and therefore R, vanish, Eq. (2.18) requires that

$$J_{ab} \equiv \chi_{;ab} = 0. \tag{2.19}$$

What constraints do these relations put on Θ and χ? We see immediately, from J_{22}, J_{23}, and J_{33}, that

$$\chi = \beta_3 x + \gamma_3 y + \delta_3, \tag{2.20}$$

where β_3, γ_3, and δ_3 are as yet arbitrary functions of p and q only. From J_{21}, J_{31}, J_{24}, and J_{34} we find that a function $\tau_3 = \tau_3(p, q)$ exists such that

$$\beta_3 = \tau_{3q}, \quad \gamma_3 = -\tau_{3p}, \quad \chi = \tau_{3q} x - \tau_{3p} y + \delta_3, \tag{2.21}$$

and the following equation must be satisfied:

$$\begin{aligned}\tau_{3q}\Theta_y + \tau_{3p}\Theta_x = P_3 \equiv{}& \tau_{3qq}x^2/2 - \tau_{3pq}xy + \tau_{3pp}y^2/2\\ &+ \sigma_{3q}x - \sigma_{3p}y + \kappa_3,\end{aligned} \tag{2.22}$$

where σ_3 and κ_3 are new functions of p and q only, and we have used the nontrivial equation $J_{14} = J_{41}$. The last triple of equations can then be manipulated to yield

$$\begin{aligned}\tau_{4q}\Theta_y + \tau_{4p}\Theta_x ={}& \tau_{4qq}x^2/2 - \tau_{4pq}xy + \tau_{4pp}y^2/2\\ &+ \mu_4 x + \nu_4 y + \kappa_4,\end{aligned} \tag{2.23}$$

where $\tau_4 \equiv -\sigma_3 + \delta_3$ and μ_4, ν_4, κ_4 are new functions of p and q.

Now suppose that τ_3 is not a constant. (We assume therefore that at least $\tau_{3q} \neq 0$.) We may then integrate Eq. (2.22) to obtain

$$\Theta = F(\chi; p, q) + (y/\tau_{3q})Q_3(x, y; p, q), \tag{2.24}$$

where F is an arbitrary, sufficiently differentiable function of three variables and Q_3 is a specific second order polynomial in x and y constructed from P_3. Notice that this implies that all fourth partial derivatives of Θ(with respect to x and y) are proportional and, therefore, that the space is of type $N\times[-]$ if χ is a nontrivial function of x or y. We may now, however, insert this equation for Θ into Eq. (2.23), obtaining

$$(\tau_{4p}\tau_{3q} - \tau_{4q}\tau_{3p})F_\chi = R_3(\chi; p, q), \tag{2.25}$$

where R_3 is a specific second order polynomial in χ. Therefore, assuming $F_{\chi\chi\chi\chi} \neq 0$ (vanishing of this would imply that the space is flat), τ_4 must be a function of τ_3. Only if the function is linear, however, can the two equations be made consistent, but, of course, the space is then either of type $N\times[-]$ or flat.

On the other hand, if τ_3 is a constant, then σ_3 and κ_3 must vanish, while τ_4 reduces to $\delta_3 = \chi = \chi(p, q)$. However, assuming χ nonconstant, one may integrate Eq. (2.23) and obtain a completely analogous equation to Eq. (2.24):

$$\Theta = G(\chi_q x - \chi_p y; p, q) + (y/\chi_q)Q_5(x, y; p, q), \tag{2.26}$$

where Q_5 is a second order polynomial in x and y. It then follows again that the space must be of type $N\times[-]$ or flat. We see therefore that if we desire a more general algebraic type only constant χ can be allowed. Therefore, taking $\chi = \chi_0$ as a constant, we may integrate the tenth and last Killing equation:

$$E_{12} + E_{34} = 4\alpha_p y - 4\alpha_q x + 4(\beta_{1p} - \gamma_{1q} + \lambda - \chi_0) = 0. \tag{2.27}$$

We see that $\alpha \equiv \alpha_0$ must be a constant. Referring back to Eqs. (2.14), we see that then D_{xy} must vanish. Together with the rest of Eq. (2.27) this requires the existence of a function $\phi_1 = \phi_1(p, q)$ such that

$$\begin{aligned}&\beta_1 = \phi_{1q} + \rho_0 p, \quad \gamma_1 = \phi_{1p} - \rho_0 q,\\ &\beta_{2p} - \gamma_{2q} = -2\xi, \quad \rho_0 \equiv (\chi_0 - \lambda_0)/2,\end{aligned} \tag{2.28}$$

with $\lambda \equiv \lambda_0$ also constrained to be a constant. Now, however, we return to Eqs. (2.17)—the rest of our consistency conditions—and consider their anti-self-dual part, which is

$$K_{\dot A\dot B;d} = S_{\dot A\dot B}{}^c{}_d\,\chi_{,c} = 0, \quad \text{with } K_{\dot A\dot B} \equiv S_{\dot A\dot B}{}^{cd}K_{c;d}. \tag{2.29}$$

We easily calculate that

$$K_{\dot1\dot1} = -4\,\xi, \quad K_{\dot1\dot2} = -4\alpha_0, \quad K_{\dot2\dot2} = 8(\rho_0 + \lambda_0). \tag{2.30}$$

These will then satisfy Eqs. (2.29) if $\xi \equiv \xi_0$ is a constant, which implies there is a further function $\phi_2 = \phi_2(p, q)$ such that

$$\beta_2 = \phi_{2q} - \xi_0 p, \quad \gamma_2 = \phi_{2p} + \xi_0 q. \tag{2.31}$$

One may now verify that the rest of Eqs. (2.17) are also satisfied. Equations (2.14) may now be integrated into just one equation:

$$\begin{aligned}\Xi + 2\alpha_0\Lambda = {}&-(x\partial_q - y\partial_p)^3\phi_1/6 + (x\partial_q - y\partial_p)^2\phi_2/2\\ &- \beta_3 x + \gamma_3 y + \epsilon,\end{aligned} \tag{2.32}$$

where ϵ is an arbitrary function of p and q and we summarize below all the relevant equations pertaining to the above master equation. The Killing vector $\mathcal{K} = K_a e^a$ is here being thought of as $\mathcal{K} = K^p\partial_p + K^q\partial_q + K^x\partial_x + K^y\partial_y$ because the coefficients are much simpler:

$$\begin{aligned}&\Xi \equiv K^p\Theta_p + K^q\Theta_q + L_1\Theta_x - L_2\Theta_y + (2\rho_0 + 6\chi_0)\Theta,\\ &K^p = \alpha_0 y + \phi_{1q} + \rho_0 p, \quad -K^q = \alpha_0 x + \phi_{1p} - \rho_0 q,\\ &K^x = L_1 + 2\alpha_0\Theta_y, \quad -K^y = L_2 + 2\alpha_0\Theta_x,\end{aligned}$$

$$L_1 \equiv -(\phi_{1pq} + \rho_0 - 2\chi_0)x + \phi_{1pp}y + \phi_{2p} + \xi_0 q, \qquad (2.33)$$

$$L_2 \equiv \phi_{1qq}x - (\phi_{1pq} - \rho_0 + 2\chi_0)y - \phi_{2q} + \xi_0 p,$$

$$\Lambda_x \equiv 2\Theta_q - \Theta_{xy}\Theta_x + \Theta_{xx}\Theta_y, \quad -\Lambda_y \equiv 2\Theta_p + \Theta_{yy}\Theta_x - \Theta_{xy}\Theta_y.$$

Considering this form, we see that all the Killing equations have been reduced to one partial differential equation relating Θ, the unknown functions ϕ_1, ϕ_2, β_3, γ_3, ϵ and the constants α_0, ρ_0, ξ_0, χ_0. It is clear, at least when $\alpha_0 = 0$, that there are no nonzero Killing vectors for the most general function Θ. On the other hand, Eqs. (2.32) and (2.33) can be very useful to determine the symmetries of a given metric, or a metric which has desired symmetries.

As a trivial example we note that in order for ∂_p to be a Killing vector we must have $K^p = 1$, $K^q = 0 = K^x = K^y$. Inserting this into our equations, we find that they integrate to

$$\Theta = f(x, y, q) + \bar{\beta}x + \bar{\gamma}y + \bar{\delta},$$

where $\bar{\beta}$, $\bar{\gamma}$, and $\bar{\delta}$ are functions of p and q only and f is arbitrary; this is just sufficient to insure that $\partial_p g_{\mu\nu} = 0$, as one would expect. It is, however, not true that there is no (implicit) dependence of the metric on the functions $\bar{\beta}$ and $\bar{\gamma}$ since Θ must still satisfy the heavenly equation (2.2a), which gives the dependence on $\bar{\beta}_p$ and $\bar{\gamma}_q$ of the function $f(x, y, q)$.[7] It is also somewhat interesting to consider the case where both ∂_p and ∂_q are Killing vectors. Equation (2.33) then shows that

$$\Theta = Z(x, y) + (\bar{\tau}_q + k^2 p/2)x - (\bar{\tau}_p - k^2 q)y + \bar{\epsilon}, \qquad (2.34)$$

and

$$Z_{xx}Z_{yy} - (Z_{xy})^2 = -k^2,$$

where k^2 is a complex constant. This case will be completely solved in Sec. 4.

For some less trivial examples we look first at a class of metrics first discussed in I:

$$\Theta = [\beta/2\alpha(\alpha - 1)]x^\alpha y^{1-\alpha}, \quad \alpha \neq 0, 1. \qquad (2.35)$$

We note that the excepted cases, $\alpha = 0, 1$, correspond to flat space, while, as is shown in I, $\alpha = 2, -1$ are of type $D \times [-]$. All other values of α lead to spaces of type $\mathrm{II}_G \times [-]$. If we first assume also that $\alpha \neq 2, -1$ and utilize Eq. (2.32), we find that there are exactly three Killing vectors:

$$A_1 = (\alpha + 1)(p\partial_p - x\partial_x) + (\alpha - 2)(q\partial_q - y\partial_y),$$

$$B_1 = \partial_p, \quad C_1 = \partial_q, \qquad (2.36)$$

with the commutation relations

$$[A_1, B_1] = -(\alpha + 1)B_1, \quad [A_1, C_1] = -(\alpha - 2)C_1, \qquad (2.37)$$

$$[B_1, C_1] = 0.$$

We note that the case $\alpha = 1/2$ is special because then the vectors can be renormalized so that the algebra is (a complex form of) the algebra for the Euclidean group in two dimensions.

The cases $\alpha = 2, -1$ are essentially the same (modulo renaming of coordinates), and so we mention only the case $\alpha = 2$. Here the group is four-dimensional:

$$A_2 = p\partial_p - x\partial_x, \quad B_2 = \partial_p, \qquad (2.38)$$

$$C_2 = \partial_q, \quad D_2 = p\partial_q - y\partial_x,$$

such that

$$[A_2, B_2] = -B_2, \quad [A_2, C_2] = 0, \quad [A_2, D_2] = D_2 \qquad (2.39)$$

$$[B_2, C_2] = 0, \quad [B_2, D_2] = C_2, \quad [C_2, D_2] = 0.$$

This is a solvable algebra with C_2 in the center.[8]

The last case to be considered here is

$$\Theta = kx^2/yq^3 - x^2y/4q. \qquad (2.40)$$

It is shown in Sec. 4 that this metric and the one in the previous paragraph are the simplest members of two branches of solutions which contain type $D \times [-]$ spaces. They are therefore of some special interest. For the space determined by Eq. (2.40) the Killing vectors are [again determined quite simply from Eq. (2.32)]

$$L_3 = -q\partial_q + y\partial_y, \quad A_3 = p\partial_p - q\partial_q - x\partial_x + y\partial_y, \qquad (2.41)$$

$$B_3 = \partial_p, \quad C_3 = p^2\partial_p/2 - pq\partial_q + (qy - px)\partial_x + py\partial_y,$$

$$[L_3, A_3] = 0, \quad [L_3, B_3] = 0, \quad [L_3, C_3] = 0, \qquad (2.42)$$

$$[A_3, B_3] = -B_3, \quad [A_3, C_3] = C_3, \quad [B_3, C_3] = A_3.$$

This algebra is isomorphic to a complex form of the algebra for the group which is the direct product of time translations and the usual spherical symmetry group. That is to say, (in a complex way) this is just the Killing algebra shared by the Schwarzschild and NUT solutions.

3. MASSLESS SPINOR FIELDS IN HEAVEN

We first consider a $D(0, s)$ object (spinorial field for spin s) subject to the usual constraint

$$\nabla^C{}_{\dot{B}}\Psi_{CA_1\cdots A_{2s-1}} = g^{aC}{}_{\dot{B}}\nabla_a\Psi_{CA_1\cdots A_{2s-1}} = 0, \qquad (3.1)$$

where $\Psi_{C_1\cdots C_{2s}}$ is totally symmetric in its indices. Such a field describes a general (massless) particle of spin s. Utilizing the connections in the Θ version of the heavenly metric [see Eqs. (2.2) and Paper I], we have, with $\dot{B} = 2$,

$$\partial_y\Psi_{1A_1\cdots A_{2s-1}} = \partial_x\Psi_{2A_1\cdots A_{2s-1}}, \qquad (3.2)$$

which implies the existence of a spinor $\xi_{A_1\cdots A_{2s-1}}$ such that

$$\Psi_{1A_1\cdots A_{2s-1}} = \partial_x\xi_{A_1\cdots A_{2s-1}} \qquad (3.3)$$

$$\Psi_{2A_1\cdots A_{2s-1}} = \partial_y\xi_{A_1\cdots A_{2s-1}}.$$

We may facilitate further matters greatly by using a "heavenly spinorial derivative"

$$\delta_A : \begin{cases} \delta_1 \equiv \partial_x, \\ \\ \delta_2 \equiv \partial_y, \end{cases} \qquad [\delta_A, \delta_B] = 0. \qquad (3.4)$$

We then have that

$$\Psi_{A_1\cdots A_{2s}} = \delta_{A_1}\xi_{A_2\cdots A_{2s}}. \qquad (3.5)$$

However, the symmetry of Ψ allows us to repeat this process:

$$\delta_{A_1}\xi_{A_2A_3\cdots A_{2s}} = \delta_{A_2}\xi_{A_1A_3\cdots A_{2s}}. \qquad (3.6)$$

Repeating this process $2s - 1$ more times, we find that there must be a single potential function[9] H such that

$$\Psi_{A_1 \cdots A_{2s}} = \delta_{A_1} \cdots \delta_{A_{2s}} H. \tag{3.7}$$

We now consider Eqs. (3.1) with $\mathring{B} = 1$, which becomes

$$(\nabla_1\nabla_2 + \nabla_4\nabla_3)\xi_{A_1 \cdots A_{2s-1}} = (\nabla_2\nabla_1 + \nabla_3\nabla_4)\xi_{A_1 \cdots A_{2s-1}} = 0, \tag{3.8}$$

where the form of the heavenly Riemann tensor guarantees that the two expressions are equal to each other. We may therefore rewrite the equation as

$$\nabla^a\nabla_a\xi_{A \cdots A_{2s-1}} = \nabla^a\nabla_a\delta_{A_1} \cdots \delta_{A_{2s-1}} H = 0, \tag{3.9}$$

which is then the subsidiary condition that H must satisfy.

We note that for the case $s = 1/2$ this merely says that H must satisfy the (curved space) d'Alembert equation[10]—$\Box H = 0$. We may, however, for larger values of s, attempt to commute $\nabla^a\nabla_a$ and δ_A. To do this, we note that the heavenly connections may be written in a most useful form by the use of our new notation:

$$\Gamma_{AB1} = \delta_A\delta_B\delta_2\Theta, \quad \Gamma_{AB4} = \delta_A\delta_B\delta_1\Theta, \tag{3.10}$$

while the other Γ's vanish. It then follows that

$$\begin{aligned}\tfrac{1}{2}\nabla^a\nabla_a\xi_{A_1 \cdots A_{2s-1}} = {} & (\partial_1\partial_2 + \partial_4\partial_3)\xi_{A_1 \cdots A_{2s-1}} \\ & + T^{CD}{}_{A_1}\delta_C\xi_{DA_2 \cdots A_{2s-1}} \\ & + \cdots + T^{CD}{}_{A_{2s-1}}\delta_C\xi_{DA_1 \cdots A_{2s-2}},\end{aligned} \tag{3.11}$$

where

$$T^{CD}{}_A = \delta^C\delta^D\delta_A\Theta \tag{3.12}$$

is just a useful way of writing the connections involved, using Eqs. (3.10). It is also useful because we easily calculate that

$$[\partial_1\partial_2 + \partial_4\partial_3, \delta_A] = -T^{CD}{}_A\delta_C\delta_D. \tag{3.13}$$

We now have that

$$\begin{aligned}0 = {} & \delta_{A_1}(\partial_1\partial_2 + \partial_4\partial_3)\delta_{A_2} \cdots \delta_{A_{2s-1}} H \\ & + T^{CD}{}_{A_2}\delta_C\delta_D\delta_{A_1} \cdots \delta_{A_{2s-1}} H \\ & + \cdots + T^{CD}{}_{A_{2s-1}}\delta_C\delta_D\delta_{A_1} \cdots \delta_{A_{2s-2}} H.\end{aligned} \tag{3.14}$$

In the case $s = 1$ (electromagnetism) this merely says

$$0 = 2\delta_A(\partial_1\partial_2 + \partial_4\partial_3)H = \delta_A\nabla^a\nabla_a H. \tag{3.15}$$

By following the "philosophy" propounded in I, a real electromagnetic field can be characterized by a 2-form

$$\begin{aligned}&\omega \equiv 2f_{AB}S^{AB}, \quad d\omega = 0, \\ &\bar{\omega} \equiv 2\bar{f}_{\mathring{A}\mathring{B}}S^{\mathring{A}\mathring{B}}, \quad d\bar{\omega} = 0,\end{aligned} \tag{3.16}$$

where we have just used f_{AB} to represent the special case of $\Psi_{A_1 \cdots A_{2s}}$ for $s = 1$. On a real manifold ω and $\bar{\omega}$ are related by complex conjugation; but, a (purely) heavenly electromagnetic field has $\bar{\omega} = 0$ (similarly $\omega = 0$ for a hellish electromagnetic field). We then note that Eq. (3.15) implies that $\Box H = f_p(p, q)$, which, regauging H by letting H go to $H + xf(p, q)$, becomes

$$0 = \Box H = 2(\partial_1\partial_2 + \partial_4\partial_3)H, \quad f_{AB} = \delta_A\delta_B H. \tag{3.17}$$

For reference we also point out that we can rewrite this directly in terms of the self-dual electromagnetic 2-form—Eq. (3.16):

$$\omega = -d(4H_y dp - 4H_x dq). \tag{3.18}$$

Also the invariant of the field is

$$\mathcal{J} \equiv 4f_{AB}f^{AB} = B[H_{xx}H_{yy} - (H_{xy})^2]. \tag{3.19}$$

Equations (3.17)—(3.19) now constitute a complete solution to the problem of a strong heaven with purely heavenly electromagnetic field. It is also worthwhile to point out that the usual electromagnetic energy—momentum tensor E_{ab} vanishes if the field is self-dual. That this is true can be seen by a direct calculation in 4-space but is much more easily seen if one writes the Einstein equations in spinor form:

$$C_{ab} = 2E_{ab} \longleftrightarrow C_{AB\mathring{C}\mathring{D}} = -8f_{AB}f_{\mathring{C}\mathring{D}}. \tag{3.20}$$

From the form of this equation it is quite clear that if a purely heavenly (or purely hellish) electromagnetic field is the only matter present, then $C_{AB\mathring{C}\mathring{D}}$ must vanish and therefore the coupling of the curvature to the electromagnetic field is eliminated. [There is, of course, coupling in the reverse direction, via the connections in Eq. (3.17).]

For spins greater than 1 the repetition of the process leading to Eq. (3.14)—commuting more than one derivative past $\partial_1\partial_2 + \partial_4\partial_3$—leads to the introduction into the formulas of derivatives of $T^{CD}{}_A$ or, if one prefers to use covariant derivatives, components of C_{ABCD}, which, in general, does not yield particularly simple equations nor does it allow convenient regauging, such as was done to obtain Eq. (3.17). Some words should be said, however, about certain special cases. We see that Eqs. (3.10) make the connections look, more or less, as if they had $s = 3/2$ although this is not exactly so because of their mixed nature. Also for $s = 2$ there is a special case, the gravitational field itself. We easily see that

$$C_{ABCD} = \delta_A\delta_B\delta_C\delta_D\Theta, \tag{3.20}$$

showing the actual role that Θ plays as the potential for the gravitational field. Of course, the heavenly equation is simply a regauged and thrice integrated form of Eq. (3.9) for this special case. Note, however, that the standard spinorial form for the Bianchi identities, when $R_{ab} = 0$ is just

$$\nabla^E{}_{\mathring{F}}C_{EBCD} = 0, \tag{3.21}$$

which is just Eq. (3.1) for the case $s = 2$. We may also note that Eq. (3.9) for this special case of a spin 2 field equal to the conformal curvature itself allows considerable simplification because the Θ in Eqs. (3.20) and (3.12) is the same:

$$\delta_{A_1}\delta_{A_2}(\partial_1\partial_2 + \partial_4\partial_3)\delta_{A_3}\Theta = 0. \tag{3.22}$$

However, Eq. (2.2a), which Θ is constrained to satisfy, implies

$$(\partial_1\partial_2 + \partial_4\partial_3)\delta_{A_3}\Theta = 0,$$

so that this is the mechanism by which the Bianchi equations are satisfied.

4. MORE PARTICULAR SOLUTIONS OF THE HEAVENLY EQUATION

Looking for interesting solutions of Eq. (2.2a) we first consider the logical special case in which $\Theta_p = \Theta_q = 0$. In this case we clearly have at least two independent Killing vectors ∂_p and ∂_q and, as we will see, the solution always describes a space which is algebraically special. The heavenly equation—Eq. (2.2a)—reduces to just the classical equation for a developable surface in two independent variables. There are[11] two first integrals describable as

$$\begin{aligned} &\text{(a) } \Theta_y - F(\Theta_x) = 0, \\ &\text{(b) } y\Theta_y + x\Theta_x + G(\Theta_x) - \Theta = 0, \end{aligned} \tag{4.1}$$

where F and G are arbitrary, sufficiently differentiable functions of one variable. The general solution may also be written in the form

$$\Theta = \Theta(x,y) = hx + F(h)y + G(h), \tag{4.2a}$$

where $h = h(x,y)$ is determined by the equation

$$x + yF'(h) + G'(h) = 0. \tag{4.2b}$$

To show that all solutions so generated are algebraically special, we calculate the components of the conformal curvature tensor, which may be written as

$$C^{(J)} = 2\partial_x\partial_x(H^{5-j}\Theta_{xx}), \quad j = 1, \ldots, 5, \tag{4.3}$$

where

$$H = H(x,y) = \begin{cases} F', & \text{solution taken from Eq. (4.1a)}, \\ -(x+G')/y, & \text{solution from Eq. (4.1b)}. \end{cases} \tag{4.4}$$

One may then calculate the invariants of the conformal tensor, with the result that [see Eq. (1.42)]

$$\begin{aligned} &\overset{2}{C} = 6(H_x\Theta_{xx})^2, \quad \overset{3}{C} = 6(H_x\Theta_{xx})^3, \\ &2\Delta \equiv (\overset{2}{C})^3 - 6(\overset{3}{C})^2 = 0, \end{aligned} \tag{4.5}$$

thus guaranteeing algebraic degeneracy; i.e., there is no possibility of type $G\times[-]$. However, we can do more by looking at the equation for the P spinor as the equation the degeneracy of whose roots determines the type of the solution [see Eq. (1.41)]. Inserting values from Eq. (4.3), we find that there is always a double root at $z = -H$. There are basically three cases:

$$\begin{aligned} &\Theta_{xx}H_x = 0 \quad \text{implies type } N\times[-] \\ &\Theta_{xx}H_x \neq 0, \\ &(\Theta_{xx}H_{xx} + 2\Theta_{xxx}H_x)^2 - 3\Theta_{xx}\Theta_{xxxx}(H_x)^2 \begin{array}{l} = 0, \quad D\times[-], \\ \neq 0, \quad \mathrm{II}_G\times[-]. \end{array} \end{aligned} \tag{4.6}$$

Having found all solutions independent of p and q, we generalize to all solutions where the metric coefficients are independent of p and q, given by Eq. (2.34). The general solution is generated by the set of equations

$$\begin{aligned} &Z = (ky - h)x + F(2ky - h) + G(h), \\ &x = G'(h) - F'(2ky - h), \end{aligned} \tag{4.7}$$

where $h = h(x,y)$ and as usual F and G are arbitrary, sufficiently differentiable functions of one variable. Note that if either F'' or G'' vanish, then it is automatic that only $C^{(5)}$ is nonvanishing and we have type $N\times[-]$ again. However, these solutions are in fact sufficiently general to include spaces of algebraically general type when $k \neq 0$. By noting that the two first integrals can be written in the form

$$y \pm iZ_x = f_\pm(x \mp iZ_y),$$

with $f_\pm$ arbitrary, the degeneracy equation may again be calculated. As it is quite complicated we content ourselves here with two examples of type $G\times[-]$.

If $F(u) = G(u) = u \ln u$ is chosen, we find that the metric components are simply (taking $k = 1$)

$$\begin{aligned} &\Theta_{xx} = -\tfrac{1}{2}\,\mathrm{sech}^2(x/2), \ \Theta_{xy} = \tanh(x/2), \\ &\Theta_{yy} = 2/y. \end{aligned} \tag{4.8}$$

The degeneracy equation then becomes

$$\begin{aligned} &w^4 + \tfrac{1}{2}\tanh^2(x/2)\,\mathrm{sech}^2(x/2)w \\ &\quad + \mathrm{sech}^2(x/2)[1 + 3\tanh^2(x/2)]/16 = 0, \end{aligned} \tag{4.9}$$

with $w = yz$, which has no multiple roots.

Another somewhat more interesting example is obtained from

$$Z = 2(x - by^3)^{3/2}y^{-1/2}, \quad b = k^{-2}/27. \tag{4.10}$$

The metric components are given by

$$\begin{aligned} &J \equiv \tfrac{3}{2}y^{-1/2}(x - by^3)^{-1/2} = \Theta_{xx}, \\ &\Theta_{xy} = -(x + 2by^3)J/y, \\ &\Theta_{yy} = (x - 4by^3)^2 J/y^2. \end{aligned} \tag{4.11}$$

Again we note that this solution is of algebraically general type, but in the limit as b goes to zero it becomes type $\mathrm{II}_G\times[-]$, being then a special case of a solution discussed in I. It is now clear that solutions of all possible algebraic types exist for the heavenly equation. It is also relevant to note that when this metric is inserted into Eq. (2.32), which determines Killing vectors, we find that ∂_p and ∂_q are the only solutions, which, of course, was obvious. However, for $b = 0$, one acquires an extra Killing vector—Eqs. (2.37) for $\alpha = \tfrac{3}{2}$.

As another example of interesting heavenly metrics we construct solutions of Eq. (2.2a) which have

$$C^{(5)} = 0 = C^{(4)} \tag{4.12a}$$

and are of type $D\times[-]$, which [given Eq. (4.12a)] is equivalent to the condition

$$3C^{(1)}C^{(3)} = 2C^{(2)}C^{(2)}. \tag{4.12b}$$

By using Eq. (3.20) for the $C^{(i)}$'s (see also I), Eq. (4.12a) requires that Θ be a third order polynomial in x such that the coefficient of x^3 is also independent of y. Inserting this form into Eq. (4.12b) leads to the following form (modulo p,q-dependent translations of x and y):

$$\Theta = \alpha x^2/y + \beta x^2 y + \gamma x y^2 + \delta y^3 + \epsilon x + \zeta y + \eta, \tag{4.13}$$

where $\alpha, \ldots, \eta$ are functions of p and q only. One then finds that

$$C^{(3)} = 8\alpha/y^3, \quad C^{(2)} = -24\alpha x/y^4, \quad C^{(1)} = 48\alpha x^2/y^5, \tag{4.14}$$

so that we must have α nonvanishing for a nontrivial solution. However, this Θ must still be constrained to satisfy Eq. (2.2a). Combining Eqs. (4.13) and (2.2a) and comparing coefficients of different powers of x and y, one finds two distinct families of solutions:

$$\begin{array}{ll}
\text{Family I} & \text{Family II} \\
\alpha = f(p), \quad \beta = 0, \quad \gamma = -\tfrac{1}{6} f'/f, & \alpha = k[q + f(p)]^{-3}, \quad \beta = -\tfrac{1}{4}(q+f)^{-1}, \\
\delta = \gamma(4\gamma - 1)q/3 + g(p), & \gamma = -2\beta f', \quad \delta = \tfrac{1}{6} f'' + \beta(f')^2 - \beta^{-1} g(p).
\end{array}$$

$$\epsilon_p + \zeta_q = -12\alpha\delta,$$

where $k \neq 0$ is a constant and $f(p)$ and $g(p)$ are arbitrary, sufficiently differentiable functions. We notice that η does not appear in these equations or in the metric and so can merely be set equal to zero without loss of generality. The metric can then be written as

$$ds^2 = 2dpdx + 2dqdy - 4\alpha y^{-3}(xdp + ydq)^2 - 4(\gamma x + 3\delta y)\,dp^2 - 4\beta y dq^2 + 8(\beta x + \gamma y)\,dp\,dq, \tag{4.16}$$

with α, β, γ and δ given by one of the sets in Eqs. (4.15). In Sec. 2 the Killing algebra was determined for the simplest members of each of these two families—$\alpha = \alpha_0$, $\beta = 0 = \gamma = \delta$ and $\alpha = -64k\beta^3$, $\beta = -\tfrac{1}{4}q^{-1}$, $\gamma = 0 = \delta$. The algebra for that member of Family II strongly suggests that it describes the heavenly version of Schwarzschild—NUT space. (See also the next section.)

5. OTHER APPROACHES TO THE QUESTION OF SOLUTIONS

If one hopes that the heavenly (hellish) solutions of the complex Einstein equations can be important as—in some sense—basic and elementary "bricks" which, through a procedure of synthesis (at present unknown), would generate physical (real) solutions, it is of some interest to reverse the question and to examine how some known physical solutions generate related complex solutions with only self-dual (or anti-self-dual) conformal curvature. Particularly useful for this purpose are the real solutions of the Einstein—Maxwell equations of type D presented by Plebański and Demiański.[12] We briefly summarize here the relevant results and then indicate how to determine the heavenly part. Let $\{p, q, \tau, \sigma\}$ be real coordinates and m, n, e_0, g_0 be real constants [interpreted as mass, NUT parameter (magnetic mass), electric charge, and magnetic charge] and ϵ and γ two real constants related to the rotation and acceleration parameters, while λ is the cosmological constant. Then, having the two polynomials

$$\begin{aligned}
\mathcal{P} &\equiv (-\lambda/6 + \gamma - g_0{}^2) + 2np - \epsilon p^2 + 2mp^3 \\
&\quad + (-\lambda/6 - \gamma - e_0{}^2)p^4, \\
\mathcal{Q} &\equiv (-\lambda/6 - \gamma + g_0{}^2) + 2nq + \epsilon q^2 + 2mq^3 \\
&\quad + (-\lambda/6 + \gamma + e_0{}^2)q^4,
\end{aligned} \tag{5.1}$$

we write down the null tetrad for the space in question:

$$\begin{aligned}
\left.\begin{matrix} e^1 \\ e^2 \end{matrix}\right\} &= \frac{1}{\sqrt{2}}\,\frac{1}{p+q}\left[\left(\frac{1+p^2q^2}{\mathcal{P}}\right)^{1/2} dp \right. \\
&\quad \left. \pm i\left(\frac{\mathcal{P}}{1+p^2q^2}\right)^{1/2} (d\sigma + q^2 d\tau)\right], \\
\left.\begin{matrix} e^3 \\ e^4 \end{matrix}\right\} &= \frac{1}{\sqrt{2}}\,\frac{1}{p+q}\left[\left(\frac{1+p^2q^2}{\mathcal{Q}}\right)^{1/2} dq \right. \\
&\quad \left. \pm \left(\frac{\mathcal{Q}}{1+p^2q^2}\right)^{1/2} (d\tau - p^2\, d\sigma)\right],
\end{aligned} \tag{5.2}$$

with metric

$$ds^2 = 2e^1e^2 + 2e^3e^4. \tag{5.3}$$

The corresponding electromagnetic field is given by

$$\begin{aligned}
\omega &= d\left(\frac{e_0 + ig_0}{1 - ipq}\,(qd\tau + ipd\sigma)\right) \\
\bar{\omega} &= d\left(\frac{e_0 - ig_0}{1 + ipq}\,(qd\tau - ipd\sigma)\right).
\end{aligned} \tag{5.4}$$

The conformal curvature tensor has only

$$\begin{aligned}
C^{(3)} &= 2\left(\frac{p+q}{1-iqp}\right)^3 \left[m + in - (e_0{}^2 + g_0{}^2)\left(\frac{p-q}{1+ipq}\right)\right], \\
\bar{C}^{(3)} &= 2\left(\frac{p+q}{1+ipq}\right)^3 \left[m - in - (e_0{}^2 + g_0{}^2)\left(\frac{p-q}{1-ipq}\right)\right]
\end{aligned} \tag{5.5}$$

as non-zero components.

In the first step we formally extend this solution onto a complex V_4 maintaining all formulas [Eqs. (5.1)—(5.5)] as they are, but interpreting the coordinates and parameters as complex. The formal Einstein—Maxwell equations over complex V_4 are thus still fulfilled, giving a solution of type $D \times D$. In the second step we now contract the space to a (weak) heavenly space of type $D \times [-]$ by just selecting

$$m - in = 0, \quad e_0 - ig_0 = 0, \tag{5.6}$$

which guarantees $\bar{C}^{(3)} = 0$ and $\bar{\omega} = 0$. Redefining $\gamma_0 = \gamma + e_0{}^2$, we then have a solution described only by five independent (complex) constants, m, e_0, ϵ, γ_0, and λ. Setting a polynomial

$$D(u) \equiv (-\lambda/6 + \gamma_0) - 2imu - \epsilon u^2 + 2mu^3 + (-\lambda/6 - \gamma_0)u^4, \tag{5.7a}$$

we now have

$$\mathcal{P} = D(p), \quad \mathcal{Q} = q^4 D(i/q), \tag{5.7b}$$

where the tetrad is still given by the form of Eqs. (5.2) with, now, $\mathcal{P}$ and $\mathcal{Q}$ from Eq. (5.7) instead of (5.1). The corresponding electromagnetic field can be written as

$$\tfrac{1}{2}\omega = d\left(\frac{e_0}{1 - ipq}\,(qd\tau + ipd\sigma)\right), \quad \bar{\omega} = 0, \tag{5.8}$$

which is, of course, purely heavenly and therefore does not couple with the gravitational field (see Sec. 3).

It is clear that this complex solution can be considered as a complex prototype of the important real solutions of the type D which contain in particular the Kerr—Newman and Taub—NUT solutions, possibly generalized by the presence of magnetic charge, acceleration parameter, and cosmological constant.

This solution is still very general. If one is interested in the complex prototype of the Schwarzschild (Reissner—Nordström) solution, he can try to make the appropriate contraction of the above complex solution (done for the real case in Ref. 12). It is much simpler, though, to complexify the contracted real solution given in Ref. 12. By imposing again the conditions

$$m_0 - in_0 = 0, \quad e_0 - ig_0 = 0 \tag{5.9}$$

the metric and electromagnetic field become

$$\begin{aligned} ds^2 &= \Psi^{-1} dq'^2 + (q'^2 + \ell_0^2)(d\theta^2 + \sin^2\theta\, d\phi^2) \\ &\quad - \Psi(dt' - 2\ell_0 \cos\theta\; d\phi)^2 \end{aligned} \tag{5.10}$$

$$\Psi \equiv 1 - 2m_0/(q' + i\,\ell_0) - (\lambda/3)(q'^2 + 5\,\ell_0{}^2),$$
$$-im_0 \equiv \ell_0 - (4\lambda/3)\;\ell_0{}^3$$

$$\tfrac{1}{2}\omega = - d\{[e_0/(q' + i\;\ell_0)]\,[dt' - i(q' - i\;\ell_0)\cos\theta\; d\phi]\},$$

while the field invariants are

$$C^{(3)} = - 4m_0/(q' + i\,\ell_0)^3, \quad \tfrac{i}{2}\mathcal{J} = - e_0^2/(q' + i\;\ell_0)^4. \tag{5.11}$$

With $\lambda = 0$ this should be considered as the complex prototype of the Schwarzschild (Reissner—Nordström) and Taub—NUT solutions. With $r \equiv q' + m_0$, $\lambda_0 = 0$, we may rewrite[13]

$$\begin{aligned} ds^2 &= \left(1 - \frac{2m_0}{r}\right)\;\left(\frac{dr^2}{(1 - 2m_0/r)^2} + r^2(d\theta^2 + \sin^2\theta\; d\phi^2)\right. \\ &\quad \left. - (dt' + 2im_0 \cos\theta\; d\phi)^2\right), \\ &\det(g_{\mu\nu}) = (1 - 2m_0/r)^2 r^4 \sin^2\theta, \\ &\tfrac{1}{2}\omega = - d\{(e_0/r)[dt' - i(r - 2m_0)\cos\theta\, d\phi]\}. \end{aligned} \tag{5.12}$$

Although, when investigating strong heavens, it is in general convenient to apply the formalism based on the key function Θ, in some subcases it is more efficient to approach the problem more directly. An interesting example of this is the following: the problem of determining all strong heavens of type $N \times [-]$.

To begin, we can assume a hellish gauge such that

$$\Gamma_{\dot{A}\dot{B}} = 0 \longleftrightarrow \Gamma_{41} = 0 = \Gamma_{32}, \quad \Gamma_{12} = \Gamma_{34}. \tag{5.13}$$

Moreover, working with spaces of type $N \times [-]$, we can fix the heavenly gauge so that only $C^{(1)}$ is different from zero. Our choice for the null tetrad is, however, still invariant with respect to two specific heavenly tetrad gauges; these are given by (specialized to the gauge choice we have already made)

$$\sigma: \begin{array}{l} e'^1 = e^\sigma e^1, \quad e'^3 = e^\sigma e^3 \\ e'^2 = e^{-\sigma} e^1, \quad e'^4 = e^{-\sigma} e^4 \end{array} \longrightarrow$$
$$\begin{cases} \Gamma'_{42} = e^\sigma \Gamma_{42}, \quad \Gamma'_{12} = \Gamma_{12} + \tfrac{1}{2}d\sigma, \;\; \Gamma'_{31} = e^{-\sigma}\Gamma_{31} \\ C'^{(5)} = C'^{(4)} = C'^{(3)} = C'^{(2)} = 0, \quad C'^{(1)} = e^{-2\sigma}C^{(1)} \end{cases} \tag{5.14}$$

$$C: \begin{array}{l} e'^1 = e^1, \quad e'^2 = e^2 + Ce^3 \\ e'^3 = e^3, \quad e'^4 = e^4 - Ce^1 \end{array} \longrightarrow$$

$$\begin{cases} \Gamma'_{42} = \Gamma_{42}, \quad \Gamma'_{12} = \Gamma_{12} + C\Gamma_{42}, \\ \Gamma'_{31} = \Gamma_{31} + 2C\Gamma_{12} + C^2\Gamma_{42} + dC \\ C'^{(5)} = C'^{(4)} = C'^{(3)} = C'^{(2)} = 0, \quad C'^{(1)} = C^{(1)}. \end{cases} \tag{5.15}$$

We may now start to integrate Cartan's structure equations:

$$\begin{aligned} de^1 &= - e^1 \wedge \Gamma_{12} - e^4 \wedge \Gamma_{42}, \qquad & de^2 &= e^2 \wedge \Gamma_{12} - e^3 \wedge \Gamma_{31}, \\ de^4 &= e^1 \wedge \Gamma_{31} + e^4 \wedge \Gamma_{12}, & de^3 &= e^2 \wedge \Gamma_{42} - e^3 \wedge \Gamma_{12}, \end{aligned} \tag{5.16}$$

$$\begin{aligned} d\Gamma_{42} + 2\Gamma_{42} \wedge \Gamma_{12} &= 0, \qquad d\Gamma_{12} + \Gamma_{42} \wedge \Gamma_{31} = 0, \\ d\Gamma_{31} + 2\Gamma_{12} \wedge \Gamma_{31} &= \tfrac{1}{2}C^{(1)}e^3 \wedge e^1. \end{aligned} \tag{5.17}$$

We distinguish two cases:

$$\text{S(special): } \Gamma_{42} = 0; \quad \text{G(general): } \Gamma_{42} \neq 0. \tag{5.18}$$

Considering first case S, we see that $d\Gamma_{12} = 0$ which implies $\Gamma_{12} = dp$. But, choosing $\sigma = - p/2$, we can (without loss of generality) take

$$\text{S:} \quad \Gamma_{12} = 0 = \Gamma_{42}. \tag{5.19}$$

Equations (5.16) then imply that there exist functions p and y such that $e^1 = dp$ and $- e^3 = dy$, and Eqs. (5.17) then require that $C^{(1)}$ is a function only of p and y, which we choose so that $C^{(1)} = F_{yy}(y, p)$, which makes $\Gamma_{31} = - \tfrac{1}{2}F_y(y, p)dp + dC$. Now, we utilize C-gauge—Eqs. (5.15)—to eliminate the dC term in Γ_{31}. Finishing the integration of Eqs. (5.16), we have

$$\begin{aligned} &e^1 = dp, \quad - e^4 = dq, \\ &e^2 = dx - \tfrac{1}{2}F(y, p)dp, \quad - e^3 = dy, \\ &\Gamma_{12} = 0 = \Gamma_{42}, \quad \Gamma_{31} = - \tfrac{1}{2}F_y(y, p)dp, \quad C^{(1)} = F_{yy}. \end{aligned} \tag{5.20}$$

(This solution was already discussed in I, with x, q and y, p interchanged, although it was not derived from such basic notions there.)

Returning now to the general case, we see that we can write $\Gamma_{42} = - e^\sigma dy \neq 0$, while the exponential factor may be regauged to 1 by using Eqs. (5.14), giving[14]

$$\Gamma_{42} = - dy \neq 0. \tag{5.21}$$

Equations (5.17) then imply that $\Gamma_{31} = - x dy$ and $- dx \wedge dy = \tfrac{1}{2}C^{(1)}e^3 \wedge e^1 \neq 0$, so that x and y can be considered as independent coordinates. Looking separately at the two pairs in Eqs. (5.16), we obtain the existence of functions f, g, u, and v such that

$$e^4 = dv + f dy, \quad e^2 = du + g dy.$$

Re-entering with these equations back into Eqs. (5.16)—for consistency—we find that

$$e^1 = d\xi + v\,dy, \quad e^3 = d\eta - u\,dy,$$

where ξ and η are two new scalar functions. We easily have that

$$2dx \wedge dy \wedge du \wedge dv = -C^{(1)} e^1 \wedge e^2 \wedge e^3 \wedge e^4 \neq 0, \tag{5.22}$$

so that x, y, u, v may be chosen as independent coordinates. Again from consistency with Eqs. (5.16) we find that

$$d(f + x\xi) = \xi dx + \lambda dy, \quad d(g - x\eta) = -\eta dx + \mu dy, \tag{5.23}$$

which we interpret as defining two functions $F(x,y) = f + x\xi$, $G(x,y) = g - x\eta$ and giving ξ, λ, η and μ in terms of partial derivatives of F and G. We may then summarize our results for this general case:

$$\begin{aligned} &e^1 = dF_x + v\,dy, \quad e^2 = du + (G - xG_x)dy, \\ &e^4 = dv + (F - xF_x)dy, \quad -e^3 = dG_x + u\,dy, \\ &C^{(1)} = 2[G_{xx}(F_{xy} + v) - F_{xx}(G_{xy} + u)]^{-1}, \end{aligned} \tag{5.24}$$

where F and G are arbitrary except that not both F_{xx} and G_{xx} may vanish. One may also observe that

$$\begin{aligned} &e^3 \wedge de^3 = -G_{xx} dx \wedge dy \wedge du, \\ &e^1 \wedge de^1 = -F_{xx} dx \wedge dy \wedge dv \end{aligned} \tag{5.25}$$

so that these two quantities—F_{xx} and G_{xx}—measure the twists of the forms e^1 and e^3, at least one of which must be nonzero. We have then, in summary, that any solution of type $N \times [-]$ is represented either by Eqs. (5.24) or the special case given by Eq. (5.20).

6. CONCLUSIONS

We consider this work as one more step toward a better understanding of the structure of self-dual solutions to the complex Einstein equations. It is to be remembered that these self-dual solutions are thought of as an intermediate step toward methods of generating general solutions of Einstein's equations on a real manifold, even though the method by which they may be so used is not clear at this moment. Yet we believe that the full discussion of the permitted symmetries (generated by Killing vectors) of these spaces given here should be of considerable value striving toward this goal. In particular, the Killing algebras for certain type $D \times [-]$ metrics, discussed in Secs. 2 and 5, are very helpful in identifying for which real metrics our complex solutions are heavenly prototypes [even though explicit coordinate transformations which, for example, connect the metric determined by the Θ in Eq. (2.40) and the metric given in Eq. (5.12) have not yet been found]. Because of the simplicity of the equation determining these Killing vectors this process should be susceptible to extension to many other relevant uses.

We hope also that further studies can utilize the heavenly spinorial (massless) fields of Sec. 3 to similar good purposes. Lastly note that the yet newer approaches to heavenly metrics, given in Sec. 5, yield complex heavenly prototypes of all solutions of type $N \times [-]$ and the most important solutions of type $D \times [-]$.

APPENDIX

Using the spinor relations

$$\tilde{C}_{AB\dot{C}\dot{D}} = \tfrac{1}{4} g^a{}_{A\dot{C}} g^b{}_{B\dot{D}} \tilde{C}_{ab}, \quad \tilde{C}_{ab} = \tilde{R}_{ab} - \tfrac{1}{4}\tilde{R} g_{ab}, \tag{A1}$$

Eqs. (1.7) and (2.2b), we have

$$\begin{aligned} &-\tilde{C}_{11\dot{2}\dot{2}} = \phi\phi_{xx}, \quad -\tilde{C}_{11\dot{1}\dot{2}} = \phi\phi_{,4x}, \\ &\quad -\tilde{C}_{11\dot{1}\dot{1}} = \phi\phi_{,44} - \Theta_{xxx}\phi_{,1} + \Theta_{xxy}\phi_{,4}, \\ &-\tilde{C}_{12\dot{2}\dot{2}} = -\phi\phi_{xy}, \quad -\tilde{C}_{12\dot{1}\dot{2}} = \tfrac{1}{2}(\phi_{,1x} + \phi_{,4y})\phi, \\ &\quad -\tilde{C}_{12\dot{1}\dot{1}} = \phi\phi_{,14} - \Theta_{xxy}\phi_{,1} + \Theta_{xyy}\phi_{,4}, \\ &-\tilde{C}_{22\dot{2}\dot{2}} = \phi\phi_{yy}, \quad -\tilde{C}_{22\dot{1}\dot{2}} = -\phi\phi_{,1y}, \\ &\quad -\tilde{C}_{22\dot{1}\dot{1}} = \phi\phi_{,11} - \Theta_{xyy}\phi_{,1} + \Theta_{yyy}\phi_{,4}, \end{aligned} \tag{A2}$$

$$-\tilde{R}/12 = \phi(\phi_{,1x} - \phi_{,4y}) - 2\phi_{,1}\phi_{,x} + 2\phi_{,4}\phi_{,y}. \tag{A3}$$

By trying to set $\tilde{C}_{AB\dot{C}\dot{D}} = 0$, the first triple of Eqs. (A2) require that

$$\phi = \beta_6 x + \gamma_6 y + \delta_6, \tag{A4}$$

where β_6, γ_6, and δ_6 are functions of p and q only. Inserting this information into the second triple, we find that

$$\begin{aligned} \beta_6\Theta_y - \gamma_6\Theta_x = P_6 \equiv \tfrac{1}{2}\beta_6 x^2 + \tfrac{1}{2}(\gamma_{6q} - \beta_{6p})xy \\ - \tfrac{1}{2}\gamma_6 y^2 + \mu_6 x + \nu_6 y + \kappa_6, \end{aligned} \tag{A5}$$

where μ_6, ν_6, and κ_6 are new functions of p and q only. (This procedure is a simpler version of the integration of triples of equations in Sec. 2.)

Using now the third triple of equations, we find that there must be a function τ_6 and a constant η_0 such that

$$\beta_6 = -\tau_{6q} + \eta_0 p, \quad \gamma_6 = \tau_{6p} + \eta_0 q, \tag{A6}$$

and a function σ_6 such that

$$\mu_6 = -(\sigma_6 - \delta_6)_q, \quad \nu_6 = (\sigma_6 - \delta_6)_p, \tag{A7}$$

and a new constraint equation:

$$\begin{aligned} 3\rho_0\Theta - \phi_{,1}\Theta_x + \phi_{,4}\Theta_y = P_7 \equiv -\tfrac{1}{2}\sigma_{6qq}x^2 + \sigma_{6qp}xy \\ - \tfrac{1}{2}\sigma_{6pp}y^2 + \mu_7 x + \nu_7 y + \kappa_7, \end{aligned} \tag{A8}$$

with μ_7, ν_7, and κ_7 again being functions of p and q only.

We are now ready to interpret Eqs. (A4), (A5), and (A8). First we consider the case where either β_6 or γ_6 is different from zero. (We assume that it is β_6, at least.) In that case Eq. (A5) may be solved to obtain

$$\Theta = G_6(\phi, p, q) + (y/\beta_6)Q_6(x, y, p, q), \tag{A9}$$

where G_6 is an arbitrary, sufficiently differentiable function of three variables, Q_6 is a second order polynomial in x and y, constructed from P_6. We may then insert this information into Eq. (A8), which implies that

$$3\rho_0 G_6 - (\rho_0\phi + \tilde{R}/24)G_{6\phi} = S_6, \tag{A10}$$

where S_6 is a second order polynomial in ϕ and we have inserted the value of the curvature scalar,

$$-\tilde{R}/24 = \rho_0(\delta_6 - p\sigma_{6p} - q\sigma_{6q}) + \sigma_{6p}\tau_{6q} - \sigma_{6q}\tau_{6p}, \tag{A11}$$

calculated from Eq. (A3), which is constant by the

Bianchi identities. We therefore see that $(\partial/\partial\phi)^4G=0$. However, Eqs. (A9) say then that all fourth derivatives of Θ with respect to x and y must vanish, and therefore the space is flat (see I also).

The only nontrivial option is to retreat and make both β_6 and γ_6 vanish. In this case $\phi=\delta_6$, $\rho_0=0$, $\tau_6=0=\mu_6=\nu_6=\kappa_6$, so that σ_6 just reduces to ϕ and Eq. (A8) remains, in the form

$$\phi_p\Theta_x+\phi_q\Theta_y=P_7, \tag{A12}$$

where P_7 is still a second order polynomial in x and y. Therefore, if either ϕ_p or ϕ_q is nonzero, we have that (assuming $\phi_q\neq 0$)

$$\Theta=G_7(\phi_qx-\phi_py,p,q)+(y/\phi_q)Q_7(x,y,p,q), \tag{A13}$$

Q_7 being a second order polynomial in x and y. Differentiating, we find that

$$\begin{aligned}&\tfrac{1}{2}C^{(j)}=(\phi_q)^{j-1}(-\phi_p)^{5-j}H,\\&H\equiv(\partial/\partial\Phi)^4G_7,\quad \Phi\equiv\phi_qx-\phi_py,\end{aligned} \tag{A14}$$

from which we see that the space must have originally been of type $N\times[-]$ (and also of course the transformed space must be of this type as well). Utilizing Eq. (A11), however, we easily see that $\tilde{R}=0$ so that the transformation is simply between one strong heaven, V_4, and another, $\tilde{V}_4$, without inducing a weak heaven—with $\tilde{C}_{ab}=0$, $\tilde{R}\neq 0$. The last possibility is that of constant ϕ which corresponds merely to a change of scale.

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[1] J.F. Plebański, J. Math. Phys. **16**, 2396 (1975).

[2] S. Hacyan and J.F. Plebański, J. Math. Phys. **16**, 2403 (1975).

[3] See, for example, E.T. Newman and A.I. Janis, J. Math. Phys. **6**, 915 (1965), and R.W. Lind and E.T. Newman, J. Math. Phys. **15**, 1103 (1974). More direct and thorough approaches to the problem can be seen in Ref. 1, as well as by E.T. Newman, in a report to the 1974 Tel Aviv Conference and a lecture at the Enrico Fermi Summer School of Varenna, 1975, and by R. Penrose in the 1975 First Award Winning Essay of the Gravity Research Foundation.

[4] We use lower case Latin indices to denote tetrad indices which run from 1 to 4, lower case Greek indices to denote coordinate indices which also run from 1 to 4, and upper case Latin indices (both undotted and dotted) to denote spinor indices which run from 1 to 2. We use a comma to indicate ordinary (tetradial) differentiation and a semicolon to indicate covariant differentiation. We also use a signature of +2 in the underlying real manifold. Our definition of duality is so arranged that for an arbitrary p-form $\omega=**\omega$: if $\omega=(p!)^{-1}\omega_{\mu_1\ldots\mu_p}dx^{\mu_1}\wedge\cdots\wedge dx^{\mu_p}$, then

$$*\omega\equiv\exp[(i\pi/2)(pp'-1)](p!p'!)^{-1}|\det(g_{\mu\nu})|^{1/2}\epsilon^{\lambda_1\ldots\lambda_p}{}_{\mu_1\ldots\mu_{p'}}\omega_{\lambda_1\ldots\lambda_p}dx^{\mu_1}\wedge\cdots\wedge dx^{\mu_{p'}}$$

with $p+p'=4$.

[5] This, of course, merely generates some solutions, not all.

[6] See, for instance, L.P. Eisenhart, *Riemannian Geometry* (Princeton U.P., Princeton, N.J., 1926), Chap. VI.

[7] We point out that if one considers two Θ's, $\Theta_1=f_1(x,y)$, $\Theta_2=f_2(x,y)+\bar{\beta}x+\bar{\gamma}y$, then Eq. (2.2a) partially determines the functions f_1 and f_2:

$$f_{1xx}f_{1yy}-(f_{1xy})^2=0,\ f_{2xx}f_{2yy}-(f_{2xy})^2=-\bar{\beta}_p-\bar{\gamma}_q\to-1,$$

where we have taken advantage of the fact that since f_2 is independent of p and q we must have $\bar{\beta}_p+\bar{\gamma}_q$ a constant (for any solution to exist at all) which we may then renormalize to 1. Looking casually at Θ_1 and Θ_2 we might say that if f_1 and f_2 were equal they would generate the same metric. This is surely true, but almost never can f_1 and f_2 be equal, as they are solutions to two quite different differential equations. See Sec. 4 for more details on these differential equations.

[8] The existence of this particular group of motions in this space suggests that there is a coordinate transformation which identifies it with the heavenly contraction of the real manifold on which a G_4I group [Petrov's notation for the group whose algebra is just given by Eqs. (2.39)] acts. See A.Z. Petrov, *Einstein Spaces* (Pergamon, New York, 1969), p. 227.

[9] We are motivated to use the symbol H for these potentials because they are actually "heavenly Hertz potentials for any spin."

[10] We use $\Box$ to indicate the action of $\nabla^a\nabla_a$ on a scalar field. Also we note that the case $s=1/2$ corresponds to a "heavenly" neutrino satisfying Weyl's equation in the heavenly space. We have here quite simply $\Psi_A=\delta_AH$, $\Box H=0$.

[11] E. Goursat, *A Course in Mathematical Analysis* (Dover, New York, 1964), Vol. III, Part I, p. 67.

[12] J.F. Plebański and M. Demiański, Cal. Tech. Preprint OAP-401, April, 1975. For a compact resumé see also New York Acad. Sci. **262**, 246 (1975); first announced in J.F. Plebański, in *Gravitational Radiation and Gravitational Collapse*, edited by C. DeWitt-Morette (Reidel, Holland, 1974), pp. 188—90. For the contraction to NUT solution see J.F. Plebański, Ann. Phys. **90**, 190 (1975).

[13] Note that the real Taub—NUT metric has determinant $(r+il_0)^2(r-il_0)^2\sin^2\theta$, nonzero for real values of r and l_0. However, in a complex space there is a more serious problem at the (allowed) point $r=il_0=m_0$.

[14] Actually what one obtains from Eq. (5.17) is $\Gamma_{31}=-xdy+dC$, but again C-gauge—Eqs. (5.15)—allows us to regauge so as to eliminate the dC term.

Correspondence rules and path integrals*

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Using the Weyl correspondence, Mizrahi has derived an expression for the transition amplitude as a path integral in phase space. It is shown that the same result follows if any correspondence rule is used.

INTRODUCTION AND CONCLUSION

Mizrahi[1] has given an interesting derivation for the transition amplitude expressed as a Feynman path integral in phase space. Particular emphasis was placed on the Weyl correspondence rule as the "royal road" in the derivation. We show that all correspondence rules lead to the same result.

There are an infinite number of correspondence rules and no particular one is forced in the Schrödinger formalism.[2] The fact that the Feynman path integral formulation does not either has been previously shown.[3-5]

The set of all possible correspondence rules is given by[2]

$$A(\mathbf{P},\mathbf{Q})=\iint \gamma(\theta,\tau)f(\theta,\tau)\times\exp(i\theta\mathbf{Q}+i\tau\mathbf{P})\,d\theta\,d\tau, \tag{1}$$

$$\gamma(\theta,\tau)=\frac{1}{4\pi^2}\int\int a(p,q)\exp(-i\theta q-i\tau p)\,dq\,dp, \tag{2}$$

where $A(\mathbf{P},\mathbf{Q})$ is the quantum mechanical operator corresponding to the classical function $a(q,p)$, and $f(\theta,\tau)$ is any function such that

$$f(\theta,0)=f(0,\tau)=1 \tag{3}$$

For simplicity we have restricted ourselves to one dimension.

Different correspondence rules are obtained by selecting different choices for f. In particular the Weyl, symmetrization, Born and Jordan rules are obtained by taking f equal to 1, $\cos\frac{1}{2}\theta\tau\hbar$ and $\sin\frac{1}{2}\theta\tau\hbar/(\frac{1}{2}\theta\tau\hbar)$, respectively.

To follow closely the derivation of Mizrahi, we rewrite (1) and (2) as

$$A(\mathbf{P},\mathbf{Q})=\frac{1}{2\pi\hbar}\int\int a(p,q)\Delta(p,q)\,dp\,dq, \tag{4}$$

where

$$\begin{aligned}\Delta(p,q)&=\frac{\hbar}{2\pi}\int\int f(\theta,\tau)\exp[i\theta(\mathbf{Q}-q)+i\tau(\mathbf{P}-p)]\,d\theta\,d\tau\\&=\frac{\hbar}{2\pi}\int\int f(\theta,\tau)\exp(\tfrac{1}{2}i\theta\tau\hbar-i\theta q-i\tau p)\\&\quad\times\exp(i\theta\mathbf{Q})\exp(i\tau\mathbf{P})\,d\theta\,d\tau.\end{aligned} \tag{5}$$

The matrix elements of Δ can readily be obtained,

$$\begin{aligned}\langle q'|\Delta(p,q)|q''\rangle&=\frac{1}{2\pi}\quad f\left(\theta,\frac{q''-q'}{\hbar}\right)\\&\quad\times\exp[-i\theta(q-\tfrac{1}{2}(q''+q'))]\exp\left(\frac{ip(q'-q'')}{\hbar}\right)d\theta\end{aligned} \tag{6}$$

We now follow the steps analogous to Mizrahi's after his equation (35).

$$\begin{aligned}&\left\langle q_{j+1}\right|\exp\left(\frac{-i(t_{j+1}-t_j)\mathbf{H}}{\hbar}\right)\left|q_j\right\rangle\\&=\left\langle q_{j+1}\right|\frac{1}{2\pi\hbar}\int\exp\left(\frac{-i(t_{j+1}-t_j)h(p,q)}{\hbar}\right)\\&\quad\times\Delta(p,q)\,dp\,dq\left|q_j\right\rangle\\&=\frac{1}{(2\pi)^2\hbar}\int f\left(\theta,\frac{q_j-q_{j+1}}{\hbar}\right)\exp[i\theta(q-\tfrac{1}{2}(q_{j+1}-q_j))]\\&\quad\times\exp\left\{\frac{i}{\hbar}\left[\frac{q_{j+1}-q_j}{t_{j+1}-t_j}p-h(p,q)\right]\right.\\&\quad\left.\times(t_{j+1}-t_j)\right\}dp\,dq\,d\theta.\end{aligned} \tag{7}$$

The transition amplitude is then

$$\begin{aligned}&\langle q_b,t_b|q_a,t_a\rangle\\&=\int dq_1\cdots dq_m\prod_{j=0}^{m}\frac{dp\,dx\,d\theta}{(2\pi)^2\hbar}f\left(\theta,\frac{q_j-q_{j+1}}{\hbar}\right)\\&\quad\times\exp[i\theta(\chi-\tfrac{1}{2}(q_{j+1}+q_j))]\\&\quad\times\exp\left[\frac{i}{\hbar}\left(\frac{q_{j+1}-q_j}{t_{j+1}-t_j}p-h(p,x)\right)(t_{j+1}-t_j)\right]\\&=\int\frac{dq_1\cdots dq_m\,dp_0\cdots dp_m}{(2\pi\hbar)^m(2\pi)^2\hbar}\int f\left(\theta,\frac{q_j-q_{j+1}}{\hbar}\right)\\&\quad\times\exp[i\theta(x-\tfrac{1}{2}(q_{j+1}+q_j))]\\&\quad\times\exp\left[\frac{i}{\hbar}\sum_{j=0}^{m}\left(\frac{q_{j+1}-q_j}{t_{j+1}-t_j}p_j-h(p_j,x)\right)\right.\\&\quad\left.\times(t_{j+1}-t_j)\right]d\theta\,dx.\end{aligned} \tag{8}$$

Passing to the limit we have

$$\begin{aligned}&\langle q_b,t_b|q_a,t_a\rangle\\&\doteq\int\frac{dp\,dq\,dx\,d\theta}{(2\pi)^2\hbar}f(\theta,0)\exp[i\theta(x-q(t))]\\&\quad\times\exp\left(\frac{i}{\hbar}\int_{ta}^{tb}[p(t)\dot{q}(t)-h(p(t),x)]\,dt\right).\end{aligned} \tag{9}$$

But, since $f(\theta,0)$ equals 1, we have for the θ integration

$$\int \exp[i\theta(x - q(t))]\,d\theta = 2\pi\delta(x - q(t)). \tag{10}$$

and hence (9) becomes

$$\langle q_b, t_b | q_a, t_a \rangle \doteq \int \frac{dp\,dq}{2\pi\hbar} \times \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} [p(t)\mathring{q}(t) - h(p(t), q(t))]\,dt\right). \tag{11}$$

That all correspondence rules yield Eq. (11) is analogous to the situation of obtaining a correspondence rule from the Feynman path integral in *configuration* space. It has been shown that no unique correspondence is forced. The reasons given in Refs. 3–5 apply equally well in the present case.

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[1] M. M. Mizrahi, J. Math. Phys. 16, 2201 (1975).

[2] L. Cohen, J. Math. Phys. 7, 781 (1966).

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[4] F. J. Testa, J. Math. Phys. 11, 1471 (1971).

[5] I. W. Mayes and J. S. Dowker, J. Math. Phys. 14, 434 (1973).

ERRATA

Erratum: Statistical theory of effective electrical, thermal, and magnetic properties of random heterogeneous materials. VI. Comment on the notion of a cell material [J. Math. Phys. 16, 1772 (1975)]

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(Received 7 November 1975)

Line 10 in the left column on p. 1772 should read as follows: "material is not. If his assertion is true, our formula-...".

Erratum: Semisimple Lie algebras [J. Math. Phys. 16, 2062 (1975)]

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(Received 11 December 1975)

The root weight theorem page 2068 should read:

Root-weight theorem: To each weight α corresponds a root a such that $a = 2\alpha$ and

$$\{V_\alpha, V_\alpha\} \neq 0 \tag{3.41}$$

or $\alpha_i \alpha^i = 0$.

The last possibility was overlooked in the paper. If the Lie algebra is simple, however, then $\alpha_i \alpha^i \neq 0$, and all the conclusions derived from the root weight theorem apply.

For further details see W. Nahm, V. Rittenberg, and M. Scheunert, "Classification of simple graded Lie algebras containing a reductive Lie algebra" (to be published).

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