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# A Lattice of Von Neumann Algebras Associated with the Quantum Theory of a Free Bose Field*

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Von Neumann algebras associated with the normal representation of canonical commutation relations are studied. Corresponding to each subspace of a real Hilbert space (test function space), a von Neumann algebra on another complex Hilbert space (the Fock space) is defined. This correspondence is proved to be an isomorphism between a certain complemented lattice of subspaces and that of the von Neumann algebras. This result has an application to the duality theorem in the theory of a free scalar field, which is to be discussed in a separate paper.

A necessary and sufficient condition on a subspace, in order that the corresponding von Neumann algebra is of type I, is obtained.

## 1. INTRODUCTION

SOME attention has recently been focused on the lattice of von Neumann algebras of local observables in quantum field theory.[1] In this context, a number of questions concerning the properties of "algebras of local observables" have arisen. The most important conjecture is the "duality theorem." Another interesting problem concerns the type of the algebras. In order to study these questions for the case of a free scalar field, we present, in this paper, a systematic investigation of von Neumann algebras associated with the normal representation of the canonical commutation relations (CCR's). The duality theorem for the free scalar field will be treated in a separate paper as an application of the present analysis.

The normal representation (or the Fock representation[2]) of CCR's can be treated at least in three different ways and each approach has its own advantage. In Sec. 2, we introduce two approaches, one using Weyl's formulation[3] and the other using Segal's formulation.[4] In Weyl's formulation, the object under consideration is specified by a real Hilbert space $K$ (the common test function space for both conjugate fields $\varphi$ and $\pi$), while in Segal's formulation it is specified by a real Hilbert space $H$ and an antisymmetric unitary operator $\beta$ on $H$. ($H$ is the direct sum of test function spaces of $\varphi$ and $\pi$ and $\beta$ is used for the purpose of remembering the different roles of test function spaces of $\varphi$ and $\pi$.) As will be seen more explicitly in a separate publication, Weyl's formulation is convenient for the description of the field at one sharp time, whereas Segal's formulation is better suited for the description of the field over all space–time.

The von Neumann algebras[5] associated with the normal representation of CCR's are introduced in Sec. 3. In Weyl's formulation, the von Neumann algebra $R_F(K_1, K_2/K)$ is determined by two subspaces $K_1$ and $K_2$ of $K$, and only the relative relation (up to unitary equivalence) of $K_1$, $K_2$, and

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[1] R. Haag, *Proceedings of the Midwest Conference on Theoretical Physics*, Minneapolis, 1961; R. Haag and B. Schroer, J. Math. Phys. **3**, 248 (1962).

[2] V. Fock, Z. Physik **75**, 622 (1932).

[3] H. Weyl, Z. Physik **46**, 1 (1927).

[4] I. E. Segal, in lecture notes of Boulder Seminar on Applied Mathematics, Boulder, Colorado, 1960 (unpublished).

[5] J. von Neumann, Math. Ann. **102**, 370 (1929).

$K$ is important for the intrinsic properties of the von Neumann algebra. In Segal's formulation, the von Neumann algebra $R_S(H_1/H)$ is determined by a subspace $H_1$ of $H$, and only the relative relation (up to unitary equivalence) of $H_1$, $H$, and $\beta$ is important for the intrinsic properties of the von Neumann algebra.

Later in Sec. 3, we introduce the structure of a complemented lattice for the set of pairs of subspaces $K_1$, $K_2$ in $K$ or for the set of subspaces $H_1$ in $H$ and also for the set of von Neumann algebras. Here the complementations are, respectively, $(K_1, K_2) \to (K_2^\perp, K_1^\perp)$, $H_1 \to \beta H_1^\perp$ for subspaces, and $R \to R'$ (the commutant of $R$) for von Neumann algebras. The main theorem then asserts that the correspondence introduced earlier between subspaces and von Neumann algebras is an isomorphism of these complemented lattices. This theorem and its proof are given in Sec. 3 except for the most difficult part concerning the isomorphism of complementation (the duality theorem), which will be proved in Secs. 8 and 9. Sections 4–7 are to a large extent preparation for this proof of the duality theorem.

In Sec. 4, the relative relations up to unitary equivalence of $H_1$, $H$, and $\beta$, as well as that of $K_1$, $K_2$, and $K$, are characterized in terms of unitary invariants and this is accomplished by casting $H_1$ and $\beta$ or $K_1$ and $K_2$ into a standard form. As a by-product, the von Neumann algebras defined in Weyl's formulation and Segal's formulation are seen to be equivalent.

The analysis of Sec. 4 allows us to decompose each von Neumann algebra into a tensor product of von Neumann algebras of very simple structure and a remainder, which has some convenient property. This will be done in Sec. 5.

In Sec. 6, we introduce another approach to the normal representation of CCR's, namely the tensorial construction, in which the particle picture plays an important role. We then define generalized creation and annihilation operators, which are, roughly speaking, homogeneous polynomials of ordinary creation and annihilation operators. Their multiplication formula is derived and will be used in Sec. 8. Any bounded operator can be expanded into a series of generalized creation and annihilation operators of increasing degrees, where the convergence of the series is assured for each matrix element between vectors in a dense set (a convergence weaker than the weak convergence). This expansion is a very important tool for the proof in Secs. 8 and 9.

In Sec. 7, the connection of the tensorial construction with the other two formulations of Sec. 2 is clarified.

In Sec. 8, we begin the proof of the duality theorem. The essential point in the proof is the observation that the duality theorem corresponds to a set of uncoupled conditions, each of which refers only to terms of the same degree in the generalized creation and annihilation operators. In Sec. 8, we treat terms of the same degree in this expansion and the subtlety of the convergence question of the expansion is dealt with by using Gårding's device in Sec. 9, where the proof of the duality theorem is completed.

In Sec. 10, we derive a necessary and sufficient condition for the von Neumann algebra to be of type I in terms of the unitary invariants for $H_1$ and $\beta$ or $K_1$ and $K_2$ considered in Sec. 4. It is remarked that the von Neumann algebras in question are, in some cases, unitarily equivalent to an example of von Neumann.[6]

## 2. NORMAL REPRESENTATION OF CCR's

A representation of CCR's over a real inner product space $K$, in Weyl's form,[3] is the structure consisting of a complex Hilbert space $\mathfrak{H}$ and a set of unitary operators $U(f)$ and $V(g)$ on $\mathfrak{H}$ for every $f$ and $g$ in $K$ such that $U(\lambda f)$ and $V(\lambda g)$ are weakly (and hence strongly) continuous in $\lambda$ and

$$U(f_1)V(g_1)U(f_2)V(g_2) = U(f_1 + f_2)V(g_1 + g_2)e^{i(f_2, g_1)}. \quad (2.1)$$

Here $(f_2, g_1)$ is the real inner product of $f_2$ and $g_1$ in $K$.

If the algebra generated by $U(f)$ and $V(g)$ has a cyclic vector $\Psi$, the expectation functional

$$E(f, g) = (\Psi, U(f)V(g)\Psi) \quad (2.2)$$

determines the cyclic representation of CCR's up to unitary equivalence.[7] The normal representation of CCR's is the cyclic representation of CCR's determined[8] by the functional

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[6] J. von Neumann, Ann. Math. 41, 94 (1940)

[7] If $E(f, g)$ satisfies a certain condition, then existence is also guaranteed. See H. Araki, J. Math. Phys. 1, 492 (1960).

[8] The existence of the representation of CCR's with the functional (2.3) can be established rather easily either by proving the positive semidefiniteness condition of reference 7 for the functional (2.3), as has been done in H. Araki, Ph.D. Thesis, Princeton University (1960), or by using the infinite direct product of J. von Neumann,[9] as has been done by H. Araki and J. S. Woods.[10]

[9] J. von Neumann, Compos. Math. 6, 1 (1938).

[10] H. Araki and J. S. Woods, J. Math. Phys. 4, 637 (1963).

$$E_F(f, g) = \exp[-\tfrac{1}{4}(f, f) - \tfrac{1}{2}i(f, g) - \tfrac{1}{4}(g, g)], \quad (2.3)$$

where the space $K$ can be taken to be a real Hilbert space.[11] The Hilbert space $\mathfrak{H}$, the cyclic vector $\Psi$, and the operators $U(f)$ and $V(g)$ in the normal representation will be denoted by $\mathfrak{H}_F(K)$, $\Psi_F(K)$, $U_F(f)$, and $V_F(g)$. The self-adjoint field operators $\varphi_F(f)$ and $\pi_F(g)$ are defined through Stone's theorem[12] by

$$U_F(\lambda f) = \exp i\lambda\varphi_F(f), \quad V_F(\lambda g) = \exp i\lambda\pi_F(g). \quad (2.4)$$

$\varphi_F(f)$ and $\pi_F(g)$ depend linearly on $f$ and $g$ and satisfy CCR's.

Another structure closely related to the above has been introduced by Segal.[4] Let $H$ be a real Hilbert space and $\beta$ be an operator on $H$ satisfying

$$\beta^* = -\beta, \qquad \beta^2 = -1. \quad (2.5)$$

Then we consider the structure consisting of a complex Hilbert space $\mathfrak{H}_S(H)$, a vector $\Psi_S(H)$ in $\mathfrak{H}_S(H)$, and a set of unitary operators $W(h)$ for every $h \in H$ such that

$$W(h_1)W(h_2) = W(h_1 + h_2)\exp[(\tfrac{1}{2}i)(h_1, \beta, h_2)], \quad (2.6)$$

$$(\Psi_S(H), W(h)\Psi_S(H)) = \exp[-\tfrac{1}{4}(h, h)], \quad (2.7)$$

and such that $\Psi_S(H)$ is a cyclic vector of the algebra generated by $W(h)$, $h \in H$.

Such a structure can be related to the Weyl form explicitly as follows. The property (2.5) for $\beta$ implies[13] the existence of a (nonunique) subspace $K$ of $H$ such that[14] $K \perp \beta K$ and $H = K \oplus \beta K$. Now take $\mathfrak{H}_S(H) = \mathfrak{H}_F(K)$, $\Psi_S(H) = \Psi_F(K)$ and

$$W(h) = U_F(f)V_F(g)\exp[(\tfrac{1}{2}i)(f, g)], \quad (2.8)$$

where $h = f + \beta g$, $f, g \in K$. Equations (2.6) and (2.7) follow immediately from (2.1) and (2.2). The cyclicity is also evident, due to the equations

$$U_F(f) = W(f), \qquad V_F(g) = W(\beta g). \quad (2.9)$$

The above structure consisting of $\mathfrak{H}_S(H)$, $\Psi_S(H)$, and $W(h)$, $h \in H$, is obviously unique up to a unitary equivalence. However, the subspace $K$ is not uniquely characterized by the operator $\beta$, and hence the correspondence between the Weyl and the Segal structures is not unique. In fact, if $\mathfrak{H}_S(H)$, $\Psi_S(H)$, and $W(h)$ are given, then different possibilities for $U_F(f)$ and $V_F(g)$ corresponding to different choices of $K$ are related to each other by the linear canonical transformations

$$\varphi'_F(f) = \varphi_F(C_{11}f) + \pi_f(C_{12}f), \quad (2.10)$$

$$\pi'_F(f) = \varphi_F(C_{21}f) + \pi_f(C_{22}f), \quad (2.11)$$

where the $C_{ij}$'s are operators on $K$ satisfying

$$\sum_{jl} \epsilon_{jl}C^*_{ij}C_{kl} = \epsilon_{ik}\cdot 1, \qquad \epsilon_{11} = \epsilon_{22} = 0,$$

$$-\epsilon_{12} = \epsilon_{21} = 1. \quad (2.12)$$

The self-adjoint field operator $\chi(h)$ is defined through Stone's theorem[12] by

$$W_S(\lambda h) = \exp i\lambda\chi(h). \quad (2.13)$$

The operator $\chi(h)$ depends linearly on $h$ and satisfies the following commutation relation:

$$[\chi(h_1), \chi(h_2)] = -i(h_1, \beta h_2). \quad (2.14)$$

According to the above identification of two structures,

$$\chi(f + \beta g) = \varphi_F(f) + \pi_F(g), \quad (2.15)$$

where $f, g \in K$, $H = K \oplus \beta K$.

### 3. VON NEUMANN ALGEBRAS[5,15] AND THE MAIN THEOREM

The set of all bounded operators commuting with every operator in a set $\mathfrak{A}$ as well as its adjoint will be called the commutant of $\mathfrak{A}$, and denoted by $\mathfrak{A}'$. One has $\mathfrak{A}'' \supset \mathfrak{A}$, $\mathfrak{A}''' = \mathfrak{A}'$. A set $\mathfrak{A}$ is called self-adjoint if $T \in \mathfrak{A}$ implies $T^* \in \mathfrak{A}$. A weakly closed self-adjoint algebra of bounded operators on a Hilbert space, containing the identity operator, is called a von Neumann algebra. The von Neumann algebra generated by a set $\mathfrak{A}$ is the smallest von Neumann algebra containing $\mathfrak{A}$ and is known to coincide with $\mathfrak{A}''$.

Let $H_1$ be a linear subset of $H$ and $K_1$, $K_2$ to be two linear subsets of $K$. We define the following von Neumann algebras:

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[11] Cf. Lemma 2.3 of H. Araki and J. S. Woods, J. Math. Phys. **4**, 637 (1963).

[12] M. H. Stone, Ann. Math. **33**, 643 (1932).

[13] Consider the complexification $H + iH$ of $H$ and extend linearly the operator $\beta$ to an operator $\beta$ on $H + iH$. $\beta$ is unitary and has eigenvalues $\pm i$. Let $H_+$ be the eigenspace belonging to $+i$. Let $\{h_j\}$ be an orthonormal basis of $H_+$ and let $h_j = f_j + ig_j$, $f_j, g_j \in H$. Since $h - i\beta h \in H_+$ for any $h \in H$, $f_j$ and $g_j$ together span the real Hilbert space $H$. Since $\beta h_j = ih_j$, $g_j = -\beta f_j$, and since $(h_i, h_j) = \delta_{ij}$, $(g_i, f_j) = 0$ and $(f_i, f_j) = 1/2\,\delta_{ij}$. Let the subspace of $H$ spanned by $f_j$ be $K$. Then $\beta K$ is spanned by $g_j$ and $K \perp \beta K$, $H = K \oplus \beta K$. An alternative way is to use the relation of $K$ and $L$ in Sec. 7.

[14] In the following, the notation $A \oplus B = C$ always means that $A$ and $B$ are subspaces, $A \perp B$, and that $C$ is the direct sum of $A$ and $B$. If $A$ is not necessarily orthogonal to $B$, then $A + B$ is used to denote the set $\{x + y; x \in A, y \in B\}$. The subspace spanned by $A$ and $B$ is then denoted by $\overline{A + B}$. If $A \perp B$, then $\overline{A + B} = A \oplus B = A + B$.

[15] Cf. J. Dixmier, *Les Algebres d'operateurs dans l'espace Hilbertien* (Gauthier-Villars, Paris, 1957), and M. A. Neumark, *Normierle Algebren* (VEB Deutscher Verlag der Wissenschaften, Berlin, 1959).

$$R_S(H_1/H) = \{W(h); h \in H_1\}'', \tag{3.1}$$

$$R_F(K_1, K_2/K) = \{U(f)V(g); f \in K_1, g \in K_2\}''. \tag{3.2}$$

Whenever there is no possibility of confusion, we write simply $R_S(H_1)$ and $R_F(K_1, K_2)$ instead of $R_S(H_1/H)$ and $R_F(K_1, K_2/K)$.

If we establish the correspondence between Weyl's formulation and Segal's formulation as in Sec. 2, we have

$$R_F(K_1, K_2/K) = R_S(K_1 + \beta K_2/K \oplus \beta K). \tag{3.3}$$

We will show in Sec. 4 that, for any subspace $H_1$ of $H$, there are subspaces $K$, $K_1$, and $K_2$ of $H$ such that $H = K \oplus \beta K$, $K_1 \subset K$, $K_2 \subset K$, and $H_1 = K_1 + \beta K_2$. Hence one can go freely from any statement about $R_S(H_1/H)$ to the corresponding statement about $R_F(K_1, K_2/K)$ and vice versa if $H_1$, $K_1$, and $K_2$ are subspaces.

The von Neumann algebras for arbitrary linear subsets $H_1$, $K_1$, and $K_2$, and those for subspaces (linear closed subsets) can be related by using the following known lemma.[16]

*Lemma 3.1.* $U_F(f)$ and $V_F(g)$ are strongly continuous in $f$ and $g$ with the strong topology of $K$ for $f$ and $g$. $W_S(h)$ is strongly continuous in $h$ with the strong topology of $H$ for $h$.

From this lemma, we immediately have

$$R_S(H_1/H) = R_S(\bar{H}_1/H), \tag{3.4}$$

$$R_F(K_1, K_2/K) = R_F(\bar{K}_1, \bar{K}_2/K). \tag{3.5}$$

In the following we assume $H_1$ to be a subspace of $H$, and $K_1$, $K_2$ to be subspaces of $K$.

There is a natural lattice structure for subspaces. We define the lattice operations $\wedge$ and $\vee$ by

$$H_1 \wedge H_2 = H_1 \cap H_2, \qquad \bigwedge_\alpha H_\alpha = \bigcap_\alpha H_\alpha, \tag{3.6}$$

$$H_1 \vee H_2 = \overline{H_1 + H_2}, \qquad \bigvee_\alpha H_\alpha = \overline{\sum_\alpha H_\alpha}, \tag{3.7}$$

where $\cap$ is the set theoretical intersection and $\sum_\alpha H_\alpha$ is the set of all finite linear combinations of vectors in $H_\alpha$. Because of (2.5), the mapping $H_1 \to \beta H_1^\perp$ is a complementation in this lattice. (The lattice can be defined by the partial ordering $H_1 \subset H_2$ in terms of the set theoretical inclusion among subspaces.)

There is also a lattice structure for von Neumann algebras. We define

$$R_1 \wedge R_2 = R_1 \cap R_2, \qquad \bigwedge_\alpha R_\alpha = \bigcap_\alpha R_\alpha, \tag{3.8}$$

$$R_1 \vee R_2 = (R_1 \cup R_2)'', \qquad \bigvee_\alpha R_\alpha = (\bigcup_\alpha R_\alpha)'', \tag{3.9}$$

where the $R_\alpha$ are von Neumann algebras. $R_1 \to R_1'$ is a complementation in this lattice.

Our main result is that $R_S(H_1/H)$ gives an isomorphism between these two complemented lattices. Namely,

*Theorem 1.*

$$(1)\quad R_S(H_1) \supset R_S(H_2) \quad \text{iff} \quad H_1 \supset H_2. \tag{3.10}$$

$$(2)\quad R_S(H_1) = R_S(H_2) \quad \text{iff} \quad H_1 = H_2. \tag{3.11}$$

$$(3)\quad R_S(\bigvee_\alpha H_\alpha) = \bigvee_\alpha R_S(H_\alpha). \tag{3.12}$$

$$(4)\quad R_S(\bigwedge_\alpha H_\alpha) = \bigwedge_\alpha R_S(H_\alpha). \tag{3.13}$$

$$(5)\quad R_S(H_1)' = R_S(\beta H_1^\perp). \tag{3.14}$$

The theorem can also be stated in terms of $R_F(K_1, K_2/K)$.

*Theorem 1'.*

$$(1)\quad R_F(K_1', K_2') \supset R_F(K_1'', K_2'') \quad \text{iff} \quad K_1' \supset K_1'', \quad K_2' \supset K_2''. \tag{3.15}$$

$$(2)\quad R_F(K_1', K_2') = R_F(K_1'', K_2'') \quad \text{iff} \quad K_1' = K_1'', \quad K_2' = K_2''. \tag{3.16}$$

$$(3)\quad R_F(\bigvee_\alpha K_1^{(\alpha)}, \bigvee_\alpha K_2^{(\alpha)}) = \bigvee_\alpha R_F(K_1^{(\alpha)}, K_2^{(\alpha)}). \tag{3.17}$$

$$(4)\quad R_F(\bigwedge_\alpha K_1^{(\alpha)}, \bigwedge_\alpha K_2^{(\alpha)}) = \bigwedge_\alpha R_F(K_1^{(\alpha)}, K_2^{(\alpha)}). \tag{3.18}$$

$$(5)\quad R_F(K_1, K_2)' = R_F(K_2^\perp, K_1^\perp). \tag{3.19}$$

The hardest part of the proof is the proof of (5). This will be carried out in Secs. 8 and 9. Here we will give a proof of (1)–(4) for Theorem 1. Theorem 1' follows from Theorem 1 through the relation (3.3).

*Proof of (3.10)–(3.13):* (1) If $H_1 \supset H_2$, obviously $R_S(H_1) \supset R_S(H_2)$. If $H_1 \not\supset H_2$, then $H_1^\perp \not\subset H_2^\perp$ and there exists $h_1 \in H_1^\perp$, $\notin H_2^\perp$. For this $h_1$, there exists $h_2 \in H_2$ with $(h_2, h_1) \neq 0$ so that

$$[W(\lambda h_2), W(\beta h_1)] = W(\beta h_1)W(\lambda h_2)(e^{-i\lambda(h_2, h_1)} - 1) \neq 0$$

for some $\lambda$. Hence $W(\beta h_1) \notin R_S(H_2)'$. Obviously,

[16] H. Araki and J. S. Woods, J. Math. Phys. 4, 637 (1963), Lemma 2.3.

$W(\beta h_1) \in R_S(H_1)'$. Therefore $R_S(H_1)' \subset R_S(H_2)'$ which implies $R_S(H_1) \supset R_S(H_2)$. (2) follows from (1). (3) Since $\vee_\alpha H_\alpha \supset H_\alpha$, $R(\vee_\alpha H_\alpha) \supset R(H_\alpha)$. On the other hand, if $h_n \in \vee_\alpha H_\alpha$, then $W(h_1 + h_2)$ and $W(h)$, if $h = \lim h_n$ exists, are in $\vee_\alpha R(H_\alpha)$ due to (2.6) and Lemma 3.1. Since elements of $\vee_\alpha H_\alpha$ can be obtained by taking a finite sum of elements in $H_\alpha$ and then taking the strong limit, we have $R(\vee_\alpha H_\alpha) \subset \vee_\alpha R(H_\alpha)$. (4) follows from (3) and (5).

### 4. THE UNITARY INVARIANTS FOR $H_1$ AND $\beta$ AND FOR $K_1$ AND $K_2$

In this section we characterize the structure of the subspace $H_1 \subset H$ and the operator $\beta$ satisfying (2.5) in terms of unitary invariants. As a byproduct, we prove that the von Neumann algebra $R_S(H_1/H)$ can also be written as $R_F(K_1, K_2/K)$ for a suitable choice of $K$, $K_1$, and $K_2$. The technique and results of this section will be used repeatedly later.

We first use the lattice structure (3.6), (3.7), and the two kinds of complementation $H_1 \to H_1^\perp$ and $H_1 \to \beta H_1^\perp$ to separate out subspaces $H^{(2)}$, $H^{(3)}$, $H^{(4)}$ from $H$. The remaining part of the space $H$, called $H^{(0)}$, will be studied by using the theory of the graph of a closed operator. The structure of $H_1$ and $\beta$ will be characterized by dimensions of subspaces $H^{(2)}$, $H^{(3)}$, and $H^{(4)}$ and by the equivalence class of the spectral measure and the multiplicity function of a certain positive-definite self-adjoint operator $\alpha(\beta H_1', H_1'/H^{(0)})$, where the multiplicity function must be even.

Now suppose a subspace $H_1 \subset H$ is given. We define

$$H^{(2)} \equiv H_1 \wedge \beta H_1, \qquad H^{(3)} \equiv H_1^\perp \wedge \beta H_1^\perp, \tag{4.1}$$

$$H^{(4)} \equiv K^{(4)} \oplus \beta K^{(4)}, \quad K^{(4)} \equiv (H_1 \wedge \beta H_1^\perp), \tag{4.2}$$

$$H^{(0)} \equiv (H^{(2)} \oplus H^{(3)} \oplus H^{(4)})^\perp, \tag{4.3}$$

$$H_1' \equiv H^{(0)} \wedge H_1 = H_1 \wedge (K^{(4)} \oplus H^{(2)})^\perp, \tag{4.4}$$

$$H_2' \equiv (H_1'^\perp \wedge H^{(0)}) = H_1^\perp \wedge H^{(0)}$$
$$= H_1^\perp \wedge (\beta K^{(4)} \oplus H^{(3)})^\perp. \tag{4.5}$$

Note that $(\beta H_1)^\perp = \beta H_1^\perp$. The subspaces $H^{(2)}$, $H^{(3)}$, $K^{(4)}$, and $\beta K^{(4)}$ are intersections of two subspaces among $H_1$, $H_1^\perp$, $\beta H_1$, $(\beta H_1)^\perp$. Obviously, $H^{(0)}$, $H^{(2)}$, $H^{(3)}$, and $H^{(4)}$ are invariant under the multiplication by $\beta$ and they are mutually orthogonal. We have the direct-sum decomposition

$$H = H^{(0)} \oplus H^{(2)} \oplus H^{(3)} \oplus H^{(4)}, \tag{4.6}$$

$$H_1 = H_1' \oplus H^{(2)} \oplus \{0\} \oplus K^{(4)}, \tag{4.7}$$

$$\beta H_1^\perp = \beta H_2' \oplus \{0\} \oplus H^{(3)} \oplus K^{(4)}. \tag{4.8}$$

We see then that the decomposition (4.6) reduces $\beta$ and at the same time reduces $H_1$ as in (4.7). The structure of the subspace $H_1$ and the operator $\beta$ is completely determined by the structure of their restrictions on each of $H^{(0)}$, $H^{(2)}$, $H^{(3)}$, and $H^{(4)}$. In $H^{(2)}$, the subspace $H_1$ occupies the whole space, while it consists only of 0 in $H^{(3)}$. In $H^{(4)}$, the subspace $H_1$ has the property of the earlier $K$. In each of these spaces, $H^{(2)}$, $H^{(3)}$, and $H^{(4)}$, the structure of $H_1$ and $\beta$ is determined by the dimension of the space up to unitary equivalence, where the dimension of $H^{(4)}$ is restricted to even numbers or infinities.

By construction, any two of $H_1'$, $H_2'$, $\beta H_1'$, $\beta H_2'$ have zero intersection,

$$H_1' \wedge \beta H_1' = H_1' \wedge \beta H_2'$$
$$= H_2' \wedge \beta H_1' = H_2' \wedge \beta H_2' = \{0\}, \tag{4.9}$$

where $H_2' \equiv H_1'^\perp \wedge H^{(0)}$. As the dual statement, we also have

$$H_2' \vee \beta H_2' = H_2' \vee \beta H_1'$$
$$= H_1' \vee \beta H_2' = H_1' \vee \beta H_1' = H^{(0)}. \tag{4.10}$$

Conversely, the above stated structure or property of $H_1$ and $\beta$ in each of $H^{(0)}$, $H^{(2)}$, $H^{(3)}$, $H^{(4)}$ uniquely defines the decomposition (4.6) and (4.7). Therefore, we now want to characterize $H_1'$ and $\beta$ in $H^{(0)}$ using (4.9) and (2.5).

We first prove a lemma concerning a graph of a closed operator.[17]

*Lemma 4.1* Given two subspaces $M_1$ and $M_2$ of a Hilbert space $M$ such that any two of $M_1$, $M_2$, $M_1^\perp$, $M_2^\perp$ have zero intersection. Then there exists a unique linear closed operator $\varphi(M_2; M_1/M)$ from $M_1$ into $M_1^\perp$ whose graph is $M_2$. Furthermore, there exists a positive-definite self-adjoint operator $\alpha(M_2; M_1/M)$ on $M_1$, and a unitary operator $\bar{U}(M_2; M_1/M)$ from $M_1$ onto $M_1^\perp$ such that

$$\varphi(M_2; M_1/M)$$
$$= \bar{U}(M_2; M_1/M)\alpha(M_2; M_1/M)^{\frac{1}{2}} \tag{4.11}$$

(the polar decomposition),

$$\varphi(M_2; M_1/M)^*$$
$$= \alpha(M_2; M_1/M)^{\frac{1}{2}}\bar{U}(M_2; M_1/M)^*, \tag{4.12}$$

[17] After completion of this work, Dr. H. J. Borchers has kindly brought the author's attention to the article by M. H. Stone, [J. Indian Math. Soc. **15**, 155 (1951)] where a similar analysis can be found.

$$P(M_1)P(M_2)P(M_1)$$
$$= [1 + \alpha(M_2; M_1/M)]^{-1} \quad \text{on} \quad M_1. \tag{4.13}$$

Here $P(M_\alpha)$ is the orthogonal projection on the subspace $M_\alpha$ as an operator on $M$.

*Proof.* The operator $\varphi(M_2; M_1/M)$ is defined by

$$\varphi(M_2; M_1/M)h = h', \tag{4.14}$$

whenever $h \in M_1$, $h' \in M_1^\perp$, and $h + h' \in M_2$. Because $M_1^\perp \wedge M_2 = \{0\}$, $h = 0$ implies $h' = 0$, and $\varphi(M_2; M_1/M)$ is a well-defined linear closed operator from $M_1$ into $M_1^\perp$ with the graph $M_2$. Because $M_1 \wedge M_2^\perp = \{0\}$, the domain $D(\varphi(M_2; M_1/M)) = P(M_1)M_2$ of $\varphi(M_2; M_1/M)$ is dense in $M_1$ and, because $M_1^\perp \wedge M_2^\perp = \{0\}$, the range $P(M_1^\perp)M_2$ of $\varphi(M_2; M_1/M)$ is also dense in $M_1^\perp$. Therefore, $\varphi(M_2; M_1/M)^* = -\varphi(M_2^\perp; M_1^\perp/M)$.

$\alpha(M_2; M_1/M)$ is defined by

$$\alpha(M_2; M_1/M)$$
$$= \varphi(M_2; M_1/M)^*\varphi(M_2; M_1/M). \tag{4.15}$$

It is well-known[18] that $\alpha(M_2; M_1/M)$ is a positive-semidefinite self-adjoint operator with the domain $D(\alpha(M_2; M_1/M)) \subset D(\varphi(M_2; M_1/M))$. Because $M_1 \wedge M_2 = \{0\}$, $\varphi(M_2; M_1/M)h = 0$ implies $h = 0$, and hence $\alpha(M_2; M_1/M)$ is positive definite.

We define

$$U(M_2; M_1/M)\Psi$$
$$= \varphi(M_2; M_1/M)\alpha(M_2; M_1/M)^{-\frac{1}{4}}\Psi, \tag{4.16}$$

where we restrict $\Psi$ to $\alpha(M_2; M_1/M)^{\frac{1}{4}}\, D(\alpha(M_2; M_1/M))$. This domain is dense in $M_1$, and on this domain $U(M_2; M_1/M)$ is clearly isometric. Hence the closure $\bar{U}(M_2; M_1/M)$ is an isometric operator from $M_1$ into $M_1^\perp$. Since the closure of the restriction of $\alpha(M_2; M_1/M)^{\frac{1}{4}}$ to $D(\alpha(M_2; M_1/M))$ is $\alpha(M_2; M_1/M)^{\frac{1}{4}}$, we have

$$\varphi_1 \equiv \overline{U(M_2; M_1/M)\alpha(M_2; M_1/M)^{\frac{1}{4}}}$$
$$= \bar{U}(M_2; M_1/M)\alpha(M_2; M_1/M)^{\frac{1}{4}}. \tag{4.17}$$

Since $\alpha(M_2; M_1/M)$ is self-adjoint, $\varphi_1^*\varphi_1 \supset \alpha(M_2; M_1/M)$[19] immediately implies

$$\varphi_1^*\varphi_1 = \alpha(M_2; M_1/M). \tag{4.18}$$

Now if $h \in D(\alpha(M_2; M_1/M))$, we have

$$[1 + \alpha(M_2; M_1/M)]h = [h + \varphi(M_2; M_1/M)h] - h',$$

$$h' \equiv \varphi(M_2; M_1/M)h$$
$$- \varphi(M_2; M_1/M)^*\varphi(M_2; M_1/M)h \in M_2^\perp,$$
$$h + \varphi(M_2; M_1/M)h \in M_2.$$

Hence

$$P(M_1)P(M_2)P(M_1)[1 + \alpha(M_2; M_1/M)]h = h.$$

For any $h' \in H_1$, we may take $h = [1 + \alpha(M_2; M_1/M)]^{-1}h' \in D(\alpha(M_2; M_1/M))$ and we have (4.13).

From (4.16) and (4.17), we have $\varphi_1 \subset \varphi(M_2; M_1/M)$. If $M_2'$ is the graph of $\varphi_1$ in $M = M_1 \oplus M_1^\perp$, this means $M_2' \subset M_2$. From (4.18) and similar argument as above, we have $P(M_1)P(M_2')P(M_1) = [1 + \alpha(M_2; M_1/M)]^{-1} = P(M_1)P(M_2)P(M_1)$. From this we have $M_2 = M_2'$ due to $M_2 \wedge M_1^\perp = \{0\}$. Hence $\varphi_1 = \varphi(M_2; M_1/M)$, and (4.11) follows from (4.17). Since $\varphi(M_2; M_1/M)M_1$ is dense in $M_1^\perp$, $\bar{U}(M_2; M_1/M)$ is unitary (i.e., onto $M_1^\perp$). (4.12) follows from (4.11). This completes the proof of Lemma 4.1.

We now define

$$\gamma(\beta; H_1') = P(H_1')\beta P(H_1') \quad \text{on} \quad H_1'. \tag{4.19}$$

Since $\beta$ is unitary, $\beta P(H_1)\beta^{-1} = P(\beta H_1)$, and since $\beta^{-1} = -\beta$, we have

$$\gamma(\beta; H_1')^2 = -[1 + \alpha(\beta H_1'; H_1'/H^{(0)})]^{-1}. \tag{4.20}$$

Since $\gamma(\beta; H_1')$ commutes with $\gamma(\beta; H_1')^2$, it commutes with the spectral projections of $\alpha(\beta H_1'; H_1'/H^{(0)})$. We define

$$\Gamma = [1 + \alpha(\beta H_1'; H_1'/H^{(0)})]^{\frac{1}{4}}\gamma(\beta; H_1'). \tag{4.21}$$

$\Gamma$ commutes with $\alpha(\beta H_1)$ and satisfies

$$\Gamma^2 = -1, \qquad \Gamma^* = -\Gamma. \tag{4.22}$$

Conversely, the operators $\alpha(\beta H_1'; H_1'/H^{(0)}) \equiv \alpha$ and $\Gamma$ on $H_1'$ and the unitary mapping $\bar{U} \equiv \bar{U}(\beta H_1'; H_1'/H^{(0)})$ from $H_1'$ onto $H_2'$ completely determines $\beta$ according to the following formulas:

$$P(H_1')\beta P(H_1') = \Gamma(1 + \alpha)^{-\frac{1}{4}}, \tag{4.23}$$

$$P(H_2')\beta P(H_1') = \varphi(\beta H_1'; H_1'/H^{(0)})P(H_1')\beta P(H_1')$$
$$= \bar{U}\Gamma\alpha^{\frac{1}{4}}(1 + \alpha)^{-\frac{1}{4}}, \tag{4.24}$$

$$P(H_1')\beta P(H_2') = -[P(H_2')\beta P(H_1')]^*$$
$$= \Gamma\alpha^{\frac{1}{4}}(1 + \alpha)^{-\frac{1}{4}}\bar{U}^*, \tag{4.25}$$

$$P(H_2')\beta P(H_2') = -\varphi(\beta H_1'; H_1'/H^{(0)})^{*-1}P(H_1')\beta P(H_2')$$
$$= -\bar{U}\Gamma(1 + \alpha)^{-\frac{1}{4}}\bar{U}^*. \tag{4.26}$$

We now analyze the structure of $\alpha$ and $\Gamma$ on $H_1'$.

[18] N. I. Aichieser and I. M. Glasmann, *Theorie der Linearen Operatoren in Hilbert Raum* (Akademie-Verlag, Berlin, 1954), p. 102, Theorem 2.

[19] For operators $A_1$ and $A_2$, $A_1 \supset A_2$ means $D(A_1) \supset D(A_2)$ and $A_1\Psi = A_2\Psi$ for any $\Psi \in D(A_2)$ where $D(A_l)$ is the domain of $A_l$.

Since $\Gamma$ commutes with $\alpha$, we have the splitting[20]

$$H_1 = K_1' \oplus \Gamma K_1', \tag{4.27}$$

where $K_1$ is invariant by spectral projections of $\alpha$. As is well-known,[21] any positive self-adjoint operator $\alpha$ is characterized by the equivalence class of the (spectral) measure on $(0, +\infty)$ and the multiplicity function.

We now see that $\beta$ and $H_1'$ are completely characterized by the spectral measure $\mu$ and the multiplicity function $d(x)$ of the positive self-adjoint operator $\alpha(\beta H_1'; H_1'/H^{(0)})$, where the multiplicity must be even. Obviously, they are unitary invariants. Furthermore, if $\mu$ and $d(x)$ are given, where $d(x)$ is even or infinite, we can construct the following standard form for $\beta$ and $H_1'$. Construct a Hilbert space $K_1$ and an operator $\alpha'$ such that the spectral measure and the multiplicity are $\mu$ and $\frac{1}{2}d$. We define $H_1'' \equiv K_1 \otimes R^2$, where $R^2$ is a two-dimensional real Hilbert space. Let $\Gamma'$ be the operator on $R^2$ of the form $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. Let $H = H_1'' \otimes R^2$ where $R^2$ is another two-dimensional real vector space, $H_1' = H_1'' \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, and

$$\beta = \begin{pmatrix} (1+\alpha')^{-\frac{1}{2}} \otimes \Gamma' & \alpha'^{\frac{1}{2}}(1+\alpha')^{-\frac{1}{2}} \otimes \Gamma' \\ \alpha'^{\frac{1}{2}}(1+\alpha')^{-\frac{1}{2}} \otimes \Gamma' & -(1+\alpha')^{\frac{1}{2}} \otimes \Gamma' \end{pmatrix}. \tag{4.28}$$

We easily verify that $\beta$ and $H_1'$ satisfy the properties (4.9) and (2.5). Furthermore, the above argument shows that any $\beta$ and $H_1'$, for which the spectral measure and multiplicity of $\alpha(\beta H_1'; H_1'/H^{(0)})$ is equivalent to $\mu$ and $d(x)$, is unitarily equivalent to this standard form. Thus we have:

*Theorem 2.* A subspace $H_1$ of a Hilbert space $H$ and the operator $\beta$ satisfying (2.5) is completely characterized (up to unitary equivalence) by the dimensions $d(H^{(2)}), d(H^{(3)}), d(K^{(4)})$ of the subspaces $H^{(2)}$, $H^{(3)}$, $K^{(4)}$ [(4.1) and (4.2)], and by the equivalence class of the spectral measure over $(0, +\infty)$ and the even multiplicity function of the positive-definite self-adjoint operator $\alpha(\beta H_1'; H_1'/H^{(0)})$ [(4.3) and (4.4); Lemma 4.1].

In the above discussion, if we define

$$K^{(0)} = K_1' \oplus \bar{U}(\beta H_1'; H_1')K_1', \tag{4.29}$$

$$K_2' = \beta \Gamma K_1', \tag{4.30}$$

then we have $H^{(0)} = K^{(0)} \oplus \beta K^{(0)}$, $H_1' = K_1' \oplus \beta K_2'$, $K_1' \subset K^{(0)}$, $K_2' \subset K^{(0)}$. For $H^{(2)}$ and $H^{(3)}$, we consider any splitting $H^{(2)} = K^{(2)} \oplus \beta K^{(2)}$, $H^{(3)} = K^{(3)} \oplus \beta K^{(3)}$. We define $K = K^{(0)} \oplus K^{(2)} \oplus K^{(3)} \oplus K^{(4)}$, $K_1 = K_1' \oplus K^{(2)} \oplus \{0\} \oplus K^{(4)}$, and $K_2 = K_2' \oplus K^{(2)} \oplus \{0\} \oplus \{0\}$. Then we have $H = K \oplus \beta K$, $H_1 = K_1 \oplus \beta K_2$, $K_1 \subset K$, and $K_2 \subset K$.

From the equations $H_1 = K_1 \oplus \beta K_2$, $\beta H_1 = K_2 \oplus \beta K_1$, $H_1^\perp = (K_1^\perp \wedge K) \oplus \beta(K_2^\perp \wedge K)$, $\beta H_1^\perp = (K_2^\perp \wedge K) \oplus \beta(K_1^\perp \wedge K)$, we see that any two of $H_1$, $H_1^\perp$, $\beta H_1$, $\beta H_1^\perp$ have zero intersection if and only if any two of $K_1$, $K_2$, $K_1^\perp \wedge K$, $K_2^\perp \wedge K$ have zero intersection.

Combining these results, we have:

*Theorem 3.* For any subspace $H_1$ of $H$, there exist subspaces $K$, $K_1$, and $K_2$ of $H$ such that $H = K \oplus \beta K$, $H_1 = K_1 \oplus \beta K_2$, $K_1 \subset K$, and $K_2 \subset K$. Any two of $H_1$, $\beta H_1$, $H_1^\perp$, $\beta H_1^\perp$ have zero intersection if and only if any two of $K_1$, $K_2$, $K_1^\perp \wedge K$, $K_2^\perp \wedge K$ have zero intersection. If this condition is satisfied, $\varphi(K_2; K_1/K)$ is the restriction of $\varphi(\beta H_1; H_1/H)$ to $K_1$.

The analogue of Theorem 2 for the space $K$ is the following:

*Theorem 2'.* Two subspaces $K_1$ and $K_2$ in $K$ are characterized up to unitary equivalence by the dimension of subspaces $K^{(2)} = K_1 \wedge K_2$, $K^{(3)} = K_1^\perp \wedge K_2^\perp$, $K_4 = K_1 \wedge K_2^\perp$, and $K_5 = K_2 \wedge K_1^\perp$ and by the spectral measure over $(0, \infty)$ and multiplicity function of the positive-definite self-adjoint operator $\alpha(K_2'; K_1'/K^{(0)})$ where $K_l' = K_l \wedge K^{(0)}$, $l = 1, 2$, $K^{(0)} = (K^{(2)} + K^{(3)} + K_4 + K_5)^\perp$, and any two of $K_1'$, $K_2'$, $K_1'^\perp \wedge K^{(0)}$, $K_2'^\perp \wedge K^{(0)}$ have zero intersection. If $H = K \oplus \beta K$, $H_1 = K_1 \oplus \beta K_2$, then $H^{(2)} = K^{(2)} \oplus \beta K^{(2)}$, $H^{(3)} = K^{(3)} \oplus \beta K^{(3)}$, $K^{(4)} = K_4 \oplus \beta K_5$, $H^{(0)} = K^{(0)} \oplus \beta K^{(0)}$, $H_1' = K_1' \oplus \beta K_2'$, $\alpha(K_2'; K_1'/K^{(0)})$ is the restriction of $\alpha(\beta H_1'; H_1'/H^{(0)})$ to $K_1'$, the spectral measure of $\alpha(\beta H_1'; H_1'/H^{(0)})$ is equivalent to that of $\alpha(K_2'; K_1'/K^{(0)})$, and the multiplicity function of the former is twice that of the latter.

## 5. PRELIMINARY ANALYSIS OF THE VON NEUMANN ALGEBRAS

In this section we consider the consequences of the splitting (4.6), (4.7), and (4.8) for the space

[20] Proof: Let $\mathfrak{A}$ be the commutative algebra generated by spectral projections of $\alpha$. If $A, B \in \mathfrak{A}$, $A^* = A$, $B^* = B$, then, due to $[A, \Gamma] = [B, \Gamma] = [A, B] = 0$, we have $(Af, B\Gamma f) = -(B\Gamma f, Af) = -(Af, B\Gamma f)$, which implies $(Af, B\Gamma f) = 0$ for any $f \in H_1'$. Let $H(\alpha, f) = \bar{R}f$ be the cyclic subspace generated by $R$ from $f$. According to the above, $H(\alpha, f) \perp H(\alpha, \Gamma f)$. Let $H(\alpha, \Gamma; f) = H(\alpha, f) \oplus H(\alpha, \Gamma f)$. $H(\alpha, \Gamma; f)$ is invariant under $\alpha$ and $\Gamma$. By transfinite induction, $H = \sum_\mu \oplus H(\alpha, \Gamma; f_\mu)$ for some $f_\mu$. Then we define $K_1' = \sum_\mu \oplus H(\alpha, f_\mu)$, and have $H_1' = K_1' \oplus \Gamma K_1'$, where $K_1'$ is invariant under $R$.

[21] For the multiplicity theory, see, for example, P. R. Halmos, *Introduction to Hilbert Space and the Theory of Spectral Multiplicity* (Chelsea Publishing Company, New York, 1957).

$\mathfrak{H}_S(H)$ and the von Neumann algebra $R_S(H_1/H)$. The following two lemmas will show that the splitting (4.6)–(4.8) can be viewed as a splitting of the degrees of freedom of the system into the part $H^{(2)}$, where the operators concerned, $W(h)$, $h \in H_1$, are complete; the part $H^{(3)}$, which is irrelevant for the operators concerned; the part $H^{(4)}$ where the center of the set of the operator concerned is maximal Abelian, and the rest $H^{(0)}$ where the operator set concerned has more complicated structure.

*Lemma 5.1.*

$$R_S(H/H) = B(\mathfrak{H}_S(H)), \tag{5.1}$$

$$R_F(K, K/K) = B(\mathfrak{H}_F(K)), \tag{5.2}$$

$$R_F(K, 0/K)' = R_F(K, 0/K), \tag{5.3}$$

$$R_F(0, K/K)' = R_F(0, K/K). \tag{5.4}$$

$\Psi_F(K)$ is a cyclic vector of $R_F(K, 0/K)$ as well as of $R_F(0, K/K)$. Here $B(\mathfrak{H})$ denotes the set of all bounded operators on $\mathfrak{H}$.

The proof of (5.2) and the cyclicity of $\Psi_F(K)$ are known.[22] (5.1) follows from (5.2). Since $R_F(K, 0/K)$ and $F_F(0, K/K)$ are Abelian and have a cyclic vector, they are maximal Abelian[22] and satisfy (5.3) and (5.4).

*Lemma 5.2.* If $H = H' \oplus H''$, there exists a unitary mapping $S$ of $\mathfrak{H}_S(H') \otimes \mathfrak{H}_S(H'')$ onto $\mathfrak{H}_S(H)$ such that $\Psi_S(H) = S(\Psi_S(H') \otimes \Psi_S(H''))$, $W(h) = S(W_F(h_1) \otimes W_F(h_2))S^{-1}$ where $h = h_1 + h_2, h_1 \in H', h_2 \in H''$. $S$ is unique. Furthermore, if $H_1 = H_1' \oplus H_1''$, $H_1' \subset H'$, $H_1'' \subset H''$, then [24]

$$R_S(H_1/H) = S(R_S(H_1'/H') \otimes R_S(H_1''/H''))S^{-1}. \tag{5.5}$$

Because of the uniqueness of $S$, we often identify $\mathfrak{H}_S(H') \otimes \mathfrak{H}_S(H'')$ with $\mathfrak{H}_S(H' \oplus H'')$ and shorten the notation by omitting $S$ in all equations.

*Proof:* $S$ is defined by

$$S(W_S(h_1)\Psi_S(H') \otimes W_S(h_2)\Psi_S(H'')) = W_S(h_1 + h_2)\Psi_S(H)$$

for any $h_1 \in H', h_2 \in H''$. $S$ is obviously isometric. Because of the cyclicity of $\Psi_S(H)$, $\Psi_S(H')$ and $\Psi_S(H'')$ [which follows from (5.1)], $S$ is unitary. $S$ satisfies all desired property in an obvious way.

*Lemma 5.2'.* If $K = K' \oplus K''$, there exists a unitary mapping $S$ of $\mathfrak{H}_F(K') \otimes \mathfrak{H}_F(K'')$ onto $\mathfrak{H}_F(K)$ such that $\Psi_F(K) = S(\Psi_F(K') \otimes \Psi_F(K''))$, $U_F(f) = S(U_F(f_1) \otimes U_F(f_2))S^{-1}$, $V_F(g) = S(V_F(g_1) \otimes V_F(g_2))S^{-1}$ where $f = f_1 + f_2$, $g = g_1 + g_2$; $f_1, g_1 \in K'$; $f_2, g_2 \in K''$. $S$ is unique. Furthermore, if $K_1 = K_1' \oplus K_1''$, $K_2 = K_2' \oplus K_2''$; $K_1', K_2' \subset K'$; $K_1'', K_2'' \subset K''$, then

$$R_F(K_1, K_2/K) = S(R_F(K_1', K_2'/K') \otimes R_F(K_1'', K_2''/K''))S^{-1}. \tag{5.6}$$

We also omit $S$ in the following equations. The proof is the same as for Lemma 5.2.

By applying the above lemmas repeatedly to (4.6)–(4.8), we obtain the following decompositions:

$$\mathfrak{H}_S(H) = \mathfrak{H}_S(H^{(0)}) \otimes \mathfrak{H}_S(H^{(2)}) \otimes \mathfrak{H}_S(H^{(3)}) \otimes \mathfrak{H}_S(H^{(4)}), \tag{5.7}$$

$$R_S(H_1/H) = R_S(H_1'/H^{(0)}) \otimes B(\mathfrak{H}_S(H^{(2)})) \otimes 1 \otimes R_S(K^{(4)}/H^{(4)}), \tag{5.8}$$

$$R_S(\beta H_1^{\perp}) = R_S(\beta H_2'/H^{(0)}) \otimes 1 \otimes B(\mathfrak{H}_S(H^{(3)})) \otimes R_S(K^{(4)}/H^{(4)}). \tag{5.9}$$

Due to (2.6) and (4.10), we have

$$R_S(H_1'/H^{(0)})' \supset R_S(\beta H_2'/H^{(0)}), \tag{5.10}$$

$$R_S(H_1'/H^{(0)}) \vee R_S(\beta H_2'/H^{(0)}) = B(\mathfrak{H}_S(H^{(0)})). \tag{5.11}$$

Therefore the pair of von Neumann algebras $R_S(H_1'/H^{(0)})$ and $R_S(\beta H_2'/H^{(0)})$ is a factorization. In Secs. 8 and 9, we will show that they are paired factors, namely,

$$R_S(H_1'/H^{(0)})' = R_S(\beta H_2'/H^{(0)}). \tag{5.12}$$

For other parts of the decomposition, we have

$$B(\mathfrak{H}_S(H^{(2)}))' = \{\lambda 1\} \quad \text{in} \quad \mathfrak{H}_S(H^{(2)}), \tag{5.13}$$

$$\{1\}' = B(\mathfrak{H}_S(H^{(3)})) \quad \text{in} \quad \mathfrak{H}_S(H^{(3)}), \tag{5.14}$$

$$R_S(K^{(4)}/H^{(4)})' = R_S(K^{(4)}/H^{(4)}) \quad \text{in} \quad \mathfrak{H}_S(H^{(4)}). \tag{5.15}$$

The last equation is due to $H^{(4)} = K^{(4)} \oplus \beta K^{(4)}$ and Eq. (5.3). The duality equation (3.14) will follow from the above equations due to the following lemma.[25]

[22] H. Araki and J. S. Woods, J. Math Phys. 4, 637 (1963), Lemma 2.4.

[23] I. E. Segal, Mem. Am. Math. Soc., No. 9, II (1951), Corollaries 1.1 and 1.2.

[24] For the definition of the tensorial product of von Neumann algebras, see, for example, J. Dixmier, reference 15.

[25] It is also possible to prove the duality equation (3.14) without using this lemma. For this, we consider full space $H$ instead of $H^{(0)}$ and with only a slight modification, which is indicated in the proof of the corollary in Sec. 9, the argument of Secs. 8 and 9 goes through. However, this complicates notation in Secs. 8 and 9, and we find it shorter to use this lemma.

*Lemma. 5.4.* Let $R_l$ be von Neumann algebras on $\mathfrak{H}_l$, $l = 1, 2$ and let $\mathfrak{H} = \mathfrak{H}_1 \otimes \mathfrak{H}_2$. If $R_2 = B(\mathfrak{H}_2)$ or if $R_2$ is maximal Abelian on $\mathfrak{H}_2$, then $(R_1 \otimes R_2)' = R_1' \otimes R_2'$.

*Proof:* If $R_2 = B(\mathfrak{H}_2)$,

$$(R_1 \otimes R_2)' \subset \{(R_1 \otimes 1) \vee (1 \otimes R_2)\}'$$
$$= (R_1 \otimes 1)' \wedge (1 \otimes B(\mathfrak{H}_2))'$$
$$= (R_1 \otimes 1)' \wedge (B(\mathfrak{H}_1) \otimes 1) = R_1' \otimes 1.$$

On the other hand, $R_1' \otimes 1 \subset (R_1 \otimes R_2)'$. Hence $(R_1 \otimes R_2)' = R_1' \otimes 1 = R_1' \otimes R_2'$. If $R_2$ is maximal Abelian, then we have a spectral decomposition $\mathfrak{H}_2 = L_2(\Xi,\mu)$, $R_2 =$ multiplication algebra of bounded $L_2$ functions $f(\xi), \xi \in \Xi$, and $\mathfrak{H} = \int \mathfrak{H}_{1\xi}\, d\mu(\xi)$, $\mathfrak{H}_{1\xi} \approx \mathfrak{H}_1$, $R_1 \otimes R_2 = \int R_{1\xi}\, d\mu(\xi)$, $R_{1\xi} \approx R_1$. By a known theorem,[26] we have $(R_1 \otimes R_2)' = \int R_{1\xi}'\, d\mu(\xi) = (R_1' \otimes R_2) = (R_1' \otimes R_2')$.

By the analysis of this section we have reduced Eq. (3.14) to (5.12).

## 6. CREATION AND ANNIHILATION OPERATORS

The original construction[27] of the normal representation of CCR's uses the tensorial construction, which will be discussed in the present section. The important notions are the total particle number $n$ and the polynomial algebra of creation and annihilation operators. We define generalized creation and anihilation operators, which correspond to a homogeneous polynomial of conventional creation and annihilation operators. Their multiplication rule is given by Lemma 6.1. Equation (6.30) gives a unique expansion of an arbitrary bounded operator in terms of homogeneous polynomials of creation and annihilation operators of ascending degrees. The connection of the tensorial construction of this section and other constructions of Sec. 2 will be discussed in the next section.

Let $L$ be a complex Hilbert space and $L^{\otimes n}$ be the tensor product of $n$ copies of $L$. If $n = 0$, $L^{\otimes n}$ is defined to be the complex one-dimensional vector space. The mapping

$$h_1 \otimes \cdots \otimes h_n \to h_{P^{-1}(1)} \otimes \cdots \otimes h_{P^{-1}(n)}$$

for any $h_i \in L$ defines a unitary operator $U(P)$ on $L^{\otimes n}$ for each permutation $P$ of $n$ indices. $\{U(P)\}$ is a unitary representation of the symmetric group $\mathfrak{S}_n$ and $L^{\otimes n}$ can be reduced into inequivalent irreducible representations. The totally symmetric part of $L^{\otimes n}$ will be denoted by Sym $L^{\otimes n}$. The projection operator on Sym $L^{\otimes n}$ is given by

$$E_n^{\mathrm{Sym}} = \frac{1}{n!} \sum_P U(P). \tag{6.1}$$

We define Sym $L^{\otimes 0} = L^{\otimes 0}$ and $E_0^{\mathrm{Sym}} = 1$.

We now consider the complex Hilbert space

$$\mathfrak{H}_T(L) = \sum_{n=0}^{\infty}{}^{\oplus} \mathrm{Sym}\, L^{\otimes n}. \tag{6.2}$$

The projection operator for the subspace Sym $L^{\otimes n}$ of $\mathfrak{H}_T(L)$ will be denoted by $E_n$. $n$ is the total particle number.

Let $A$ be a bounded operator mapping Sym $L^{\otimes n}$ into Sym $L^{\otimes m}$. Let $\hat{A}$ be the extension of $A$ to an operator from $L^{\otimes n}$ into $L^{\otimes m}$, being $A$ on Sym $L^{\otimes n}$ and 0 on the orthogonal complement of Sym $L^{\otimes n}$. Let $1_t$ be an identity operator on $L^{\otimes t}$. Then $\hat{A} \otimes 1_t$ is an operator from $L^{\otimes(n+t)} = L^{\otimes n} \otimes L^{\otimes t}$ into $L^{\otimes(m+t)} = L^{\otimes m} \otimes L^{\otimes t}$, and $E_{m+t}^{\mathrm{Sym}}(\hat{A} \otimes 1_t)E_{n+t}^{\mathrm{Sym}}$ can be considered as an operator from Sym $L^{\otimes(n+t)}$ into Sym $L^{\otimes(m+t)}$. We denote by Sym $(A \otimes 1_t)$ the operator on $\mathfrak{H}_T(L)$ which is $E_{m+t}^{\mathrm{Sym}}(\hat{A} \otimes 1_t)E_{n+t}^{\mathrm{Sym}}$ on Sym $L^{\otimes(n+t)}$ and 0 on its orthogonal complement in $\mathfrak{H}_T(L)$. Finally the generalized creation and annihilation operator is defined by[28]

$$(a^{\dagger m}Aa^n) = \sum_{t=0}^{\infty} [(n+t)!\,(m+t)!/t!^2]^{\frac{1}{2}} \times \mathrm{Sym}\,(A \otimes 1_t). \tag{6.3}$$

We define this operator only on the domain

$$D = \bigcup_N \sum_{n=0}^{N} \mathrm{Sym}\, L^{\otimes n}. \tag{6.4}$$

The right-hand side of (6.3) is effectively a finite sum on $D$. $(a^{\dagger m}Aa^n)$ with domain $D$ is not closed.

If $m = 0$, $n = 1$, we write $(f^*, a)$ where $f \in L$ and $f^*$ is the mapping from $L$ into complex numbers given by $g \in L \to (f, g)$. If $m = 1$, $n = 0$, we write $(a^\dagger, f)$ where $f \in L$. They are conventional annihilation and creation operators.

*Lemma 6.1.*[29]

$$(a^{\dagger m}Aa^n)^* \supset (a^{\dagger n}A^*a^m), \tag{6.5}$$

$$(a^{\dagger m}A_1a^n)(a^{\dagger k}A_2a^l) = \sum_{t=0}^{\min(k,n)} \binom{n}{t}\binom{k}{t} t!\,(a^{\dagger(m+k-t)}F_ta^{(n+l-t)}), \tag{6.6}$$

[26] J. Dixmier, reference 15, p. 184.

[27] See reference 2. See also J. M. Cook, Trans. Am. Math. Soc. **74**, 222 (1953).

[28] This definition is obtained by considering the integral operator $B$ with the kernel function $B(x_1 \cdots x_m; y_1 \cdots y_n)$ and by substituting a well-known definition of creation and annihilation operators $a(x)$ and $a^\dagger(x)$ into the expression $\int a^\dagger(x_1) \cdots a^\dagger(x_m)B(x_1 \cdots x_m; y_1 \cdots y_n)a(y_1) \cdots a(y_n)\, dx\, dy$.

[29] The formula in this theorem can be obtained by a formal calculation using the expression of footnote (28) and applying the well-known commutation relation (6.12).

$$F_t = E^{\mathrm{Sym}}_{m+k-t}(\hat{A}_1 \otimes \mathbf{1}_{k-t})(\mathbf{1}_{m-t} \otimes \hat{A}_2)E^{\mathrm{Sym}}_{n+l-t}. \quad (6.7)$$

In (6.7) it is important that the operator $\hat{A}_1$ meets with $\mathbf{1}_{m-t}$ on its right, the operator $\hat{A}_2$ meets with $\mathbf{1}_{k-t}$ on its left and only $t$ legs of $\hat{A}_1$ meet with those of $\hat{A}_2$.

*Proof:* For (6.5), we have to prove

$$(\Psi, (a^{\dagger m}Aa^n)\Phi)^* = (\Phi, (a^{\dagger n}A^*a^m)\Psi) \quad (6.8)$$

for all $\Phi, \Psi \in D$. Since $(\hat{A} \otimes \mathbf{1}_t)^* = (\hat{A}^* \otimes \mathbf{1}_t) = \widehat{(A^* \otimes \mathbf{1}_t)}$, we have

$$(\Psi, \mathrm{Sym}\,(A \otimes \mathbf{1}_t)\Phi)^* = (\Phi, \mathrm{Sym}\,(A^* \otimes \mathbf{1}_t)\Psi)$$

for any $\Psi$ and $\Phi$ in $\mathfrak{H}_T(L)$. Hence (6.8) follows.

For (6.6), it is enough to prove the matrix elements of the equation between states $\Psi \in \mathrm{Sym}\, L^{\otimes\rho}$ and $\Phi \in \mathrm{Sym}\, L^{\otimes\sigma}$ for arbitrary $\rho$ and $\sigma$. If $\rho - \sigma \neq (m + k) - (n + l)$, or $\sigma < l$ or $\rho < m$, both sides of Eq. (6.6) vanishes and therefore the equality holds for such a case. If $\rho - \sigma = m + k - n - l$, $\sigma \geqq l$, $\rho \geqq n$, then the left-hand side becomes

$$[(\rho+n-m)!\,\rho!\,(\sigma+k-l)!\,\sigma!/(\rho-m)!^2(\sigma-l)!^2]^{\frac{1}{2}}$$
$$\times (\Psi, (\hat{A}_1 \otimes \mathbf{1}_{\rho-m})E^{\mathrm{Sym}}_{\sigma-l+k}(\hat{A}_2 \otimes \mathbf{1}_{\sigma-l})\Phi). \quad (6.9)$$

We now substitute $E^{\mathrm{Sym}}_{\sigma-l+k} = (\sigma - l + k)!^{-1}\sum_P U(P)$. If $P$ brings $S$ of last $(\sigma - l)$ indices again into the set of last $(\rho - m)$ indices while bringing other $(\sigma - l - S)$ of last $(\sigma - l)$ indices into the set of first $n$ indices, then that term gives

$$(\Psi, [(\hat{A}_1 \otimes \mathbf{1}_{\rho-m-S})(\mathbf{1}_{\sigma-l-S} \otimes \hat{A}_2) \otimes \mathbf{1}_S]\Phi)$$

because $\hat{A}_2$ and $\Phi$ are already symmetrized. The number $d_S$ of the permutation $P$ which fits the above description is given by

$$d_S = \begin{pmatrix} \sigma - l \\ S \end{pmatrix}\begin{pmatrix} \rho - m \\ S \end{pmatrix} S!$$
$$\times \begin{pmatrix} n \\ \sigma - l - S \end{pmatrix}(\sigma - l - S)!\,k!$$
$$= (\sigma - l)!\,(\rho - m)!\,m!\,k!/S!$$
$$\times (\rho - m - S)!\,(\sigma - l - S)!\,(\sigma - l - n - S)!.$$

Therefore (6.9) is equal to

$$\sum_{S=\sigma-n-l}^{\min(\rho-m,\sigma-l)} C_S(\Psi[(\hat{A}_1 \otimes \mathbf{1}_{\rho-n-S})$$
$$\times (\mathbf{1}_{\sigma-l-S} \otimes \hat{A}_2) \otimes \mathbf{1}_S]\Phi), \quad (6.10)$$

where

$$C_S = d_S[(\rho + n - m)!\,\rho!\,(\sigma - l + k)!$$
$$\times \sigma!/(\rho - m)!^2(\sigma - l)!^2]^{\frac{1}{2}}(\sigma - l + k)!^{-1}$$
$$= [\rho!\,\sigma!/S!^2]^{\frac{1}{2}}\begin{pmatrix} n \\ S + l + n - \sigma \end{pmatrix}$$
$$\times \begin{pmatrix} k \\ S + l + n - \sigma \end{pmatrix}(S + l + n - \sigma)!.$$

By setting $t \equiv S + l + n - \sigma = S + k + m - \rho$, we see that (6.10) is the same as the right-hand side of (6.6). This completes the proof of Lemma 6.1.

*Corollary 1.* If $f = E^{\mathrm{Sym}}_m f_1 \otimes \cdots \otimes f_m$, $g = E^{\mathrm{Sym}}_n g_1 \otimes \cdots \otimes g_n$, $f_i, g_i \in L$ and $A = fg^*$ [i.e., $Ag' = (g, g')f$ for any $g' \in \mathrm{Sym}\, L^{\otimes n}$], then

$$(a^{\dagger m}Aa^n) = (a^\dagger, f_1) \cdots (a^\dagger f_m)(g_1^* a) \cdots (g_n^* a). \quad (6.11)$$

By repeated applications of (6.6), we obtain (6.11).

*Corollary 2.*[30] If $f, g \in L$,

$$[(g^*, a), (a^\dagger f)] = (g, f), \quad (6.12)$$
$$(a^\dagger, f)^* = \overline{(f^*, a)}, \quad (6.13)$$
$$(g^*, a)\Psi_0 = 0 \quad \text{if} \quad \Psi_0 \in \mathrm{Sym}\, L^{\otimes 0}. \quad (6.14)$$

$(a^\dagger, f)$ is linear in $f$, and $(g^*a)$ is antilinear in $g$. $\Psi_0 \in \mathrm{Sym}\, L^{\otimes 0}$ is in the domain of any polynomial of operators $(a^\dagger f_i)$, $f_i \in L$ and is cyclic vector of the set of all such polynomials. The foregoing properties, where (6.13) may be weakened to $(a^\dagger, f)^* \supset (f^*, a)$, determines the structure consisting of the Hilbert space $\mathfrak{H}_T(L)$, the cyclic vector $\Psi_0$ and the closed operators $\overline{(a^\dagger f)}$, $\overline{(g^* a)}$ up to unitary equivalence.

*Proof:* The stated properties except for (6.13) are trivial consequences of definitions and the Lemma 6.1. Equation (6.13) will be proved shortly. The uniqueness of the structure consisting of $\mathfrak{H}_T(L)$, $\Psi_0$ and the restriction of $\overline{(a^\dagger f)}$, $\overline{(g^* a)}$ to the domain $D$ is well-known. The property (6.13) will then guarantee the uniqueness of the closed operators $\overline{(a^\dagger f)}$ and $\overline{(g^* a)}$.

We now prove (6.13). From (6.5), $(a^\dagger, f)^* \supset (f^*, a)$. We have only to prove $D[(a^\dagger, f)^*] = D[(f^*, a)]$. Let $L(f, n)$ be the subspace spanned by vectors $(a^\dagger f)^n Q\Psi_0$ where $Q$ is an arbitrary polynomial of $(a^\dagger f_i)$, $f_i \perp f$. We easily see that $L(f, m) \perp L(f, n)$ for $m \neq n$, and

$$L = \sum_{n=0}^{\infty \oplus} L(f, n).$$

Let $E(f, n)$ be the projection on $L(f, n)$. If $\Psi \in$

[30] We follow the physicists's convention that the inner product $(g, f)$ in a complex Hilbert space is linear in $f$ and antilinear in $g$.

$L(f, n) \cap D$, then $(a^\dagger, f)\Psi \in L(f, n+1)$ $(f^*, a)\Psi \in L(f, n-1)$ $(=0$ if $n=0)$, and $||(f^*, a)\Psi||^2 = n(f, f)\,||\Psi||^2$. Since $L(f, n) \cap D$ is dense in $L(f, n)$ and since $(f^*, a)$ is bounded on $L(f, n)$, $L(f, n)$ is in the domain of $\overline{(f^*, a)}$. If $\Psi = \sum \Psi_n$, $\Psi_n \in L(f, n)$ and $\sum n\,||\Psi_n||^2 < \infty$, then

$$\Psi_N = \sum_{n=0}^{N} \Psi_n \to \Psi \quad \text{and} \quad \overline{(f^*, a)}\Psi_N \to \sum_{n=0} \overline{(f^*, a)}\Psi_n.$$

Hence

$$D[\overline{(f^*, a)}] \supset \left\{\Psi;\ \sum_{n=0}^{\infty} n\,||E(f, n)\Psi||^2 < \infty\right\}. \tag{6.15}$$

On the other hand, if $\Psi \in D[(a^\dagger, f)^*]$, and $\Psi_n = E(f, n)\Psi$, then $E(f, n)(a^\dagger, f)^*\Psi = E(f, n)(a^\dagger, f)^*\Psi_{n+1}$ due to $(a^\dagger, f)L(f, n) \subset L(f, n+1)$ and $E(f, n)(a^\dagger, f)^*\Psi_{n+1} = (f^*, a)\Psi_{n+1}$ due to $(a^\dagger, f)^* \supset (f^*, a)$ and $D[(f^*, a)] \supset L(f, n+1)$. Since $\sum_n ||E(f, n)\Phi||^2 < \infty$ for any $\Phi$, we have

$$\sum_{n=0} ||\overline{(f^*, a)}\Psi_{n+1}||^2 = \sum_{n=0} (n+1)\,||\Psi_{n+1}||^2 < \infty.$$

Hence

$$D[(a^\dagger, f)^*] \subset \left\{\Psi;\ \sum_{n=0}^{\infty} n\,||E(f, n)\Psi||^2 < \infty\right\}. \tag{6.15'}$$

Since $(f^*, a) \subset (a^\dagger, f)^*$, (6.15) and (6.15′) imply (6.13).

*Remark:* The above proof and a similar argument also show that

$$D(\overline{(a^\dagger, f)}) = D(\overline{(f^*, a)}) = \left\{\Psi;\ \sum_{n=0}^{\infty} n\,||E(f, n)\Psi||^2 < \infty\right\}. \tag{6.16}$$

For the sake of application in Sec. 10, we add a further definition. Let $v$ be an operator on $L$ with $||v|| \leqq 1$. $v^{\otimes n}$ is then an operator on $L^{\otimes n}$ which leaves Sym $L^{\otimes n}$ invariant and $||v^{\otimes n}|| \leqq 1$. (This can be proved in a similar manner as the proof of Lemma 10.4.) We use the same notation $v^{\otimes n}$ for its restriction to Sym $L^{\otimes n}$. Then the tensorial extension of $v$ on $\mathfrak{H}_T(L)$ is defined by

$$T(v) = \sum_{n=0}^{\infty}{}^{\oplus} v^{\otimes n} \qquad (||v|| \leqq 1). \tag{6.17}$$

Here, $v^{\otimes 0}$ is defined to be 1. $||T(v)|| = 1$ and $T(v)$ commutes with $E_n$. Furthermore,

$$T(v_1)T(v_2) = T(v_1 v_2), \tag{6.18}$$

$$T(v)^* = T(v^*), \tag{6.19}$$

$$\lim_{n\to\infty} T(v_n) = T(\lim v_n), \tag{6.20}$$

where the limit is in strong sense and $\lim v_n$ is assumed to exist. Equations (6.18), (6.19), and (6.20) can be checked easily on each subspace $E_n\mathfrak{H}_T(L)$. Since $||T(v_n)|| \leqq 1$ independent of $n$, and since

$$\mathfrak{H}_T(L) = \sum_n{}^{\oplus} E_n\mathfrak{H}_T(L),$$

(6.20) holds on the entire space $\mathfrak{H}_T(L)$.

If $v$ is unitary, then $T(v)$ is unitary and we have

$$T(v)(a^{\dagger m}Aa^n)T(v^*) = (a^{\dagger m}v^{\otimes m}A(v^*)^{\otimes n}a^n). \tag{6.21}$$

If $K$ is a self-adjoint operator on $L$, then $T(e^{i\lambda K})$ is a one-parameter family of unitary operators and we define the self-adjoint operator $Q(K)$ by

$$T(e^{i\lambda K}) = e^{i\lambda Q(K)}. \tag{6.22}$$

$Q(K)$ coincides with $(a^\dagger Ka)$ on $D$ if $K$ is bounded, and essentially self-adjoint on $D$.

Finally, we discuss an expansion of an arbitrary bounded operator $B$ on $\mathfrak{H}_T(L)$ into generalized creation and annihilation operators. We define

$$B_{mn} = E_m B E_n. \tag{6.23}$$

Furthermore, we define an operator $[B]_{kl}$ from Sym $L_\otimes{}^l$ into Sym $L_\otimes{}^k$ by the following recursive formula:

$$B_{mn} = \sum_{t=0}^{\min(k,l)} [m!\,n!/t!^2]^{\frac{1}{2}} \times \mathrm{Sym}\,([B]_{m-t,n-t} \otimes 1_t). \tag{6.24}$$

This can be solved explicitly and we obtain[31]

$$[B]_{k,l} = \sum_{t=0}^{\min(k,l)} \alpha(k, l; t)\,\mathrm{Sym}\,(B_{k-t,l-t} \otimes 1_t), \tag{6.25}$$

$$\alpha(k, l; t) = C_t[(k-t)!\,(l-t)!]^{-\frac{1}{2}}, \tag{6.26}$$

$$C_t = \sum_n (-1)^n \sum_{t_1+\cdots+t_n=t,\ t_j\geqq 1} [t_1!\cdots t_n!]^{-1} = \frac{1}{t!}\left(\frac{d}{dx}\right)^t e^{1-e^x}\Big|_{x=0} \qquad (C_0 = 1). \tag{6.27}$$

It is also convenient to define

$$[B]_N = \sum_{k+l=N} (a^{\dagger k}[B]_{k,l}a^l). \tag{6.28}$$

Because $\sum E_n = 1$, we have from (6.3) and (6.24) the following expansion:

$$(\Phi B\Psi) = \sum_{k,l} (\Phi(a^{\dagger k}[B]_{k,l}a^l)\Psi) \tag{6.29}$$

$$= \sum_N (\Phi[B]_N\Psi), \tag{6.30}$$

where $\Phi$ and $\Psi$ are restricted to $D$. (The summation terminates at finite $k$, $l$ and $N$.)

## 7. THE CONNECTION OF THE SPACE $\mathfrak{H}_T(L)$ WITH $\mathfrak{H}_F(K)$ AND $\mathfrak{H}_S(H)$

Let $L = K + iK$ be the complexification of a real Hilbert space $K$. It is easy to show, that

[31] In (6.25), $B_{k-t,t-t}$ and $\mathrm{Sym}(B_{k-t,\tau-t} \otimes 1_t)$ are used as operators on Sym $L^\otimes$ instead of operators on $\mathfrak{H}_T(L)$.

in $\mathfrak{H}_F(K)$, $\varphi_F(f)$ and $\pi_F(g)$ can be operated on $\Psi_F(K)$ repeatedly. Let $D_F$ be the subset of $\mathfrak{H}_F(K)$ consisting of vectors $Q\Psi_F(K)$ where $Q$ is an arbitrary polynomial of $\varphi_F(f_i)$ and $\pi_F(g_j)$. For any $h = f + ig$; $f, g \in K$, we now define the operators $(a_F^\dagger, h)$ and $(h^*, a_F)$ on $D_F$ by

$$(a_F^\dagger, h)\Psi = 2^{-\frac{1}{2}}(\varphi_F(f) + i\varphi_F(g) + \pi_F(g) - i\pi_F(f))\Psi, \tag{7.1}$$

$$(h^*, a_F)\Psi = 2^{-\frac{1}{2}}(\varphi_F(f) - i\varphi_F(g) + \pi_F(g) + i\pi_F(f))\Psi, \tag{7.2}$$

where we restrict $\Psi$ to $D_F$. Obviously $(a_F^\dagger, h)$ and $(h^*, a_F)$ can be applied on $\Psi_F(K)$ repeatedly. $\varphi_F(f)$ and $\pi_F(g)$ can be written as

$$\varphi_F(f)\Psi = 2^{-\frac{1}{2}}((a_F^\dagger, f) + (f^*, a_F))\Psi, \tag{7.3}$$

$$\pi_F(g)\Psi = 2^{-\frac{1}{2}}i((a_F^\dagger, g) - (g^*, a_F))\Psi. \tag{7.4}$$

Therefore, any vector in $D_F$ can be obtained by applying a polynomial of $(a_F^\dagger, h_i)$ and $(h_j^*, a_F)$ on $\Psi_F(K)$. Because $U_F(f)\Psi_F(K) = \sum n!^{-1}\varphi(f)^n\Psi_F(K)$, $D_F$ is dense in $\mathfrak{H}_F(K)$. (Cf. Lemma 5.1.) Other properties required for $(a^\dagger, h)$ and $(h^*, a)$ in the Corollary 2 to the Lemma 6.1 follow immediately from the definition (7.1) and (7.2) and from the linearity in $f$ and $g$, Hermiticity, and CCR's of $\varphi(f)$ and $\pi(g)$. Therefore we have the unitary equivalence: $\mathfrak{H}_F(K) = \mathfrak{H}_T(K + iK)$, $\Psi_F(K) = \Psi_0$, $(a_F^\dagger, h) = (a^\dagger, h)$, $(h^*, a_F) = (h^*, a)$. Since $D_F \subset D$, we may also write $(a_F^\dagger, h) \subset (a^\dagger, h)$ and $(h^*, a_F) \subset (h^*, a)$. It is rather easy to prove[32]

$$\varphi_F(f) = 2^{-\frac{1}{2}}\overline{((a_F^\dagger, f) + (f^*, a_F))} \supset 2^{-\frac{1}{2}}\overline{((a_F^\dagger, f)} + \overline{(f^*, a_F))}, \tag{7.5}$$

$$\pi_F(g) = 2^{-\frac{1}{2}}i\overline{((a_F^\dagger, g) - (g^*, a_F))} \supset 2^{-\frac{1}{2}}i(\overline{(a_F^\dagger, g)} - \overline{(g^*, a_F)}). \tag{7.6}$$

For a given $L$, the choice of $K$ is not unique. On the other hand, for a given $K$, we have a canonical way of constructing $L$ and $H$ by $L = K + iK$ and $H = K \otimes R^2$, where $K$ may be identified with $K \otimes \begin{pmatrix}1\\0\end{pmatrix}$, and $\beta$ with $\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}$, so that $H = K \oplus \beta K$. These two, $L$ and $H$, are uniquely interrelated and this relation can be formulated in the following way without going through $K$.

For a given $L$, we introduce a new real inner product $(\ )_{\hat{L}}$ by

$$(f, g)_{\hat{L}} = \mathrm{Re}\,(f, g), \quad f, g \in L. \tag{7.7}$$

[32] This is a particular case of (7.12).

$(f, g)_{\hat{L}}$ is real linear in $f$ and g, symmetric and positive-definite and $L$ is complete with respect to this real inner product. Therefore $L$, with this inner product, is a real Hilbert space, which we shall denote by $\hat{L}$. The multiplication of $i$ in $L$ induces an operator on $\hat{L}$, which will be denoted by $\beta$. This $\beta$ satisfies (2.5), and

$$(\hat{f}, \beta\hat{g})_{\hat{L}} = -\mathrm{Im}\,(f, g), \tag{7.8}$$

where $\hat{f}$ and $\hat{g}$ are $f$ and $g$ considered as an element in $\hat{L}$.

Conversely, if $H$ is given, we define a new complex inner product $(\ )_{\hat{H}}$ by

$$(h_1, h_2)_{\hat{H}} = (h_1, h_2) - i(h_1, \beta h_2). \tag{7.9}$$

We also define the multiplication of the complex number $a + ib$ by the multiplication of $a + \beta b$. Then $(h_1, h_2)_{\hat{H}}$ is linear in $h_2$, antilinear in $h_1$, Hermitian and positive-definite, and $H$ is complete. $H$ becomes a complex Hilbert space which we denote by $\hat{H}$. If $H = \hat{L}$, then $\hat{H}$ returns to $L$ and vice versa. The correspondence is uniquely defined by (7.7)–(7.9).

In $\mathfrak{H}_S(H)$, $\chi(h)$ can be operated on $\Psi_S(H)$ repeatedly and we define $D_S$ to be the subset of $\mathfrak{H}_S(H)$ consisting of all vectors $Q\Psi_S(H)$, where $Q$ is an arbitrary polynomial of $\chi(h_i)$. If $\mathfrak{H}_S(H)$ is identified with $\mathfrak{H}_F(K)$, with $K \oplus \beta K = H$, then $D_S = D_F$. On $D_S$, we define operators $(a_S^\dagger h)$ and $(h^*, a_S)$,

$$(a_S^\dagger h)\Psi = 2^{-\frac{1}{2}}(\chi(h) - i\chi(\beta h))\Psi, \tag{7.10}$$

$$(h^*, a_S)\Psi = 2^{-\frac{1}{2}}(\chi(h) + i\chi(\beta h))\Psi, \tag{7.11}$$

where $\Psi \in D_S$. With the help of the identification $\mathfrak{H}_S(H) = \mathfrak{H}_F(K) = \mathfrak{H}_T(K + iK)$, we see the unitary equivalence, $\mathfrak{H}_S(H) = \mathfrak{H}_T(H)$, $\Psi_S(H) = \Psi_0$, $(a_S^\dagger, h) \subset (a^\dagger, h)$, $(h^*, a_S) \subset (h^*, a)$. It is easy to prove[33]

[33] From the proof of the Corollary 2 of the Lemma 6.1, the last inclusion in (7.12) is easily obtained. To prove the first equality of (7.12), let $\chi_1 = (a^\dagger, h) + (h^*, a)$, $\Psi \in D(\chi_1^*)$, and $\Psi_n = E(h, n)\Psi$. Since $D(\bar{\chi}_1) \supset L(h, n)$ and $\bar{\chi}_1 = \chi_1^*$ on $L(h, n)$, we see that $E(h, n)\chi_1^*\Psi = E(h, n)\bar{\chi}_1(\Psi_{n+1} + \Psi_{n-1})$. Since $(a^\dagger h)(h^* a) = n$ on $L(h, n)$, $||E(h, n)\bar{\chi}_1\Psi_{n+1}||^2 = (n + 1)\,||\Psi_{n+1}||^2$. For a given $\epsilon$, there exists $N$ such that $\sum_{n=N}^\infty ||E(h, n)\chi_1^*\Psi||^2 < \epsilon^2$ and $\sum_{n=N}^\infty ||\Psi_n||^2 < \epsilon^2$. For these $\epsilon$ and $N$, there exists $k$ and $l$ such that $k > N$, $l > N$, $2k\,||\Psi_{2k}||^2 < \epsilon^2$, $(2l + 1)\,||\Psi_{2l+1}||^2 < \epsilon^2$ because $\sum_n ||\Psi_n||^2 < \infty$ and $\sum_{k>N} 1/2k = \sum_{l>N} 1/(2l + 1) = \infty$. Then $\Psi_\epsilon \equiv \sum_{n=0}^{k-1}\Psi_{2n} + \sum_{n=0}^{l-1}\Psi_{2n+1}$ satisfies $||\Psi - \Psi_\epsilon|| < \epsilon$ and $||\chi_1^*\Psi - \bar{\chi}_1\Psi_\epsilon|| < 3\epsilon$. Hence $D(\bar{\chi}_1) = D(\chi_1^*)$ and $\bar{\chi}_1 = \chi_1^*$, which proves (7.12). If we define $\Psi_0^n = [n!(h, h)^n]^{-\frac{1}{2}}(h^*, a)^n\Psi_n$, we easily see that $D(\chi_1^*) = \{\Psi;\ \sum ||(n + 1)^{\frac{1}{2}}\Psi_0^{n+1} + n\Psi_0^{n-1}||^2 < \infty\}$. From this we have $D(\chi_1(h)) \cap D(\chi(\beta h)) = D(\overline{(a^\dagger, h)}) = D(\overline{(h^*, a)})$ and (7.13) and (7.14) follows. The equality of (7.12) can also be obtained by calculating the defect indices of $\chi_1$.

$$\chi(h) = 2^{-\frac{1}{2}}\overline{((a_S^\dagger, h) + (h^*, a_S))}$$
$$\supset 2^{-\frac{1}{2}}(\overline{(a_S^\dagger, h)} + \overline{(h^*, a_S)}), \quad (7.12)$$
$$\overline{(a_S^\dagger, h)} = 2^{-\frac{1}{2}}(\chi(h) - i\chi(\beta h)), \quad (7.13)$$
$$\overline{(h^*, a)} = 2^{-\frac{1}{2}}(\chi(h) + i\chi(\beta h)). \quad (7.14)$$

Let $v$ be a unitary operator on $L$ and we identify $\mathfrak{H}_S(\hat{L})$ and $\mathfrak{H}_T(L)$ as above. By using $W(h)\Psi_S(\hat{L}) = \sum_{n=0}^{\infty} 1/n!\, \chi(h)^n\Psi_S(L)$, we can directly prove

$$T(v)W(h)\Psi_S(\hat{L}) = W(\hat{v}h)\Psi_S(\hat{L}). \quad (7.15)$$

From this we have

$$T(v)W(h)T(v)^{-1} = W(\hat{v}h), \quad (7.16)$$
$$T(v)U_F(f)V_F(g)T(v)^{-1}$$
$$= CU_F(\mathrm{Re}\, vf - \mathrm{Im}\, vg)V_F(\mathrm{Re}\, vg + \mathrm{Im}\, vf), \quad (7.17)$$
$$C = \exp i[\tfrac{1}{2}(\mathrm{Re}\, vf, \mathrm{Im}\, vf)$$
$$- \tfrac{1}{2}(\mathrm{Re}\, vg, \mathrm{Im}\, vg) - (\mathrm{Im}\, vf, \mathrm{Im}\, vg)], \quad (7.18)$$

where Re and Im refer to the decomposition $L = K + iK$, and we omitted the $\wedge$ symbol in (7.17) and (7.18).

## 8. PROOF OF THE DUALITY THEOREM (1)

We now prove (3.14) in this and the following sections. In Sec. 5, we have already seen that it is enough to prove Eq. (5.12). We use the unitary equivalence $\mathfrak{H}_S(H^{(0)}) = \mathfrak{H}_T(\hat{H}^{(0)})$ considered in Sec. 7.

If $R_1$ commutes with $R_2$ and $R_1'$ commutes with $R_2'$, then the two von Neumann algebras $R_1$ and $R_2$ are the commutant of each other. Therefore, we take an arbitrary element $B$ from $R(H_1')'$ and an arbitrary element $C$ from $R(\beta H_2')'$ and see whether they commute with each other. In this section, we will prove that $C$ commutes with $[B]_N$ for every $N$. In the next section, we will prove that $C$ commutes with $B$.

Since $B$ commutes with $W(\lambda h)$ for any $h \in H_1'$ and real $\lambda$, $BD(\chi(h)) \subset D(\chi(h))$ and $(B, \chi(h))\Psi = 0$ for any $\Psi \in D(\chi(h))$. Since $D(\chi(h)) \supset D$, we have

$$\{\Phi, (B\chi(h) - \chi(h)B)\Psi\} = 0 \quad (8.1)$$

for any $\Phi, \Psi \in D$. By using the Lemma 6.1, we have

$$\sqrt{2}\,[B\chi(h) - \chi(h)B]_{m,n}$$
$$= (n+1)[B]_{m,n+1}\hat{h} - (m+1)\hat{h}^*[B]_{m+1,n}, \quad (8.2)$$

where the notation on the right-hand side is defined by $([B]_{m,n+1}\hat{h})g = [B]_{m,n+1}E_{n+1}^{\mathrm{Sym}}\hat{h} \otimes g$ for any $g \in \mathrm{Sym}\, L^{\otimes n}$, and $\hat{h}^*[B]_{m+1,n} = ([B]_{m+1,n}^*\hat{h})^*$. Thus (8.1) implies

$$(n+1)[B]_{m,n+1}\hat{h} = (m+1)\hat{h}^*[B]_{m+1,n} \quad (8.3)$$

for any $h \in H_1'$. Similarly, for any $h \in \beta H_2'$,

$$(n+1)[C]_{m,n+1}\hat{h} = (m+1)\hat{h}^*[C]_{m+1,n}. \quad (8.4)$$

We note that the conditions (8.3) and (8.4) separate into independent conditions on each $[B]_N$ and $[C]_N$. As a simple corollary of this observation, we obtain

$$[[B]_N, \chi(h)]\Psi = 0 \quad (8.5)$$

for $\Psi \in D$ and $h \in H_1$.

We now use the definition (6.28) and Lemma 6.1,

$$[[B]_N, [C]_L]$$
$$= \sum_{\rho=0}^{N+L} \sum_{t=0}^{\min(\rho, N+L-\rho)} [a^{\dagger(\rho-t)}Q(\rho, t)a^{N+L-\rho-t}],$$
$$Q(\rho, t) = E_{\rho-t}^{\mathrm{Sym}}\Big[\sum_{m+k=\rho}\binom{N-m}{t}\binom{k}{t}t!$$
$$\times ([B]_{m,N-m} \otimes \mathbf{1}_{k-t})(\mathbf{1}_{N-m-t} \otimes [C]_{k,L-k})$$
$$- \sum_{m+k=\rho}\binom{m}{t}\binom{L-k}{t}t!\,([C]_{k,L-k} \otimes \mathbf{1}_{m-t})$$
$$\times (\mathbf{1}_{L-k-t} \otimes [B]_{m,N-m})]E_{N+L-\rho-t}^{\mathrm{Sym}}, \quad (8.7)$$

where $m$ runs from $\max(0, \rho - L)$ to $\min(N - t, \rho - t)$ in the first summation, and from $\max(t, \rho - L + t)$ to $\min(N, \rho)$ in the second summation.

In order to utilize the properties (8.3) and (8.4), we consider the following device. Due to the Theorem 3, there exist subspaces $K^{(0)}$, $K_1'$, and $K_2'$ of $H^{(0)}$ such that $H^{(0)} = K^{(0)} \oplus \beta K^{(0)}$, $K_1', K_2' \subset K^{(0)}$, $H_1' = K_1' \oplus \beta K_2'$, and any two of $K_1'$, $K_2'$, $K_1'^{\perp} \cap K^{(0)}$, $K_2'^{\perp} \cap K^{(0)}$ have zero intersection. $\beta H_2'$ is then $K_2'^{\perp} \oplus \beta K_1'^{\perp}$.

In terms of operators $\alpha(K_2'; K_1'/K^{(0)})$ and $\bar{U}(K_2'; K_1'/K^{(0)})$, introduced in Sec. 4, we define two nonorthogonal projections $E_1'$ and $E_2'$ by

$$E_1' = P(K_1') - \bar{U}(K_2'; K_1'/K^{(0)})$$
$$\times \alpha(K_2'; K_1'/K^{(0)})^{-\frac{1}{2}}P(K_1'), \quad (8.8)$$
$$E_2' = P(K_1'^{\perp} \cap K^{(0)}) + \bar{U}(K_2'; K_1'/K^{(0)})$$
$$\times \alpha(K_2'; K_1'/K^{(0)})^{-\frac{1}{2}}P(K_1'). \quad (8.9)$$

They satisfy $E_1'^2 = E_1'$, $E_2'^2 = E_2'$, $E_1' + E_2' \subset P(K^{(0)})$, and if

$$x \in K^{(0)} \cap D[\alpha(K_2'; K_1'/K^{(0)})^{-\frac{1}{2}}P(K_1')],$$
$$x = E_1'x + E_2'x, \quad E_1'x \in K_2'^{\perp} \cap K^{(0)},$$
$$E_2'x \in K_1'^{\perp} \cap K^{(0)}. \quad (8.10)$$

The adjoint of $E_1'$ and $E_2'$ satisfies for any

$$x \in K^{(0)} \cap D[\alpha(K_2'; K_1'^{\perp} \cap K^{(0)}/K^{(0)})^{\frac{1}{2}} \times P(K_1'^{\perp} \cap K^{(0)})],$$

$$x = E_1'^* x + E_2'^* x, \quad E_1'^* x \in K_1', \quad E_2'^* x \in K_2'. \tag{8.11}$$

We now introduce the spectral projection of $\alpha(K_2'; K_1'/K^{(0)})$,

$$\alpha(K_2'; K_1'/K^{(0)}) = \int \lambda \, dE(\lambda), \tag{8.12}$$

where $E(\Delta) = \int_\Delta dE(\lambda)$ are the spectral projections of $\alpha(K_2'; K_1'/K^{(0)})$ acting on $K_1'$ for any Borel set $\Delta$. We define the projection operator $E_\epsilon$ on $K^{(0)} = K_1' \oplus (K_1'^{\perp} \cap K^{(0)})$ by

$$E_\epsilon = E((\epsilon, \infty)) + \bar{U}(K_2'; K_1'/K^{(0)}) \times E((\epsilon, \infty))\bar{U}(K_2'; K_1'/K^{(0)})^*. \tag{8.13}$$

Furthermore, we define two operators on $K^{(0)}$ by

$$E_{1\epsilon} = E_1' E_\epsilon, \qquad E_{2\epsilon} = E_2' E_\epsilon. \tag{8.14}$$

They are bounded operators and satisfy

$$E_{1\epsilon} + E_{2\epsilon} = E_\epsilon, \tag{8.15}$$

$$\lim_{\epsilon \to 0} E_\epsilon = 1 \qquad (\text{on } K^{(0)}). \tag{8.16}$$

Any linear bounded operator on a real Hilbert space $K^{(0)}$ can be uniquely extended to a linear bounded operator on its complexification $K^{(0)} + iK^{(0)} = \hat{H}^{(0)}$. We denote the extended operators by $\hat{E}_{1\epsilon}$, $\hat{E}_{2\epsilon}$ and $\hat{E}_\epsilon$. Let $\{f_\mu^{1\epsilon}\}$, $\{f_\mu^{2\epsilon}\}$, $\{g_\mu^{1\epsilon}\}$, $\{g_\mu^{2\epsilon}\}$ be orthonormal bases for $E_\epsilon K_1'$, $E_\epsilon K_2'$, $E_\epsilon(K_2'^{\perp} \cap K^{(0)})$, and $E_\epsilon(K_1'^{\perp} \cap K^{(0)})$, respectively. Then $\{\hat{f}_\mu^{1\epsilon}\}$, etc., are orthonormal bases for $\hat{E}_\epsilon(K_1' + iK_1')$, etc. Furthermore,

$$\hat{E}_{1\epsilon} = \sum_\nu \sum_\mu d_{\nu\mu}^{1\epsilon} \hat{g}_\nu^{1\epsilon} (\hat{f}_\mu^{1\epsilon})^*, \tag{8.17}$$

$$\hat{E}_{1\epsilon}^* = \sum_\nu \sum_\mu d_{\nu\mu}^{1\epsilon} \hat{f}_\mu^{1\epsilon} (\hat{g}_\nu^{1\epsilon})^*, \tag{8.18}$$

where

$$d_{\nu\mu}^{l\epsilon} = (\hat{g}_\nu^{l\epsilon}, \hat{E}_{l\epsilon} \hat{f}_\mu^{l\epsilon}) = (g_\nu^{l\epsilon}, E_{l\epsilon} f_\mu^{l\epsilon}), \tag{8.19}$$

$l = 1, 2$, and the summation converges in strong sense. [$\hat{g}_\nu \hat{f}_\mu^*$ is an operator such that $\hat{g}_\nu \hat{f}_\mu^* x = (\hat{f}_\mu, x)\hat{g}_\nu$.] Note that $d_{\nu\mu}^{l\epsilon}$ is real.

We further introduce the following notation:

$$d_{\{\nu\}\{\mu\}}^{\{l\}\epsilon} = \prod_{j=1}^{t} d_{\nu_j \mu_j}^{l_j \epsilon}, \tag{8.20}$$

$$\hat{f}_{\{\mu\}}^{\{l\}\epsilon} = \hat{f}_{\mu_1}^{l_1 \epsilon} \otimes \cdots \otimes \hat{f}_{\mu_t}^{l_t \epsilon}, \tag{8.21}$$

$$\hat{g}_{\{\nu\}}^{\{l\}\epsilon} = \hat{g}_{\nu_1}^{l_1 \epsilon} \otimes \cdots \otimes \hat{g}_{\nu_t}^{l_t \epsilon}. \tag{8.22}$$

We then have the following equations on $H^{\otimes t}$ with strong operator topology:

$$\sum_{\{l\}} \sum_{\nu_1} \sum_{\mu_1} \cdots \sum_{\nu_t} \sum_{\mu_t} d_{\{\nu\}\{\mu\}}^{\{l\}\epsilon} \hat{g}_{\{\nu\}}^{\{l\}\epsilon} (\hat{f}_{\{\mu\}}^{\{l\}\epsilon})^* = \hat{E}_\epsilon^{\otimes t} \tag{8.23}$$

$$= \sum_{\{l\}} \sum_{\nu_1} \sum_{\mu_1} \cdots \sum_{\nu_t} \sum_{\mu_t} d_{\{\nu\}\{\mu\}}^{\{l\}\epsilon} \hat{f}_{\{\mu\}}^{\{l\}\epsilon} (\hat{g}_{\{\nu\}}^{\{l\}\epsilon})^*. \tag{8.24}$$

We now return to (8.6) and consider the following operator $A_\epsilon$:

$$A_\epsilon \equiv ([C]_{k, L-k} \otimes 1_{m-t})(1_{L-k-t} \otimes \hat{E}_\epsilon^{\otimes t} \otimes 1_{m-t}) \times (1_{L-k-t} \otimes [B]_{m, N-m}). \tag{8.25}$$

We insert (8.23) for $\hat{E}_\epsilon^{\otimes t}$ and use the following equation which follows from (8.3), (8.4), and $\widehat{\beta g}_\nu = i\hat{g}_\nu$, $\widehat{\beta g}_\nu^* = -i\hat{g}_\nu^*$, etc. :

$$\frac{(n+t)!}{n!} [B]_{m, n+t} \hat{f}_{\{\mu\}}^{\{l\}\epsilon} = \frac{(m+t)!}{m!} (-1)^{t + \sum l_i} (\hat{f}_{\{\mu\}}^{\{l\}\epsilon})^* [B]_{m+t, n}, \tag{8.26}$$

$$\frac{(n+t)!}{n!} [C]_{m, n+t} \hat{g}_{\{\nu\}}^{\{l\}\epsilon} = \frac{(m+t)!}{m!} (-1)^{t + \sum l_i} (\hat{g}_{\{\nu\}}^{\{l\}\epsilon})^* [C]_{m+t, n}. \tag{8.27}$$

With the aid of (8.24), we now have

$$A_\epsilon = G(1_k \otimes [B]_{m-t, N-m+t})(1_k \otimes \hat{E}_\epsilon^{\otimes t} \otimes 1_{N-m}) \times ([C]_{k+t, L-k-t} \otimes 1_{N-m}), \tag{8.28}$$

where

$$G = \binom{N-m+t}{t}\binom{k+t}{t} t! \Big/ \binom{m}{t}\binom{L-k}{t} t!. \tag{8.29}$$

Because of (8.16) (which implies $\lim_{\epsilon \to 0} \hat{E}_\epsilon = 1$ on $K^{(0)} + iK^{(0)}$),

$$([C]_{k, L-k} \otimes 1_{m-t})(1_{L-k-t} \otimes [B]_{m, N-m}) = G(1_k \otimes [B]_{m-t, N-m+t}) \times ([C]_{k+t, L-k-t} \otimes 1_{N-m}). \tag{8.30}$$

If we use the equality

$$E_{\rho-t}^{\mathrm{Sym}}(1_k \otimes [B]_{m-t, N-m+t})([C]_{k+t, L-k+t} \otimes 1_{N-m}) E_{N+\rho-t}^{\mathrm{Sym}} = E_{\rho-t}^{\mathrm{Sym}}([B]_{m-t, N-m+t} \otimes 1_k) \times (1_{N-m} \otimes [C]_{k+t, L-k-t}) E_{N+\rho-t}^{\mathrm{Sym}}, \tag{8.31}$$

we see that the term with $m$ and $k$ in the second summation in the bracket of (8.7) cancels the term with $m - t$ and $k + t$ in the first summation. As $m$ runs from $\max(t, \rho - L + t)$ to $\min(N, \rho)$, $m - t$ runs from $\max(0, \rho - L)$ to $\min(N - t, \rho - t)$. Therefore the second summation exactly cancels the

first summation in (8.7) and we have

$$\{[B]_N, [C]_L\}\Psi = 0 \tag{8.32}$$

for any $\Psi \in D$. By (6.30), we have

$$([B]_N^*\Phi, C\Psi) = (\Phi, C[B]_N\Psi) \tag{8.33}$$

for any $\Phi, \Psi \in D$.

### 9. PROOF OF THE DUALITY THEOREM (2)

We now prove $[B, C] = 0$ from (8.33). Since $C\Psi$ and $C^*\Phi$ may be outside of $D$, we cannot use (6.30). It is enough to prove

$$(\Psi, [B, C]\Phi) = 0 \tag{9.1}$$

for $\Psi$ and $\Phi$ in a total set (i.e., a set whose linear hull is dense). We use vectors of the type $\Psi = A\Psi_S(H^{(0)})$, $\Phi = A'\Psi_S(H^{(0)})$, where

$$\begin{aligned} A &= \chi(h_1) \cdots \chi(h_n), \\ A' &= \chi(h_1') \cdots \chi(h_m'), \end{aligned} \tag{9.2}$$

with $h_i, h_j' \in H_1'$.

*Lemma 9.1.* The set of $\Psi_S(H^{(0)})$ and $A\Psi_S(H^{(0)})$, where $A$ is given by (9.2) with $h_i \in H_1'$ and arbitrary $n$, is a total set in $\mathfrak{H}_S(H^{(0)})$.

*Proof:* Let $\mathfrak{K}$ be the set under consideration. Let $\mathfrak{H}_n = \operatorname{Sym} H^{(0)\otimes n}$ $\mathfrak{H}_N' = \sum_{n=0}^N \mathfrak{H}_n$ and $\mathfrak{K}_N = \mathfrak{K} \cap \mathfrak{H}_N'$. It is enough to prove $\bar{\mathfrak{K}}_n = \mathfrak{H}_n$ for $n < N$ implies the same for $n = N$, because $\mathfrak{K}_0 = \mathfrak{H}_0$. As is easily seen, the vectors $(a^\dagger, h)\Psi$ with $\Psi \in \mathfrak{H}_{N-1}$ and $\hat{h} \in \hat{H}^{(0)}$ span $\mathfrak{H}_N$. Since $(a^\dagger, h)$ is bounded on any $\mathfrak{H}_n$ and continuous in $h$, and since $\overline{H_1' + \beta H_1'} = H^{(0)}$ by (4.10), and $\bar{\mathfrak{K}}_{N-1} = \mathfrak{H}_{N-1}$ by inductive assumption, $(a^\dagger h)\Psi$ with $\Psi \in \mathfrak{H}_{N-1}$ and $h \in H_1' + \beta H_1'$ span $\mathfrak{H}_N$. If $h = h_1 + \beta h_2$, $h_1 \in H_1'$, $h_2 \in H_1'$, then $(a^\dagger \hat{h})\Psi = \sqrt{2}\,[\chi(h_1) + i\chi(h_2)]\Psi + \Psi'$ where $\Psi \in \mathfrak{K}_{N-1}$ and $\Psi' = (\hat{h}_1^* - i\hat{h}_2^*, a)\Psi \in \bar{\mathfrak{K}}_{N-2}$. Hence $(a^\dagger, \hat{h})\Psi \in \bar{\mathfrak{K}}_N$ and we have $\bar{\mathfrak{K}}_N = \mathfrak{H}_N$ and $\bar{\mathfrak{K}} = \mathfrak{H}_S(H^{(0)})$.

We now use the device of Gårding.[34]

*Lemma 9.2.* If $\varphi(\lambda_1 \cdots \lambda_n) \in \mathcal{S}_n$ (the set of infinitely differentiable fast decreasing functions in the sense of Schwartz), $\Psi'$ is an arbitrary vector, $A$ is given by (9.2) and

$$W_\varphi = \int W(\lambda_1 h_1) \cdots W(\lambda_n h_n) \times \varphi(\lambda_1 \cdots \lambda_n)\, d\lambda_1 \cdots d\lambda_n, \tag{9.3}$$

then $W_\varphi\Psi'$ is in the domain of $A^*$ (as well as that of $A$) and

$$A^*W_\varphi\Psi' = W_{\varphi_1}\Psi', \tag{9.4}$$

where

$$\varphi_1(\lambda_1 \cdots \lambda_n) = \left(i\frac{\partial}{\partial\lambda_n} - \sum_{j<n} \lambda_j(h_j\beta h_n)\right) \cdots \times \left(i\frac{\partial}{\partial\lambda_2} - \lambda_1(h_1\beta h_2)\right)\left(i\frac{\partial}{\partial\lambda_1}\right)\varphi. \tag{9.5}$$

*Proof:* The integral of (9.3) converges in the uniform topology of operators and $W_\varphi$ is a bounded operator for any $\varphi \in \mathcal{S}_n$ and is continuous in $\varphi \in \mathcal{S}_n$. It is known that, if $\lambda^{-1}(W(\lambda h_j) - 1)\Psi_2$ has a strong limit as $\lambda \to 0$, $\Psi_2$ is in the domain of $\chi(h_j)$ and the limit is $i\chi(h_j)\Psi_2$. By the change of integration variables, we easily see

$$\lim_{\lambda\to 0} \lambda^{-1}(W(\lambda h_1) - 1)W_\varphi\Psi_1 = W_{-(\partial\varphi/\partial\lambda_1)}\Psi_1 = i\chi(h_1)W_\varphi\Psi_1.$$

For $\chi(h_j)$, we first bring $W(\lambda_j h_j)$ in (9.3) to the extreme left by using $W(\lambda_i h_i)W(\lambda_j h_j) = W(\lambda_j h_j) \times W(\lambda_i h_i)e^{i\lambda_i\lambda_j(h_i\beta h_j)}$. Then we use the similar calculation as above and bring $W(\lambda_j h_j)$ back to the original position. We then obtain (9.4) with (9.5). This completes the proof of Lemma 9.2.

If $\varphi_\epsilon(\lambda) \in \mathcal{S}_1$, $\varphi_\epsilon(\lambda) = 0$ for $|\lambda| < \epsilon$, $\varphi_\epsilon(\lambda) \geq 0$ and $\int \varphi_\epsilon(\lambda)\, d\lambda = 1$, then we easily see that $W_{\varphi_\epsilon} \to 1$ strongly as $\epsilon \to 0$. [$W(\lambda h)$ is strongly continuous so that, for any given $\Psi$ and $\delta > 0$, $\|(W(\lambda h) - 1)\Psi\| < \delta$ for sufficiently small $\lambda$, for example, for $|\lambda| < \epsilon$, and $\|(W_{\varphi_\epsilon} - 1)\Psi\| < \delta$.] We use the following notation:

$$\varphi_{\epsilon n} = \prod_{j=1}^n \varphi_\epsilon(\lambda_j), \tag{9.6}$$

$$W_\epsilon = W_{\varphi_{\epsilon n}}, \tag{9.7}$$

$$W_\epsilon' = \int W(\lambda_1 h_1') \cdots W(\lambda_m h_m') \times \varphi_{\epsilon m}(\lambda_1' \cdots \lambda_m')\, d\lambda_1' \cdots d\lambda_m'. \tag{9.8}$$

We then have the properties

$$\lim_{\epsilon\to 0} W_\epsilon = \lim_{\epsilon'\to 0} W_{\epsilon'}' = 1. \tag{9.9}$$

[Note that $\int W(\lambda h)\varphi_\epsilon(\lambda)\, d\lambda$ is uniformly bounded with norm 1.] Furthermore, for any vectors $\Phi_1$ and $\Psi_1$, $W_\epsilon\Psi_1$ is in the domain of $A^*$ and $W_{\epsilon'}'^*\Psi_2$ is in the domain of $A'^*$.

Since $W_\epsilon, W_\epsilon' \in R_S(H_1'/H^{(0)}) \subset R_S(\beta H_2'/H^{(0)})'$, $W_\epsilon C W_{\epsilon'}' \in R_S(\beta H_2'/H^{(0)})'$. Replacing $C$ by $W_\epsilon C W_{\epsilon'}'$ in (8.33), we have

$$([B]_L^*\Psi, W_\epsilon C W_{\epsilon'}'\Phi) = (\Psi, W_\epsilon C W_{\epsilon'}'[B]_L\Phi), \tag{9.10}$$

where $\Psi = A\Psi_S(H^{(0)})$ and $\Phi = A'\Psi_S(H^{(0)})$. Due to (8.5), we have

[34] L. Gårding, Proc. Nat. Acad. Sci. US 33, 331 (1947).

$$([B]_L^* \Psi_0(H^{(0)}),\ A^* W_\epsilon C W'^*_{\epsilon'} \Phi)$$
$$= (A'^* W'^*_{\epsilon'} C^* W^*_\epsilon \Psi,\ B_L \Psi_0(H^{(0)})). \quad (9.11)$$

Since $[B]_L^* \Psi_S(H^{(0)}) = E_L B^* \Psi_S(H^{(0)})$, $[B]_L \Psi_0(H^{(0)}) = E_L B \Psi_0(H^{(0)})$, and $\sum_L E_L = 1$ in strong sense, we obtain, by summing up (9.11) for $L = 0, 1, \cdots$,

$$(B^* \Psi_0(H^{(0)}),\ A^* W_\epsilon C W'^*_{\epsilon'} \Phi)$$
$$= (A'^* W'^*_{\epsilon'} C^* W^*_\epsilon \Psi,\ B \Psi_0(H^{(0)})) \quad (9.12)$$

Since $B$ and $B^*$ commute with each $\chi(h_i)$, $h_i \in H_1'$ [by the assumption $B \in R(H_1'/H^{(0)})'$], we obtain

$$(B^* \Psi,\ W_\epsilon C W'^*_{\epsilon'} \Phi) = (\Psi,\ W_\epsilon C W'^*_{\epsilon'} B \Phi).$$

By taking the limit $\epsilon \to 0$ and $\epsilon' \to 0$, we have

$$(B^* \Psi,\ C\Phi) = (\Psi,\ CB\Phi). \quad (9.13)$$

Since $\Psi$ and $\Phi$ form a total set in $\mathfrak{H}_S(H^{(0)})$ by Lemma 9.1, we have $[C, B] = 0$ and the duality equation (3.14) is proved.

## 10. THE TYPE OF THE VON NEUMANN ALGEBRAS

In this section we will prove the following theorems:

*Theorem 4.* $R_S(H_1/H)$ is type I if and only if $\alpha(\beta H_1';\ H_1'/H^{(0)})$ is in the trace class, where $H_1'$ and $H^{(0)}$ are defined by (4.1)–(4.4) and the operator $\alpha$ on $H_1'$ is defined in Lemma 4.1.

*Theorem 4'.* $R_F(K_1,\ K_2/K)$ is type I if and only if $\alpha(K_2';\ K_1'/K^{(0)})$ is in the trace class where notations are the same as in Theorem 2'.

Because of Theorem 3, Theorem 2', and (3.3), Theorem 4 and Theorem 4' are equivalent; therefore, we prove Theorem 4'.

As has been seen in Sec. 5, $R_S(K^{(4)}/H)$ is the center of $R_S(H_1/H)$ and $R_S(H_1/H)$ is type I by definition if and only if the factor $R_S(H^{(2)} \oplus H_1'/H^{(2)} \oplus H^{(3)} \oplus H^{(0)})$ is type I. Therefore, we look for the necessary and sufficient condition that $R_F(K_1' \oplus K^{(2)},\ K_2' \oplus K^{(2)}/K^{(0)} \oplus K^{(2)} \oplus K^{(3)})$ is type I.

We use the criterion for the factor of type I given by the following lemma.[35]

*Lemma 10.1.* A von Neumann algebra $R$ on a Hilbert space $\mathfrak{H}$ is a factor of type I if and only if there exists a tensor product decomposition $\mathfrak{H} = \mathfrak{H}_1 \otimes \mathfrak{H}_2$ such that $R = B(\mathfrak{H}_1) \otimes 1$ and $R' = 1 \otimes B(\mathfrak{H}_2)$. (Here "=" is always in the sense of the unitary equivalence.)

We now consider the decomposition of the spectrum of $\alpha(K_2';\ K_1'/K^{(0)})$ into continuous and discrete parts. Correspondingly we have the decomposition

$$K_1' = K_{1c} \oplus K_{1d}, \quad K_2' = K_{2c} \oplus K_{2d},$$
$$K^{(0)} = K_c \oplus K_d, \quad (10.1)$$
$$\alpha(K_2';\ K_1'/K^{(0)}) = \alpha_{1c} \oplus \alpha_{1d}, \quad (10.2)$$

where $\alpha_{1c}$ is the continuous part of $\alpha(K_2';\ K_1'/K^{(0)})$ operating on $K_{1c}$, $\alpha_{1d}$ is the discrete part of $\alpha(K_2';\ K_1'/K^{(0)})$ operating on $K_{1d}$, and the rest of the notation is defined by

$$K_c = K_{1c} \oplus \tilde{U}(K_2';\ K_1'/K^{(0)}) K_{1c}, \quad (10.3)$$
$$K_d = K_{1d} \oplus \tilde{U}(K_2';\ K_1'/K^{(0)}) K_{1d}, \quad (10.4)$$
$$K_{2c} = K_c \cap K_2', \quad K_{2d} = K_d \cap K_2'. \quad (10.5)$$

By Lemma 5.2 we have the corresponding tensor product decomposition:

$$\mathfrak{H}_F(K^{(0)} \oplus K^{(2)} \oplus K^{(3)})$$
$$= \mathfrak{H}_F(K_c) \otimes \mathfrak{H}_F(K_d) \otimes \mathfrak{H}', \quad (10.6)$$
$$R_F(K_1' \oplus K^{(2)};\ K_2' \oplus K^{(2)})$$
$$= R_F(K_{1c},\ K_{2c}) \otimes R_F(K_{1d},\ K_{2d}) \otimes R_0, \quad (10.7)$$

where

$$\mathfrak{H}' = \mathfrak{H}_F(K^{(2)}) \otimes \mathfrak{H}_F(K^{(3)}), \quad (10.8)$$
$$R_0 = B(\mathfrak{H}_1(K^{(2)}) \otimes 1. \quad (10.9)$$

We first investigate the continuous part $R_F(K_{1c},\ K_{2c}/K_c)$. We have

*Lemma 10.2.* $R_F(K_{1c},\ K_{2c}/K_c)$ is not type I (unless $K_c = \{0\}$).

For the proof of this lemma, we use the following known lemma.[36]

*Lemma 10.2.* If a von Neumann algebra $R$ on $\mathfrak{H}$ is a factor of type I and if a unitary operator $u$, having a unique discrete eigenvector $\Psi_0$, satisfies $uRu^{-1} = R$ (i.e., $Q \in R$ implies $uQu^{-1} \in R$ and vice versa), then $\Psi_0$ is of the form $\Psi_{01} \otimes \Psi_{02}$ in the tensorial decomposition $\mathfrak{H} = \mathfrak{H}_1 \otimes \mathfrak{H}_2$ in Lemma 10.1. In particular, $\Psi_0$ cannot be a cyclic vector of $R$ unless $R = B(\mathfrak{H})$ (and $\mathfrak{H}_2$ is one-dimensional).

Since $\Psi_F(K_c)$ is the cylic vector of $R_F(K_{1c}, K_{2c}/K_c)$

[35] J. Dixmier, reference 15, p. 124.

[36] This lemma follows from Lemma 4.2 and Lemma 4.1 of H. Araki and J. S. Woods, J. Math. Phys. 4, 637(1963). Namely, $uRu^{-1} = R$ implies $uR'u^{-1} = (uRu^{-1})' = R'$ and the condition of Lemma 4.2 of H. Araki and J. S. Woods is satisfied. If $\Psi_0 = \Psi_{01} \otimes \Psi_{02}$, then $|R\Psi_0 = \mathfrak{H}_1 \otimes \Psi_{02}$, from which $\mathfrak{H}_2$ must be one-dimensional if $\Psi_0$ is a cyclic vector of $R$ and hence $R = B(\mathfrak{H})$.

due to Lemma 9.1, we prove the Lemma 10.2 by finding a unitary operator $u$, having the unique discrete eigenvector $\Psi_F(K)$ and satisfying $uR_F(K_{1c}, K_{2c}/K_c)u^{-1} = R_F(K_{1c}, K_{2c}/K_c)$.

We define the following operator on $K_c$:

$$\alpha_c = \alpha_{1c} \oplus \tilde{U}(K_{2c}; K_{1c}/K_c) \times \alpha_{1c}\tilde{U}(K_{2c}; K_{1c}/K_c)^*, \tag{10.10}$$

$$\mathrm{c}(t) \equiv \cos t(1 + \alpha_c)^{\frac{1}{2}}, \tag{10.11}$$

$$\mathrm{s}(t) \equiv s_0 \sin t(1 + \alpha_c)^{\frac{1}{2}}, \tag{10.12}$$

$$s_0 \equiv [\{1 + \varphi(K_{2c}; K_{1c}/K_c)\}P(K_{1c}) + \{-1 + \varphi(K_{2c}; K_{1c}/K_c)^*\} \times P(K_{1c}^{\perp} \cap K_c)](1 + \alpha_c)^{-\frac{1}{2}}. \tag{10.13}$$

Since $s_0$ is bounded, commutes with $\alpha_c$, $s_0^* = s_0$, and $s_0^2 = 1$, we see that $\mathrm{c}(t)$ and $\mathrm{s}(t)$ are bounded, commute with $\alpha_c$, are Hermitian, satisfy the addition laws $\mathrm{s}(t_1 + t_2) = \mathrm{s}(t_1)\mathrm{c}(t_2) + \mathrm{s}(t_2)\mathrm{c}(t_1)$, $\mathrm{c}(t_1 + t_2) = \mathrm{c}(t_1)\mathrm{c}(t_2) - \mathrm{s}(t_1)\mathrm{s}(t_2)$, and commute with other $\mathrm{c}(t')$ and $\mathrm{s}(t')$. Furthermore,

$$\mathrm{c}(t)K_l \subset K_l, \qquad l = 1, 2, \tag{10.14}$$

$$\mathrm{s}(t)K_l \subset K_{3-l}, \qquad l = 1, 2. \tag{10.15}$$

Therefore, $u(t) = c(t) + is(t)$ on $L_c = K_c + iK_c$ is a one-parameter family of commuting unitary operators, and the corresponding operator $\hat{u}(t)$ on $\hat{L}_c = K_c \oplus \beta K_c$ has the property

$$\hat{u}(t)H_{1c} = H_{1c}, \tag{10.16}$$

where $H_{1c} = K_{1c} \oplus \beta K_{2c}$.

Now the desired unitary operator on $\mathfrak{H}_F(K^c)$ is given by

$$T_t = T[u(t)], \tag{10.17}$$

where the definition (6.17) is used. Since $u(t)$ has continuous spectrum, $u(t)^{\otimes_n}$ with $n \neq 0$ has continuous spectrum[37] and $T_t$ has the unique discrete eigenvector $\Psi_F(K_c)$. By (7.15) and (10.16), $T_t R_F(K_{1c}; K_{2c}/K^{(0)})T_t^{-1} = R_F(K_{1c}, K_{2c}/K^{(0)})$. Therefore, $T_t$ satisfy the property required and this completes the proof of Lemma 10.2.

We now investigate the discrete part. Let $\{f_\alpha\}$ be the orthonormal basis of $K_{1d}$ such that $\alpha_{1d}f_\alpha = \lambda_\alpha^2 f_\alpha$ where $\lambda_\alpha > 0$ and $\lambda_\alpha$ may be the same for different $\alpha$. Let $f'_\alpha = \tilde{U}(K_{2d}, K_{1d}/K_d)f_\alpha$. Let $K_{1\alpha}$ be the space spanned by $f_\alpha$, $K_{2\alpha}$ be that spanned by $f_\alpha + \lambda_\alpha f'_\alpha$, and $K_\alpha$ be that spanned by $f_\alpha$ and $f'_\alpha$ for each $\alpha$. We have the decomposition

$$K_\alpha = \sum_\alpha{}^{\oplus} K_\alpha, \tag{10.18}$$

$$K_{1d} = \sum_\alpha{}^{\oplus} K_{1d}, \tag{10.19}$$

$$K_{2d} = \sum_\alpha{}^{\oplus} K_{2d}. \tag{10.20}$$

Correspondingly we have the following decomposition[38]:

$$\mathfrak{H}_F(K_d) = \prod_\alpha{}^{\otimes} \mathfrak{H}_F(K_\alpha), \tag{10.21}$$

$$R_F(K_{1d}, K_{2d}/K_d) = \prod_\alpha{}^{\otimes} R_F(K_{1\alpha}, K_{2\alpha}/K_\alpha), \tag{10.22}$$

where $\prod^{\otimes}$ in (10.21) is the incomplete infinite direct product[9] containing the infinite product of vectors $\prod_\alpha^{\otimes} \Psi_F(K_\alpha)$. The $\prod_\alpha^{\otimes} R_\alpha$ for infinite number of $\alpha$ is, in general, defined by

$$\prod_\alpha{}^{\otimes} R_\alpha \equiv \bigvee_\alpha (R_\alpha \otimes \prod_{\beta \neq \alpha}{}^{\otimes} \mathbf{1}_\beta), \tag{10.23}$$

($\mathbf{1}_\beta$ is the unit operator in $\mathfrak{H}_\beta$), and the correspondence of the right- and left-hand sides of (10.21) and (10.22) is uniquely specified by the following correspondence:

$$\Psi_F(K_d) = \prod_\alpha{}^{\otimes} \Psi_F(K_\alpha), \tag{10.24}$$

$$U_F(f) = \prod_\alpha{}^{\otimes} U_F(E_\alpha f), \tag{10.25}$$

$$V_F(g) = \prod_\alpha{}^{\otimes} V_F(E_\alpha g) \tag{10.26}$$

($E_\alpha$ is the projection on $K_\alpha$).

We now prove

*Lemma 10.4.* $R_F(K_{1\alpha}, K_{2\alpha}/K_\alpha)$ is a factor of type I for each $\alpha$.

*Proof:* As is well-known, $\mathfrak{H}_F(K_\alpha)$ for two-dimensional $K_\alpha$ can be realized by

$$\mathfrak{H}_F(K_\alpha) = L_2(R^2) = \left\{\Psi(x_\alpha^1, x_\alpha^2); \int |\Psi|^2 \, dx_\alpha^1 \, dx_\alpha^2 < \infty\right\}, \tag{10.27}$$

$$\Psi_F(K_\alpha) = \pi^{-1} \exp -\tfrac{1}{2}[(x_\alpha^1)^2 + (x_\alpha^2)^2], \tag{10.28}$$

$$(U_F(f)\Psi)(x_\alpha^1, x_\alpha^2) = \Psi(x_\alpha^1, x_\alpha^2) \times \exp i[(f, f_\alpha)x_\alpha^1 + (f, f'_\alpha)x_\alpha^2], \tag{10.29}$$

$$(V_F(g)\Psi)(x_\alpha^1, x_\alpha^2) = \Psi(x_\alpha^1 + (g, f_\alpha), x_\alpha^2 + (g, f'_\alpha)). \tag{10.30}$$

We define a one-parameter family of unitary operators $U_\alpha(\rho)$ by

[37] H. Araki and J. S. Woods, J. Math. Phys. 4, 637 (1963), Lemma 4.1.

[38] This decomposition can be proved trivially by an argument similar to that before Lemma 2.4 in H. Araki and J. S. Woods, J. Math. Phys. 4, 637(1963).

$$(U_\alpha(\rho)\Psi)(x_\alpha^1, x_\alpha^2) = \Psi(x_\alpha^1, x_\alpha^2 + \rho x_\alpha^1). \quad (10.31)$$

We easily verify

$$[U_\alpha(\rho), U_F(cf_\alpha)] = [U_\alpha(\rho), V_F(cf'_\alpha)] = 0, \quad (10.32)$$

$$U_\alpha(\rho)U_F(cf'_\alpha)U_\alpha(\rho)^{-1} = U_F(cf'_\alpha + \rho cf_\alpha), \quad (10.33)$$

$$U_\alpha(\rho)V_F(cf_\alpha)U_\alpha(\rho)^{-1} = V_F(cf_\alpha - \rho cf'_\alpha). \quad (10.34)$$

If we define

$$R_\alpha^{(1)}(\lambda) = \{U_F(cf_\alpha)V_F(df_\alpha + \lambda\, df'_\alpha); c, d \text{ real}\}'', \quad (10.35)$$

$$R_\alpha^{(2)}(\lambda) = \{U_F(cf'_\alpha - \lambda cf_\alpha)V_F(df'_\alpha); c, d \text{ real}\}'', \quad (10.36)$$

then we have

$$U_\alpha(\rho)R_\alpha^{(l)}(\lambda)U_\alpha(\rho)^{-1} = R_\alpha^{(l)}(\lambda - \rho), \quad l = 1, 2. \quad (10.37)$$

By Lemmas 5.1 and 5.2, $\mathfrak{H}_F(K_\alpha) = \mathfrak{H}_F(K_{1\alpha}) \otimes \mathfrak{H}_F(K_{1\alpha}^\perp \cap K_\alpha)$, $R_\alpha^{(1)}(0) = B(\mathfrak{H}_F(K_{1\alpha})) \otimes \mathbf{1}$, and $R_\alpha^{(2)}(0) = \mathbf{1} \otimes B(\mathfrak{H}_F(K_{1\alpha}^\perp \cap K_\alpha))$. Hence $R_\alpha^{(l)}(0)$ is a factor of type I and the same is true for $R_\alpha^{(l)}(\lambda)$. Since $R_F(K_{1\alpha}, K_{2\alpha}/K_\alpha) = R_\alpha^{(l)}(\lambda_\alpha)$, this proves Lemma 10.4.

We now need a criterion to tell us whether or not $\prod_\alpha^\otimes R_\alpha$ is type I when $R_\alpha$ is type I. Such a criterion is given by the following theorem.

*Theorem 5.* Let $\mathfrak{H} = \mathfrak{H}_a \otimes \mathfrak{H}_b$, $\mathfrak{H}_b$ be the incomplete infinite direct product of $\mathfrak{H}_\alpha$ containing $\prod_\alpha^\otimes \Psi_{0\alpha}$, $\Psi_{0\alpha} \in \mathfrak{H}_\alpha$, $||\Psi_{0\alpha}|| = 1$, $\mathfrak{H}_\alpha = \mathfrak{H}_\alpha^1 \otimes \mathfrak{H}_\alpha^2$, $R_\alpha^{(1)} = B(\mathfrak{H}_\alpha^1) \otimes \mathbf{1}$, $R_a$ be a factor on $\mathfrak{H}_a$, $R_b = \prod_\alpha^\otimes R_\alpha^{(1)}$, and $R = R_a \otimes R_l$. Then $R$ is type I if and only if $R_a$ is type I and

$$\sum_\alpha |1 - d(\Psi_{0\alpha}; \mathfrak{H}_\alpha^1, \mathfrak{H}_\alpha^2)| < \infty \quad (10.38)$$

(i.e., $\prod_\alpha d(\Psi_{0\alpha}; \mathfrak{H}_\alpha^1, \mathfrak{H}_\alpha^2)$ is absolutely convergent), where

$$d(\Psi; \mathfrak{H}_1, \mathfrak{H}_2) = \sup_{\Phi_i \in \mathfrak{H}_i} |(\Psi, \Phi_1 \otimes \Phi_2)|\, ||\Phi_1||^{-1}\, ||\Phi_2||^{-1}. \quad (10.39)$$

For the proof of this theorem, we need three lemmas.

*Lemma 10.5.* Let $A_l$ be bounded antilinear operators from $\mathfrak{H}_l^1$ into $\mathfrak{H}_l^2$, and $\prod_{l=1}^{N\otimes} A_l$ be their tensor product transforming $\prod_{l=1}^{N\otimes} \mathfrak{H}_l^1$ into $\prod_{l=1}^{N\otimes} \mathfrak{H}_l^2$. Then

$$\left|\left|\prod_{l=1}^{N\otimes} A_l\right|\right| = \prod_{l=1}^{N} ||A_l||.$$

*Proof:* If we prove the case $N = 2$, then we obtain the general case by associative law. Taking $\Psi = \Psi_1^1 \otimes \Psi_2^1$, $\Psi_l^1 \in \mathfrak{H}_l^1$ in $||A_1 \otimes A_2|| = \sup ||(A_1 \otimes A_2)\Psi|| \cdot ||\Psi||^{-1}$, we have $||A_1 \otimes A_2|| \geqq ||A_1|| \cdot ||A_2||$. On the other hand, $||A_1 \otimes A_2|| \leqq ||A_1 \otimes T|| \times ||1 \otimes TA_2||$ where $T$ is any conjugation on $\mathfrak{H}_2^2$ ($T^2 = 1$, $Ti = -iT$, $||T\Psi|| = ||\Psi||$), $1 \otimes TA_2$ maps $\mathfrak{H}_1^1 \otimes \mathfrak{H}_2^1$ into $\mathfrak{H}_1^1 \otimes \mathfrak{H}_2^2$ linearly, and then $A_1 \otimes T$ maps $\mathfrak{H}_1^1 \otimes \mathfrak{H}_2^2$ into $\mathfrak{H}_1^2 \otimes \mathfrak{H}_2^2$ antilinearly. Let $\Psi_\nu$ be an orthonormal basis for $\mathfrak{H}_2^2$ with $T\Psi_\nu = \Psi_\nu$. Then any $\Psi \in \mathfrak{H}_1^1 \otimes \mathfrak{H}_2^2$ has the expansion $\Psi = \sum_\nu \Psi_\nu^{(1)} \otimes \Psi_\nu$ with $||\Psi||^2 = \sum_\nu ||\Psi_\nu^{(1)}||^2$ and $||(A_1 \otimes T)\Psi||^2 = \sum_\nu ||A_1\Psi_\nu^{(1)}||^2 \leqq ||A_1||^2 \cdot ||\Psi||^2$. Hence, $||A_1 \otimes T|| \leqq ||A_1||$. Similarly, $||1 \otimes TA_2|| \leqq ||TA_2|| = ||A_2||$. Therefore, $||A_1 \otimes A_2|| = ||A_1|| \cdot ||A_2||$.

*Lemma 10.6.* Let $\mathfrak{H} = \prod_{l=1}^{N\otimes} \mathfrak{H}_l$, $\mathfrak{H}_l = \mathfrak{H}_l^1 \otimes \mathfrak{H}_l^2$, $\mathfrak{H}^i = \prod_{l=1}^{N\otimes} \mathfrak{H}_l^i$, $\Psi = \prod_{l=1}^{N\otimes} \Psi_l$, $\Psi_l \in \mathfrak{H}_l$. Then

$$d(\Psi; \mathfrak{H}^1, \mathfrak{H}^2) = \prod_{l=1}^{N} d(\Psi_l; \mathfrak{H}_l^1, \mathfrak{H}_l^2). \quad (10.40)$$

*Proof:* $(\Psi_l, \Phi_{l1} \otimes \Phi_{l2}) = (\chi_l(\Phi_{l1}), \Phi_{l2})$ defines a vector $\chi_l(\Phi_{l1})$ in $\mathfrak{H}_l^2$ depending antilinearly on $\Phi_{l1}$, and $\chi_l(\Phi_{l1}) = \rho_{12}^l(\Psi_l)\Phi_{l1}$ defines an antilinear operator from $\mathfrak{H}_l^1$ into $\mathfrak{H}_l^2$. We have

$$||\rho_{12}^l|| = \sup |(\Phi_{l2}, \rho_{12}^l\Phi_{l1})|\, ||\Phi_{l1}||^{-1}\, ||\Phi_{l2}||^{-1} = d(\Psi_l; \mathfrak{H}_l^1\mathfrak{H}_l^2).$$

Similarly we define $\rho_{12}(\Psi)$ from $\mathfrak{H}^1$ into $\mathfrak{H}^2$. Obviously, $\rho_{12}(\Psi) = \prod_{l=1}^{N\otimes} \rho_{12}^l(\Psi_l)$ and $||\rho_{12}|| = d(\Psi; \mathfrak{H}_l^1, \mathfrak{H}_l^2)$. From the previous lemma, we have (10.40).

*Lemma 10.7.* If $\mathfrak{H} = \mathfrak{H}^1 \otimes \mathfrak{H}^2$, then, for any given $\Psi \in \mathfrak{H}$, there exists normalized $\Phi^l \in \mathfrak{H}^l$, $l = 1, 2$, such that

$$d(\Psi; \mathfrak{H}^1, \mathfrak{H}^2) = (\Psi, \Phi^1 \otimes \Phi^2). \quad (10.41)$$

*Proof:* We consider the operator $\rho_{12}(\Psi)$ introduced in the proof of the Lemma 10.6. We define a positive-semidefinite Hermitian form $K$ on $\mathfrak{H}^1$ by $(\rho_{12}\Phi_1, \rho_{12}\Phi'_1) = (\Phi'_1, K\Phi_1)$. We see that $K$ is a bounded operator with $||K|| = ||\rho_{12}||^2$. Furthermore, for any complete set $\Phi_{\mu_l}^l$ in $\mathfrak{H}^l$, $l = 1, 2$, we have

$$\operatorname{tr} K = \sum_{\mu_1\mu_2} |(\Phi_{\mu_2}^2, \rho_{12}\Phi_{\mu_1}^1)|^2 = ||\Psi||^2 < \infty.$$

Hence $K$ is in the trace class and has a discrete spectral decomposition

$$K = \sum \lambda_\mu P_\mu, \quad (10.42)$$

where $\lambda_\mu > 0$ has no accumulation point except possibly at 0. Let $\Phi^1$ be a unit eigenvector of $K$ belonging to $\lambda_0 = \max \lambda_\mu$ and $\Phi^2 = \lambda_0^{-\frac{1}{2}}\rho_{12}(\Psi)\Phi^1$. We see that $||\Phi^l|| = 1$, $(\Psi, \Phi^1 \otimes \Phi^2) = \lambda_0^{\frac{1}{2}}$ and $||\rho_{12}(\Psi)|| = \lambda_0^{\frac{1}{2}}$, which implies (10.41).

Before proceeding to the proof of Theorem 5, we state a few basic properties of the incomplete infinite direct product. Let $\chi_{\nu\alpha}$ be an orthonormal basis of $\mathfrak{H}_\alpha$ containing $\Psi_{0\alpha}$ as its member. Then

$$\chi_{\{\nu\}} = \prod_\alpha{}^{\otimes} \chi_{\nu_\alpha \alpha} \tag{10.43}$$

with only finite number of $\nu_\alpha \neq 0$, constitutes an orthonormal basis for the incomplete infinite direct product $\prod_\alpha^\otimes \mathfrak{H}_\alpha$ containing $\Psi_0 = \prod_\alpha^\otimes \Psi_{0\alpha}$ (Lemma 4.1.4 of reference 9). If $\sum_\alpha | \, ||\Psi^{(\alpha)}|| - 1| < \infty$, and $\sum_\alpha |(\Psi^{(\alpha)}, \Psi_{0\alpha}) - 1| < \infty$, then $\prod_\alpha^\otimes \Psi^{(\alpha)}$ is in the space with the expansion coefficient in the basis (10.43) given by $\prod_\alpha (\chi_{\nu_\alpha \alpha}, \Psi^{(\alpha)})$. If $U^{(\alpha)}$ is a unitary operator on $\mathfrak{H}_\alpha$, and if

$$\sum_\alpha |1 - (\Psi_{0\alpha}, U^{(\alpha)}\Psi_{0\alpha})| < \infty, \tag{10.44}$$

then $U = \prod_\alpha^\otimes U_\alpha$ can be defined by $U\chi_\nu = \prod_\alpha^\otimes U_\alpha \chi_{\nu_\alpha \alpha}$ and is unitary. If the index set $\{\alpha\}$ is divided into two parts $I$ and $J$, and if $\mathfrak{H}_I$ and $\mathfrak{H}_J$ are incomplete infinite direct products of $\mathfrak{H}_\alpha$, $\alpha \in I$ and $\mathfrak{H}_\alpha$, $\alpha \in J$, containing $\Psi_{0I} = \prod_{\alpha\in I}^\otimes \Psi_{0\alpha}$, and $\Psi_{0J} = \prod_{\alpha\in J}^\otimes \Psi_{0\alpha}$, respectively, then $\mathfrak{H} = \mathfrak{H}_I \otimes \mathfrak{H}_J$, $\Psi_0 = \Psi_{0I} \otimes \Psi_{0J}$ and $\chi_{\{\nu\}} = \chi_{\{\nu\}I} \otimes \chi_{\{\nu\}J}$, where $\chi_{\{\nu\}I} = \prod_{\alpha\in I}^\otimes \chi_{\nu_\alpha \alpha}$ and $\chi_{\{\nu\}J} = \prod_{\alpha\in J}^\otimes \chi_{\nu_\alpha \alpha}$. Finally,

$$B(\mathfrak{H}) = \prod_\alpha{}^{\otimes} B(\mathfrak{H}_\alpha) \tag{10.45}$$

for any incomplete infinite direct product $\mathfrak{H} = \prod_\alpha^\otimes \mathfrak{H}_\alpha$.

*Proof of Theorem 5:* First we prove that $R$ is a factor. Define $R_\alpha^{(2)} = 1 \otimes R(\mathfrak{H}_\alpha^2)$, $R_b^{(2)} = \prod_\alpha^\otimes R_\alpha^{(2)}$, $R^{(2)} = R_a' \otimes R_b^{(2)}$. Obviously, $R$ commutes with $R^{(b)}$. By (10.45), $R_b \vee R_b^{(2)} = B(\mathfrak{H}_b)$ and hence $R \vee R^{(2)} = B(\mathfrak{H})$. Therefore $R$ is a factor.

Next we show that, if $R$ is type I, $\sum_\alpha (1 - d(\Psi_{0\alpha}, \mathfrak{H}_\alpha^1, \mathfrak{H}_\alpha^2)) = \infty$ leads to a contradiction. If $R$ is type I, then $\mathfrak{H} = \mathfrak{H}^1 \otimes \mathfrak{H}^2$, $R = B(\mathfrak{H}^1) \otimes 1$, $R' = 1 \otimes B(\mathfrak{H}^2)$ for some $\mathfrak{H}^1$ and $\mathfrak{H}^2$. Consider a vector $\Psi \in \mathfrak{H}$ of the form $\Psi = \Psi^1 \otimes \Psi^2$, $||\Psi^1|| = ||\Psi^2|| = 1$, $\Psi^l \in \mathfrak{H}^l$. We prove that

$$(\Psi, \Phi \otimes \chi_{\{\nu\}}) = 0 \tag{10.46}$$

for all $||\Phi|| = 1$, $\Phi \in \mathfrak{H}_a$, and the orthonormal basis $\chi_{\{\nu\}}$ of $\mathfrak{H}_b = \prod_\alpha^\otimes \mathfrak{H}_\alpha$ given in (10.43). This, of course, is a contradiction to $\Psi \neq 0$. Let $I$ be any finite set of $\alpha$ such that $\nu_\alpha = 0$ for a given set $\{\nu_\alpha\}$. Let

$$R_I^{(1)} = 1_a \otimes \prod_{\alpha\in J}^\otimes 1_\alpha \otimes \prod_{\alpha\in I}^\otimes R_\alpha^{(1)},$$

$$R_\gamma^{(1)} = R_a \otimes \prod_{\alpha\in J}^\otimes R_\alpha^{(1)} \otimes \prod_{\alpha\in I}^\otimes 1_\alpha,$$

$$R_\gamma^{(2)} = R_a' \otimes \prod_{\alpha\in J}^\otimes R_\alpha^{(2)} \otimes \prod_{\alpha\in I}^\otimes 1_\alpha,$$

where $J$ is the complement index set of $I$. We see that $(R_\gamma^{(1)}, R_I^{(1)})$ is a factorization of $R = B(\mathfrak{H}^1) \otimes 1$ and $(R_\gamma^{(2)}, R_I^{(2)})$ is a factorization of $R = 1 \otimes B(\mathfrak{H}^2)$. Since $R_I^{(1)}$ is type I for a finite set $I$, we have further decomposition: $\mathfrak{H}^1 = \mathfrak{H}_\gamma^1 \otimes \mathfrak{H}_I^1$, $\mathfrak{H}^2 = \mathfrak{H}_\gamma^2 \otimes \mathfrak{H}_I^2$; $R_\gamma^{(1)} = B(\mathfrak{H}_\gamma^1) \otimes 1$, $R_I^{(1)} = 1 \otimes B(\mathfrak{H}_I^1)$. By comparing with the decomposition, $\mathfrak{H} = \mathfrak{H}_\gamma \otimes \mathfrak{H}_I$, $\mathfrak{H}_I = \prod_{\alpha\in I}^\otimes \mathfrak{H}_\alpha$, $\mathfrak{H}_\gamma = \mathfrak{H}_a \otimes \prod_{\alpha\in J} \otimes \mathfrak{H}_\alpha$, $R_I^{(1)} \vee R_I^{(2)} = 1 \otimes B(\mathfrak{H}_I)$, we see the unitary equivalence $\mathfrak{H}_\gamma = \mathfrak{H}_\gamma^1 \otimes \mathfrak{H}_\gamma^2$, $\mathfrak{H}_I = \mathfrak{H}_I^1 \otimes \mathfrak{H}_I^2$. By applying definition (10.39) and the Lemma 10.6, we have

$$\begin{aligned} |(\Psi, \Phi \otimes \chi_{\{\nu\}})| &\leqq d(\Phi \otimes \chi_{\{\nu\}}; \mathfrak{H}^1, \mathfrak{H}^2) \\ &= d(\Phi \otimes \prod_{\alpha\neq I} \chi_{\nu_\alpha \alpha}; \mathfrak{H}_\gamma^1, \mathfrak{H}_\gamma^2) \\ &\quad \times \prod_{\alpha\in I} d(\Psi_{0\alpha}; \mathfrak{H}_\alpha^1, \mathfrak{H}_\alpha^2). \end{aligned} \tag{10.47}$$

The first factor on the right-hand side is not larger than 1. If $\sum_\alpha (1 - d(\Psi_{0\alpha}; \mathfrak{H}_\alpha^1, \mathfrak{H}_\alpha^2))$ diverges, then $\prod_\alpha d(\Psi_{0\alpha}; \mathfrak{H}_\alpha^1 \mathfrak{H}_\alpha^2) = 0$ [note that $0 \leqq d(\Psi_{0\alpha}; \mathfrak{H}_\alpha^1, \mathfrak{H}_\alpha^2) \leqq 1$], and therefore, by suitably choosing $I$, the right-hand side of (10.47) can be made smaller than any given $\epsilon > 0$. Therefore we have (10.45), which is a contradiction to $\Psi \neq 0$. Hence, if $R$ is type I, (10.38) holds.

Now assume (10.38). According to the Lemma 10.7, we consider unit vectors $\Phi_\alpha^l$, $l = 1, 2$ such that

$$(\Psi_{0\alpha}, \Phi_\alpha^1 \otimes \Phi_\alpha^2) = d(\Psi_{0\alpha}; \mathfrak{H}_\alpha^1, \mathfrak{H}_\alpha^2).$$

By (10.38), $\prod_\alpha^\otimes (\Phi_\alpha^1 \otimes \Phi_\alpha^2)$ is a unit vector in $\mathfrak{H}_b$. Let $\mathfrak{H}_b^l$ be the incomplete infinite direct product $\prod_\alpha^\otimes \mathfrak{H}_\alpha^l$ containing $\prod_\alpha^\otimes \Phi_\alpha^l$. Then we have the decomposition $\mathfrak{H}_b = \mathfrak{H}_b^1 \otimes \mathfrak{H}_b^2$ and, due to (10.45), $R_b = B(\mathfrak{H}_b^1) \otimes 1$. Namely, $R_b$ is type I.

Finally, if $R$ is type I, then we have (10.38), and hence $R_b$ is type I. Because the pair $(R_a, R_b)$ is a factorization of $R = B(\mathfrak{H}^1) \otimes 1$, $R_a$ must also be a factor of type I.[35] Conversely, if $R_a$ is type I and (10.38) holds, then $R_b$ is also type I and hence $R$ is type I. This completes the proof of Theorem 5.

*Proof of Theorems 4 and 4':* We now apply the Theorem 5 to the tensorial decomposition (10.6), (10.7), (10.21), and (10.22), where $\mathfrak{H}_F(K_c)$ and $R_F(K_{1c}, K_{2c})$ is taken to be $\mathfrak{H}_a$, and $R_a$ and $\mathfrak{H}'$ and $R_0$ are considered as one member in the infinite direct product over $\alpha$. Other members of the infinite direct product over $\alpha$ are, of course, $\mathfrak{H}_F(K_\alpha)$ and $R_F(K_{1\alpha}, K_{2\alpha}/K_\alpha)$. The decomposition $\mathfrak{H}_\alpha^1 \otimes \mathfrak{H}_\alpha^2$ for $\mathfrak{H}'$ is given by (10.8) and (10.9), and the decomposition for $\mathfrak{H}_F(K_\alpha)$ is given by Lemma 10.4 as

$$\mathfrak{H}_F(K_\alpha) = U_\alpha(\lambda_\alpha)^{-1}(\mathfrak{H}_F(K_{1\alpha}) \otimes \mathfrak{H}_F(K_{1\alpha}^\perp \cap K_\alpha)). \quad (10.48)$$

We first calculate $d(\Psi_{0\alpha};\ \mathfrak{H}_\alpha^1,\ \mathfrak{H}_\alpha^2)$ which is given for $\mathfrak{H}_F(K_\alpha)$ by $d(U_\alpha(\lambda_\alpha)\Psi_F(K_\alpha);\ \mathfrak{H}_F(K_{1\alpha}),\ \mathfrak{H}_F(K_{1\alpha}^\perp \cap K_\alpha))$. In the realization (10.27) of $\mathfrak{H}_F(K_{1\alpha})$, $\mathfrak{H}_F(K_{1\alpha}) \approx \{\Psi(x_\alpha^1);\ \int |\Psi|^2\, dx_\alpha^1 < \infty\}$ and the operator $K$ introduced in the proof of the Lemma 10.7 is given by an integral operator with the following kernel function:

$$K(x_1, x_1') = \int (U_\alpha(\lambda_\alpha)\Psi_F(K_\alpha))(x_1, y) \times (U_\alpha(\lambda_\alpha)\Psi_F(K_\alpha))(x_1' y)^*\, dy$$
$$= \pi^{-\frac{1}{4}} \exp\{-\tfrac{1}{2}(1 + \tfrac{1}{2}\lambda_\alpha^2)(x_1^2 + x_1'^2) + \tfrac{1}{2}\lambda_\alpha^2 x_1 x_1'\}. \quad (10.49)$$

By using the formula

$$\pi^{-\frac{1}{4}}\gamma^{\frac{1}{4}}(\cosh t) \exp\{-\tfrac{1}{2}(\cosh 2t)(x^2 + y^2) + xy \sinh 2t\}\gamma = \sum_{n=0}^{\infty} (\tanh t)^n f_n(x) f_n(y)^*, \quad (10.50)$$

$$f_n(x) = \gamma^{\frac{1}{4}}(\pi^{\frac{1}{2}} 2^n n!)^{-\frac{1}{2}} H_n(\gamma^{\frac{1}{2}} x) \exp(-\tfrac{1}{2}\gamma x^2), \quad (10.51)$$

we obtain

$$K(x_1, x_1') = \left(\frac{1 + (1 + \lambda_\alpha^2)^{\frac{1}{2}}}{2}\right)^{-1} \times \sum_{n=0}^{\infty} \left(\frac{(1 + \lambda_\alpha^2)^{\frac{1}{2}} - 1}{(1 + \lambda_\alpha^2)^{\frac{1}{2}} + 1}\right)^n f_n(x_1) f_n(x_1')^*. \quad (10.52)$$

Since $\{f_n\}$ is an orthonormal basis for $\mathfrak{H}_F(K_{1\alpha})$, we have

$$d(U_\alpha(\lambda_\alpha)\Psi_F(K_\alpha); \mathfrak{H}_F(K_{1\alpha}), \mathfrak{H}_F(K_{1\alpha}^\perp \cap K)) = ||K||^{\frac{1}{2}} = \left(\frac{1 + (1 + \lambda_\alpha^2)^{\frac{1}{2}}}{2}\right)^{-\frac{1}{2}}. \quad (10.53)$$

Now applying the Theorem 5 to the present situation, the von Neumann algebra $R_F(K_1, K_2/K)$ is type I if and only if $R_F(K_{1c}, K_{2c}/K_c)$ is type I, and

$$\sum_\alpha (1 - [\tfrac{1}{2}\{1 + (1 + \lambda_\alpha^2)^{\frac{1}{2}}\}]^{-\frac{1}{2}}) < \infty. \quad (10.54)$$

Due to the Lemma 10.2, $R_F(K_{1c}, K_{2c}/K_c)$ is type I if and only if $K_c = 0$, and (10.54) holds if and only if $\sum_\alpha \lambda_\alpha^2 < \infty$. Therefore, we have type I if and only if $\alpha(K_2', K_1'/K^{(0)})$ is in the trace class. This completes the proof of Theorem 4′, and hence that of Theorem 4.

*Theorem 6.* $R_F(K_1, K_2/K)$ is infinite type.

*Proof:* We prove that the factor $R_F(K_1' \oplus K^{(2)}, K_2' \oplus K^{(2)}/K^{(0)} \oplus K^{(2)} \oplus K^{(3)})$ is infinite type. Let $f \in K_1' \oplus K^{(2)}$ and let $E(\Delta)$ for a Borel set $\Delta$ be the spectral projection of $U_F(\lambda f)(U_F(\lambda f) = \int e^{i\lambda t}\, dE(t))$. There exists $g \in K_2' \oplus K^{(2)}$ such that $a \equiv (f, g) \neq 0$. For such $g$, $V(\lambda g)E(\Delta)V(\lambda g)^{-1} = E(\Delta + \lambda a)$. For any interval $\Delta = [b, c)$, $E(\Delta)$ is nonzero because $\sum_{n=-\infty}^{\infty} E(\Delta + n(c - b)) = 1$. For $\Delta = (-\infty, b)$ and $\lambda a > 0$, $E(\Delta) \neq E(\Delta + \lambda a)$, $E(\Delta) < E(\Delta + \lambda a)$. Hence $E(\Delta)$ must have the relative dimension $\infty$. Hence $R_F(K_1, K_2/K)$ is infinite type.

Because of Theorem 6, $R_F(K_1, K_2/K)$ is either type $\mathrm{II}_\infty$ or $\mathrm{III}_\infty$ if it is not type I. The discrete part $R_F(K_{1d}, K_{2d}/K_d)$ can be mapped unitarily to an example of von Neuman,[6] and whether this algebra is type $\mathrm{II}_\infty$ or $\mathrm{III}_\infty$ can be decided by seeing whether a certain measure is equivalent to an invariant measure or not. We will not pursue this problem any further in this paper. The unitary mapping to an example of von Neumann just mentioned also gives another proof of the duality equation for the discrete part $R_F(K_{1d}, K_{2d}/K_d)$.

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# Method for Construction of Unitary Operators in Quantum Field Theory

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A method for the construction of explicit representations of unitary Hilbert-space operators in the particle-number representation is presented and illustrated by application to several examples.

## 1. INTRODUCTION

IT is true that methods for the construction of explicit representations of symmetry operators are already available in field theory. Indeed, there is a well-known method for constructing the generator of any continuous transformation in terms of field operators when it is defined in terms of its action on field components (and when the Lagrangian and variations of coordinates are known)[1]; and Berger, Foldy, and Osborn have given a method which is more general in being applicable also to discrete transformations.[2] However, these methods lead only indirectly to representations in terms of annihilation and creation operators of the field expansions ("AO's" and "CO's" for short); and we find, in fact, that representations of discrete operators have usually been constructed by simpler *ad hoc* methods.[3]

The purpose of the present paper is to describe a convenient method for the construction of representations of both continuous and discrete unitary Hilbert-space operators directly in terms of AO's and CO's. The method is useful when (1) the transformations are known in terms of their action on the AO's or CO's (or, equivalently, on one-particle states), and (2) the AO's and CO's satisfy the customary commutation or anticommutation relations[4,5]

$$[a_\alpha, a^*_\beta]_\mp = \delta_{\alpha\beta}, \quad [a_\alpha, a_\beta]_\mp = [a^*_\alpha, a^*_\beta]_\mp = 0. \quad (1.1)$$

The present method thus enjoys the same generality as that of reference 2; however, it deals directly with the AO's and CO's, which have a more immediate physical interpretation than the field operators.

## 2. METHOD

Unitary transformations are generally divided into two types, continuous and discrete. A continuous transformation acting on the AO's can be written $a_\alpha \rightarrow \sum_\beta c_{\alpha\beta} a_\beta$, where the $c_{\alpha\beta}$ are parameters of the transformation. A discrete (or discontinuous) transformation exchanges pairs of AO's in such a way that its double application yields only the factor $\pm 1$; that is, $a_\alpha \rightarrow \eta a_\beta \rightarrow \pm a_\alpha$, where $\eta$ is a unimodular phase factor. If we let $A$ denote a column matrix of AO's $a_\alpha$ which (with their Hermitian conjugates) satisfy Eqs. (1.1),

$$A \equiv \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ \vdots \end{pmatrix}, \quad (2.1)$$

then a unitary transformation of either type can be defined by means of a unitary matrix $\mathfrak{U}$ of complex numbers such that

$$A \rightarrow A' \equiv \begin{pmatrix} a'_1 \\ a'_2 \\ \vdots \\ \vdots \end{pmatrix} = \mathfrak{U} A. \quad (2.2)$$

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[1] See, e.g., P. Roman, *Theory of Elementary Particles* (Interscience Publishers, Inc., New York 1961), 2nd ed., pp. 220–223.

[2] J. M. Berger, L. L. Foldy, and R. K. Osborn, Phys. Rev. **87**, 1061 (1952). These authors have stated their Theorem I for anticommuting fields, but both theorem and proof are equally valid for commuting fields.

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[4] The subscripts $\alpha$ and $\beta$ refer to a complete set of dynamic and intrinsic variables such as momentum, spin, isospin, and baryon number, with each index generally standing for more than one variable.

[5] We shall not follow the conventional practice of using $a$'s and $b$'s to denote the $AO$'s of particles and antiparticles, respectively, but rather use the letter $a$ for both, with indices 1 and 2, respectively.

*Theorem.*[6] If a matrix $\mathfrak{B}$ is known such that

$$\exp(-i\mathfrak{B}) = \mathfrak{U}, \tag{2.3}$$

then it is possible to construct a unitary Hilbert-space operator $U$ which performs the transformation according to

$$UAU^{-1} \equiv \begin{pmatrix} Ua_1U^{-1} \\ Ua_2U^{-1} \\ \vdots \end{pmatrix} = A'. \tag{2.4}$$

The construction is given by

$$U = e^{iB}, \tag{2.5}$$

where[7]

$$B \equiv A^\dagger \mathfrak{B} A. \tag{2.6}$$

*Proof:* Upon expanding the exponentials we find that

$$UAU^{-1} = e^{iB}Ae^{-iB} = \sum_{n=0}^{\infty} \frac{i^n}{n!}[B, A]_n, \tag{2.7}$$

where

$$[B, A]_n \equiv [B, [B, A]_{n-1}]_- \quad \text{for} \quad n \neq 0, \tag{2.8}$$

and

$$[B, A]_0 \equiv A.$$

Using the definition (2.6) for $B$, we find the $\alpha$th component of the column $[B, A]_-$ to be

$$\begin{aligned}[B, a_\alpha]_- &= \sum_{\beta\gamma} \mathfrak{B}_{\beta\gamma}[a_\beta^* a_\gamma, a_\alpha]_- \\ &= \sum_{\beta\gamma} \mathfrak{B}_{\beta\gamma}[(a_\beta^* a_\gamma a_\alpha \mp a_\beta^* a_\alpha a_\gamma) \\ &\quad - (a_\alpha a_\beta^* a_\gamma \mp a_\beta^* a_\alpha a_\gamma)] = -\sum_\gamma \mathfrak{B}_{\alpha\gamma} a_\gamma,\end{aligned} \tag{2.9}$$

where we have used the commutation (anticommutation) relations, corresponding to the upper (lower) signs. Thus $[B, A]_1 = -\mathfrak{B}A$, from which we obtain by induction that

$$[B, A]_n = (-\mathfrak{B})^n A. \tag{2.10}$$

Substituting this result into (2.7), we find

$$\begin{aligned}UAU^{-1} &= e^{iB}Ae^{-iB} \\ &= \sum_{n=0}^{\infty} \frac{(-i\mathfrak{B})^n}{n!} A = \exp(-i\mathfrak{B})A.\end{aligned} \tag{2.11}$$

Equation (2.11) shows that the unitary transformation which mixes or permutes the AO's of $A$ corresponds to a Hilbert-space operator constructed from the same set of AO's as is $A$.

[6] Cf. Theorem I of reference 2.
[7] We define $A^\dagger \equiv (a_1^*, a_2^*, \cdots)$.

Under any given transformation the operators $a_\alpha$ fall naturally into subsets such that the transformation leads to mixing only within subsets—not between subsets. This property is useful because it allows us to construct the total unitary operator $U$ as a product of partial unitary operators acting on these subsets.[8] That is, we can write

$$U = \prod_\rho U_\rho = \prod_\rho e^{iB_\rho}, \tag{2.12}$$

where $U_\rho = \exp(iB_\rho)$ is the partial unitary operator which transforms the AO's of the $\rho$th subset; from (2.6), (2.3), and (2.2), we find

$$B_\rho = A_\rho^\dagger \mathfrak{B}_\rho A_\rho, \tag{2.13}$$

provided

$$\exp(-i\mathfrak{B}_\rho) = \mathfrak{U}_\rho, \text{ where } A_\rho \to A_\rho' = \mathfrak{U}_\rho A_\rho \tag{2.14}$$

under the given transformation, and $A_\rho$ is the column formed from the AO's of the $\rho$th subset. The proof of (2.12) follows easily from the observation that the AO's in any $A_\tau$ commute with all $B_\rho$ for which $\rho \neq \tau$. Since the operators $B_\rho$ also commute with one another, (2.12) can be rewritten as

$$U = e^{iB}, \quad \text{where} \quad B = \sum_\rho B_\rho. \tag{2.15}$$

In many applications, the matrices $\mathfrak{U}_\rho$ and $\mathfrak{B}_\rho$ turn out to be the same for each $\rho$, so that the index on these matrices is superfluous.

For discrete transformations, which permute pairs of AO's, it is generally necessary to determine the matrix $\mathfrak{B}_\rho$ from a known matrix $\mathfrak{U}_\rho$. But this is easily done, since in this case $\mathfrak{U}_\rho$ is a $2 \times 2$ unitary matrix which can always be written as an exponential function of a Hermitian matrix. Thus we set

$$\begin{aligned}\mathfrak{U}_\rho &= \exp(-i\mathfrak{B}_\rho) = \exp[i(\lambda \mathfrak{s} + \mu \mathbf{b}\cdot\boldsymbol{\sigma})] \\ &= e^{i\lambda}(\mathfrak{s}\cos\mu + i\mathbf{b}\cdot\boldsymbol{\sigma}\sin\mu),\end{aligned} \tag{2.16}$$

where $\mathfrak{s}$ is the $2 \times 2$ identity, the $\sigma_i$ $(i = 1, 2, 3)$ are Pauli matrices, and $\lambda$, $\mu$ and $b_i$ are real parameters satisfying $\mathbf{b}\cdot\mathbf{b} = 1$. Explicitly, the matrices of (2.16) are

$$\mathfrak{U}_\rho = e^{i\lambda}\begin{pmatrix} \cos\mu + ib_3\sin\mu & (b_2 + ib_1)\sin\mu \\ (-b_2 + ib_1)\sin\mu & \cos\mu - ib_3\sin\mu \end{pmatrix}, \tag{2.17a}$$

and

$$\mathfrak{B}_\rho = -\begin{pmatrix} \lambda + \mu b_3 & \mu(b_1 - ib_2) \\ \mu(b_1 + ib_2) & \lambda - \mu b_3 \end{pmatrix}. \tag{2.17b}$$

[8] See, e.g., L. Wolfenstein and D. G. Ravenhall, Phys. Rev. **88**, 279 (1952).

Comparison of the known matrix $\mathfrak{U}_\rho$ with the corresponding matrix of (2.17) now permits one to determine the allowed values of the parameters[9] and hence the matrix $\mathfrak{G}_\rho$.

## 3. APPLICATIONS

### A. Isorotation of an isovector field

This is an example of a continuous operator, applicable to the pion field, in which $\mathfrak{G}$ is known. Let us define[10]

$$\varphi_\pi \equiv \begin{pmatrix}\varphi_{\pi 1}\\ \varphi_{\pi 2}\\ \varphi_{\pi 3}\end{pmatrix} \quad \text{and} \quad A_{\mathbf{k}} \equiv \begin{pmatrix}a_{\mathbf{k}1}\\ a_{\mathbf{k}1}\\ a_{\mathbf{k}3}\end{pmatrix}, \tag{3.1}$$

where the AO's $a_{\mathbf{k}i}$ are those which occur in the corresponding Hermitian fields $\varphi_{\pi i}$. These Cartesian components $a_{\mathbf{k}i}$ are defined by $(a_{\mathbf{k}1} \mp ia_{\mathbf{k}2})/\sqrt{2} \equiv a_{\mathbf{k}\pm}$ and $a_{\mathbf{k}3} \equiv a_{\mathbf{k}0}$, where the latter are AO's for $\pi^\pm$ and $\pi^0$ mesons, respectively; a similar definition holds for the $\varphi_{\pi i}$. An isorotation through the angle $|\boldsymbol{\alpha}|$ about the direction of $\boldsymbol{\alpha}$ is then given by

$$\varphi'_\pi = \exp(-i\boldsymbol{\alpha}\cdot\boldsymbol{\vartheta})\varphi_\pi, \text{ or } A'_{\mathbf{k}} = \exp(-i\boldsymbol{\alpha}\cdot\boldsymbol{\vartheta})A_{\mathbf{k}}, \tag{3.2}$$

where the $\vartheta_i$ are $3 \times 3$ "angular momentum" matrices in the Cartesian representation.[11] For simplicity, we shall take $\alpha_1 = \alpha_3 = 0$. We then have, according to (3.2) and (2.14),

$$\mathfrak{G}_{\mathbf{k}} = \alpha_2\vartheta_2 = \alpha_2\begin{pmatrix}0 & 0 & i\\ 0 & 0 & 0\\ -i & 0 & 0\end{pmatrix}. \tag{3.3}$$

From (2.13),

$$\begin{aligned}B_{\mathbf{k}} &= A^\dagger_{\mathbf{k}}\mathfrak{G}_{\mathbf{k}}A_{\mathbf{k}} = i\alpha_2(a^*_{\mathbf{k}1}a_{\mathbf{k}3} - a^*_{\mathbf{k}3}a_{\mathbf{k}1})\\ &= (i/\sqrt{2})\alpha_2(a^*_{\mathbf{k}+}a_{\mathbf{k}0} + a^*_{\mathbf{k}-}a_{\mathbf{k}0}\\ &\qquad - a^*_{\mathbf{k}0}a_{\mathbf{k}+} - a^*_{\mathbf{k}0}a_{\mathbf{k}-});\end{aligned} \tag{3.4}$$

and $U = e^{iB}$, with $B = \sum_{\mathbf{k}} B_{\mathbf{k}}$, according to (2.15).

### B. Space inversion of a Dirac field

This is a discrete transformation for which $U^2 = \pm 1$; the upper sign leads to the "real parity class" (with phase factor $\eta_R = \pm 1$), and the lower sign to the "imaginary parity class" (with phase factor $\eta_I = \pm i$). We consider first the real class which can be defined on particle and antiparticle AO's, respectively, by[5,12]

$$a_{\pm\mathbf{k}s1} \to \eta_R a_{\mp\mathbf{k}s1} \quad \text{and} \quad a_{\pm\mathbf{k}s2} \to -\eta_R a_{\mp\mathbf{k}s2}. \tag{3.5}$$

Letting

$$A_{\mathbf{k}s1} \equiv \begin{pmatrix}a_{\mathbf{k}s1}\\ a_{-\mathbf{k}s1}\end{pmatrix} \quad \text{and} \quad A_{\mathbf{k}s2} \equiv \begin{pmatrix}a_{\mathbf{k}s2}\\ a_{-\mathbf{k}s2}\end{pmatrix}, \tag{3.6}$$

we get

$$\mathfrak{U}_{\mathbf{k}s1} = \begin{pmatrix}0 & \eta_R\\ \eta_R & 0\end{pmatrix} \quad \text{and} \quad \mathfrak{U}_{\mathbf{k}s2} = \begin{pmatrix}0 & -\eta_R\\ -\eta_R & 0\end{pmatrix}. \tag{3.7}$$

Referring to Eqs. (2.17), we choose for $\mathfrak{U}_{\mathbf{k}s1}$ the parameters $\mu = -\frac{1}{2}\pi = -\lambda$, $b_2 = b_3 = 0$, and $b_1 = \eta_R(= \pm 1)$; and the same for $\mathfrak{U}_{\mathbf{k}s2}$, except that $\lambda = -\frac{1}{2}\pi$. Thus we get, from (2.17),

$$\mathfrak{G}_{\mathbf{k}s1} = \frac{\pi}{2}\begin{pmatrix}-1 & \eta_R\\ \eta_R & -1\end{pmatrix} \quad \text{and} \quad \mathfrak{G}_{\mathbf{k}s2} = \frac{\pi}{2}\begin{pmatrix}1 & \eta_R\\ \eta_R & 1\end{pmatrix}; \tag{3.8}$$

from (2.13),

$$\begin{aligned}B_{\mathbf{k}sn} = \tfrac{1}{2}\pi[(-1)^n(a^*_{\mathbf{k}sn}a_{\mathbf{k}sn} + a^*_{-\mathbf{k}sn}a_{-\mathbf{k}sn})\\ + \eta_R(a^*_{\mathbf{k}sn}a_{-\mathbf{k}sn} + a^*_{-\mathbf{k}sn}a_{\mathbf{k}sn})]\end{aligned} \tag{3.9}$$

for $n = 1$ or 2; and $B = \sum'_{\mathbf{k}sn} B_{\mathbf{k}sn}$ from (2.15).[13]

For the imaginary parity class, space inversion is defined by[12]

$$a_{\pm\mathbf{k}sn} \to \eta_I a_{\mp\mathbf{k}sn} \tag{3.10}$$

for both particle and antiparticle AO's. Here we find

$$\mathfrak{U}_{\mathbf{k}sn} = \begin{pmatrix}0 & \eta_I\\ \eta_I & 0\end{pmatrix}; \tag{3.11}$$

choosing the parameters in (2.17) to be[9] $\mu = \frac{1}{2}\pi$, $\lambda = b_2 = b_3 = 0$, and $b_1 = -i\eta_I(= \pm 1)$, we get

$$\mathfrak{G}_{\mathbf{k}sn} = \frac{i\pi}{2}\begin{pmatrix}0 & \eta_I\\ \eta_I & 0\end{pmatrix}; \tag{3.12}$$

and

$$\begin{aligned}B = \sum_{\mathbf{k}sn}{}' B_{\mathbf{k}sn} = \sum_{\mathbf{k}sn}{}' \tfrac{1}{2}\pi i\eta_I(a^*_{\mathbf{k}sn}a_{-\mathbf{k}sn}\\ + a^*_{-\mathbf{k}sn}a_{\mathbf{k}sn}).\end{aligned} \tag{3.13}$$

[9] Among the allowed values, the best choice is generally that for which the matrix (2.17b), and hence the operator $B$, is simplest; this occurs, for example, when that matrix has two zero elements. Note that the nonuniqueness of the operator $B$ is not reflected in the action of $U$. That is, the effect of $U$ on the AO's (and hence on the CO's) is unique, by the above theorem; the uniqueness on states then follows from expressing the latter as products of CO's acting on the vacuum, since the vacuum is invariant under any $U$ of the form (2.5) and (2.6).

[10] Reference 1, p. 501.

[11] Reference 1, pp. 427 and 429.

[12] R. E. Marshak and E. C. G. Sudarshan, *Introduction to Elementary Particle Physics* (Interscience Publishers, Inc., New York, 1961), p. 53.

[13] The prime indicates summation over only half of k space (say, $k_3 > 0$). This restriction arises because the permuted indices happen to be k and $-$k, so that a summation over all of k space would include each term twice.

Equations (3.9) and (3.13) show that the space-inversion operators for the two parity classes are quite distinct.[14] Because of the particle-number-operator terms which appear in (3.9), we see that these two operators will behave differently under particle–antiparticle conjugation.[15]

### C. *R* inversion of baryon fields

As a final example, we shall construct the operator for an $R$ inversion[16] of the baryon fields. (The corresponding operator for the meson fields is quite similar, and will not be worked out here.) In this example, we shall change our notation and denote the AO's by the symbols of the particles annihilated; the equation $A'_{\mathbf{k}s1} = \mathcal{K}_{\mathbf{k}s1}A_{\mathbf{k}s1}$ defining this transformation can then be written out explicitly as

$$\begin{bmatrix} \Xi^- \\ p \\ \Xi^0 \\ n \\ \Sigma^- \\ \Sigma^+ \\ \Sigma^0 \\ \Lambda \end{bmatrix} = \begin{bmatrix} 0 & 1 & & & & & & \\ 1 & 0 & & & & & & \\ & & 0 & 1 & & & & \\ & & 1 & 0 & & & & \\ & & & & 0 & 1 & & \\ & & & & 1 & 0 & & \\ & & & & & & 1 & 0 \\ & & & & & & 0 & 1 \end{bmatrix} \begin{bmatrix} p \\ \Xi^- \\ n \\ \Xi^0 \\ \Sigma^+ \\ \Sigma^- \\ \Sigma^0 \\ \Lambda \end{bmatrix}. \tag{3.14}$$

The indices $\mathbf{k}$ and $s$ have been suppressed in (3.14); the particle symbols take the place of subscripts denoting hypercharge and the third component of isospin, which are reversed by this transformation. The column $A_{\mathbf{k}s1}$ has been ordered in such a way that $\mathfrak{U}_{\mathbf{k}s1}$ consists simply of $2 \times 2$ submatrices along the diagonal, so that (2.17) can be applied as before to yield

$$\mathfrak{G}_{\mathbf{k}s1} = \frac{\pi}{2}\begin{bmatrix} -1 & 1 & & & & & & \\ 1 & -1 & & & & & & \\ & & -1 & 1 & & & & \\ & & 1 & -1 & & & & \\ & & & & -1 & 1 & & \\ & & & & 1 & -1 & & \\ & & & & & & 0 & 0 \\ & & & & & & 0 & 0 \end{bmatrix}. \tag{3.15}$$

From this we obtain

$$\begin{aligned} B_{\mathbf{k}s1} = \tfrac{1}{2}\pi[&(-p^*p + p^*\Xi^- + \Xi^{-*}p - \Xi^{-*}\Xi^-) \\ &+ (p \to n, \Xi^- \to \Xi^0) \\ &+ (p \to \Sigma^+, \Xi^- \to \Sigma^-)]_{\mathbf{k}s}, \end{aligned} \tag{3.16}$$

where the last two terms are obtained from the first by means of the indicated substitutions, and the AO's and CO's each carry the indices $\mathbf{k}$ and $s$. The operator $B_{\mathbf{k}s2}$ which acts on the antibaryon column $A_{\mathbf{k}s2}$ is obtained from (3.16) by substituting antiparticle AO's and CO's for all particle AO's and CO's; and, finally, substitution of the operator $B = \sum_{\mathbf{k}sn} B_{\mathbf{k}sn}$ into (2.15) yields the desired unitary operator.


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[14] Note that the explicit representation of the space-inversion operator given in reference 12 is valid only for the real parity class.

[15] Cf., for example, B. P. Nigam and L. L. Foldy, Phys. Rev. **102**, 1410 (1956).

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# Modified Langevin Equation for the Description of Brownian Motion

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A modified Langevin equation for the description of Brownian motion is shown to give results equivalent to those of the Langevin equation in some physical situations. The Smoluchowski equation for the probability density of the displacement of a Brownian particle is derived from the modified Langevin equation with the aid of assumptions weaker than those needed to derive the Smoluchowski equation from the ordinary Langevin equation. Sufficient conditions for the applicability of the modified Langevin equation to the calculation of configuration-space averages are obtained. Then the modified Langevin equation is applied to three simple systems, and the results are compared with those of the Langevin equation.

## INTRODUCTION

THE starting point for investigations into the theory of the Brownian motion of a particle immersed in a fluid is usually the Langevin equation

$$\dot{\mathbf{u}} = -\beta\mathbf{u} + \mathbf{A}(t) + \mathbf{K}(\mathbf{r}), \tag{1}$$

where $\mathbf{r}$ is the position and $\mathbf{u}$ the velocity of the particle. The effect of the medium is assumed to be separable into two parts, a dynamical friction, $-\beta\mathbf{u}$, and a rapidly fluctuating term, $\mathbf{A}(t)$, which is assumed to be independent of $\mathbf{u}$. The last term in the equation represents the acceleration caused by any fields of force acting on the particle. The fluctuating term has only statistically defined properties. A convenient formulation of its properties was given by Chandrasekhar.[1] Let $\Delta t$ be any time which is long compared with the times of fluctuation of $\mathbf{A}(t)$. If we let

$$\mathbf{B}(\Delta t) = \int_t^{t+\Delta t} \mathbf{A}(\xi)\, d\xi,$$

then the probability density for the values of $\mathbf{B}(\Delta t)$ is

$$W[\mathbf{B}(\Delta t)] = (4\pi q \Delta t)^{-\frac{3}{2}} \exp\left(-|\mathbf{B}(\Delta t)|^2/4q\Delta t\right), \tag{2}$$

where $q = \beta kT/m$. The mass of the particle is $m$, and $k$ is Boltzmann's constant.

Chandrasekhar[1] also proved the following useful lemma. Let

$$\mathbf{R} = \int_0^t \psi(\xi)\mathbf{A}(\xi)\, d\xi.$$

Then the probability density for the values of $\mathbf{R}$ is

$$W(\mathbf{R}) = \left(4\pi q \int_0^t \psi^2(\xi)\, d\xi\right)^{-\frac{3}{2}} \times \exp\left(-|\mathbf{R}|^2/4q \int_0^t \psi^2(\xi)\, d\xi\right). \tag{3}$$

If we arbitrarily remove the $\dot{\mathbf{u}}$ term from the Langevin equation we obtain the modified Langevin equation

$$0 = -\beta\mathbf{u} + \mathbf{A}(t) + \mathbf{K}(\mathbf{r})$$

or

$$\mathbf{u} = \beta^{-1}\mathbf{A}(t) + \beta^{-1}\mathbf{K}(\mathbf{r}). \tag{4}$$

Equation (4) can only apply in a coarse-grained sense, since it implies that the particle is at all instants of time moving with the friction-limited velocity consistant with its instantaneous forces. Equation (4) is not valid for times of the order of or less than $\beta^{-1}$, since it gives results which are qualitatively different from those of the (physically reasonable) Langevin equation. However, for times much larger than $\beta^{-1}$, the predictions of this equation are often the same as those of the Langevin equation for certain types of external fields $\mathbf{K}$. The modified Langevin equation has the advantage that, since it is a first-order stochastic differential equation, it is easier to solve than the Langevin equation, which is a second-order stochastic differential equation or the various second-order partial differential equations which have been used to describe Brownian motion. The purpose of this article is to derive conditions for the validity of the modified Langevin equation.

## DERIVATION OF THE SMOLUCHOWSKI EQUATION FROM THE MODIFIED LANGEVIN EQUATION

Let us assume that there is a time $\Delta t$ which is both long compared with the time of fluctuation

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of $\mathbf{A}(t)$ and short compared with the times during which the position of the particle changes appreciably. When Eq. (4) is integrated from time $t_0$ to $t_0 + \Delta t$, the result is

$$\Delta\mathbf{r} = \mathbf{r}(t_0 + \Delta t) - \mathbf{r}(t_0)$$
$$= \beta^{-1}\mathbf{B}(\Delta t) + \beta^{-1}\mathbf{K}[\mathbf{r}(t_0)]\Delta t + O(\Delta t)^2, \quad (5)$$

where we have made use of the fact that

$$\mathbf{K}[\mathbf{r}(t)] - \mathbf{K}[\mathbf{r}(t_0)] = O(\Delta t) \quad \text{for} \quad t_0 \leq t \leq t_0 + \Delta t.$$

We make use of Eq. (5) and Eq. (2) to calculate the probability density that a particle originally at position $\mathbf{r}$ at time $t$ will be at position $\mathbf{r} + \Delta\mathbf{r}$ at time $t + \Delta t$.

$$\psi(\mathbf{r};\, \Delta\mathbf{r}) = \beta^3(4\pi q\Delta t)^{-\frac{3}{2}} \exp\left(-|\beta\Delta\mathbf{r} - \mathbf{K}\Delta t|^2/4q\Delta t\right).$$

Since $\Delta t$ is long compared with the fluctuations of $\mathbf{A}(t)$ we expect the following equation to be valid:

$$W(\mathbf{r},\, t + \Delta t)$$
$$= \int W(\mathbf{r} - \Delta\mathbf{r},\, t)\psi(\mathbf{r} - \Delta\mathbf{r};\, \Delta\mathbf{r})\, d(\Delta\mathbf{r}), \quad (6)$$

where $W(\mathbf{r},\, t)$ is the probability density that the particle is at position $\mathbf{r}$ at time $t$.

When each of the factors in Eq. (6) is expanded in a Taylor series, we obtain

$$W(\mathbf{r},\, t) + \frac{\partial W}{\partial t}\Delta t + O(\Delta t)^2$$
$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left\{W(\mathbf{r},\, t) - \sum_{i=1}^{3}\frac{\partial W}{\partial r_i}\Delta r_i\right.$$
$$\left. + \tfrac{1}{2}\sum_{i=1}^{3}\frac{\partial^2 W}{\partial r_i^2}(\Delta r_i)^2 + \sum_{i<j}\frac{\partial^2 W}{\partial r_i\,\partial r_j}\Delta r_i\,\Delta r_j + \cdots\right\}$$
$$\cdot\left\{\psi(\mathbf{r},\, \Delta\mathbf{r}) - \sum_{i=1}^{3}\frac{\partial\psi}{\partial r_i}\Delta r_i + \tfrac{1}{2}\sum_{i=1}^{3}\frac{\partial^2\psi}{\partial r_i^2}(\Delta r_i)^2\right.$$
$$\left. + \sum_{i<j}\frac{\partial^2\psi}{\partial r_i\,\partial r_j}\Delta r_i\,\Delta r_j + \cdots\right\} d(\Delta r_1)\, d(\Delta r_2)\, d(\Delta r_3), \quad (7)$$

where $r_1$, $r_2$, and $r_3$ are the components of the vector $\mathbf{r}$. If we define

$$\langle\Delta r_i\rangle = \iiint_{-\infty}^{\infty}\Delta r_i\psi(\mathbf{r};\, \Delta\mathbf{r})\, d(\Delta\mathbf{r}),$$

$$\langle\Delta r_i^2\rangle = \iiint_{-\infty}^{\infty}(\Delta r_i)^2\psi(\mathbf{r};\, \Delta\mathbf{r})\, d(\Delta\mathbf{r}),$$

$$\langle\Delta r_i\,\Delta r_j\rangle = \iiint_{-\infty}^{\infty}\Delta r_i\,\Delta r_j\psi(\mathbf{r};\, \Delta\mathbf{r})\, d(\Delta\mathbf{r}),$$

Eq. (7) can be simplified to

$$\frac{\partial W}{\partial t}\Delta t + O(\Delta t)^2 = -\sum_{i=1}^{3}\frac{\partial}{\partial r_i}(W\langle\Delta r_i\rangle)$$
$$+ \tfrac{1}{2}\sum_{i=1}^{3}\frac{\partial^2}{\partial r_i^2}(W\langle\Delta r_i^2\rangle) + \sum_{i<j}\frac{\partial^2}{\partial r_i\,\partial r_j}$$
$$\times(W\langle\Delta r_i\Delta r_j\rangle) + O(\langle\Delta r_i\Delta r_j\Delta r_k\rangle). \quad (8)$$

The averages are

$$\langle\Delta r_i\rangle = \beta^{-1}K_i\Delta t,$$
$$\langle\Delta r_i^2\rangle = 2q\beta^{-2}\Delta t + O(\Delta t)^2,$$
$$\langle\Delta r_i\Delta r_j\rangle = O(\Delta t)^2,$$
$$\langle\Delta r_i\Delta r_j\Delta r_k\rangle = O(\Delta t)^2 \quad \text{(for any choice of } i,\, j,\, k).$$

Equation (8) then becomes

$$\frac{\partial W}{\partial t}\Delta t + O(\Delta t)^2 = -\beta^{-1}\Delta t\nabla\cdot(W\mathbf{K}) + q\beta^{-2}\Delta t\nabla^2 W.$$

Dividing this equation by $\Delta t$, and neglecting terms of order $\Delta t$, we obtain

$$\frac{\partial W}{\partial t} = \nabla\cdot(q\beta^{-2}\nabla W - \beta^{-1}\mathbf{K}W),$$

which is the Smoluchowski equation.

The assumptions made in this derivation are the same as those made in the derivation[1] of the phase-space Fokker–Planck equation from the Langevin equation. With the aid of additional assumptions about $\mathbf{K}(\mathbf{r})$ and about the velocity distribution of the Brownian particle, the Smoluchowski equation can be derived[1] from the Fokker–Planck equation, for times much larger than $\beta^{-1}$. Thus, whenever the Smoluchowski equation follows from the Langevin equation, it also follows from the modified Langevin equation. This leads to the conjecture that the modified Langevin equation is at least as valid as Smoluchowski's equation. In fact, for several simple systems, such as the free particle and the particle in a centrifugal or harmonic potential (see below), the modified Langevin equation and the Smoluchowski equation give identical results.

## SUFFICIENT CONDITIONS FOR THE VALIDITY OF THE MODIFIED LANGEVIN EQUATION

When solving a stochastic differential equation such as the Langevin Eq. (1) or the modified Langevin Eq. (4) for a single particle, one assumes that $\mathbf{A}(t)$ is a definite function of time and solves the equation for $\mathbf{r}(t)$ as an initial-value problem in the usual manner. The answer will involve $\mathbf{A}(t)$, and from the statistical properties of $\mathbf{A}(t)$ one calculates the statistical properties of $\mathbf{r}(t)$. This is

equivalent to imagining an ensemble of particles, each of which has the same initial conditions. The functions $\mathbf{A}(t)$ are "distributed" in some manner in the ensemble, and each member of the ensemble has a definite $\mathbf{A}(t)$ acting upon it.

Let us consider two ensembles, $L$ and $M$. $L$ consists of particles $L_1, L_2, \cdots L_N$, and $M$ consists of particles $M_1, M_2, \cdots M_N$, where $N$ is an extremely large number. Let each of them have an $\mathbf{A}(t)$ assigned to it such that $L_1$ and $M_1$ have $\mathbf{A}_1(t)$, $L_2$ and $M_2$ have $\mathbf{A}_2(t)$, $\cdots$ etc. Let each of the particles in the $L$ ensemble start at $t = 0$ at point $\mathbf{r}_0$ with velocity $\mathbf{u}_0$ and then move according to Langevin's equation. Let each of the particles in the $M$ ensemble start at $t = 0$ at the point $\mathbf{r}_0$ and move according to the modified Langevin equation. (We cannot specify the initial velocities for the particles in the $M$ ensemble because the modified Langevin equation is a first-order differential equation.) Thus, the equation of motion of particle $L_i$ is

$$\dot{\mathbf{u}} = -\beta\mathbf{u} + \mathbf{A}_i(t) + \mathbf{K}(\mathbf{r}), \qquad i = 1, 2, \cdots N,$$

while the equation of motion of particle $M_i$ is

$$\mathbf{u} = \beta^{-1}\mathbf{A}_i(t) + \beta^{-1}\mathbf{K}(\mathbf{r}), \qquad i = 1, 2, \cdots N.$$

Particles $L_i$ and $M_i$ will, of course, not follow the same trajectory, even though they both have the same $\mathbf{A}_i(t)$ acting on them. Their trajectories will differ by

$$\mathbf{y}_i(t) = \mathbf{r}_{L_i}(t) - \mathbf{r}_{M_i}(t), \qquad i = 1, 2, \cdots N.$$

This defines a new random variable $\mathbf{y}(t)$, whose statistical properties are described by the combined ensemble.

Suppose the ensemble averages $\langle|\mathbf{y}(t)|\rangle_{\text{av}}$ and $\langle\mathbf{y}^2(t)\rangle_{\text{av}}^{\frac{1}{2}}$ are small compared with distances which we wish to measure. This would imply that at all times, for almost all $i$,

$$\mathbf{r}_{L_i}(t) = \mathbf{r}_{M_i}(t)$$

to within experimental accuracy. If we wanted to calculate the ensemble average of any function of $\mathbf{r}$, such as $\mathbf{r} - \mathbf{r}_0$ or $(\mathbf{r} - \langle\mathbf{r}\rangle_{\text{av}})^2$, the two ensembles would give the same result to within experimental accuracy. This implies that the Langevin equation and the modified Langevin equation are equivalent, as far as a description of the positions of the particles is concerned. Thus, to demonstrate the equivalence of the Langevin and modified Langevin equations we need only demonstrate that $\langle|\mathbf{y}(t)|\rangle_{\text{av}}$ and $\langle\mathbf{y}^2(t)\rangle_{\text{av}}^{\frac{1}{2}}$ are small.

For simplicity in the following discussion let us just consider the case of one-dimensional motion. Let $x_{L_i}(t)$ be the position of particle $L_i$, and let $x_{M_i}(t)$ be that of $M_i$. The equation for $x_{L_i}$ is

$$\ddot{x}_{L_i} = -\beta\dot{x}_{L_i} + A_i(t) + K(x_{L_i}), \tag{9}$$

subject to the conditions that

$$x_{L_i}(0) = x_0 \quad \text{and} \quad \dot{x}_{L_i}(0) = u_0.$$

The equation for $x_{M_i}$ is

$$\dot{x}_{M_i} = \beta^{-1}A_i(t) + \beta^{-1}K(x_{M_i}), \tag{10}$$

subject to the condition that

$$x_{M_i}(0) = x_0.$$

We define $y_i = x_{L_i} - x_{M_i}$. (From this point on we shall omit use of the subscript $i$ since it will never be necessary to distinguish between two members of the ensemble.)

Equation (9) can be rewritten in the form

$$e^{-\beta t}(d/dt)(e^{\beta t}\dot{x}_L) = A(t) + K(x_L).$$

Integration of this equation twice results in

$$x_L(t) = \beta^{-1}\int_0^t (1 - e^{-\beta(t-\xi)})(A(\xi) + K[x_L(\xi)])\,d\xi + \beta^{-1}u_0(1 - e^{-\beta t}) + x_0.$$

Equation (10) can be immediately integrated to give

$$x_M(t) = \beta^{-1}\int_0^t (A(\xi) + K[x_M(\xi)])\,d\xi + x_0.$$

From these two expressions we see that

$$y(t) \equiv x_L(t) - x_M(t) = \beta^{-1}\int_0^t (K[x_L(\xi)] - K[x_M(\xi)])\,d\xi - \beta^{-1}\int_0^t e^{-\beta(t-\xi)}(A(\xi) + K[x_L(\xi)])\,d\xi + \beta^{-1}u_0(1 - e^{-\beta t}). \tag{11}$$

We make use of the mean-value theorem to write

$$K[x_L(\xi)] - K[x_M(\xi)] = (x_L(\xi) - x_M(\xi))K^1[z(\xi)],$$

where $z(\xi)$ is between $x_L(\xi)$ and $x_M(\xi)$ and $K^1(x)$ denotes the first derivative of $K(x)$. Equation (11) becomes

$$y(t) = \beta^{-1}\int_0^t K^1[z(\xi)]y(\xi)\,d\xi - \beta^{-1}\int_0^t e^{-\beta(t-\xi)} \times (A(\xi) + K[x_L(\xi)])\,d\xi + \beta^{-1}u_0(1 - e^{-\beta t}). \tag{12}$$

This equation may be written in the simple form

$$y(t) = \beta^{-1}\int_0^t K^1[z(\xi)]y(\xi)\,d\xi + S(t), \tag{13}$$

where

$$S(t) = -\beta^{-1}\int_0^t e^{-\beta(t-\xi)}(A(\xi) + K[x_L(\xi)])\,d\xi + \beta^{-1}u_0(1 - e^{-\beta t}). \quad (14)$$

Equation (13) is an integral equation for $y(t)$. The solution of Eq. (13) is

$$y(t) = S(t) + \beta^{-1}\int_0^t d\xi K^1[z(\xi)]S(\xi) \times \exp\left(\beta^{-1}\int_\xi^t K^1[z(\eta)]\,d\eta\right). \quad (15)$$

Using this result the statistical properties of $y(t)$ may be determined from those of $S(t)$.

$S(t)$ is the sum of three terms. The first term,

$$S_1(t) = -\beta^{-1}\int_0^t e^{-\beta(t-\xi)}A(\xi)\,d\xi,$$

is a random variable whose probability density may be calculated with the aid of Eq. (3). The distribution is Gaussian with a mean of zero and a variance of $(kT/m\beta^2)(1 - e^{-2\beta t})$, which is small for most physical situations. For example, in the experiments by Westgren,[2] $kT/m\beta^2$ is about $10^{-19}$ cm$^2$.

The second term in $S(t)$,

$$S_2(t) = -\beta^{-1}\int_0^t K[x_L(\xi)]e^{-\beta(t-\xi)}\,d\xi,$$

is also a random variable. Let us assume that in the physical situation under consideration, $K(x)$ is bounded; i.e. $|K(x)| < P$ for all $x$ of physical interest. In this case,

$$|S_2(t)| < \beta^{-1}P\int_0^t e^{-\beta(t-\xi)}\,d\xi < \beta^{-2}P,$$

and $|S_2(t)|$ is bounded uniformly in time by an amount which in most physical situations is much smaller than $\langle|S_1|\rangle_{av}$. We shall neglect this term.

The third term in $S(t)$,

$$S_3(t) = \beta^{-1}u_0(1 - e^{-\beta t}),$$

is also small. When $u_0$ is a thermal velocity, $S_3$ is of the same order of magnitude as $S_1$.

$S(t)$ is then a random variable with a mean of $\beta^{-1}u_0(1 - e^{-\beta t})$ and a variance of $(kT/m\beta^2)(1 - e^{-2\beta t})$. We may now investigate the statistical properties of $y(t)$ in various cases.

Case I. If $K^1(x) = 0$ for all $x$, i.e., if the external force on the particle is independent of position, Eq. (15) states that $y(t) = S(t)$. Thus, $y(t)$ has a Gaussian distribution with small mean and variance. We expect, therefore, that the Langevin and modified Langevin equations are equivalent in this case.

Case II. Let us assume that $|K^1(x)|$ is bounded by $R$, a constant. Then

$$\langle|y(t)|\rangle_{av} < \langle|S(t)|\rangle_{av} + \beta^{-1}R\langle|S(t)|\rangle_{av} \times \int_0^t \exp\left[\beta^{-1}R(t-\xi)\right]d\xi < \langle|S(t)|\rangle_{av}\,e^{Rt/\beta}$$

where we have used the fact that $\langle|S(t)|\rangle_{av} > \langle|S(\xi)|\rangle_{av}$ for $t > \xi$. Also used twice is the theorem that

$$\langle|fg|\rangle_{av} \leq f_{max}\langle|g|\rangle_{av},$$

where $f$ and $g$ are any two random variables and $f_{max}$ is the maximum value of $|f|$.

When Eq. (15) is squared, an expression for $y^2(t)$ is obtained. From this it is easily shown that $\langle y^2(t)\rangle_{av} \leq \langle S^2(t)\rangle_{av}(4 + e^{2Rt/\beta})$.

For $t < \beta R^{-1}$, $\langle|y(t)|\rangle_{av}$ and $\langle y^2(t)\rangle_{av}^{\frac{1}{2}}$ are small, and for such times we should expect Eqs. (1) and (4) to be equivalent. For larger times, these averages may increase indefinitely. An example of such a deviation of the results of the two equations is given below in the centrifugal potential problem. We note that solutions of the stochastic equations for $t > \beta R^{-1}$ are rarely of physical interest.

Case III. Suppose $K^1(x)$ is bounded and less than a negative constant, i.e.,

$$-R \leq K^1(x) \leq -Q < 0 \quad (16)$$

for all $x$ of physical interest. $R$ and $Q$ are positive numbers. This implies that

$$\langle|y(t)|\rangle_{av} < \langle|S(t)|\rangle_{av} + \beta^{-1}R\langle|S(t)|\rangle_{av} \times \int_0^t \exp\left[-\beta^{-1}Q(t-\xi)\right]d\xi < \langle|S(t)|\rangle_{av}(1 + RQ^{-1}).$$

Similarly it can be shown that

$$\langle y^2(t)\rangle_{av} < \langle S^2(t)\rangle_{av}(1 + RQ^{-1})^2.$$

If $(1 + RQ^{-1})\langle|S(t)|\rangle_{av}$ and $(1 + RQ^{-1})\langle S^2(t)\rangle_{av}^{\frac{1}{2}}$ are small compared with measurable distances, $\langle|y(t)|\rangle_{av}$ and $\langle y^2(t)\rangle_{av}^{\frac{1}{2}}$ will be small for all times. The above conditions (16) on $K^1(X)$ imply that there is one minimum of potential energy. An example of such a case is given below in the harmonic-oscillator problem.

We have demonstrated that if the external force and the space derivative of the external force on a Brownian particle are bounded and if these bounds satisfy certain numerical requirements, then for $t \leq \beta R^{-1}$, the Langevin and modified

Langevin equations are equivalent for the calculation of averages over the positions of the particles. If, in addition, the derivative of the force is always less than a negative constant, the equivalence holds for all times.

## APPLICATION OF THE MODIFIED LANGEVIN EQUATION TO SIMPLE SYSTEMS

### The Free Particle

The modified Langevin equation for the free particle is

$$\mathbf{u} = \beta^{-1}\mathbf{A}(t),$$

which can be integrated immediately to give

$$\mathbf{r} = \beta^{-1}\int_0^t \mathbf{A}(\xi)\,d\xi + \mathbf{r}_0.$$

Applying Eq. (3), with $\psi = \beta^{-1}$, we see that

$$W(\mathbf{r}, t; \mathbf{r}_0) = (\beta^2/4\pi qt)^{\frac{3}{2}} \exp(-\beta^2|\mathbf{r} - \mathbf{r}_0|^2/4qt).$$

If we let $D = q/\beta^2 = kT/m\beta$, this becomes

$$W(\mathbf{r}, t; \mathbf{r}_0) = (4\pi Dt)^{-\frac{3}{2}} \exp(-|\mathbf{r} - \mathbf{r}_0|^2/4Dt), \quad (17)$$

which is identical to the result[1] of the Langevin equation for $t \gg \beta^{-1}$.

The Smoluchowski equation for this problem is

$$\partial W/\partial t = \beta^{-2}q\nabla^2 W,$$

which is satisfied identically by Eq. (17).

### The Harmonic Oscillator

The modified Langevin equation for a harmonic oscillator with frequency $\omega$ is (for one dimension)

$$\dot{x} = \beta^{-1}A(t) - \beta^{-1}\omega^2 x,$$

the solution of which is

$$x = x_0 e^{-\omega^2 t/\beta} + \beta^{-1}\int_0^t e^{-\omega^2(t-\xi)/\beta}A(\xi)\,d\xi.$$

Use of Eq. (3) in its one-dimensional form gives

$$W(x, t; x_0) = \left(\frac{m\omega^2}{2\pi kT(1 - e^{-2\omega^2 t/\beta})}\right)^{\frac{1}{2}} \times \exp\left(-\frac{m\omega^2(x - x_0 e^{-\omega^2 t/\beta})^2}{2kT(1 - e^{-2\omega^2 t/\beta})}\right). \quad (18)$$

Equation (18) is a Gaussian for which

$$\langle x\rangle_{\text{av}} = x_0 e^{-\omega^2 t/\beta}$$

and

$$\langle x^2\rangle_{\text{av}} = \langle x\rangle_{\text{av}}^2 + (kT/m\omega^2)(1 - e^{-2\omega^2 t/\beta}).$$

The Langevin equation also predicts[1] a Gaussian for which

$$\langle x\rangle_{\text{av}} = x_0 e^{-\beta t/2}[\cosh(\beta_1 t/2) + \beta\beta_1^{-1}\sinh(\beta_1 t/2)] + 2\beta_1^{-1}u_0 e^{-\beta t/2}\sinh(\beta_1 t/2)$$

$$\langle x^2\rangle = \langle x\rangle_{\text{av}}^2 + (kT/m\omega^2)[1 - e^{-\beta t}(2\beta_1^{-2}\beta^2 \times \sinh^2(\beta_1 t/2) + \beta_1^{-1}\beta\sinh(\beta_1 t) + 1)],$$

where $\beta_1 = (\beta^2 - 4\omega^2)^{\frac{1}{2}}$. For $\beta t \gg 1$ and $\omega \ll \beta$, these expressions reduce to

$$\langle x\rangle_{\text{av}} = [x_0 + O(u_0/\beta)]e^{-\omega^2 t/\beta}[1 + O(\omega^2/\beta^2)]$$

$$\langle x\rangle_{\text{av}} = \langle x\rangle_{\text{av}}^2 + (kT/m\omega^2)[1 - e^{-2\omega^2 t/\beta}(1 + O(\omega^2/\beta^2))].$$

Thus, the modified Langevin equation is correct to first order in $\omega/\beta$ when $t \gg \beta^{-1}$. (The $u_0/\beta$ term is small compared with any macroscopic $x$.)

For $t \gg \beta/\omega^2$, both the modified Langevin equation and the Langevin equation predict that

$$W(x, t; x_0) \to (m\omega^2/2\pi kT)^{\frac{1}{2}} \exp(-m\omega^2 x^2/2kT),$$

which is the equilibrium Boltzmann distribution.

The Smoluchowski equation for this problem is

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial x}\left(\frac{q}{\beta^2}\frac{\partial W}{\partial x} + \frac{\omega^2 x W}{\beta}\right),$$

of which Eq. (18) is a solution.

### The Centrifugal Potential

The apparent acceleration of a particle in a centrifuge rotating with with angular frequency $\omega$ is $\omega^2 x$. Thus the modified Langevin equation is

$$\dot{x} = \beta^{-1}A(t) + \beta^{-1}\omega^2 x,$$

the solution of which is

$$x = x_0 e^{\omega^2 t/\beta} + \beta^{-1}\int_0^t \exp[\omega^2(t - \xi)/\beta]A(\xi)\,d\xi.$$

Application of Eq. (3) in its one-dimensional form gives

$$W(x, t; x_0) = \left(\frac{m\omega^2}{2\pi kT(e^{2\omega^2 t/\beta} - 1)}\right)^{\frac{1}{2}} \times \exp\left(-\frac{m\omega^2(x - x_0 e^{\omega^2 t/\beta})^2}{2kT(e^{2\omega^2 t/\beta} - 1)}\right). \quad (19)$$

This is a Gaussian with

$$\langle x\rangle_{\text{av}} = x_0 e^{\omega^2 t/\beta}$$

and

$$\langle x^2\rangle_{\text{av}} = \langle x\rangle_{\text{av}}^2 + (kT/m\omega^2)(e^{2\omega^2 t/\beta} - 1).$$

The Langevin equation for this problem is

$$\ddot{x} = -\beta\dot{x} + A(t) + \omega^2 x,$$

the solution of which may be obtained by the "variation of parameters" method:

$$x = x_0 e^{-\beta t/2} \cosh(\beta_1 t/2) + \beta_1^{-1}(\beta x_0 + 2u_0)e^{-\beta t/2} \times \sinh(\beta_1 t/2) + 2\beta_1^{-1} \int_0^t e^{-\beta(t-\xi)/2} \times \sinh[\beta_1(t-\xi)/2] A(\xi)\, d\xi,$$

where $\beta_1 = (\beta^2 + 4\omega^2)^{\frac{1}{2}}$. This, combined with Eq. (3), predicts that the probability distribution is a Gaussian with

$$\langle x\rangle_{av} = x_0 e^{-\beta t/2} \cosh(\beta_1 t/2) + \beta_1^{-1}(\beta x_0 + 2u_0)e^{-\beta t/2} \sinh(\beta_1 t/2)$$

and

$$\langle x^2\rangle_{av} = \langle x\rangle_{av}^2 + 2\beta kT(m\beta_1^2)^{-1}[(\beta_1 - \beta)^{-1}e^{(\beta_1-\beta)t} - 2\beta^{-1}(1 - e^{-\beta t}) + (\beta_1 + \beta)^{-1}(1 - e^{-(\beta_1+\beta)t})].$$

When $t \gg \beta/\omega^2$, the modified Langevin equation predicts that $\langle x^2\rangle - \langle x\rangle^2$ increases as $e^{2\omega^2 t/\beta}$, but the Langevin equation predicts $e^{(\beta_1-\beta)t}$. Thus, for large enough times, the two results diverge. However, if

$$t \ll \beta^3\omega^{-4}e^{-2\omega^2 t/\beta}$$

and $\omega \ll \beta$, the Langevin results become

$$\langle x\rangle_{av} = [x_0 + O(u_0/\beta)]e^{\omega^2 t/\beta}[1 + O(\omega^2/\beta^2)],$$

$$\langle x^2\rangle_{av} = \langle x\rangle_{av}^2 + (kT/m\omega^2)[1 + O(\omega^2/\beta^2)] \times \{e^{2\omega^2 t/\beta}[1 + O(\omega^4 t/\beta^3)] - 1 + O(\omega^2/\beta^2)\},$$

which is similar to the results of the modified Langevin equation.

The solution to the modified Langevin equation, Eq. (19), is the exact solution of the Smoluchowski equation for this problem.

## CONCLUSIONS

1. The modified Langevin equation is, in some cases, easier to solve than the other equations which are used to describe Brownian motion. Therefore, it is useful to know under which conditions the equation is valid.

2. Under certain restrictions (given above) about the force acting on a Brownian particle and about the time, the modified Langevin equation is equivalent to the Langevin equation for the calculation of configuration space averages. The conditions given are sufficient, but not necessary, to imply the validity of the modified Langevin equation.

3. When the Smoluchowski equation is valid, the modified Langevin equation is probably valid, and in some situations they give identical results.

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# Comparison of Two Generalizations of Maxwell's Equations Involving Creation of Charge

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A comparison is made of the Lyttleton–Bondi, and the Watson theories for the electromagnetic fields produced when charge is created. It is shown that, except when dimensions of the order of the radius of the Universe are involved, the difference is negligible and that consequently the Watson theory, being mathematically more simple, is the better.

## 1. INTRODUCTION

CLASSICALLY, Maxwell's equations of the electric field assume the conservation of charge.[1] However, the hypotheses have been made that the absolute values of the charges of the proton and electron are not equal, and that there is creation of hydrogen atoms (and hence charge). Two different generalizations of Maxwell's equations have been put forward which discuss this.[2,3] One of the generalizations is due to Lyttleton and Bondi,[2] and the other to Watson.[4]

In both theories, two of Maxwell's equations remain unchanged:

$$\nabla \times \mathbf{E} + \partial \mathbf{B}/\partial t = 0, \tag{1.1}$$

$$\nabla \cdot \mathbf{B} = 0. \tag{1.2}$$

The solution to these is given by

$$\mathbf{E} = -\nabla V - \partial \mathbf{A}/\partial t, \qquad \mathbf{B} = \nabla \times \mathbf{A}, \tag{1.3}$$

$\mathbf{A}$ and $V$ being the vector and scalar potentials, respectively. The charge creation is however introduced in different ways. In the Lyttleton–Bondi theory, the generalization is made by feeding the potentials back into the remaining Maxwell equations which take the form

$$\nabla \times \mathbf{H} - \partial \mathbf{D}/\partial t = \mathbf{J} - (1/\mu_0 l^2)\mathbf{A}, \tag{1.4}$$

$$\nabla \cdot \mathbf{D} = \rho - (\epsilon_0/l^2)V, \tag{1.5}$$

where $l$ is of the dimensions length and is suggested by Lyttleton and Bondi to be of the order of the radius of the Universe. [This is the reason for the negative signs on the right-hand sides of Eqs. (1.4) and (1.5)]. On the other hand, Watson's modification introduces a new potential $N$, and the modification is given by

$$\nabla \times \mathbf{H} - \partial \mathbf{D}/\partial t = \mathbf{J} - \nabla N, \tag{1.6}$$

$$\nabla \cdot \mathbf{D} = \rho + \mu_0 \epsilon_0 (\partial N/\partial t). \tag{1.7}$$

It will now be convenient to discuss the implications of these two formulations and make comparisons of the fields which would be generated by the creation of a charge at zero time at the origin. Clearly, any charge creation can be obtained from this. Similarly, the fields associated with an elementary current creation will be calculated.

## 2. THE LYTTLETON–BONDI FORMULATION

It is fairly easily seen[5] that

$$\nabla^2 \mathbf{A} - \frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} - \frac{\mathbf{A}}{l^2} = -\mu_0 \mathbf{J}, \tag{2.1}$$

$$\nabla^2 V - \frac{1}{c^2}\frac{\partial^2 V}{\partial t^2} - \frac{V}{l^2} = -\frac{\rho}{\epsilon_0}, \tag{2.2}$$

and the creation rate of charge density is given by

$$\nabla \cdot \mathbf{J} + \frac{\partial \rho}{\partial t} = \frac{1}{\mu_0 l^2}\left(\nabla \cdot \mathbf{A} + \frac{1}{c^2}\frac{\partial V}{\partial t}\right). \tag{2.3}$$

Consider now the creation of a charge $Q$ at the origin at time $t = 0$. The equation governing this is

$$\nabla^2 V - \frac{1}{c^2}\frac{\partial^2 V}{\partial t^2} - \frac{V}{l^2} = \frac{-Q\delta(\mathbf{r})H(t)}{\epsilon_0}, \tag{2.4}$$

$\delta(\mathbf{r})$ being the three-dimensional delta function with pole at the origin, and $H(t)$ the Heaviside unit function. Clearly, the only field this will generate will be $E_r = -\partial V/\partial r$.

The Green's function associated with Eqs. (2.1) and (2.2) is the solution of

$$\nabla^2 G - \frac{1}{c^2}\frac{\partial^2 G}{\partial t^2} - \frac{1}{l^2}G = \delta(\mathbf{r})\delta(t), \tag{2.5}$$

[1] J. A. Stratton, *Electromagnetic Theory* (McGraw-Hill Book Company, Inc., New York, 1941), p. 6.
[2] R. A. Lyttleton and H. Bondi, Proc. Roy. Soc. (London), **A252**, 313 (1959).
[3] Ll. G. Chambers, Nature **191**, 262 (1961).
[4] W. H. Watson, *Proceedings of the Second Symposium on Applied Mathematics* (American Mathematics Society, 1950), p. 49.
[5] Reference 1, p. 24.

and is[6]

$$-\frac{1}{4\pi r}\left\{\delta\left(t-\frac{r}{c}\right)-H\left(t-\frac{r}{c}\right)\frac{r}{l}\frac{J_1[(c/l)(t^2-r^2/c^2)^{\frac{1}{2}}]}{(t^2-r^2/c^2)^{\frac{1}{2}}}\right\}. \tag{2.6}$$

Thus the solution of Eq. (2.4) is

$$\frac{Q}{4\pi\epsilon_0 r}\left\{H\left(t-\frac{r}{c}\right)\left[1-\frac{r}{l}\int_{r/c}^{t}\frac{J_1[(c/l)(\tau^2-r^2/c^2)^{\frac{1}{2}}]}{(\tau^2-r^2/c^2)^{\frac{1}{2}}}d\tau\right]\right\}, \tag{2.7}$$

which may be rewritten in the form

$$\frac{Q}{4\pi\epsilon_0 r}H\left(t-\frac{r}{c}\right)-\frac{Q}{4\pi\epsilon_0 l}H\left(t-\frac{r}{c}\right)\int_{r/c}^{t}\frac{J_1[(c/l)(\tau^2-r^2/c^2)^{\frac{1}{2}}]}{(\tau^2-r^2/c^2)^{\frac{1}{2}}}d\tau.$$

The associated electric field is

$$\begin{aligned}E_r &= -\partial V/\partial r\\ &= \frac{Q}{4\pi\epsilon_0 r^2}H\left(t-\frac{r}{c}\right)+\frac{Q}{4\pi\epsilon_0 cr}\delta\left(t-\frac{r}{c}\right)\\ &\times\frac{-Q}{4\pi\epsilon_0 cl}\delta\left(t-\frac{r}{c}\right)\int_{r/c}^{t}\frac{J_1[(c/l)(\tau^2-r^2/c^2)^{\frac{1}{2}}]}{(\tau^2-r^2/c^2)^{\frac{1}{2}}}d\tau\\ &+\frac{-Q}{4\pi\epsilon_0 l}H\left(t-\frac{r}{c}\right)\left\{-\frac{1}{c}\lim_{\tau\to r/c}\frac{J_1[(c/l)(\tau^2-r^2/c^2)^{\frac{1}{2}}]}{(\tau^2-r^2/c^2)^{\frac{1}{2}}}\right.\\ &\left.+\int_{r/c}^{t}\frac{\partial}{\partial r}\left[\frac{J_1[(c/l)(\tau^2-r^2/c^2)^{\frac{1}{2}}]}{(\tau^2-r^2/c^2)^{\frac{1}{2}}}\right]d\tau\right\}.\end{aligned} \tag{2.8}$$

The third term clearly vanishes, and the limit in the fourth term is $\frac{1}{2}(c/l)$.

Also, $(d/dx)\{(1/x)J_1(\alpha x)\} = (-\alpha/x)J_2(\alpha x)$. The integral in the last term thus assumes the form

$$\begin{aligned}&\int_{r/c}^{t}\frac{\partial}{\partial r}\left(\tau^2-\frac{r^2}{c^2}\right)^{\frac{1}{2}}\cdot-\frac{c}{l}\frac{J_2[(c/l)(\tau^2-r^2/c^2)^{\frac{1}{2}}]}{(\tau^2-r^2/c^2)^{\frac{1}{2}}}d\tau\\ &=\int_{r/c}^{t}-\frac{r/c^2}{(\tau^2-r^2/c^2)^{\frac{1}{2}}}\cdot-\frac{c}{l}\frac{J_2[(c/l)(\tau^2-r^2/c^2)^{\frac{1}{2}}]}{(\tau^2-r^2/c^2)^{\frac{1}{2}}}d\tau.\end{aligned}$$

Thus the electric field becomes

$$\frac{Q}{4\pi\epsilon_0 r^2}H\left(t-\frac{r}{c}\right)+\frac{Q}{4\pi\epsilon_0 cr}\delta\left(t-\frac{r}{c}\right)+\frac{Q}{8\pi\epsilon_0 l^2}H\left(t-\frac{r}{c}\right)-\frac{Q}{4\pi\epsilon_0 cl^2}H\left(t-\frac{r}{c}\right)\int_{r/c}^{t}\frac{J_2[(c/l)(\tau^2-r^2/c^2)^{\frac{1}{2}}]}{(\tau^2-r^2/c^2)}d\tau. \tag{2.9}$$

The third term is of order $l^{-2}$, and the fourth of order $l^{-4}$. The creation of current may be dealt with in a similar manner. Consider the current defined by

$$\mathbf{J} = m\delta(\mathbf{r})\delta(t)\mathbf{k}, \qquad \rho = 0. \tag{2.10}$$

This represents a current density in the $z$ direction which vanishes everywhere except at the origin and at zero time. ($m$ is of the dimensions of electric dipole.) Any arbitrary current creation can be obtained by integration of fields derived from current densities of this type.

The only one of Eqs. (2.1) and (2.2) which is involved is

$$\nabla^2 A_z-\frac{1}{c^2}\frac{\partial^2 A_z}{\partial t^2}-\frac{1}{l^2}A_z = -\mu_0 m\delta(\mathbf{r})\delta(t), \tag{2.11}$$

where $A_z = -\mu_0 mG$. The associated fields are

$$\mathbf{B} = \nabla\times\mathbf{A}, \qquad \mathbf{E} = -\partial\mathbf{A}/\partial t.$$

Writing $r^2 = z^2+\tilde{\omega}^2$, it follows that the only fields which are nonzero are (if $\tilde{\omega}$, $\phi$, $z$ are cylindrical coordinates)

$$\begin{aligned}H_\phi &= m\frac{\partial G}{\partial\tilde{\omega}} = m\frac{\partial\tilde{\omega}}{\partial r}\frac{\partial G}{\partial r} = m\frac{\tilde{\omega}}{r}\frac{\partial G}{\partial r}\\ &= m\sin\theta\frac{\partial G}{\partial r}\text{ in spherical coordinates,}\end{aligned} \tag{2.12}$$

and

$$E_z = \mu_0 m\frac{\partial G}{\partial t}. \tag{2.13}$$

Clearly, Eq. (2.12) can be written as

$$\begin{aligned}H_\phi &= m\sin\theta\frac{\partial}{\partial r}\left[-\frac{1}{4\pi r}\delta\left(t-\frac{r}{c}\right)\right]\\ &+\frac{m\sin\theta}{4\pi l}\frac{\partial}{\partial r}\left\{H\left(t-\frac{r}{c}\right)\frac{J_1[(c/l)(t^2-r^2/c^2)^{\frac{1}{2}}]}{(t^2-r^2/c^2)^{\frac{1}{2}}}\right\}\\ &= +\frac{m\sin\theta}{4\pi r^2}\delta\left(t-\frac{r}{c}\right)+\frac{m\sin\theta}{4\pi cr}\delta'\left(t-\frac{r}{c}\right)\\ &-\frac{m\sin\theta}{4\pi l}\frac{1}{c}\delta\left(t-\frac{r}{c}\right)\frac{J_1[(c/l)(t^2-r^2/c^2)^{\frac{1}{2}}]}{(t^2-r^2/c^2)^{\frac{1}{2}}}\\ &+\frac{m\sin\theta}{4\pi l}H\left(t-\frac{r}{c}\right)\frac{\partial}{\partial r}[(t^2-r^2/c^2)^{\frac{1}{2}}]\\ &\times-\frac{c}{l}\frac{J_2[(c/l)(t^2-r^2/c^2)^{\frac{1}{2}}]}{(t^2-r^2/c^2)^{\frac{1}{2}}}\\ &= \frac{m\sin\theta}{4\pi r^2}\delta\left(t-\frac{r}{c}\right)+\frac{m\sin\theta}{4\pi rc}\delta'\left(t-\frac{r}{c}\right)\\ &-\frac{m\sin\theta}{8\pi l^2}\delta\left(t-\frac{r}{c}\right)\\ &+\frac{m\sin\theta}{4\pi l^2 c}\frac{J_2[(c/l)(t^2-r^2/c^2)^{\frac{1}{2}}]}{(t^2-r^2/c^2)}H\left(t-\frac{r}{c}\right).\end{aligned} \tag{2.14}$$

Here again the third and fourth terms are of order $l^{-2}$, and $l^{-4}$, respectively.

The associated value of $E_z$ is given by

$$E_z = \mu_0 m\frac{\partial}{\partial t}\left[\frac{-\delta(t-r/c)}{4\pi r}\right]+\frac{\mu_0 m}{4\pi l}\frac{\partial}{\partial t}\left\{H\left(t-\frac{r}{c}\right)\frac{J_1[(c/l)(t^2-r^2/c^2)^{\frac{1}{2}}]}{(t^2-r^2/c^2)^{\frac{1}{2}}}\right\}$$

[6] P. M. Morse and H. Feshbach, *Methods of Mathematical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1.

$$= -\mu_0 m \frac{\delta'(t - r/c)}{4\pi r}$$

$$+ \frac{\mu_0 m}{4\pi l} \delta\left(t - \frac{r}{c}\right) \frac{J_1[(c/l)(t^2 - r^2/c^2)^{\frac{1}{2}}]}{(t^2 - r^2/c^2)^{\frac{1}{2}}}$$

$$+ \frac{\mu_0 m}{4\pi l} H\left(t - \frac{r}{c}\right) \frac{\partial}{\partial t} \frac{J_1[(c/l)(t^2 - r^2/c^2)^{\frac{1}{2}}]}{(t^2 - r^2/c^2)^{\frac{1}{2}}}$$

$$= (-\mu_0 m/4\pi r)\delta'(t - r/c)$$

$$- (\mu_0 m/8\pi l^2) c\delta(t - r/c)$$

$$+ (\mu_0 m/4\pi l) H(t - r/c)$$

$$\times -\frac{c}{l} \frac{J_2[(c/l)(t^2 - r^2/c^2)^{\frac{1}{2}}]}{(t^2 - r^2/c^2)^{\frac{1}{2}}} \frac{t}{(t^2 - r^2/c^2)^{\frac{1}{2}}}$$

$$= -(\mu_0 m/4\pi r)\delta'(t - r/c)$$

$$+ (\mu_0 mc/8\pi l^2)\delta(t - r/c)$$

$$- \frac{\mu_0 mc}{4\pi l^2} H\left(t - \frac{r}{c}\right) \frac{t}{(t^2 - r^2/c^2)}$$

$$\times J_2[(c/l)(t^2 - r^2/c^2)^{\frac{1}{2}}]. \tag{2.15}$$

Here the second and third terms are, respectively, of order $l^{-2}$, and $l^{-4}$.

### 3. THE WATSON FORMULATION

If charge is conserved, Maxwell's equations lead to

$$\nabla^2 \mathbf{E} - \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2} = \mu_0 \frac{\partial \mathbf{J}}{\partial t} + \frac{\nabla \rho}{\epsilon_0}, \tag{3.1}$$

and

$$\nabla^2 \mathbf{H} - \mu_0 \epsilon_0 (\partial^2 \mathbf{H}/\partial t^2) = -\nabla \times \mathbf{J}. \tag{3.2}$$

Clearly, replacing $\mathbf{J}$ by $\mathbf{J} - \nabla N$, and $\rho$ by $\rho + \mu_0 \epsilon_0 (\partial N/\partial t)$, these equations retain the same form, and so it follows that any field due to nonconservation of charge must satisfy

$$\nabla^2 \mathbf{E} - \mu_0 \epsilon_0 (\partial^2 \mathbf{E}/\partial t^2) = 0,$$

$$\nabla^2 \mathbf{H} - \mu_0 \epsilon_0 (\partial^2 \mathbf{H}/\partial t^2) = 0.$$

That this will be the case follows also from the following.

From Eqs. (1.6) and (1.7) it is possible to write

$$\nabla \cdot \mathbf{J} + \partial \rho/\partial t$$

$$= \nabla^2 N - \mu_0 \epsilon_0 (\partial^2 N/\partial t^2) = Q\delta(\mathbf{r})\, \delta(t) \tag{3.3}$$

if a charge $Q$ is created at the origin at zero time. Solving,

$$N = -(Q/4\pi r)\delta(t - r/c). \tag{3.4}$$

From Eq. (1.7), the field due to $N$ is given by

$$\epsilon_0 \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 E_r) = \mu_0 \epsilon_0 \frac{\partial N}{\partial t}. \tag{3.5}$$

Integrating and remembering that $E$ must be zero at infinity,

$$E_r = \frac{Q}{4\pi\epsilon_0 r^2} \cdot H\left(t - \frac{r}{c}\right) + \frac{Q}{4\pi\epsilon_0 rc} \cdot \delta\left(t - \frac{r}{c}\right). \tag{3.6}$$

Considering now an elementary current creation as indicated in Eq. (2.10),

$$\mathbf{J} = m\delta(\mathbf{r})\delta(t)\mathbf{k}, \qquad \rho = 0, \tag{3.7}$$

$$\nabla^2 N - \mu_0 \epsilon_0 \frac{\partial^2 N}{\partial t^2} = \frac{\partial J_z}{\partial z} = m\delta(t) \frac{\partial}{\partial z} \delta(\mathbf{r}).$$

It follows that

$$N = \frac{-m}{4\pi} \frac{\partial}{\partial z} \left[\frac{\delta(t - r/c)}{r}\right]. \tag{3.8}$$

The appropriate solution of Eqs. (1.1), (1.2), (1.6), and (1.7) is given by

$$\mathbf{H} = H\boldsymbol{\phi}, \qquad \mathbf{E} = E\mathbf{k},$$

$$\epsilon_0(\partial E/\partial z) = \mu_0 \epsilon_0 (\partial N/\partial t),$$

whence

$$E = -(\mu_0 m/4\pi)[\delta'(t - r/c)/r]. \tag{3.9}$$

In an exactly similar manner,

$$H = (m \sin\theta/4\pi r^2)\delta(t - r/c)$$

$$+ (m \sin\theta/4\pi r)\delta'(t - r/c). \tag{3.10}$$

### 4. CONCLUSION

It will be seen that, in both cases, the difference between the fields obtained is of order $l^{-2}$ at the most. Any fields which involve charge creation may be calculated by integration of the fields of the type considered, and so the statement is true more generally. Now if $l$ is of the order of the radius of the Universe, this difference is negligibly small, it would not be possible to measure it, and so for all practical purposes the two formulations would be equivalent. (This of course would not be true when the system is of the order of the size of the Universe as in the origin Lyttleton–Bondi paper.[2]) The difference between the fields does, in fact, represent a tail of negligible proportions.

Because of the equivalence of the fields produced on the two different formulations, it is desirable to use the simpler formulation, and this is the Watson formulation, since the differential equation involved —the wave equation—is much simpler than that associated with the Lyttleton–Bondi formulation, namely the Proca equation. Thus, for any system on a scale smaller than that of the Universe, the Watson formulation is the better.

# Existence and Uniqueness Theorems for the Neutron Transport Equation*

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In an attempt to understand the conditions under which the neutron transport equation has solutions, and the properties of those solutions, a number of existence and uniqueness theorems are proved. One finds that the properties of the solution are closely related to the boundedness of the source as well as to certain velocity-space integrals of the scattering kernel. Both time-dependent and time-independent equations are considered as are also the time-dependent and time-independent adjoint equations. Although only a very few of all possible existence and uniqueness theorems for these equations are considered here, the work may serve as a guide to the treatment of similar problems.

## I. INTRODUCTION

VARIOUS theorems concerning the existence and uniqueness of solution to the neutron transport equation have appeared in the literature. For example, Case[1] has proved uniqueness for the one-speed, time-dependent equation under the assumption that the kernel is rotationally invariant. He has, in addition, shown that under the same assumptions the solution of the time-*independent* equation is unique if $c(\mathbf{r})$, the mean number of neutrons emitted per collision, is everywhere less than one. Olhoeft[2] has considered the more general velocity-dependent case, and has shown, subject to the same restriction on $c$, that a unique, integrable solution exists for the time-independent equation. Davison[3] has made some rather general remarks concerning existence and uniqueness for the time-dependent case, but has only outlined the methods of proof and has actually said little about the restrictions which must be imposed in order that the theorems be true.

Basically, the situation is the following: There are a number of possible restrictions which one can imagine might be applied to the cross sections and sources appearing in the neutron transport equation. For certain of these restrictions it is possible to prove that continuous solutions exist; for other sets of restrictions the solutions may not be continuous but still integrable functions of one or more of the independent variables involved [i.e., position, velocity, and (in the time-dependent case) time]. For other restrictions, it may be impossible to prove anything. We have investigated a large number of possible restrictions which might reasonably be imposed upon the cross sections and sources, and investigated the existence of unique solutions for each case. In this way, we have tried to bring some order into the chaos of "obvious" or partially proved results which at the present exist in the literature.

In addition, we consider not only the transport equation but the time-dependent and time-independent "adjoint equations," and investigate the sufficient conditions that unique solutions exist for those equations. It turns out that there are many cases in which existence and uniqueness theorems can be proved for one or the other, but not both.

In Sec. II of this paper, we convert the transport and adjoint equations to integral equations in the usual manner. Then, in Sec. III, we discuss the restrictions on the sources and cross sections which will, for physical reasons, be applied in all cases.

Then, in Secs. IV and V we consider various existence and uniqueness theorems for the time-dependent transport and adjoint equations. In Sec. VI we consider theorems for the time-independent equations (both transport and adjoint) and finally, in Sec. VII, we discuss certain "by-products" of the theorems—a formula for the minimum critical size of a reactor and a proof that the time-dependence of the solutions of the time-dependent equations must obey certain restrictions.

We have made no attempt to be comprehensive

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[1] K. M. Case, Rev. Mod. Phys. 29, 651 (1957).

[2] Jack E. Olhoeft, "The Doppler Effect for Non-Uniform Temperatures," University of Michigan Ph.D. Thesis (1962).

[3] B. Davison, *Neutron Transport Theory* (Oxford University Press, London, 1957).

in our treatment of the existence and uniqueness problem. Indeed, one can imagine virtually an infinite number of possible theorems similar to those which we prove. However, we have presented some of those which we feel have the most intrinsic interest and, in addition, demonstrate well the method of proof. In this way, if any of the conditions which we consider are not met in a particular problem, our work may serve as a guide to the correct treatment.

## II. INTEGRAL EQUATION FORMULATION

### A. The Transport Equations

The time-dependent transport equation is

$$\partial\psi(\mathbf{r}, \mathbf{v}, t)/\partial t + v(\boldsymbol{\Omega}\cdot\nabla + \sigma(\mathbf{r}, \mathbf{v}))\psi(\mathbf{r}, \mathbf{v}, t) = q(\mathbf{r}, \mathbf{v}, t) + \int v'\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})\psi(\mathbf{r}, \mathbf{v}', t)\, d^3v', \tag{1a}$$

while, in the stationary limit, we have

$$v(\boldsymbol{\Omega}\cdot\nabla + \sigma(\mathbf{r}, \mathbf{v}))\psi(\mathbf{r}, \mathbf{v}) = q(\mathbf{r}, \mathbf{v}) + \int v'\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})\psi(\mathbf{r}, \mathbf{v}')\, d^3v'. \tag{1b}$$

Here $\psi$ is the neutron angular density (i.e., the one-particle distribution function); $\mathbf{v} = v\boldsymbol{\Omega}$ is the neutron velocity; $\sigma(\mathbf{r}, \mathbf{v})$ is the total cross section, and the kernel $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ is the cross section for a neutron of velocity $\mathbf{v}'$ to be emitted into $d^3v$ about $\mathbf{v}$.

Equation (1) may be converted into intergal equations in the usual way, i.e., by introducing the Green's function of the left-hand side. This Green's function is well known.[4] We obtain for the integral equation equivalent to (1a)

$$\psi(\mathbf{r}, \mathbf{v}, t) = Q(\mathbf{r}, \mathbf{v}, t) + \int_0^t dt' \int d^3v'v'\sigma(\mathbf{r} - \mathbf{v}(t - t'), \mathbf{v}' \to \mathbf{v}) \times \psi(\mathbf{r} - \mathbf{v}(t - t''), \mathbf{v}', t') \times \exp\left[-\int_{t'}^{t} v\sigma(\mathbf{r} - \mathbf{v}(t - t''), \mathbf{v})\, dt''\right], \tag{2a}$$

where

$$Q(\mathbf{r}, \mathbf{v}, t) = \psi(\mathbf{r} - \mathbf{v}t, \mathbf{v}, 0) \times \exp\left[-\int_0^t v\sigma(\mathbf{r} - \mathbf{v}(t - t'), \mathbf{v})\, dt'\right] + \int_0^t dt' q(\mathbf{r} - \mathbf{v}(t - t'), \mathbf{v}, t') \times \exp\left[-\int_{t'}^{t} v\sigma(\mathbf{r} - \mathbf{v}(t - t''), \mathbf{v})\, dt''\right]. \tag{2b}$$

Actually, we shall prove theorems involving the esistence and uniqueness of solutions within a given volume of space $V$ bounded by a surface $S$ when the incoming (or, in the case of the adjoint equations, the outgoing) angular distribution is specified on $S$. The simplest way to modify Eq. (2) to describe this situation is to define $q(\mathbf{r}, \mathbf{v}, t)$, $\psi(\mathbf{r}, \mathbf{v}, 0)$, $\sigma(\mathbf{r}, \mathbf{v})$, and $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ to vanish for $\mathbf{r} \notin V$. Then the specified incident angular distribution $\psi_1(\mathbf{r}_s, \mathbf{v}, t)$ is replaced by a surface source $q_s(\mathbf{r}_s, \mathbf{v}, t)$ on $S$ in the usual manner:[4]

$$q_s(\mathbf{r}_s, \mathbf{v}, t) = v\,|\boldsymbol{\Omega}\cdot\mathbf{n}_0|\,\psi_i(\mathbf{r}_s, \mathbf{v}, t), \quad \boldsymbol{\Omega}\cdot\mathbf{n}_0 < 0, \quad t > 0, \quad = 0 \quad \text{otherwise}, \tag{3}$$

where $\mathbf{n}_0$ is the outward normal to $S$. Then Eq. (2) still applies [understanding the redefinitions of $q$, $\psi$, $\sigma$, and $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ mentioned above] with an additional term $Q_s$ added to $Q$, Eq. (2b), to account for the surface source:

$$Q_s = \frac{1}{v}\, q_s(\mathbf{r}_s, \mathbf{v}, t - R_s/v) \times \exp\left[-\alpha(\mathbf{r}, \mathbf{r} - R_s\boldsymbol{\Omega}, \mathbf{v})\right]. \tag{4}$$

Here $\alpha$ is the usual optical path

$$\alpha(\mathbf{r}, \mathbf{v}', \mathbf{v}) = \int_0^R ds\sigma\left(\mathbf{r} - s\frac{\mathbf{R}}{R}\right), \tag{5}$$

where $R_s$ is the distance from $\mathbf{r}$ to the surface $S$ along the direction $-\Omega$ (See Fig. 1). Note: $R_s = R_s(\mathbf{r}, \boldsymbol{\Omega})$.

Equation (2), thus modified, is the general integral equation formulation of the time-dependent neutron transport problem with which we shall be concerned. It is convenient to rewrite it in the somewhat more tractable form:

$$\psi(\mathbf{r}, \mathbf{v}, t) = Q'(\mathbf{r}, \mathbf{v}, t) + K\psi(\mathbf{r}, \mathbf{v}, t), \tag{6a}$$

where $K$ is the integral operator

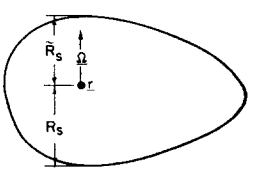


FIG. 1.

[4] K. M. Case, F. de Hoffmann, and G. Placzek, *Introduction to the Theory of Neutron Diffusion* (U. S. Government Printing Office, Washington, D. C., 1953).

$$Kf(\mathbf{r}, \mathbf{v}, t)$$
$$= \int_0^t dt' \int d^3r' \int d^3v'\ \delta(\mathbf{r}' - \mathbf{r} + \mathbf{v}(t - t'))$$
$$\times \exp\left[-\int_{t'}^t v\sigma(\mathbf{r} - \mathbf{v}(t - t''), \mathbf{v})\, dt''\right]$$
$$\times v'\sigma(\mathbf{r}', \mathbf{v}' \to v)f(\mathbf{r}', \mathbf{v}', t'), \tag{6b}$$

and

$$Q'(\mathbf{r}, \mathbf{v}, t) = Q(\mathbf{r}, \mathbf{v}, t) + Q_s(\mathbf{r}, \mathbf{v}, t). \tag{6c}$$

The integral equation formulation of the time-independent transport equation (1b) is obtained in just the same way, i.e., by introducing the Green's function of the left side of Eq. (1b). We obtain

$$\phi(\mathbf{r}, \mathbf{v}) = Q'(\mathbf{r}, \mathbf{v}) + \Lambda\phi(\mathbf{r}, \mathbf{v}), \tag{7a}$$

where $\Lambda$ is the integral operator

$$\Lambda f(\mathbf{r}, \mathbf{v}) = \int_0^{R_s} dR \int d^3r' \int d^3v'\ \delta(\mathbf{r}' - \mathbf{r} + R\boldsymbol{\Omega})$$
$$\times \exp\left[-\alpha(\mathbf{r}, \mathbf{r}', \mathbf{v})\right]v'\sigma(\mathbf{r}', \mathbf{v}' \to \mathbf{v})f(\mathbf{r}', \mathbf{v}'), \tag{7b}$$
$$Q'(\mathbf{r}, \mathbf{v}) = q_s(\mathbf{r}_s, \mathbf{v}) \exp\left[-\alpha(\mathbf{r}, \mathbf{r} - R_s\boldsymbol{\Omega}, \mathbf{v})\right]$$
$$+ \int_0^{R_s} q(\mathbf{r} - R\boldsymbol{\Omega}, \mathbf{v}) \exp\left[-\alpha(\mathbf{r}, \mathbf{r} - R\boldsymbol{\Omega}, \mathbf{v})\right] dR, \tag{7c}$$

and

$$\phi(\mathbf{r}, \mathbf{v}) = v\psi(\mathbf{r}, \mathbf{v}). \tag{7d}$$

Again we mention that the cross sections and sources have been defined to vanish for $\mathbf{r} \notin V$ (or for $t < 0$).

### B. The Adjoint Equations

The time-dependent adjoint equation is defined to be

$$\frac{\partial\tilde{\psi}(\mathbf{r}, \mathbf{v}, t)}{\partial t} + v(-\boldsymbol{\Omega}\cdot\nabla + \sigma(\mathbf{r}, \mathbf{v}))\tilde{\psi}(\mathbf{r}, \mathbf{v}, t)$$
$$= \tilde{q}(\mathbf{r}, \mathbf{v}, t) + v\int d^3v'\sigma(\mathbf{r}, \mathbf{v} \to \mathbf{v}')\tilde{\psi}(\mathbf{r}, \mathbf{v}'), \tag{8a}$$

while the time-independent adjoint equation is

$$v(-\boldsymbol{\Omega}\cdot\nabla + \sigma(\mathbf{r}, \mathbf{v}))\tilde{\psi}(\mathbf{r}, \mathbf{v}) = \tilde{q}(\mathbf{r}, \mathbf{v})$$
$$+ v\int d^3v'\sigma(\mathbf{r}, \mathbf{v} \to \mathbf{v}')\tilde{\psi}(\mathbf{r}, \mathbf{v}'). \tag{8b}$$

The adjoint of a solution of Eqs. (1a) and (1b) will be taken to be the solution of Eqs. (8a) and (8b) subject to appropriate boundary conditions.

These boundary conditions are that the *outgoing* density on $S$, $\psi_0(\mathbf{r}_s, \mathbf{v}, t)$, rather than the incoming, will be specified. As before, we replace the boundary conditions by a surface source:

$$\tilde{q}_s(\mathbf{r}_s, \mathbf{v}, t)$$
$$= v\,|\boldsymbol{\Omega}\cdot\mathbf{n}_0|\,\psi_0(\mathbf{r}_s, \mathbf{v}, t), \quad \boldsymbol{\Omega}\cdot\mathbf{n}_0 > 0, \quad t > 0,$$
$$= 0 \quad \text{otherwise.} \tag{9}$$

We now convert Eqs. (8) into integral equations just as for the case of transport equations, obtaining for the time-dependent equation

$$\tilde{\psi}(\mathbf{r}, \mathbf{v}, t) = \tilde{Q}'(\mathbf{r}, \mathbf{v}, t) + \tilde{K}\tilde{\psi}(\mathbf{r}, \mathbf{v}, t), \tag{10a}$$

where $\tilde{K}$ is the integral operator

$$\tilde{K}f(\mathbf{r}, \mathbf{v}, t)$$
$$= v\int_0^t dt' \int d^3v' \int d^3v'\ \delta(\mathbf{r}' - \mathbf{r} - \mathbf{v}(t - t'))$$
$$\times \exp\left[-\int_{t'}^t v\sigma(\mathbf{r} + \mathbf{v}(t - t''), \mathbf{v})\, dt''\right]$$
$$\times \sigma(\mathbf{r}', \mathbf{v} \to \mathbf{v}')f(\mathbf{r}', \mathbf{v}', t'), \tag{10b}$$

and

$$\tilde{Q}'(\mathbf{r}, \mathbf{v}, t) = \tilde{\psi}(\mathbf{r} + \mathbf{v}t, \mathbf{v}, 0)$$
$$\times \exp\left[-\int_0^t v\sigma(\mathbf{r} + \mathbf{v}(t - t''), \mathbf{v})\, dt''\right]$$
$$+ \int_0^t dt'\tilde{q}(\mathbf{r} + \mathbf{v}(t - t'), \mathbf{v}, t')$$
$$\times \exp\left[-\int_{t'}^t v\sigma(\mathbf{r} + \mathbf{v}(t - t''), \mathbf{v})\, dt''\right]$$
$$+ (1/v)q_s(\mathbf{r}_s, \mathbf{v}, t - \tilde{R}_s/v)$$
$$\times \exp\left[-\alpha(\mathbf{r}, \mathbf{r} + \tilde{R}_s\boldsymbol{\Omega}, \mathbf{v})\right]. \tag{10c}$$

As before, cross sections and the initial distribution are defined to vanish for $\mathbf{r} \notin V$. Also, $\tilde{R}_s = \tilde{R}_s(\mathbf{r}, \boldsymbol{\Omega})$ is the distance from $\mathbf{r}$ to the surface along the direction $+\boldsymbol{\Omega}$ (rather than along the direction $-\boldsymbol{\Omega}$ as in the case of the transport equation). See Fig. 1.

For the time-*independent* adjoint equation we obtain similarly

$$\tilde{\psi}(\mathbf{r}, \mathbf{v}) = (1/v)\tilde{Q}'(\mathbf{r}, \mathbf{v}) + \tilde{\Lambda}\tilde{\psi}(\mathbf{r}, \mathbf{v}), \tag{11a}$$

where $\tilde{\Lambda}$ is defined by

$$\tilde{\Lambda}f(\mathbf{r}, \mathbf{v}) = \int_0^{\tilde{R}_s} dR \int d^3r' \int d^3v'\ \delta(\mathbf{r}' - \mathbf{r} - R\boldsymbol{\Omega})$$
$$\times \exp\left[-\alpha(\mathbf{r}, \mathbf{r}', \mathbf{v})\right]\sigma(\mathbf{r}', \mathbf{v} \to \mathbf{v}')f(\mathbf{r}', \mathbf{v}'), \tag{11b}$$

and

$$\tilde{Q}'(\mathbf{r}, \mathbf{v}) = \tilde{q}_s(\mathbf{r}_s, \mathbf{v}) \exp [-\alpha(\mathbf{r}, \mathbf{r} + \tilde{R}_s\boldsymbol{\Omega}, \mathbf{v})] + \int_0^{\tilde{R}_s} \tilde{q}(\mathbf{r} + R\boldsymbol{\Omega}, \mathbf{v}) \exp [-\alpha(\mathbf{r}, \mathbf{r} + R\boldsymbol{\Omega}, \mathbf{v})]\, dR. \quad (11c)$$

## III. BASIC DEFINITIONS AND ASSUMPTIONS

In all of our subsequent discussions we shall assume that the source functions $Q'(\mathbf{r}, \mathbf{v}, t)$ and $\tilde{Q}'(\mathbf{r}, \mathbf{v}, t)$ as well as the cross sections $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$, and $\sigma(\mathbf{r}, \mathbf{v})$, obey certain physically reasonable conditions.

(1) $Q'$ and $\tilde{Q}'$ are positive for all values of their arguments.

(2) Either $Q'$ and $\tilde{Q}'$ are bounded or they can be written as the product of bounded functions multiplied by delta functions in one or more of their arguments.

(3) There exists a $v_0 < \infty$ such that for $|\mathbf{v}| > v_0$, $Q'$ and $\tilde{Q}'$ vanish identically.

(4) There exists a $v_1 < \infty$ such that $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) \equiv 0$, for $v > v' > v_1$.

Assumptions (3) and (4) permit us to avoid any difficulties that the infinite range of the velocity variable might otherwise introduce since together they imply that there are no neutrons present with speeds greater than $v_m = \max(v_0, v_1)$. Then the integrals over $v'$ in any of the integral equations can be written as

$$\int d^3v' \to \int d\boldsymbol{\Omega}' \int_0^{v_m} v'^2\, dv'. \quad (12)$$

These restrictions can actually be relaxed to some extent; we might assume that $Q'$ and $\tilde{Q}'$ go to zero sufficiently rapidly as $v \to \infty$ that, if other restrictions are obeyed, the infinite range of $v$ need not cause any trouble. However, assumptions (3) and (4) are physically reasonable, and so we shall make no attempts to relax them.

(5) $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ can be written in the form

$$\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) = \sum N_i(\mathbf{r}) \sigma_i(\mathbf{v}' \to \mathbf{v}), \quad (13)$$

where $N_i(\mathbf{r})$ is bounded. [Actually $N_i(\mathbf{r})$ represents a density of nuclei, and $\sigma_i$ is a microscopic cross-section, so we are merely assuming that there are no infinite concentrations of atoms present in the systems that we consider.]

(6) The cross-section $\sigma(\mathbf{r}, \mathbf{v})$ can be written in the same form:

$$\sigma(\mathbf{r}, \mathbf{v}) = \sum_i N_i(\mathbf{r}) \sigma_i(\mathbf{v}). \quad (14)$$

(7) $v\sigma_i(\mathbf{v})$ is bounded. We expect $\sigma_i(\mathbf{v})$ to be bounded except possibly for $v \to 0$, in which case we admit $\sigma_i(v) \sim 1/v$.

(8) $\sigma_i(\mathbf{r}, \mathbf{v})$, $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$, $\sigma_i(\mathbf{v})$, and $\sigma_i(\mathbf{v}' \to \mathbf{v})$ are all positive.

(9) The function

$$c(\mathbf{r}, \mathbf{v}) = \int \sigma(\mathbf{r}, \mathbf{v} \to \mathbf{v}')\, d^3v'/\sigma(\mathbf{r}, \mathbf{v}) \quad (15)$$

is positive. This assumption is also physically reasonable, since $c(\mathbf{r}, \mathbf{v})$ represents the mean number of neutrons emitted per collision. We define a similar microscopic quantity $\xi_i(\mathbf{v})$ which is also bounded

$$\xi_i(\mathbf{v}) = \int \sigma_i(\mathbf{v} \to \mathbf{v}')\, d^3v'/\sigma_i(\mathbf{v}). \quad (16)$$

We shall also have occasion to use two further functions,

$$c'(\mathbf{r}, \mathbf{v}) = \int \sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})\, d^3v'/\sigma(\mathbf{r}, \mathbf{v}), \quad (17a)$$

and

$$c''(\mathbf{r}, \mathbf{v}) = \int v'\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})\, d^3v'/\sigma(\mathbf{r}, \mathbf{v}). \quad (17b)$$

It may be noted that $c'$ and $c''$ may not always be bounded but they (like $c$) are always positive. Similarly the functions

$$\xi_i'(\mathbf{v}) = \int \sigma_i(\mathbf{v}' \to \mathbf{v})\, d^3v'/\sigma_i(\mathbf{v}) \quad (18a)$$

and

$$\xi_i''(\mathbf{v}) = \int v'\sigma_i(\mathbf{v}' \to \mathbf{v})\, d^3v'/\sigma_i(\mathbf{v}) \quad (18b)$$

may not be bounded but, like $\xi_i(\mathbf{v})$, they *are* positive.

## IV. THE TIME-DEPENDENT TRANSPORT EQUATION

Bearing in mind the restrictions discussed in Sec. III, we consider now various existence and uniqueness theorems for the time-dependent transport equation.

*Theorem 1.* Let $Q'(\mathbf{r}, \mathbf{v}, t)$ be bounded. Then if $c''(\mathbf{r}, \mathbf{v})$ is bounded, a unique, positive, and continuous solution to the time-dependent transport equation exists.

We prove the theorem by constructing the Neumann series solution to Eq. (6):

$$\psi(\mathbf{r}, \mathbf{v}, t) = \sum_{n=0}^{\infty} \psi_n(\mathbf{r}, \mathbf{v}, t), \quad (19)$$

where

$$\psi_0(\mathbf{r}, \mathbf{v}, t) = Q'(\mathbf{r}, \mathbf{v}, t), \quad (20a)$$

and

$$\psi_n(\mathbf{r}, \mathbf{v}, t) = K\psi_{n-1}(\mathbf{r}, \mathbf{v}, t). \tag{20b}$$

By hypothesis,

$$0 \leqq \psi_0 \leqq M < \infty. \tag{21}$$

Furthermore,

$$\psi_1(\mathbf{r}, \mathbf{v}, t) = KQ'(\mathbf{r}, \mathbf{v}, t) \leqq Mc''_{\max}\sigma_{\max}t. \tag{22}$$

Continuing the iteration we find

$$\psi_n(\mathbf{r}, \mathbf{v}, t) \leqq M(c''_{\max}\sigma_{\max})^n(t^n/n!). \tag{23}$$

Thus, the Neumann series converges pointwise, and the theorem is proved. The fact that $\psi(\mathbf{r}, \mathbf{v}, t)$ is positive follows from the fact that every term in the series is positive.

Next, assume that $c''(\mathbf{r}, \mathbf{v})$ is not bounded. Then we can state:

*Theorem 2.* Let $Q'(\mathbf{r}, \mathbf{v}, t)$ be bounded. Then a unique, positive solution to the transport equation exists which is a continuous function of $t$ and $\mathbf{r}$ and an integrable function of $\mathbf{v}$.

*Proof:* The proof proceeds along the lines of Theorem 1; however, it is sufficient to show that the series

$$\sum_n \int d^3v\psi_n(\mathbf{r}, \mathbf{v}, t) \tag{24}$$

converges pointwise. Consider first

$$\int d^3v\psi_1(\mathbf{r}, \mathbf{v}, t) \leqq M \int_0^t dt' \int v'\, d^3v' \times \int d^3v\sigma(\mathbf{r} - \mathbf{v}(t - t'), \mathbf{v}' \to \mathbf{v}). \tag{25}$$

However, we have assumed in Sec. III that $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ could be written in the form

$$\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) = \sum N_i(\mathbf{r})\sigma_i(\mathbf{v}' \to \mathbf{v}), \tag{26}$$

where the $N_i(\mathbf{r})$ are bounded, say by $N_{i0}$. Then

$$\int d^3v\psi_1(\mathbf{r}, \mathbf{v}, t) \leqq Mt \sum N_{i0} \int v'\, d^3v'\xi_i(\mathbf{v}')\sigma_i(\mathbf{v}'). \tag{27}$$

But $\xi_i(\mathbf{v}')$ and $\sigma_i(\mathbf{v}')$ are assumed in Sec. III to be bounded, say by $\xi_{i0}$ and $\sigma_{i0}$. Then

$$\int d^3v\psi_1(\mathbf{r}, \mathbf{v}, t) \leqq Mt \sum N_{i0}\xi_{i0}\sigma_{i0} \int v'\, d^3v', \tag{28}$$

and since $v' \leqq v_m$ (cf. Sec. III), we have

$$\int d^3v\psi_i(\mathbf{r}, \mathbf{v}, t) \leqq Kt, \qquad 0 \leqq K < \infty. \tag{29}$$

Similarly, we find

$$\int d^3v\psi_n(\mathbf{r}, \mathbf{v}, t) \leqq \frac{K't^n}{n!}, \qquad 0 \leqq K' < \infty, \tag{30}$$

and the theorem is proved. Again each term is positive, so that the solution is positive.

Next consider the case that $Q'(\mathbf{r}, \mathbf{v}, t)$ is not bounded, but integrable. The following theorems are simple to prove by straightforward construction of the Neumann series, as above.

*Theorem 3.* If $Q'(\mathbf{r}, \mathbf{v}, t) = Q_0(\mathbf{r}, \mathbf{v})\delta(t)$, where $Q_0(\mathbf{r}, \mathbf{v})$ is bounded, then, for the time-dependent transport equation:

(a) If $c''(\mathbf{r}, \mathbf{v})$ is bounded, a unique, positive solution $\psi(\mathbf{r}, \mathbf{v}, t)$, exists. $\psi(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $\mathbf{r}$ and $\mathbf{v}$, and $\psi(\mathbf{r}, \mathbf{v}, t) - Q'(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $t$.

(b) If $c''(\mathbf{r}, \mathbf{v})$ is not bounded, then the solution $\psi(\mathbf{r}, \mathbf{v}, t)$ may be an integrable rather than a continuous function of $\mathbf{v}$. Otherwise the conclusions are unchanged.

*Theorem 4.* If $Q'(\mathbf{r}, \mathbf{v}, t) = Q_1(\mathbf{r}, t)\delta(\mathbf{v} - \mathbf{v}_0)$, where $Q_1(\mathbf{r}, t)$ is bounded, then:

(a) If $v\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ is bounded, a unique, positive solution $\psi(\mathbf{r}, \mathbf{v}, t)$ exists. $\psi(\mathbf{r}, \mathbf{v}, t)$ is a continuous function $\mathbf{r}$ and $t$, and $\psi(\mathbf{r}, \mathbf{v}, t) - Q'(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $\mathbf{v}$.

(b) If $v\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ is not bounded, then $\psi(\mathbf{r}, \mathbf{v}, t) - Q'(\mathbf{r}, \mathbf{v}, t)$ may be an integrable rather than a continuous function of $\mathbf{v}$. [In proving part (b) we make use of the fact (cf. Sec. III) that $v$ and $\xi_i(\mathbf{v})$ have both been assumed bounded.]

*Theorem 5.* If $Q'(\mathbf{r}, \mathbf{v}, t) = Q'_2(\mathbf{v}, t)\delta(\mathbf{r} - \mathbf{r}_0)$, where $Q'_2(\mathbf{r}, t)$ is bounded, then:

(a) If $c''(\mathbf{r}, \mathbf{v})$ is bounded, a positive, unique solution $\psi(\mathbf{r}, \mathbf{v}, t)$ exists. $\psi(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $\mathbf{v}$ and $t$, and an integrable function of $\mathbf{r}$.

(b) If $c''(\mathbf{r}, \mathbf{v})$ is not bounded, then $\psi(\mathbf{r}, \mathbf{v}, t)$ may be an integrable rather than a continuous function of $\mathbf{v}$.

The theorems for the cases in which $Q'(\mathbf{r}, \mathbf{v}, t)$ involves a delta function in more than a single variable, may easily be constructed by appropriately combining the above theorems. We shall not state them separately.

## V. THE TIME-DEPENDENT "ADJOINT" EQUATION

Here we deal with Eq. (10). The theorems will all be stated without proof, since the proofs are

completely analogous to those given in the previous section.

*Theorem 6.* If $\tilde{Q}'(\mathbf{r}, \mathbf{v}, t)$ is bounded, then a continouous, unique, positive solution exists. [Note that in proving this theorem it is necessary to make use of the fact that $c(\mathbf{r}, \mathbf{v})$ is bounded (cf. Sec. III).]

*Theorem 7.* If $\tilde{Q}'(\mathbf{r}, \mathbf{v}, t) = \tilde{Q}_0(\mathbf{r}, \mathbf{v})\delta(t)$, where $\tilde{Q}_0$ is bounded, then a unique, positive solution exists. $\tilde{\psi}(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $\mathbf{r}$ and $\mathbf{v}$, and $\tilde{\psi}(\mathbf{r}, \mathbf{v}, t) - \tilde{Q}'(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $t$.

*Theorem 8.* If $\tilde{Q}'(\mathbf{r}, \mathbf{v}, t) = \tilde{Q}_1(\mathbf{r}, t)\delta(\mathbf{v} - \mathbf{v}_0)$, where $\tilde{Q}_1$ is bounded, then:

(a) If $v\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ is bounded, a unique, positive solution $\tilde{\psi}(\mathbf{r}, \mathbf{v}, t)$ exists. $\tilde{\psi}(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $\mathbf{r}$ and $t$, and $\tilde{\psi}(\mathbf{r}, \mathbf{v}, t) - \tilde{Q}'(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $\mathbf{v}$.

(b) If $v\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ is unbounded but $\xi_i''(\mathbf{r}, \mathbf{v})$ is bounded, then the conditions above hold except that $\tilde{\psi}(\mathbf{r}, \mathbf{v}, t) - \tilde{Q}'(\mathbf{r}, \mathbf{v}, t)$ may be an integrable, rather than a continuous, function of $\mathbf{v}$.

*Theorem 9.* If $\tilde{Q}'(\mathbf{r}, \mathbf{v}, t) = \tilde{Q}_2(\mathbf{v}, t)\delta(\mathbf{r} - \mathbf{r}_0)$, where $\tilde{Q}_2$ is bounded, then a unique, positive solution $\tilde{\psi}(\mathbf{r}, \mathbf{v}, t)$ exists. $\tilde{\psi}(\mathbf{r}, \mathbf{v}, t)$ is a continuous function of $\mathbf{v}$ and $t$, and an integrable function of $\mathbf{r}$.

Again, when $\tilde{Q}'$ involves delta functions in more than a single variable, the appropriate theorems can be constructed by appropriately combining the results above, and so we shall avoid stating them explicitly.

## VI. THE TIME-INDEPENDENT TRANSPORT AND ADJOINT EQUATIONS

In certain rather restrictive cases, it can be proved that unique, positive solutions of the time-independent transport and adjoint equations exist. In general, the restrictions are much more severe than is the case for the time-dependent equations; we shall see later that this is to be expected.

*Theorem 10.* Let $Q'(\mathbf{r}, \mathbf{v})$ be bounded and positive. Then if $c'(\mathbf{r}, \mathbf{v}) < 1$, a unique, positive, and continuous solution to the time-independent transport equation [Eq. (7)] exists.

We note that the integral equation (7) differs from Eq. (1b) in that in the former, the dependent variable is the angular *flux* $\phi(\mathbf{r}, \mathbf{v})$ rather than the angular *density* $\psi(\mathbf{r}, \mathbf{v})$. Thus all theorems which we shall prove involving the time-independent transport equation may not apply to the angular density unless $\psi(\mathbf{r}, \mathbf{v})$ vanishes sufficiently rapidly as $v \to 0$. This is not a real worry, since one is generally interested in the flux rather than the angular density.

As usual, we prove the theorem by constructing the Neumann series:

$$\phi(\mathbf{r}, \mathbf{v}) = \sum \phi_n(\mathbf{r}, \mathbf{v}), \tag{31a}$$

with

$$\phi_0(\mathbf{r}, \mathbf{v}) = Q'(\mathbf{r}, v), \tag{31b}$$

and

$$\phi_n(\mathbf{r}, \mathbf{v}) = \Lambda^n\phi(\mathbf{r}, \mathbf{v}) = \Lambda\phi_{n-1}(\mathbf{r}, \mathbf{v}). \tag{31c}$$

By hypothesis, $\phi_0(\mathbf{r}, \mathbf{v})$ is bounded and positive:

$$0 \leqq \phi_0(\mathbf{r}, \mathbf{v}) \leqq M < \infty. \tag{32}$$

Next assume $\phi_{n-1}(\mathbf{r}, \mathbf{v})$ is bounded by $M'$, say. Then

$$\phi_n(\mathbf{r}, \mathbf{v}) = \Lambda\phi_{n-1}(\mathbf{r}, \mathbf{v}) \leqq M'c'_{\max}\int_0^\infty dR$$

$$\times \exp\left[-\alpha(\mathbf{r}, \mathbf{r} - R\boldsymbol{\Omega}, \mathbf{v})\right]\sigma(\mathbf{r} - R\boldsymbol{\Omega}, \mathbf{v}). \tag{33}$$

The integral is easily shown to be equal to unity. Thus

$$\phi_n(\mathbf{r}, \mathbf{v}) \leqq M'c'_{\max} < M', \tag{34}$$

since we have assumed $c'(\mathbf{r}, \mathbf{v}) < 1$. This proves the theorem since the Neumann series converges pointwise, and each term is seen to be positive.

The next theorem is readily proved in essentially the same manner.

*Theorem 11.* If $Q'(\mathbf{r}, \mathbf{v} = Q_1(\mathbf{r}, \mathbf{v})\delta(\mathbf{v} - \mathbf{v}_0)$, where $Q_1(\mathbf{r})$ is bounded, then if $c'(\mathbf{r}, \mathbf{v}) < 1$ and $\sigma(\mathbf{r}, \mathbf{v}_0 \to \mathbf{v})$ is bounded, a unique, positive solution $\psi(\mathbf{r}, \mathbf{v})$ exists. $\psi(\mathbf{r}, \mathbf{v})$ is a continuous function of $\mathbf{r}$ and $\psi(\mathbf{r}, \mathbf{v}) - Q'(\mathbf{r}, \mathbf{v})$ is a continouus function of $\mathbf{v}$.

*Theorem 12.* If $\sigma(\mathbf{r}, \mathbf{v})Q'(\mathbf{r}, \mathbf{v})$ is *integrable*, then if $c(\mathbf{r}, \mathbf{v}) < 1$, a unique, positive, integrable solution exists.

This is the theorem proved by Olhoeft.[2] The procedure is to construct the Neumann series for the collision density $\chi(\mathbf{r}, \mathbf{v})$ defined by

$$\chi(\mathbf{r}, \mathbf{v}) = \sigma(\mathbf{r}, \mathbf{v})\phi(\mathbf{r}, \mathbf{v}), \tag{35}$$

and prove that

$$\int d^3v\, d^3rK\chi_n(\mathbf{r}, \mathbf{v}) \leqq \int d^3r\, d^3v\chi_n(\mathbf{r}, \mathbf{v}). \tag{35}$$

Since the details are given in reference 2, they will be omitted here.

We next turn our attention to the time-independent adjoint equation. Here the theorems are quite analogous to Theorems 10–12 proved for the transport equation, except that the roles of $c$ and $c'$ are reversed. Since the proofs are so similar, we simply state the theorems.

*Theorem 13.* Let $(1/v)\tilde{Q}'(\mathbf{r}, \mathbf{v})$ be bounded and positive. Then if $c(\mathbf{r}, \mathbf{v}) < 1$, a unique, positive, continuous solution exists to the time-independent adjoint equation.

*Theorem 14.* Let $(1/v)\tilde{Q}'(\mathbf{r}, \mathbf{v}) = \tilde{Q}_1(\mathbf{r})\delta(\mathbf{v} - \mathbf{v}_0)$, where $\tilde{Q}_1(\mathbf{r})$ is bounded and positive. Then if $c(\mathbf{r}, \mathbf{v}) < 1$ and $\sigma(\mathbf{r}, \mathbf{v} \to \mathbf{v}_0)$ is bounded, a unique, positive solution $\tilde{\psi}(\mathbf{r}, \mathbf{v})$ exists. $\tilde{\psi}(\mathbf{r}, \mathbf{v})$ is a continuous function of $\mathbf{r}$ and $\tilde{\psi} - (1/v)\tilde{Q}$ is a continuous function of $\mathbf{v}$.

*Theorem 15.* If $c'(\mathbf{r}, \mathbf{v}) < 1$, and if $(1/v)\sigma(\mathbf{r}, \mathbf{v})\tilde{Q}'(\mathbf{r}, \mathbf{v})$ is integrable, then a unique, positive, integrable solution exists.

Note that in each of these theorems we have placed restrictions on $(1/v)\tilde{Q}'$ rather than on $\tilde{Q}'$. If we make the reasonable assumption that no zero-energy source neutrons are introduced into the system, then the conditions can equally well be stated as conditions on $\tilde{Q}'$ rather than on $(1/v)\tilde{Q}'$.

Next we prove a uniqueness theorem for cases in which existence has not been proved.

*Theorem 16*: If a solution of class $L^2$ of the time-independent adjoint equation exists, then an $L^2$ solution to the time-independent transport equation, if it exists, will be unique.

We sketch the proof. Suppose there are two solutions to the transport equation, $\psi_1$ and $\psi_2$. Then $\psi \equiv \psi_1 - \psi_2$ obeys the equation

$$v(\mathbf{\Omega}'\nabla + \sigma(\mathbf{r}, \mathbf{v}))\psi(\mathbf{r}, \mathbf{v}) = \int v'\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})\psi(\mathbf{r}, \mathbf{v}')\, d^3v', \tag{37}$$

with

$$\psi(\mathbf{r}_s, \mathbf{v}) = 0, \qquad \mathbf{\Omega}\cdot\mathbf{n}_0 < 0. \tag{38}$$

Consider the adjoint equation with zero outgoing angular density:

$$v(-\mathbf{\Omega}\cdot\nabla + \sigma(\mathbf{r}, \mathbf{v}))\tilde{\psi}(\mathbf{r}, \mathbf{v}) = \tilde{q}(\mathbf{r}, \mathbf{v}) + \int v\sigma(\mathbf{r}, \mathbf{v} \to \mathbf{v}')\tilde{\psi}(\mathbf{r}, \mathbf{v}')\, d^3v', \tag{39}$$

$$\tilde{\psi}(\mathbf{r}_s, \mathbf{v}) = 0, \qquad \mathbf{\Omega}\cdot\mathbf{n}_0 > 0. \tag{40}$$

(We have hypothesized that such a solution exists.)

If we now multiply Eq. (37) by $\tilde{\psi}(\mathbf{r}, \mathbf{v})$, and multiply Eq. (39) by $\psi(\mathbf{r}, \mathbf{v})$, subtract and integrate over $\mathbf{r}$ and $\mathbf{v}$, we obtain

$$\int d^3v \int dS\mathbf{\Omega}\cdot\mathbf{n}_0\psi(\mathbf{r}, \mathbf{v})\tilde{\psi}(\mathbf{r}, \mathbf{v}) = \int d^3r \int d^3v \int d^3v'v'\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) \times \psi(\mathbf{r}, \mathbf{v}')\tilde{\psi}(\mathbf{r}, \mathbf{v}) - \int d^3r \int d^3v \int d^3v'v\sigma(\mathbf{r}, \mathbf{v} \to \mathbf{v}')\tilde{\psi}(\mathbf{r}, \mathbf{v}')\psi(\mathbf{r}, \mathbf{v}) - \int d^3r \int d^3v\psi(\mathbf{r}, \mathbf{v})\tilde{q}(\mathbf{r}, \mathbf{v}). \tag{41}$$

The left-hand side of this equation has been obtained with the help of Gauss' Theorem, and by virtue of Eqs. (38) and (40), it vanishes. Similarly, the first two terms on the right side of Eq. (41) cancel, and we obtain

$$\int d^3r \int d^3v\psi(\mathbf{r}, \mathbf{v})\tilde{q}(\mathbf{r}, \mathbf{v}) = 0. \tag{42}$$

Since $\tilde{q}(\mathbf{r}, \mathbf{v})$ is arbitary (and positive), it follows that

$$\psi(\mathbf{r}, \mathbf{v}) \equiv 0, \tag{43}$$

proving the theorem.

We note that the conditions of this theorem are satisfied for (among other cases) $c(\mathbf{r}, \mathbf{v}) < 1$; thus, Eq. (39) can possess no solution for $c(\mathbf{r}, \mathbf{v}) < 1$ subject to the boundary conditions (38). Since these are precisely the equations satisfied by the neutron density in a reactor, we have succeeded in proving, as a byproduct, the not surprising result that a reactor cannot be critical if fewer neutrons are emitted than absorbed following each collision ($c < 1$). A simpler proof of this theorem (and of the following theorem) for the case that only scattering and pure absorption are present (i.e., no fission), is given in the Appendix.

The analog of Theorem (16) is:

*Theorem 17.* If an $L^2$ solution of the time-independent transport equation exists, then an $L^2$ solution of the time-independent adjoint equation, if it exists, will be unique.

The proof of this theorem is essentially identical with that of Theorem 16. The implication of this theorem is that a reactor cannot be critical if $c'(\mathbf{r}, \mathbf{v}) < 1$. This can be seen from a slight modification of the arguments used above to show the same result for $c(\mathbf{r}, \mathbf{v}) < 1$.

## VII. SOME MISCELLANEOUS RESULTS

In the previous section we have pointed out that the uniqueness of the time-independent solution is equivalent to the statement that a reactor cannot be critical. Thus we have shown (Theorem 16) that no reactor can be critical for $c(\mathbf{r}, \mathbf{v}) < 1$, which is, of course, physically obvious. However, such a condition is somewhat too stringent since it is clear that, for a system of finite size, neutron leakage may prevent a reactor from becoming critical even for $c$ somewhat larger than one.

We can obtain an estimate of the minimum value of $c$ for which a reactor of a given size will become critical from Theorem 12. The proof, which we omitted in Sec. VI, involves the construction of the Neumann series solution to the following integral equation for the collision density $\chi \equiv \sigma\phi$:

$$\chi(\mathbf{r}, \mathbf{v}) = \sigma(\mathbf{r}, \mathbf{v})Q'(\mathbf{r}, \mathbf{v}) + \tilde{\Lambda}\chi(\mathbf{r}, \mathbf{v}), \tag{44a}$$

where $\tilde{\Lambda}$ is the integral operator

$$\tilde{\Lambda}f(\mathbf{r}, \mathbf{v}) = \int_0^{R_s} dR \int d^3v'v' \, v \, d^3r' \times \exp\,[-\alpha(\mathbf{r}, \mathbf{r}', \mathbf{v})]\sigma(\mathbf{r}, \mathbf{v}) \, \delta(\mathbf{r}' - \mathbf{r} + R\boldsymbol{\Omega}) \times \frac{\sigma(\mathbf{r}', \mathbf{v}' \to \mathbf{v})}{\sigma(\mathbf{r}', \mathbf{v}')} f(\mathbf{r}', \mathbf{v}'). \tag{44b}$$

In the proof, one shows that if

$$\iint d^3v \, d^3r\chi_n(\mathbf{r}, \mathbf{v}) \leqq M, \tag{45a}$$

then

$$\iint d^3v \, d^3r\chi_{n+1}(\mathbf{r}, \mathbf{v}) \leqq c_{\max}M. \tag{45b}$$

Actually, a somewhat stronger condition holds, since from Eq. (44b) it follows immediately that

$$\iint d^3v \, d^3r\Lambda\chi_{n+1}(\mathbf{r}, \mathbf{v}) = \int d^3r \int d^3v \int d^3v' \times (1 - \exp\,[-\alpha(\mathbf{r}, \mathbf{r} + R_s\boldsymbol{\Omega}, \mathbf{v})]) \times \sigma(\mathbf{r}, \mathbf{v}' \to v) \frac{\chi_n(\mathbf{r}, \mathbf{v}')}{\sigma(\mathbf{r}, \mathbf{v})}. \tag{46}$$

In obtaining (45b), the exponential in Eq. (46) was set equal to zero. If instead we approximate Eq. (46) by the expression

$$(1 - e^{-\bar{\tau}})\bar{c} \iint \chi_n(\mathbf{r}, \mathbf{v}') \, d^3r \, d^3v', \tag{47}$$

we see that an approximate limit for the convergence of the Neuman series is

$$\bar{c} < (1 - e^{-\bar{\tau}})^{-1}. \tag{48}$$

Here $\bar{\tau}$ is the average optical chord length of the system and $\bar{c}$ is the average value of $c(\mathbf{r}, \mathbf{v})$.

This expression should give a rough estimate of critical size since one can write

$$\bar{\tau} = \bar{\sigma}\bar{l}, \tag{49}$$

where $\bar{\sigma}$ is the average cross section and $\bar{l}$ is the average chord length $(4V/S)$. The averages of $c$ and $\sigma$ are taken both with respect to $\mathbf{r}$ and $\mathbf{v}$.

A second result which follows from the theorems proved in the earlier section is that the solution of the time-dependent transport or adjoint equations can increase no faster than exponentially if the source is of exponential order or less. Consider first the transport equation. Let us write the source in the form

$$Q''(\mathbf{r}, \mathbf{v}, t) = Q_0(\mathbf{r}, \mathbf{v})f(t). \tag{50}$$

For simplicity we shall assume that $Q_0$ and $c''$ are bounded. Then we wish to examine the time-dependence of the Neumann series, Eq. (19). Since $Q_0$ is bounded we have

$$\psi_0 \leqq Mf(t), \tag{51}$$

$$\psi_1 \leqq Mc''_{\max}\sigma_{\max} \int_0^t tf(t) \, dt, \tag{52}$$

and in general

$$\psi_n \leqq M(c''_{\max}\sigma_{\max})^n \times \int_0^t dt_1 \int^{t_1} dt_2 \cdots \int_0^{t_{n-1}} t_nf(t_n) \, dt_n. \tag{53}$$

Now from Euler's identity

$$\int_0^t dt_1 \cdots \int_0^{t_{n-1}} t_nf(t_n) \, dt_n = \int_5^t \frac{(t - t')^{n-1}}{(n - 1)!} f(t') \, dt', \tag{54}$$

we have

$$\psi_n \leqq M(c''_{\max}\sigma_{\max})^n f_{\max}(t^n/n!). \tag{55}$$

Thus

$$\psi \leqq Mf_{\max} \sum_{n=0}^{\infty} \frac{(c''_{\max}\sigma_{\max}t)^n}{n!}, \tag{56}$$

or

$$\psi \leqq Mf_{\max} \exp\,(c''_{\max}\sigma_{\max}t). \tag{57}$$

Thus the time behavior of $\psi$ is asymptotically given either by $f(t)$ or by the exponential $\exp\,(c''_{\max}\sigma_{\max}t)$, whichever is more important at large times.

If $f(t) = e^{\alpha t}$, the integral in (54) can be evaluated explicitly:

$$I_n(t) = \int_0^t \frac{(t-t')^{n-1}}{(n-1)!} e^{\alpha t'}\, dt' = e^{\alpha t} \int_0^t \frac{\tau^{n-1}}{(n-1)!} e^{-\alpha\tau}\, d\tau. \quad (58)$$

Clearly,

$$I_n(t) = \frac{e^{\alpha t}}{(n-1)!} (-1)^{n-1} \frac{\partial}{\partial \alpha^{n-1}} \left(\frac{1-e^{-\alpha t}}{\alpha}\right), \quad (59)$$

so that

$$\psi_n \leqq M \frac{(c''_{\max}\sigma_{\max})^n (-1)^{n-1}}{(n-1)!} \frac{\partial^{n-1}}{\partial \alpha^{n-1}} \left(\frac{1-e^{-\alpha t}}{\alpha}\right), \quad (60)$$

for $n > 0$. Then

$$\psi \leqq M\Big[1 + c''_{\max}\sigma_{\max} e^{\alpha t} \times \sum_{n=0} \frac{(c''_{\max}\sigma_{\max})^n}{n!} (-1)^n \frac{\partial^n}{\partial \alpha^n} \left(\frac{1-e^{-\alpha t}}{\alpha}\right)\Big], \quad (61)$$

or

$$\psi \leqq M[1 + c''_{\max}\sigma_{\max}/(\alpha - c''_{\max}\sigma_{\max}) \times (e^{\alpha t} - e^{c''_{\max}\sigma_{\max} t})], \quad (62)$$

where Taylor's theorem has been used to perform the sum. We note that this limit is always positive.

A very similar argument can be used to delimit the time behavior of the adjoint equation; we shall omit it here.

## APPENDIX

Theorems 16 and 17 may be proved in a different manner from that used in the text if we assume that no mechanism is present for neutron regeneration other than ordinary elastic and/or inelastic scattering. [We note that in this case $c(\mathbf{r}, \mathbf{v}) \leqq 1$.] In such a case, we expect that the kernel $\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})$ obeys the principle of detailed balance

$$v'M(v')\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) = vM(v)\sigma(\mathbf{r}, \mathbf{v} \to \mathbf{v}'), \quad (A1)$$

since in the absence of sources and sinks of neutrons, an equilibrium should be approached. The equilibrium spectrum $M(v)$ is the Maxwell–Boltzmann distribution

$$M(v) \sim v^2 \exp\left[-\tfrac{1}{2}(Mv^2/kT)\right]. \quad (A2)$$

Consider now Eq. (37) of the text, with the boundary condition, Eq. (38). Define a new dependent variable by the relation

$$\phi(\mathbf{r}, \mathbf{v}) = F(\mathbf{r}, \mathbf{v})\psi(\mathbf{r}, \mathbf{v}), \quad (A3)$$

where $F(\mathbf{r}, \mathbf{v})$ is some well-behaved but otherwise arbitrary function to be chosen later. Then Eq. (37) becomes

$$\mathbf{v}\cdot\nabla \frac{\phi}{F} + \frac{v\sigma\phi}{F} = \int v'\sigma(\mathbf{v}' \to \mathbf{v}) \frac{\phi(\mathbf{v}')}{F(\mathbf{v}')}\, d^3v', \quad (A4)$$

with

$$\phi(\mathbf{r}_s, \mathbf{v}) = 0, \qquad \boldsymbol{\Omega}\cdot\mathbf{n}_0 < 0. \quad (A5)$$

[The function $F$ must be chosen so that Eq. (A5) is still satisfied.]

If Eq. (A4) is multiplied by $\phi(\mathbf{r}, \mathbf{v})$ and integrated over $\mathbf{r}$ and $\mathbf{v}$ we obtain, with the aid of Gauss' Theorem,

$$\frac{1}{2}\int dS \int d^3v \mathbf{n}_0\cdot\mathbf{v} \frac{\phi^2(\mathbf{r}, \mathbf{v})}{F(\mathbf{r}, \mathbf{v})}, + \int d^3r \int d^3v v\sigma(\mathbf{r}, \mathbf{v}) \frac{\phi^2(\mathbf{r}, \mathbf{v})}{F(\mathbf{r}, \mathbf{v})} = \iint d^3v\, d^3v' v' \sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) \frac{\phi(\mathbf{r}, \mathbf{v})\phi(\mathbf{r}, \mathbf{v}')}{F(\mathbf{r}, \mathbf{v}')}. \quad (A6)$$

Next consider the identity

$$[\phi(\mathbf{r}, \mathbf{v}) - \phi(\mathbf{r}, \mathbf{v}')]^2 \geqq 0, \quad (A7)$$

or

$$\phi(\mathbf{r}, \mathbf{v})\phi(\mathbf{r}, \mathbf{v}') \leqq \tfrac{1}{2}\{\phi^2(\mathbf{r}, \mathbf{v}) + \phi(\mathbf{r}, \mathbf{v}')^2\}. \quad (A8)$$

Then, by virtue of (A8), the right side of Eq. (A6) may be written

$$\iint d^3v\, d^3v' v' \sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) \frac{\phi(\mathbf{r}, \mathbf{v})\phi(\mathbf{r}, \mathbf{v}')}{F(\mathbf{r}, \mathbf{v}')} \leqq \frac{1}{2}\iint d^3v\, d^3v' v' \frac{\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})}{F(\mathbf{r}, \mathbf{v}')} \{\phi^2(\mathbf{r}, \mathbf{v}) + \phi^2(\mathbf{r}, \mathbf{v}')\} \quad (A9)$$

$$= \frac{1}{2}\int d^3v' v' \sigma(\mathbf{r}, \mathbf{v}') c(\mathbf{r}, \mathbf{v}') \frac{\phi^2(\mathbf{r}, \mathbf{v}')}{F(\mathbf{r}, \mathbf{v}')} + \frac{1}{2}\iint d^3v\, d^3v' v' \frac{\sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v})}{F(\mathbf{r}, \mathbf{v}')} \phi^2(\mathbf{r}, \mathbf{v}). \quad (A10)$$

If we now choose $F(\mathbf{r}, \mathbf{v}') = 1/M(v')$, the second term on the right of Eq. (A10) becomes

$$\frac{1}{2}\int\int d^3v\, d^3v' v' M(v') \sigma(\mathbf{r}, \mathbf{v}' \to \mathbf{v}) \phi^2(\mathbf{r}, \mathbf{v}) = \frac{1}{2}\int\int d^3v\, d^3v' v M(v) \sigma(\mathbf{r}, \mathbf{v} \to \mathbf{v}') \phi^2(\mathbf{r}, \mathbf{v}), \quad (A11)$$

by Eq. (A1). This becomes, upon integration over $v'$,

$$\frac{1}{2}\int d^3v v M(v) \sigma(\mathbf{r}, \mathbf{v}) c(\mathbf{r}, \mathbf{v}) \phi^2(\mathbf{r}, \mathbf{v}). \quad (A12)$$

writing $M(v)$ for $1/F(\mathbf{r}, \mathbf{v})$ throughout Eq. (A6),

and using (A9), (A10), and (A12), we find

$$\frac{1}{2}\int dS \int d^3v\mathbf{n}_0\cdot\mathbf{v}\phi^2(\mathbf{r},\mathbf{v})M(v) + \int d^3r \int d^3vM(v)\sigma(\mathbf{r},\mathbf{v})\phi^2(\mathbf{r},\mathbf{v}) - \int d^3vv\sigma(\mathbf{r},\mathbf{v})c(\mathbf{r},\mathbf{v})vM(v)\phi^2(\mathbf{r},\mathbf{v}) \leqq 0. \quad \text{(A13)}$$

The first term on the left side of Eq. (A13) is, by virtue of (A5), nonnegative. The other two terms combine to give

$$\int d^3r \int d^3vM(v)\sigma(\mathbf{r},\mathbf{v})\phi^2(\mathbf{r},\mathbf{v})[1 - c(\mathbf{r},\mathbf{v})], \quad \text{(A14)}$$

which is always nonnegative since $c(\mathbf{r},\mathbf{v}) < 1$. However, Eq. (A13) tells us that the sum of these terms is nonpositive. Thus

$$\phi(\mathbf{r},\mathbf{v}) \equiv 0, \quad \text{(A15)}$$

and the theorem is proved. We see that a reactor with no fuel can never be critical.

The uniqueness of the time-independent adjoint equation for the case of no reproduction can be proved in an entirely analogous fashion. This method is a slight generalization of that used in reference 1 for proving uniqueness of the one-speed equations.

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# Fundamental Properties of Perturbation-Theoretical Integral Representations. II

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In the first part of this paper, it is investigated, apart from the perturbation-theoretical basis, under what conditions the perturbation-theoretical integral representations can be derived, and two theorems are given concerning this problem. In the second part, the asymptotic behavior of the weight function in the integral representation is investigated in perturbation theory. It is proved that the weight function vanishes at infinity for an infinite sum over certain graphs which are much more general than the ladderlike graphs. This result gives the analyticity in the right half-plane of complex angular momentum.

## I. INTRODUCTION

IN a previous paper,[1] which is quoted as I, we have investigated various analyticity and uniqueness properties of the perturbation-theoretical integral representations. The purpose of the present paper is to make some further investigation on analytic properties and to examine the asymptotic behavior of weight functions.

In Sec. II the Deser–Gilbert–Sudarshan–Ida (DGSI)-type integral representation[2] is investigated. The conditions under which it can be derived are given in a practically more convenient form than that given in I.

The integral representation for the scattering amplitude[3] consists of three terms, each of which is nothing but the DGSI-type integral representation for two variables among $s$, $t$, and $u$. Hence the analyticity domain $D$ of the former is the intersection of those of the latter. In Sec. III it is proved that a function holomorphic in $D$ can always be written as a sum of three functions holomorphic in the analyticity domain of the DGSI-type integral

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[2] S. Deser, W. Gilbert, and E. C. G. Sudarshan, Phys. Rev. 115, 731 (1959). M. Ida, Progr. Theoret. Phys. (Kyoto) 23, 1151 (1960). See also N. Nakanishi, Progr. Theoret. Phys. (Kyoto) Suppl. 18, 1 (1961), Part III.

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and using (A9), (A10), and (A12), we find

$$\frac{1}{2}\int dS \int d^3v\mathbf{n}_0\cdot\mathbf{v}\phi^2(\mathbf{r},\mathbf{v})M(v) + \int d^3r \int d^3vM(v)\sigma(\mathbf{r},\mathbf{v})\phi^2(\mathbf{r},\mathbf{v}) - \int d^3vv\sigma(\mathbf{r},\mathbf{v})c(\mathbf{r},\mathbf{v})vM(v)\phi^2(\mathbf{r},\mathbf{v}) \leqq 0. \quad \text{(A13)}$$

The first term on the left side of Eq. (A13) is, by virtue of (A5), nonnegative. The other two terms combine to give

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representation. Some remarks are made on the temperedness of the weight function for each term.

In Sec. IV we investigate the asymptotic behavior of the weight function of the integral representation for scattering amplitude in perturbation theory. It is proved that the weight function vanishes at infinity for an infinite sum over certain graphs which are much more general than the ladderlike graphs. In Sec. V it is remarked that the above result gives the analyticity of partial-wave amplitude in the right half-plane of complex angular momentum according to Khuri's theorem.[4]

## II. DGSI-TYPE INTEGRAL REPRESENTATION

In this section we discuss the DGSI-type integral representation[2]:

$$\int_0^1 dz \int_{-\infty}^{\infty} d\alpha \frac{\rho(\alpha, z)}{\alpha - zs - (1-z)t}, \tag{2.1}$$

where $\rho(\alpha, z)$ vanishes unless

$$\alpha \geq za + (1-z)b, \tag{2.2}$$

$a$ and $b$ being certain constants. Replacing $s - a$ by $\hat{s}$ and $t - b$ by $\hat{t}$, we get a simpler form

$$\int_0^1 dz \int_0^{\infty} d\alpha \frac{\hat{\rho}(\alpha, z)}{\alpha - z\hat{s} - (1-z)\hat{t}}. \tag{2.3}$$

For simplicity, we hereafter omit the hat $\hat{}$.

Let $D_{st}^*$ be the set of all points $(s, t)$ such that $zs + (1-z)t$ can become real and nonnegative for some $z$ where $0 \leq z \leq 1$. More explicitly, we can write

$$D_{st}^* = D^*[s, t] \cup D^*[t, s] \cup D^*[s] \cup D^*[t], \tag{2.4}$$

where

$$D^*[s, t] \equiv \{s, t;\ \mathrm{Im}\, s > 0,\ \mathrm{Im}\, t < 0,\ \mathrm{Im}\, st^* \geq 0\},$$
$$D^*[s] \equiv \{s, t;\ \mathrm{Im}\, s = 0,\ \mathrm{Re}\, s \geq 0\}. \tag{2.5}$$

Let $D_{st}$, $D[s, t]$, $D[s]$ be the complements of $D_{st}^*$, $D^*[s, t]$, $D^*[s]$, respectively. Then every function represented as (2.3) is holomorphic in $D_{st}$. It was proved in I that $D_{st}$ is a domain of holomorphy. It was also shown in I that if a function $f(s, t)$ is holomorphic in $D_{st}$, and if it satisfies a certain boundedness condition, then $f(s, t)$ can always be represented as (2.3). This theorem can be generalized to the following form, which will be more convenient for practical applications.

*Theorem I.* If $f(s, t)$ satisfies the following three conditions, then it can be represented as (2.3) uniquely.

(i) It is holomorphic in

$$D_+ \equiv \{s, t;\ \mathrm{Im}\, s > 0,\ \mathrm{Im}\, t > 0\},$$

and in

$$D_- \equiv \{s, t;\ \mathrm{Im}\, s < 0,\ \mathrm{Im}\, t < 0\}. \tag{2.6}$$

(ii) Both boundary values on

$$E \equiv \{s, t;\ \mathrm{Im}\, s = \mathrm{Im}\, t = 0,\ \mathrm{Re}\, s < 0,\ \mathrm{Re}\, t < 0\}, \tag{2.7}$$

from $D_+$ and from $D_-$ coincide with each other.

(iii) There exist some positive numbers $M$ and $\delta$ such that

$$|f(s, t)| < (|s| + |t|)^{-\delta} \tag{2.8}$$

in $D_+$ and in $D_-$ whenever $|s| + |t| > M$ except for the neighborhoods of $D^*[s]$ and $D^*[t]$.

*Proof:* For an arbitrary point $(s, t) \in D_+$, Cauchy's theorem leads to

$$f(s, t) = \frac{1}{(2\pi i)^2} \oint \frac{ds'}{s' - s} \oint \frac{dt'}{t' - t} f(s', t'), \tag{2.9}$$

where the contours lie in the upper half-planes. Using the Feynman identity, we have

$$f(s, t) = \int_0^1 dz \psi(zs + (1-z)t, z), \tag{2.10}$$

where

$$\psi(v, z) \equiv \frac{1}{(2\pi i)^2} \oint ds' \oint dt' \frac{f(s', t')}{[zs' + (1-z)t' - v]^2}. \tag{2.11}$$

We infinitely enlarge the $s'$ contour in the upper half-plane. Then, because of the condition (iii), (2.11) becomes

$$\psi(v, z) \equiv \frac{1}{(2\pi i)^2} \times \int_{-\infty+i\epsilon}^{+\infty+i\epsilon} ds' \oint dt' \frac{f(s', t')}{[zs' + (1-z)t' - v]^2}, \tag{2.12}$$

with $\epsilon > 0$ (infinitesimal) except for $z = 0$.

The integral (2.10) is rewritten as

$$f(s, t) = \lim_{h \to 0+} \int_h^{1-h} dz \psi(zs + (1-z)t, z), \tag{2.13}$$

since $\psi(zs + (1-z)t, z)$ is a continuous function of $z$ in $0 \leq z \leq 1$. Hence we consider $\psi$ in the region $h \leq z \leq 1 - h$, $(h > 0)$. We transform the integration variable $t'$ into

$$w \equiv zs' + (1-z)t'. \tag{2.14}$$

Then the $w$ contour is dependent on $s'$. However, since the integrand is holomorphic in $\mathrm{Re}\, w \geq \epsilon$ except at $w = v$ because of the condition (i), we can

[4] See Sec. V.

deform the $w$ contour so as to become independent of $s'$. Thus after integrating by parts we can exchange the order of integrations[5] to get

$$\psi(v, z) = \oint dw \frac{g(w, z)}{w - v}, \tag{2.15}$$

with

$$g(w, z) \equiv \frac{1}{(2\pi i)^2} \frac{1}{1 - z} \int_{-\infty+i\epsilon}^{+\infty+i\epsilon} ds' \frac{\partial}{\partial w} f\left(s', \frac{w - zs'}{1 - z}\right), \tag{2.16}$$

provided that (2.16) is uniformly convergent. The last statement can be shown in the following way. For $s$ nonreal, $f(s, t)$ satisfies a dispersion relation with respect to $t$ because of the conditions (i) and (iii). Hence $(\partial/\partial t)\, f(s, t)$ vanishes at infinity faster than $|t|^{-1-\delta}$ uniformly. This fact gives the convergence of (2.16).

Now, on account of the conditions (i) and (ii), the edge-of-the-wedge theorem[6] tells us that $f(s, t)$ is holomorphic in a neighborhood of $E$. Hence we can analytically continue $g(w, z)$ to

$$\{w; \quad \text{Re } w < 0, \quad |\text{Im } w| < \epsilon\} \tag{2.17}$$

by shifting down the $s'$ contour for Re $s' < 0$. We can further continue $g(w, z)$ to the lower half-plane of $w$ by deforming the $s'$ contour because of the analyticity of $f(s, t)$ in $D_-$. Thus we see that $g(w, z)$ is holomorphic except for $w \geq 0$. Moreover, from the dispersion argument mentioned above, we see that $g(w, z)$ vanishes at infinity. Thus enlarging the $w$ contour infinitely, we obtain

$$\psi(v, z) = \int_0^\infty d\alpha \frac{\rho(\alpha, z)}{\alpha - v}, \tag{2.18}$$

with

$$\rho(\alpha, z) \equiv \lim_{\epsilon \to 0+} [g(\alpha + i\epsilon, z) - g(\alpha - i\epsilon, z)]. \tag{2.19}$$

Substituting (2.18) in (2.13), we see that $f(s, t)$ can be written as (2.3). The uniqueness of the representation was proved in I. Q.E.D.

*Remark 1.* From (2.15) we see

$$\psi(w, z) \equiv 2\pi i g(w, z). \tag{2.20}$$

*Remark 2.* For evaluating (2.16), let $w$ be *real and negative*. Since we have shown that $f(s, t)$ is holomorphic in $D_{s\epsilon}$, the integrand is holomorphic with respect to $s'$ in Im $s' < 0$ because

$$\text{Im } \frac{w - zs'}{1 - z} s'^* = \frac{w}{1 - z} \text{Im } s'^* < 0 \tag{2.21}$$

[see (2.4) with (2.5)]. We thus obtain[7]

$$g(w, z) = \frac{1}{2\pi i} \frac{1}{1 - z} \int_0^\infty ds' \frac{\partial}{\partial w} f_s\left(s', \frac{w - zs'}{1 - z}\right), \tag{2.22}$$

where $f_s(s, t)$ is the absorptive part of $f(s, t)$, i.e.,

$$f_s(s, t) \equiv (2\pi i)^{-1} \lim_{\epsilon \to 0+} [f(s + i\epsilon, t) - f(s - i\epsilon, t)]. \tag{2.23}$$

*Remark 3.* The condition (iii) excludes the single dispersion terms. It also excludes such a function as

$$f(s, t) = -(s + t)^{-1}, \tag{2.24}$$

because (2.24) remains finite if $s$ and $t$ become infinite along a straight line parallel to the real axis but in such a way that Re $s$ + Re $t$ = 0. Indeed, for this example the integral (2.16) does not converge for $z = \frac{1}{2}$. However, (2.22) still gives the correct result if we take it into account the contribution from the infinity appropriately. Namely, putting $s' = 1/x$ in

$$g(w, z) = (2\pi i)^{-1} \int_0^\infty ds'\ \delta'(w + (1 - 2z)s'), \tag{2.25}$$

we have

$$\begin{aligned} g(w, z) &= (2\pi i)^{-1} \int_0^\infty dx\ \delta'(wx + 1 - 2z) \\ &= -(2\pi i)^{-1} w^{-1}\ \delta(1 - 2z). \end{aligned} \tag{2.26}$$

The above situation can happen in (2.3) only when $\rho(\alpha, z)$ contains a ($\delta$-like) singularity, independent of $\alpha$ in $0 < z < 1$. Fortunately, such a situation cannot occur in perturbation theory.

*Remark 4.* If instead of the condition (iii), $|f(s, t)|$ does not exceed $(|s| + |t|)^{N-\delta}$, then in (2.11), $\psi(v, z)$ should be subtracted by $N$ times. The final result is given in (4.11) of I.

## III. INTEGRAL REPRESENTATION FOR SCATTERING AMPLITUDE[8]

In this section we consider the integral representation for scattering amplitude:

$$\int_0^1 dz \int_{-\infty}^\infty d\alpha \frac{\rho_{12}(\alpha, z)}{\alpha - zs - (1 - z)t}$$

[5] If the $s'$ contour is retained to a finite one, the $w$ contour is essentially dependent on $s'$ and then the order exchange of the integrations becomes impossible. On this point the previous proof given in I was incomplete.

[6] H. J. Bremermann, R. Oehme, and J. G. Taylor, Phys. Rev. **109**, 2178 (1958); F. J. Dyson, Phys. Rev. **110**, 579 (1958). The variables in the theorem should be identified with $s + t$ and $s - t$.

[7] This formula was given also in I.

[8] Main results in this section were reported in "Integral Representation for the Scattering Amplitude" (Institute for Advanced Study, Princeton, New Jersey, 1963) (unpublished). The author was indebted to Dr. H. Araki for valuable discussion on the proof of Theorem II.

$$+\int_0^1 dz \int_{-\infty}^{\infty} d\beta \frac{\rho_{23}(\beta, z)}{\beta - zt - (1-z)u}$$
$$+\int_0^1 dz \int_{-\infty}^{\infty} d\gamma \frac{\rho_{31}(\gamma, z)}{\gamma - zu - (1-z)t}, \quad (3.1)$$

where the weight functions $\rho_{12}$, $\rho_{23}$, and $\rho_{31}$ vanish unless

$$\alpha \geq za + (1-z)b,$$
$$\beta \geq zb + (1-z)c,$$
$$\gamma \geq zc + (1-z)a, \quad (3.2)$$

$a$, $b$, and $c$ being certain constants. As is well known, between $s$, $t$, and $u$ there holds an identity

$$s + t + u = d, \quad (3.3)$$

where $d$ stands for the sum of the squared external masses.

As before, we put

$$\hat{s} \equiv s - a, \quad \hat{t} \equiv t - b, \quad \hat{u} \equiv u - c,$$
$$\lambda \equiv a + b + c - d, \quad (3.4)$$

and omit the hat for simplicity. Then (3.1) reduces to

$$F(s, t) \equiv \int_0^1 dz \int_0^{\infty} d\alpha \frac{\rho_{12}(\alpha, z)}{\alpha - zs - (1-z)t}$$
$$+\int_0^1 dz \int_0^{\infty} d\beta \frac{\rho_{23}(\beta, z)}{\beta - zt - (1-z)u}$$
$$+\int_0^1 dz \int_0^{\infty} d\gamma \frac{\rho_{31}(\gamma, z)}{\gamma - zu - (1-z)s}, \quad (3.5)$$

with

$$s + t + u = -\lambda. \quad (3.6)$$

We assume

$$\lambda > 0, \quad (3.7)$$

which is satisfied in almost all practical cases (e.g., equal-mass, $N - N$, $\pi - N$, etc.).[3]

It is evident that the function $F(s, t)$ defined by (3.5) is holomorphic in

$$D \equiv D_{st} \cap D_{tu} \cap D_{us}. \quad (3.8)$$

Our purpose in this section is to investigate its inverse problem as in Sec. II.

*Lemma 1.* $D^*[s, t]$, $D^*[t, s]$, $D^*[t, u]$, $D^*[u, t]$, $D^*[u, s]$, $D^*[s, u]$, and

$$D_0^* \equiv D^*[s] \cup D^*[t] \cup D^*[u] \quad (3.9)$$

are mutually disjoint with one another.

*Proof:* It is evident that $D^*[s, t]$ is disjoint with $D^*[t, s]$, $D^*[t, u]$, $D^*[u, s]$, $D^*[s]$, and $D^*[t]$. First, consider $D^*[s, t] \cap D^*[u, t]$. For any point $(s, t)$ belonging to it, we have

$$\text{Im } t < 0, \quad \text{Im } st^* \geq 0, \quad \text{Im } ut^* \geq 0, \quad (3.10)$$

on account of (2.5). Hence

$$0 \leq \text{Im } (s + u)t^*$$
$$= -\text{Im } (t + \lambda)t^* = -\lambda \text{ Im } t^* < 0. \quad (3.11)$$

This is self-inconsistent. Thus $D^*[s, t] \cap D^*[u, t] = \phi$. $D^*[s, t] \cap D^*[s, u]$ is quite similar. Finally, consider $D^*[s, t] \cap D^*[u]$, for which we have

$$\text{Im } s > 0, \quad \text{Im } t < 0, \quad \text{Im } st^* \geq 0,$$
$$\text{Im } u = -\text{Im } (s + t) = 0, \quad \text{Re } u \geq 0. \quad (3.12)$$

Hence

$$s = s_0 + iv, \quad t = t_0 - iv, \quad v > 0, \quad (3.13)$$

and

$$\text{Im } st^* = \text{Im } (s_0 + iv)(t_0 + iv) = v(s_0 + t_0) \geq 0, \quad (3.14)$$

so that

$$s_0 + t_0 \geq 0. \quad (3.15)$$

On the other hand, Re $u \geq 0$ leads to

$$-\lambda - (s_0 + t_0) \geq 0, \quad (3.16)$$

which is evidently incompatible with (3.15). Thus $D^*[s, t] \cap D^*[u] = \phi$. Q.E.D.

*Lemma 2.*

$$D_{st} \cup (D_{tu} \cap D_{us}) = D[s] \cap D[t]. \quad (3.17)$$

*Proof:* Consider the complement of the left-hand side:

$$D_{st}^* \cap (D_{tu}^* \cup D_{us}^*) = (D_{st}^* \cap D_{tu}^*) \cup (D_{st}^* \cap D_{us}^*). \quad (3.18)$$

Using (2.4) and Lemma 1, we can easily see

$$D^*[t] \subset D_{st}^* \cap D_{tu}^* \subset D^*[s] \cup D^*[t],$$
$$D^*[s] \subset D_{st}^* \cap D_{us}^* \subset D^*[s] \cup D^*[t]. \quad (3.19)$$

From (3.18) and (3.19) we get

$$D_{st}^* \cap (D_{tu}^* \cup D_{us}^*) = D^*[s] \cup D^*[t], \quad (3.20)$$

which is equivalent to (3.17). Q.E.D.

*Theorem II.* If $F(s, t)$ is holomorphic in $D$, it can be decomposed into

$$F = f_{12} + f_{23} + f_{31}, \quad (3.21)$$

where $f_{12}$, $f_{23}$, and $f_{31}$ are holomorphic in $D_{st}$, in $D_{tu}$, and in $D_{us}$, respectively.

*Proof:* We shall make use of the following theorem

which follows from Cartan and Serre's Theorem B and Leray's lemma on the Čech cohomology.[9]

If $f$ is holomorphic in $D_1 \cap D_2$, and if $D_1$, $D_2$, and $D_1 \cup D_2$ are domains of holomorphy, then there exist such functions $f_1$ and $f_2$ that

$$f = f_1 + f_2, \tag{3.22}$$

where $f_1$ and $f_2$ are holomorphic in $D_1$ and in $D_2$, respectively.

From I we know that $D_{st}$ and $D_{tu} \cap D_{us}$ are domains of holomorphy. Furthermore, because of (3.17), $D_{st} \cup (D_{tu} \cap D_{us})$ is also a domain of holomorphy. We can therefore decompose $F$ into

$$F = f'_{12} + f'_3, \tag{3.23}$$

where $f'_{12}$ and $f'_3$ are holomorphic in $D_{st}$ and in $D_{tu} \cap D_{us}$, respectively.

In next step, we must use some trick because $D_{tu} \cup D_{us}$ is *not* a domain of holomorphy. Since $f'_3$ is naturally holomorphic in $D$, it can be decomposed into

$$f'_3 = f'_{23} + f''_{31}, \tag{3.24}$$

where $f'_{23}$ and $f''_{31}$ are holomorphic in $D_{tu}$ and in $D_{us} \cap D_{st}$, respectively. Accordingly $f''_{31}$ is holomorphic in

$$\begin{aligned}(D_{tu} \cap D_{us}) \cup (D_{us} \cap D_{st}) &= D_{us} \cap D[t] \\ &= D_{us} \cap D_0,\end{aligned} \tag{3.25}$$

on account of (3.17) and (2.4), where $D_0$ stands for the Mandelstam domain $D[s] \cap D[t] \cap D[u]$. Since $D_{us}$, $D_0$ and

$$D_{us} \cup D_0 = D[s] \cap D[u] \tag{3.26}$$

are domains of holomorphy, $f''_{31}$ can be decomposed into

$$f''_{31} = f'_{31} + f^{(0)}, \tag{3.27}$$

where $f'_{31}$ and $f^{(0)}$ are holomorphic in $D_{us}$ and in $D_0$, respectively. Finally, it is well known that $f^{(0)}$ can be decomposed into

$$f^{(0)} = f^{(0)}_{12} + f^{(0)}_{23} + f^{(0)}_{31}, \tag{3.28}$$

where $f^{(0)}_{12}$, $f^{(0)}_{23}$, and $f^{(0)}_{31}$ are holomorphic in $D[s] \cap D[t]$, $D[t] \cap D[u]$, and $D[u] \cap D[s]$, respectively. Thus, putting

$$f_{ij} \equiv f'_{ij} + f^{(0)}_{ij}, \tag{3.29}$$

we get the desired result (3.21). Q.E.D.

Unfortunately, we do not yet succeed in proving that, if $F$ vanishes at infinity in $D$, then $f_{ij}$ vanishes at infinity *separately*. Hence, at present the temperedness of $\rho_{ij}(\alpha, z)$ is an additional requirement to the function $F$.

We give the following remarks on the temperedness of $\rho_{ij}$.

(i) For a renormalizable theory, they are bounded in any *finite* order of perturbation theory.

(ii) If they are positive definite, then their behavior at infinity is the same as that of the absorptive parts of the scattering amplitude in the physical regions. This is easily seen from the relations

$$\begin{aligned}&F_s(s, t) \\ &= \pi^{-1} \int_0^1 dz\theta(zs + (1-z)t)\rho_{12}(zs + (1-z)t, z) \\ &+ \pi^{-1} \int_0^1 dz\theta(zu + (1-z)s)\rho_{31}(zu + (1-z)s, z),\end{aligned} \tag{3.30}$$

for $s > 0$, $t < 0$, $u < 0$, etc.

(iii) If the Mandelstam representation[10] is assumed, $\rho_{ij}$ are, of course, tempered because of Theorem I.

## IV. ASYMPTOTIC BEHAVIOR OF THE WEIGHT FUNCTION

It will be an important problem to find the asymptotic behavior of the weight function, which we investigate by means of perturbation theory in this section. It is well known, however, that the whole, unrenormalized perturbation series containing scalar propagators only is divergent for any nontrivial value of the coupling constant.[11] Hence, we must content ourselves with considering some subseries which contains infinitely many Feynman graphs.

The following argument will be equally applicable to the vertex function, the production amplitude, etc., but for definiteness we consider the scattering amplitude. Let $G$ be a connected Feynman graph, in which $N$ is the number of internal lines, $m$ being the number of vertices. Then the number of independent circuits is given by

$$n = N - m + 1. \tag{4.1}$$

If there are scalar particles only, the scattering

[9] H. Cartan and J. P. Serre, "Séminaire sur les fonctions de plusieurs variables," (Paris, 1951–1952, 1953–1954) (unpublished). See also reference 9 of I.

[10] S. Mandelstam, Phys. Rev. **112**, 1344 (1958); **115**, 1741, 1752 (1959).

[11] C. A. Hurst, Proc. Roy. Soc. (London) **A214**, 44 (1952); Proc. Cambridge Phil. Soc. **48**, 625 (1952). W. Thirring, Helv. Phys. Acta **26**, 33 (1953). M. A. Petermann, Helv. Phys. Acta **26**, 291 (1953). See also N. Nakanishi, Progr. Theoret. Phys. (Kyoto) **17**, 401 (1957).

amplitude corresponding to $G$ is given by[12]

$$F^G(s, t) = c\cdot(N - 2n - 1)! \int dx U^{-2}(V - i\epsilon)^{-N+2n} \tag{4.2}$$

in the Feynman parametric form. Here we have assumed $N > 2n$, and the notations are as follows:

$$0 < c \leq \lambda^m/(4\pi)^{2n}, \tag{4.3}$$

where $\lambda$ is the largest coupling constant;

$$\int dx \equiv \int_0^1 dx_1 \cdots \int_0^1 dx_N\, \delta\Big(1 - \sum_{i=1}^N x_i\Big), \tag{4.4}$$

where $x_i$ is a Feynman parameter corresponding to an internal line $i$;

$$U \equiv \sum x_{\nu_1} x_{\nu_2} \cdots x_{\nu_n}, \tag{4.5}$$

where the summation goes over all possible sets $\{\nu_1, \nu_2, \cdots, \nu_n\}$ such that the corresponding Feynman integration momenta $p_{\nu_1}, p_{\nu_2}, \cdots, p_{\nu_n}$ are linearly independent;

$$V \equiv \sum_{i=1}^N x_i m_i^2 - \sum_{I=A}^D \zeta_I M_I^2 - \zeta_{AB} s - \zeta_{AC} t - \zeta_{AD} u, \tag{4.6}$$

with

$$s + t + u = \sum_{I=A}^D M_I^2, \tag{4.7}$$

and

$$0 \leq \zeta_h \leq 1, \quad (h = A, B, C, D, AB, AC, AD), \tag{4.8}$$

where $m_i$ and $M_I$ are an internal mass and an external one, respectively.

The corresponding weight function $\rho_{12}^G(\alpha, z)$ is defined by

$$\rho_{12}^G(\alpha, z) \equiv c \int dx \frac{\varphi}{(g + h)^{N-2n}} \times \delta^{(N-2n-1)}\Big(\alpha - \frac{f}{g + h}\Big)\, \delta\Big(z - \frac{g}{g + h}\Big), \tag{4.9}$$

with

$$\begin{aligned} f &\equiv \sum_i x_i m_i^2 - \sum_I (\zeta_I + \zeta_{AD}) M_I^2, \\ g &\equiv \zeta_{AB} - \zeta_{AD}, \\ h &\equiv \zeta_{AC} - \zeta_{AD}, \\ \varphi &\equiv \theta(\zeta_{AB} - \zeta_{AD})\theta(\zeta_{AC} - \zeta_{AD}) U^{-2}. \end{aligned} \tag{4.10}$$

[12] Original Proofs are: N. Nakanishi, Progr. Theoret. Phys. (Kyoto) **17**, 401 (1957); Y. Nambu, Nuovo Cimento **6**, 1064 (1957); K. Symanzik, Progr. Theoret. Phys. (Kyoto) **20**, 690 (1958). Reviews and further proofs are: N. Nakanishi, Progr. Theoret. Phys. (Kyoto) Suppl. **18**, 1 (1961), Part I; Progr. Theoret. Phys. (Kyoto) **26**, 337 (1961); T. Kinoshita, J. Math. Phys. **3**, 650 (1962); Y. Shimamoto, Nuovo Cimento **25**, 1292 (1962).

Let $\psi(z)$ be an arbitrary function continuous in $0 \leq z \leq 1$. Then we have

$$\int_0^1 dz \psi(z) \int_0^\infty \frac{d\alpha}{\alpha}\, \rho_{12}^G(\alpha, z) = c\cdot(N - 2n - 1)! \int dx \frac{\varphi}{f^{N-2n}} \psi\Big(\frac{g}{g + h}\Big), \tag{4.11}$$

if $f > 0$, or more precisely, if we introduce the following assumption for an infinite set, $\Phi$, of graphs.

*Assumption A.* There is a positive constant $a$ such that

$$\forall G \in \Phi : f \geq a, \quad \text{when} \quad \varphi \not\equiv 0. \tag{4.12}$$

Now, let

$$b \equiv \max |\psi(z)|. \tag{4.13}$$

Then we have

$$\Big|\int_0^1 dz \psi(z) \int_0^\infty \frac{d\alpha}{\alpha}\, \rho_{12}^G(\alpha, z)\Big| \leq \frac{\lambda^m b}{(4\pi)^{2n} a^{N-2n}} (N - 2n - 1)! \int \frac{dx}{U^2}. \tag{4.14}$$

We further impose the following conditions on $\Phi$.

*Assumption B.* There is a constant $\sigma$ for all $G \in \Phi$ such that

$$\text{(i)} \quad \forall H \subset G : 2n(H)/N(H) \leq \sigma < 1, \tag{4.15}$$

where $H$ stands for a nontrivial subgraph of $G$, $N(H)$ and $n(H)$ being the $N$ and the $n$ of $H$, respectively;

$$\text{(ii)} \quad \exists k : \sigma N - 2n \leq k, \tag{4.16}$$

where $k$ is an integer independent of the order $m$.

*Lemma.* If $G$ satisfies (4.15), then one has

$$U^2 \geq \prod_{i=1}^N x_i^\sigma \quad \text{for} \quad 0 \leq x_i \leq 1. \tag{4.17}$$

*Proof:* Since numbering of lines is not specified, we may assume

$$1 \geq x_N \geq x_{N-1} \geq \cdots \geq x_1 \geq 0, \tag{4.18}$$

without loss of generality. We choose a set of lines $\{\nu_1, \nu_2, \cdots, \nu_n\}$ in such a way that $\nu_1 = N$, and $\nu_j$ is the largest number among those in which $p_{\nu_j}$ is linearly independent of $p_{\nu_1}, \cdots, p_{\nu_{j-1}}$. Then, of course, $p_{\nu_1}, p_{\nu_2}, \cdots, p_{\nu_n}$ are linearly independent so that

$$x_{\nu_1} x_{\nu_2} \cdots x_{\nu_n} \in U, \tag{4.19}$$

namely,

$$U^2 \geq x_{\nu_1}^2 x_{\nu_2}^2 \cdots x_{\nu_n}^2. \tag{4.20}$$

Let $C_1, C_2, \cdots, C_n$ be the circuits along which $p_{\nu_1}, p_{\nu_2}, \cdots, p_{\nu_n}$ flow, respectively. Let

$$H_j \equiv \bigcup_{i=0}^{j-1} C_{n-i}. \tag{4.21}$$

By assumption we know

$$2j = 2n(H_j) \leq \sigma \cdot N(H_j) \quad (j = 1, 2, \cdots, n), \tag{4.22}$$

so that

$$x_{\nu_1}^2 \cdots x_{\nu_{n-1}}^2 x_{\nu_n}^2 \geq [x_{\nu_1}^{\alpha_n} \cdots x_{\nu_{n-1}}^{\alpha_2} x_{\nu_n}^{\alpha_1}]^\sigma, \tag{4.23}$$

with

$$\alpha_j \equiv N(H_j) - N(H_{j-1}) \quad (j = 2, \cdots, N), \qquad \alpha_1 \equiv N(H_1). \tag{4.24}$$

Furthermore, we have

$$\forall i \in H_j : x_{\nu_j} \geq x_i, \tag{4.25}$$

because if $\exists i : x_{\nu_j} < x_i$, then $i > \nu_j$, and $i \notin G - H_j$, i.e., $p_i$ is independent of $p_{\nu_1}, \cdots, p_{\nu_{j-1}}$; and the existence of such a line $i$ is inconsistent with our choice of $\nu_j$. Hence

$$x_{\nu_1}^{\alpha_n} \cdots x_{\nu_{n-1}}^{\alpha_2} x_{\nu_n}^{\alpha_1} \geq \prod_{i=1}^{N} x_i. \tag{4.26}$$

Collecting (4.20), (4.23), and (4.26), we get the desired result (4.17). Q.E.D.

We thus have

$$\int dx U^{-2} \leq \int dx \prod_{i=1}^{N} x_i^{-\sigma}. \tag{4.27}$$

The generalized beta-function formula leads to

$$\int dx \prod_{i=1}^{N} x_i^{-\sigma} = [\Gamma(1-\sigma)]^N / \Gamma(N(1-\sigma)). \tag{4.28}$$

Accordingly, we obtain

$$(N-2n-1)! \int \frac{dx}{U^2} \leq [\Gamma(1-\sigma)]^N \frac{\Gamma(N-2n)}{\Gamma(N-\sigma N)} < [\Gamma(1-\sigma)]^N (N-2n)^k \tag{4.29}$$

on account of (4.16). Since

$$N < m/(1 - \tfrac{1}{2}\sigma), \tag{4.30}$$

and

$$(N-2n)^k < m^k < 2^m,$$

for $m$ large, from (4.29) we can see that the right-hand side of (4.14) behaves at most (const)$^m$. Therefore, if the number of $m$th-order graphs belonging to $\Phi$ increases at most as (const)$^m$, and if the coupling constant $\lambda$ is sufficiently small, then we have

$$\left| \int_0^1 dz \psi(z) \int_0^\infty \frac{d\alpha}{\alpha} \rho_{12}^{\Phi}(\alpha, z) \right| \leq \sum_{G \in \Phi} \left| \int_0^1 dz \psi(z) \int_0^\infty \frac{d\alpha}{\alpha} \rho_{12}^{G}(\alpha, z) \right| < \infty, \tag{4.31}$$

where

$$\rho_{12}^{\Phi}(\alpha, z) \equiv \sum_{G \in \Phi} \rho_{12}^{G}(\alpha, z). \tag{4.32}$$

The above inequality shows

$$\rho_{12}^{\Phi}(\alpha, z) = o(1), \tag{4.33}$$

for $\alpha \to \infty$ if we assume that $\rho_{12}^{\Phi}(\alpha, z)$ does not oscillate infinitely. Without such an assumption, exactly in the same way as for (4.31), we can prove

$$\left| \int_0^\infty dz \psi(z) \int_0^\infty d\alpha \frac{\rho_{12}^{\Phi}(\alpha, z)}{[\alpha - zs - (1-z)t]^r} \right| < \infty, \tag{4.34}$$

where Re $r \geq 1$ and $|\alpha - zs - (1-z)t| \geq a > 0$ for $\rho_{12}^{G}(\alpha, z) \not\equiv 0$. It will turn out that (4.34) is sufficient for practical applications.

Now, it remains to investigate in what cases Assumptions A and B are satisfied. Assumption A is certainly satisfied if a nonforward dispersion relation can be proved in perturbation theory. For instance, in the equal-mass case we know an inequality[13]:

$$\sum_{i=1}^{N} x_i \mu^2 - \sum_{I=A}^{D} (\zeta_I + \zeta_{AD}) \cdot 2\mu^2 - (\zeta_{AB} - \zeta_{AD}) \cdot 4\mu^2 - (\zeta_{AC} - \zeta_{AD}) \cdot 4\mu^2 \geq 0. \tag{4.35}$$

Hence when $g \geq 0$ and $h \geq 0$, we have

$$2f \geq \sum_i x_i \mu^2 = \mu^2, \tag{4.36}$$

so that $a \equiv \frac{1}{2}\mu^2$.

Assumption B is satisfied if for any $G$ of $\Phi$ there are 3-vertices only and no self-energy parts. Let $r(H)$ be the number of external lines of $H$. Then, in the present case, we have

$$N(H) = \tfrac{3}{2} m(H) - \tfrac{1}{2} r(H), \qquad n(H) = \tfrac{1}{2} m(H) - \tfrac{1}{2} r(H) + 1. \tag{4.37}$$

Since $r(H) \geq 3$,

$$2n(H)/N(H) \leq \tfrac{2}{3} \equiv \sigma. \tag{4.38}$$

Furthermore,

$$\sigma N - 2n = \tfrac{2}{3} < 1 \equiv k. \tag{4.39}$$

Thus Assumption B is satisfied. Even if there are 4-vertices, Assumption B can be still satisfied if there are also 2-vertices so as to prevent $n/N$ from increasing.

[13] For instance, N. Nakanishi, Progr. Theoret. Phys. (Kyoto) Suppl. **18**, 1 (1961), Part III. See also reference 3.

## V. ANALYTICITY IN COMPLEX ANGULAR-MOMENTUM PLANE

Recently, it has become of special interest to investigate the analyticity in complex angular-momentum plane of the relativistic scattering amplitude. A number of authors[14] have made use of the Mandelstam representation,[10] which is known to be valid only for very special kinds of graphs. On the other hand, Polkinghorne[15] and Federbush and Grisaru[16] have obtained the Regge behavior by summing the generalized ladder graphs in perturbation theory. They assume that the asymptotic behavior of the sum is given by the sum of the leading terms, but plausible counterexamples against this assumption can be easily found.[17] Under the same assumption, Bjorken and Wu[18] have obtained a non-Regge behavior by summing the so-called truss–bridge graphs in which three-particle intermediate states are important.

Now, in Sec. IV we have rigorously proved that when the Lagrangian density is given by

$$L = -\tfrac{1}{2}[(\partial\phi/\partial x_\nu)^2 + \mu^2\phi] + \tfrac{1}{3}\lambda\phi^3, \qquad (5.1)$$

an approximate scattering amplitude $F^\Phi(s, t)$ can be represented as (3.1) with $\alpha, \beta, \gamma \geq 4\mu^2$,[3] if $\lambda$ is sufficiently small. Here $F^\Phi(s, t)$ is a sum over such a subseries that there are no graphs containing self-energy parts and that the number of $m$th-order graphs increases at most as $(\text{const})^m$. It is evident from (3.1) that

$$F^\Phi(s, t) \to 0 \quad \text{as} \quad |t| \to \infty, \qquad (5.2)$$

when $s$ is fixed. According to the Regge analysis, (5.2) suggests that the partial-wave amplitude corresponding to $F^\Phi(s, t)$ is a holomorphic function of the angular momentum $l$ in the right half-plane. Khuri has pointed out that this is indeed the case as is shown by applying his theorem,[19] from which the following statement follows.

The rightmost singularity of the partial-wave amplitude in $\text{Re}\ l > -\frac{1}{2}$ is located at the same position as that of the coefficient in the power-series expansion with respect to $t$.

In our case we have[20]

$$F^\Phi(s, t) = \sum_{l=0}^{\infty} f_t^\Phi(s, l)t^l + \sum_{l=0}^{\infty} f_u^\Phi(s, l)u^l, \qquad (5.3)$$

except for a neighborhood of $s \geq 4\mu^2$, where

$$f_t^\Phi(s, l) \equiv \int_0^1 dz \int_{4\mu^2}^\infty d\alpha \frac{(1-z)^l \rho_{12}^\Phi(\alpha, z)}{(\alpha - zs)^{l+1}}$$

$$+ \int_{\frac{1}{2}}^1 dz \int_{4\mu^2}^\infty d\beta \frac{(2z-1)^l \rho_{23}^\Phi(\beta, z)}{[\beta - (1-z)(4\mu^2 - s)]^{l+1}}, \qquad (5.4)$$

$f_u^\Phi(s, l)$ being similar. It is evident from (4.33) or (4.34) that $f_t^\Phi$ and $f_u^\Phi$ are holomorphic in $\text{Re}\ l \geq 0$ when continued in the natural way.

Clearly our subseries is much more general than that of Polkinghorne and others. Especially, graphs in the former may contain many intermediate states for the crossed channels. Our result is, however, not inconsistent with the conclusion of Bjorken and Wu because their example does not satisfy Assumption B and our analysis does not give the exact location of the rightmost singularity in the $l$ plane. But we may say that the three-or-more-particle intermediate states do not have a very important effect on the analyticity in the $l$ plane.

*Note added in proof.* The envelope of holomorphy of $D_+ \cup D_- \cup E$ was investigated by Glaser by using a parametric dispersion relation under the assumption of boundedness. [See A. Bottino, A. M. Longoni, and T. Regge, Nuovo Cimento **23**, 954 (1962); A. Bottino and A. M. Longoni, Nuovo Cimento **24**, 353 (1962)]. It is easily shown that his result is naturally identical with $D_{st}$.


### ACKNOWLEDGMENTS

The author is much indebted to Dr. N. N. Khuri for a helpful suggestion, and to Professor F. J. Dyson for kind interest. He would also like to express his thanks both to Professor J. R. Oppenheimer for the hospitality extended to him at the Institute for Advanced Study, and to the National Science Foundation for financial support.


[14] For instance, V. N. Gribov, Zh. J. Eksperim i Theor. Fiz. **41**, 1962 (1961) [English transl.: Soviet Phys.—JETP **14** 1395 (1962)]. M. Froissart, unpublished talk at La Jolla Conference (1961); Phys. Rev. **123**, 1053 (1961); A. O. Barut and D. E. Zwanziger, Phys. Rev. **127**, 974 (1962).

[15] J. C. Polkinghorne, J. Math. Phys. **4**, 503 (1963).

[16] P. G. Federbush and M. T. Grisaru, Ann. Phys. (N. Y.) **22**, 263, 299 (1963).

[17] For example,

$$\sum_{m=0}^{\infty} \frac{(\log t)^m}{m!\, t}\left(1 + \frac{3^m}{t!}\right).$$

[18] J. D. Bjorken and T. T. Wu, Phys. Rev. **130**, 2566 (1963).

[19] N. N. Khuri, Phys. Rev. Letters **10**, 420 (1963), and Phys. Rev. **130** 429 (1963).

[20] The first and the second term in (5.3) correspond to the direct, and exchange scattering, respectively.

# Singularities of Regge Trajectories and Asymptotes to Landau Curves*

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A new class of singularities associated with the trajectories and residues of particular Regge poles is investigated. It is shown that the singularities are associated with properties of asymptotes to Landau curves. One of the singularities corresponds to the singularity of the Regge amplitude discovered recently by Islam, Landshoff, and Taylor. The only singularities affecting physical asymptotic behavior correspond to diagrams which have all three Mandelstam spectral functions.

## 1. INTRODUCTION

SERIES expansions have recently been given[1,2,3,4] for Regge-pole trajectories $\alpha(s)$ which are derived from evaluating the asymptotic behavior of Feynman diagrams. The terms in these series consist of integrals having a structure similar to that associated with self-energy diagrams. They therefore exhibit the expected $s$-channel normal threshold singularities. However, extra factors occur in the integrands which have no counterpart in the Feynman integrals associated with self-energy diagrams. These factors produce further singularities of $\alpha(s)$, some of which are on the physical sheet. This is discussed in Sec. 2.

Recently Islam, Landshoff, and Taylor[5] have found an unexpected singularity of the Regge amplitude $a(l, s)$. Their argument is based on the properties of the asymptotes of a certain Landau curve, the leading curve of the tetrahedron diagram. In Sec. 3 it is shown that this is a particular example of the class of singularities discussed in Sec. 2. The equivalence is established by means of an algorithm for calculating asymptotes to Landau curves.

In Sec. 4 the analytic properties of the coefficient function $\beta(s)$ are discussed. The terms in its series expansion contain integrals with structures similar to those of vertex parts. The singularities will, therefore, include $s$-channel normal thresholds and, in appropriate circumstances, anomalous thresholds. In addition, there are further singularities which again can be associated with the asymptotes to Landau curves.

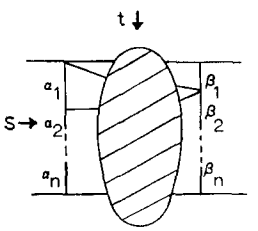


FIG. 1. A typical diagram considered.

## 2. SINGULARITIES OF REGGE TRAJECTORIES

We consider those contributions to the series expansions of Regge-pole trajectories which are associated with ladderlike iterations[6] since it is these which produce singularities which are most simply associated with four-point Landau curves.

A typical contribution is associated with a Feynman diagram like Fig. 1. The $\alpha$'s and $\beta$'s are the Feynman parameters associated with the two $n$ lines[3] and the remaining Feynman parameters are denoted by $\gamma_i$. The blob must not contain within itself an $m$ line with $m \leq n$. The number of lines joining each point of an $n$ line to the blob can be arbitrary. The coefficient of $t$ in the denominator of the Feynman integral associated with Fig. 1 is denoted by $g(\alpha, \beta, \gamma)$. This diagram gives a contribution to $\alpha(s)$ which contains the function

$$A_n(s) = \int_0^1 \frac{d\bar{\alpha}\, d\bar{\beta}\, d\gamma\ \delta(\sum \bar{\alpha} - 1)\ \delta(\sum \bar{\beta} - 1)\ \delta(\sum \gamma - 1)}{[\bar{g}(\bar{\alpha}, \bar{\beta}, \gamma)]^n} \times \frac{[c(\gamma)]^x}{[d(\gamma, s)]^y}, \qquad (1)$$

where $\bar{g}$ is formed from $g$ by deleting all products involving more than one $\alpha$ and one $\beta$, and $c$ and $d$ are the numerator and denominator functions asso-

* The research reported in this document has been sponsored in part by the Air Force Office of Scientific Research, OAR, through the European Office, Aerospace Research, United States Air Force.

[1] J. C. Polkinghorne, J. Math. Phys. 4, 503 (1963).
[2] P. G. Federbush and M. T. Grisaru, Ann. Phys. (N. Y.) 22, 263, 299 (1963).
[3] I. G. Halliday, to be published (Department of Applied Mathematics and Theoretical Physics, Cambridge University preprint).
[4] N. H. Fuchs, J. Math. Phys. 4, 617 (1963).
[5] J. N. Islam, P. V. Landshoff, and J. C. Taylor, Phys. Rev. 130, 2560 (1963).

[6] More complicated iterations also give Regge poles; see references 3 and 4.

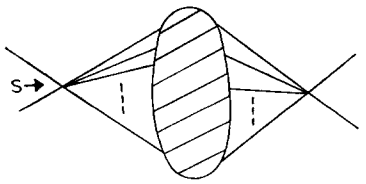
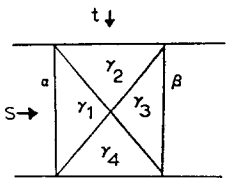



FIG. 2. The self-energy part corresponding to Fig. 1.

FIG. 3. The tetrahedron diagram.




ciated with the self-energy part, Fig. 2. The exponents $x$ and $y$ can be calculated but are irrelevant to our discussion.

In addition to normal threshold and second-type singularities, $A_n(s)$ has singularities given by

$$\lambda\bar{g}(\bar{\alpha}, \bar{\beta}, \gamma) = 0, \tag{2}$$

$$d(\gamma, s) = 0, \tag{3}$$

$$\lambda\bar{\alpha}_i(\partial\bar{g}/\partial\bar{\alpha}_i) = 0, \qquad i = 1, 2, \cdots, n, \tag{4}$$

$$\lambda\bar{\beta}_i(\partial\bar{g}/\partial\bar{\beta}_i) = 0, \qquad i = 1, 2, \cdots, n, \tag{5}$$

$$\gamma_i(\lambda(\partial\bar{g}/\partial\gamma_i) + (\partial d/\partial\gamma_i)) = 0, \quad i = 1, 2, \cdots, \tag{6}$$

where $\lambda$ is a Lagrange multiplier.[7] A singularity can only occur in a Regge trajectory associated with the physical asymptotic behavior if it corresponds to positive values of $\bar{\alpha}$, $\bar{\beta}$, $\gamma$. In order to satisfy Eq. (2), in these circumstances it is necessary that Fig. 1 should be a diagram not having a proper dual (i.e., it should have all its three Mandelstam spectral functions nonzero). A simple diagram which will give a singularity of this type for physical $\alpha(s)$ is given by Fig. 3 for which

$$\bar{g} = \bar{\alpha}\bar{\beta}(\gamma_1\gamma_3 - \gamma_2\gamma_4). \tag{7}$$

This is the diagram considered by Islam, Landshoff and Taylor.[5]

### 3. ASYMPTOTES TO LANDAU CURVES

The asymptotes of some simple Landau curves are given by their normal threshold contractions but it is known that not all asymptotes are normal thresholds. In this section we will develop a method for finding asymptotes of the leading Landau curve associated with Fig. 1.

The denominator function of the corresponding Feynman integral can be written in the form

$$D = g(\xi)t + \delta(\xi, s), \tag{8}$$

where $\xi$ is used as a generic symbol for the $\alpha$'s, $\beta$'s, and $\gamma$'s. The leading Landau curve is given by

$$\partial D/\partial\xi_i = 0, \qquad i = 1, 2, \cdots, \tag{9}$$

which has as a consequence

$$D = 0. \tag{10}$$

If (9) is to be satisfied as $t$ tends to infinity, then either some $\xi$'s tend to infinity, or the $g_i(\xi)$ tend to zero. We consider the latter possibility.

We write

$$t = t'/z^2, \tag{11}$$

$$\alpha_i = \bar{\alpha}_i z, \tag{12}$$

$$\beta_i = \bar{\beta}_i z. \tag{13}$$

Then

$$D = \tilde{g}t' + \delta, \tag{14}$$

where

$$\tilde{g} = g/z^2. \tag{15}$$

Equations (9) may be written

$$t'(\partial\tilde{g}/\partial\bar{\alpha}_i) + z(\partial\delta/\partial\alpha_i) = 0, \tag{16}$$

$$t'(\partial\tilde{g}/\partial\bar{\beta}_i) + z(\partial\delta/\partial\beta_i) = 0, \tag{17}$$

$$t'(\partial\tilde{g}/\partial\gamma_i) + (\partial\delta/\partial\gamma_i) = 0. \tag{18}$$

Putting $z = 0$ to correspond to $t$ infinite, $\tilde{g}$ and its derivatives become identical with $\bar{g}$ and its derivatives, and $\delta$ and its $\gamma$ derivatives become identical with $d$ and its $\gamma$ derivatives. Thus a point at infinity in $t$ on the Landau curve is given by

$$t'(\partial\bar{g}/\partial\bar{\alpha}_i) = 0, \tag{19}$$

$$t'(\partial\bar{g}/\partial\bar{\beta}_i) = 0, \tag{20}$$

$$t'(\partial\bar{g}/\partial\gamma_i) + (\partial d/\partial\gamma_i) = 0. \tag{21}$$

The function $\bar{g}$ is homogeneous of degree one in $\bar{\alpha}_i$ (and also in $\bar{\beta}_i$), so that (19) [or (20)] implies

$$\bar{g} = 0. \tag{22}$$

Then from the analogue of (10) we deduce also that

$$d = 0. \tag{23}$$

Equations (19)–(23) reproduce the leading singularity of Eqs. (2)–(6) with $\lambda = t'$. The other singu-

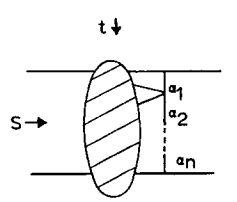



FIG. 4. A diagram contributing to $\beta(s)$.

[7] See lectures by J. C. Polkinghorne in *1961 Brandeis Summer Institute Lectures in Theoretical Physics* (W. A. Benjamin Company, Inc., New York, 1962), Vol. I.

larities correspond to asymptotes of lower-order Landau curves.

Normal threshold asymptotes correspond to $t' = 0$, that is, to writing

$$t = t''/z, \qquad \alpha_i = \bar{\alpha}_i z, \qquad \beta_i = \bar{\beta}_i z. \tag{24}$$

This method can also be used to search for asymptotes not parallel to the $s$, $t$, or $u$ axes since the function $D$ is linear in $s$, $t$, $u$, and so it is equally possible to consider any linear combination of $s$, $t$, $u$ tending to infinity.

## 4. SINGULARITIES OF $\beta(s)$

A typical diagram contributing to $\beta(s)$ is shown in Fig. 4. It is bounded by an $n$ line, and the blob must not contain within itself an $m$ line with $m \leq n$. The coefficient of $t$ in denominator of the Feynman integral associated with Fig. 4 is denoted by $g(\alpha, \gamma)$, where $\alpha$ denotes the Feynman parameters of the $n$ line and $\gamma$ the remaining Feynman parameters. This diagram gives a contribution to $\beta(s)$ which contains the function

$$B_n(s) = \int_0^1 \frac{d\bar{\alpha}\, d\gamma\, \delta(\sum \bar{\alpha} - 1)\, \delta(\sum \gamma - 1)}{[\bar{g}(\bar{\alpha}, \gamma)]^n} \times \frac{[c(\gamma)]^x}{[d(\gamma, s)]^y}, \tag{25}$$

where $c$ and $d$ refer to the vertex part obtained by contracting the $n$ line, and $\bar{g}$ is formed from $g$ by omitting products with more than one $\alpha$. In addition to the normal, anomalous, and second-type singularities of the associated vertex part, $B_n(s)$ has singularities given by

$$\lambda \bar{g} = 0, \tag{26}$$

$$d = 0, \tag{27}$$

$$\lambda \bar{\alpha}_i (\partial \bar{g}/\partial \bar{\alpha}_i) = 0, \quad i = 1, 2, \cdots n, \tag{28}$$

$$\gamma_i (\lambda (\partial \bar{g}/\partial \gamma_i) + (\partial d/\partial \gamma_i)) = 0, \quad i = 1, 2, \cdots . \tag{29}$$

These can be associated with asymptotes of the Landau curves associated with Fig. 4 and calculated by writing

$$t = t'/z, \tag{30}$$

$$\alpha_i = \bar{\alpha}_i z. \tag{31}$$

## 5. DISCUSSION

It is not difficult to see from a more general view point how the singularities discussed in this paper arise. The Froissart–Gribov definition[8] of $a(\ell, s)$ contains integrals of the form

$$\int_{z_1}^{\infty} \rho(s, z) Q_\ell(z)\, dz, \tag{32}$$

where $z$ is the scattering angle and $\rho$ is a $t$- or $u$-channel discontinuity. The expression (32) will have an end-point singularity for a value of $s$ for which a singularity of $\rho$ occurs at $z = \infty$. Such values of $s$ correspond to asymptotes to Landau curves. The normal threshold singularities in $s$ occur in this way since $\rho$ itself does not have $s$-channel normal thresholds. The singularities of $\rho$ on the physical sheet include the curves of virtual singularity[7] which are the boundaries of Mandelstam spectral functions. It is known that these correspond to positive $\alpha$'s.[9]

The analysis of this paper confirms the existence of the singularity discovered by Islam, Landshoff, and Taylor[5] and shows that it is a member of a wide class of singularities. We are also able to show that these singularities occur in the trajectories and residues of particular Regge poles.

The only singularities which are relevant to physical asymptotic behavior correspond to Feynman diagrams which have three Mandelstam spectral functions. They provide, therefore, another example of a phenomenon associated with a relativistic theory which will not have a counterpart in nonrelativistic potential models.

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[8] M. Froissart, Proceedings of the La Jolla Conference 1961 (unpublished); V. Gribov, Zh. Eksperim. i Teor. Fiz. **41**, 1221 (1961) [English transl.: Soviet Phys.—JETP **14**, 871 (1962)].

[9] This follows from the work of T. T. Wu, Phys. Rev. **123**, 678 (1961).

# High-Energy Behavior in Perturbation Theory. II*

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Contributions to the asymptotic behavior of Feynman integrals are evaluated which correspond to pinches in the interior of the hypercontour of integration. It is shown that they give the Gribov–Pomeranchuk phenomenon and Regge cuts. A set of diagrams is investigated which gives a Regge cut on the physical sheet.

## 1. INTRODUCTION

HIGH-energy behavior which is Regge pole-like has recently been discovered in a wide class of perturbation-theory diagrams.[1-4] The method has been used to extend Regge behavior to production processes[5] and to exhibit a new class of singularities of particular Regge trajectories.[6]

Feynman integrals only give a significant high-energy contribution from regions of the hypercontour of integration over the Feynman parameters in which $g(\alpha)$, the coefficient of the asymptotic variable $t$, vanishes. Moreover, these must be regions which cannot be avoided by some permissible distortion of the hypercontour. In $I$ the regions discussed were edges of the hypercontour given by the vanishing of a number of $\alpha$'s. All Regge-pole behavior that has been discovered in perturbation theory corresponds to these edge contributions. Since the edges are always fixed parts of the hypercontour, the corresponding asymptotic behavior will be found on all Riemann sheets of the Feynman amplitude.

In addition to the edges, there may be other regions of the hypercontour in which the coefficient $g(\alpha)$ vanishes and which give a contribution to the asymptotic behavior because the hypercontour is trapped there by pinches as $t \to \infty$. It is characteristic of pinching configurations that they only contribute to certain Riemann sheets of the function so that the corresponding asymptotic behavior will not be found on all sheets of the Feynman amplitude. The Feynman integrals which give *physical* asymptotic behavior correspond to integrations over undistorted positive $\alpha$ contours. In these circumstances $g(\alpha)$ can only vanish away from an edge for diagrams not possessing a proper dual, a class which includes all amplitudes with all three Mandelstam spectral functions nonzero. These are just the diagrams which do not have a simple analogy to potential theory, and it is therefore not surprising that the corresponding asymptotic behavior corresponds to fixed singularities[7] and moving cuts.[8-10]

On a given Riemann sheet of the amplitude, its asymptotic behavior is given by the combination of the contributions from the edges and the pinch contributions. The problem of determining what contributions occur on a given Riemann sheet is equivalent to determining what Landau singularities[11] occur at $t = \infty$ for all $s$ on this sheet.

In this paper we analyze the form of some typical pinch contributions. In Sec. 2 the simplest illustrative example is given, and this is used to show how the Gribov–Pomeranchuk (G–P) phenomenon[7] occurs in perturbation theory. In Sec. 3 it is pointed out that the A–F–S-type cut[8,9,12] must occur on unphysical sheets, and it is shown how this arises in perturbation theory. Finally in Sec. 4 the analysis is used to show the existence on the physical sheet of cuts arising from a set of diagrams which has also been discussed by Mandelstam.[10]

## 2. THE GRIBOV-POMERANCHUK PHENOMENON

A simple but instructive example is provided by

$$I = \int_{x_1}^{x_2} dx \int_{y_1}^{y_2} dy \, \frac{1}{[xyt + d]^{n+2}}. \qquad (1)$$

* The research reported in this document has been sponsored in part by the Air Force Office of Scientific Research, OAR, through the European Office, Aerospace Research, United States Air Force.

[1] J. C. Polkinghorne, J. Math. Phys. 4, 503 (1963). Referred to as I.

[2] P. G. Federbush and M. T. Grisaru, Ann. Phys. (N. Y.) 22, 263, 299 (1963).

[3] I. G. Halliday, Nuovo Cimento (to be published).

[4] N. H. Fuchs, J. Math. Phys. 4, 617 (1963).

[5] I. G. Halliday and J. C. Polkinghorne, Phys. Rev. 132, 852 (1963).

[6] J. C. Polkinghorne, J. Math. Phys. 4, 1393 (1963), previous paper.

[7] V. N. Gribov and I. Ya Pomeranchuk, Phys. Letters 2, 239 (1962).

[8] D. Amati, S. Fubini, and A. Stanghellini, Nuovo Cimento 26, 896 (1962).

[9] J. C. Polkinghorne, Phys. Rev. 128, 2459 (1962).

[10] S. Mandelstam (to be published).

[11] See lectures by R. J. Eden and J. C. Polkinghorne in *1961 Brandeis Summer Institute Lectures in Theoretical Physics* (W. A. Benjamin and Company, New York, 1962), Vol. I.

[12] J. C. Polkinghorne, Phys. Letters 4, 24 (1963).

If none of the end points of integration are zero, it might appear that $I \sim t^{-n-2}$ as $t \to \infty$. It is not difficult to evaluate $I$ exactly. The answer has the form

$$-\frac{1}{(n+1)td^{n+1}} \log \frac{(x_1y_1t+d)(x_2y_2t+d)}{(x_1y_2t+d)(x_2y_1t+d)} + R(t), \quad (2)$$

where $R(t)$ is a rational function of $t$ which need not be given here explicitly. As $t \to \infty$, the logarithm tends to log 1. If the principal branch of the logarithm is chosen, cancellations between the first and second terms of (2) make $I \sim t^{-n-2}$ as $t \to \infty$, as expected. However, if a branch is chosen on which log 1 $= 2\pi mi$ ($m$ a nonzero integer), the leading asymptotic behavior is

$$I \sim -[2\pi mi/(n+1)d^{n+1}]t^{-1}. \quad (3)$$

If the lower limits $x_1$ and $y_1$ are both greater than zero, so that the $x$ and $y$ integrations are over positive values only, the principal branch is the correct choice. If, however, $x_1$ and $y_1$ are both less than zero so that both $x$ and $y$ integrations pass through their origins, then as $t \to +\infty + i\epsilon$, the two factors in the numerator of the logarithm both tend to $+\infty + i\epsilon$, and the two factors in the denominator both tend to $-\infty - i\epsilon$. The correct branch is then given by $m = -1$, and the asymptotic form is changed.

It is not difficult to understand why this is so. In order to discuss $t = \infty$, we make the change of variable

$$t = t'/z.$$

A pinch singularity of $I$ occurs when

$$\begin{aligned} xyt' + zd &= 0, \\ yt' &= 0, \\ xt' &= 0. \end{aligned} \quad (4)$$

These conditions are satisfied by $z = 0$ (or $t = \infty$), and $x = y = 0$. If the contours of $x$ and $y$ integrations pass through their origins, the contour will actually be trapped at $x = y = 0$ as $t \to \infty$, and the resulting singularity manifests itself in the change of asymptotic behavior.

This pinch can be readily verified explicitly. After the $y$ integration has been performed, we obtain

$$-\frac{1}{(n+1)t}\int_{x_1}^{x_2} dx\left[\frac{1}{x(xy_2t+d)^{n+1}} - \frac{1}{x(xy_1t+d)^{n+1}}\right]. \quad (5)$$

The integrand of (5) has no pole at $x = 0$, but if its two terms are considered separately, a convention for avoiding the seeming pole must be chosen. For definiteness we choose a detour in the upper half-plane. The first term has a pole at $-dy_2^{-1}t^{-1}$ in the upper half-plane which gives a pinch as $t \to \infty + i\epsilon$. If the contour is pulled over the pole at $x = 0$ to avoid the pinch, the residual contribution is

$$2\pi i/(n+1)td^{n+1}.$$

No pinch occurs in the second term whose other pole is in the lower half-plane. Had we chosen the opposite convention for the $x$ integration, the second term would have given the pinch but the contribution would have been the same.

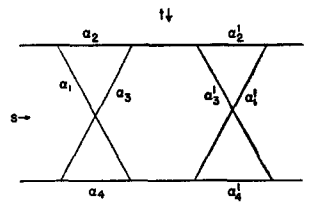


FIG. 1. A diagram relevant to the G–P phenomenon.

This result is the principal analytic tool used in this paper. It can be applied immediately to exhibit in perturbation theory the Gribov–Pomeranchuk phenomenon,[7] which states that complete scattering amplitudes never go to zero more rapidly than $t^{-1}$ in a fully relativistic theory. In order to apply the G–P argument to asymptotic behavior in $t$ at fixed $s$, it is necessary that: (i) the amplitude should have a nonzero $tu$ spectral function; (ii) it should satisfy two-particle unitarity in $s$ in some region. One might expect therefore that the Feynman integral corresponding to Fig. 1, which contains the two-particle iteration of a diagram with a $tu$ spectral function, would $\sim t^{-1}$ as $t \to \infty$ at fixed $s$. However, the edge contributions to such a diagram's asymptotic behavior only give a contribution $\sim t^{-2} \log^5 t$.[13] The coefficient of $t$ in the Feynman denominator corresponding to Fig. 1 is $xy$, where

$$\begin{aligned} x &= \alpha_1\alpha_3 - \alpha_2\alpha_4, \\ y &= \alpha_1'\alpha_3' - \alpha_2'\alpha_4'. \end{aligned} \quad (6)$$

The physically relevant integrations are over positive $\alpha$'s, and so points with $x = y = 0$ occur in the interior of the hypercontour. The behavior of the Feynman integral in the neighborhood of such points may be approximated by an integral of the form (1) for large values of $t$ and so one obtains the expected $t^{-1}$ behavior.

Further iterations give asymptotic behaviors

[13] This point has also been noticed by P. G. Federbush and M. T. Grisaru (private communication), and by G. Tiktopoulos, Phys. Rev. **131**, 2373 (1963).

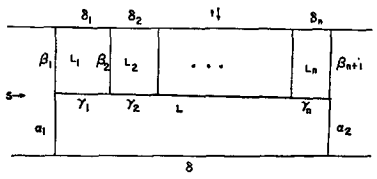

FIG. 2. A diagram of A–F–S type.

$t^{-1}$ $(\log t)^n$ which do not sum up into Regge poles. These represent the occurrence of $(n+1)$-fold poles at $l=-1$. The total effect is an essential singularity at $l=-1$.

### 3. CUTS ON UNPHYSICAL SHEETS

The type of Regge cut proposed by Amati, Fubini, and Stanghellini[8] is obtained by combining together two Regge poles, or a Regge pole and an ordinary pole. The simplest set of perturbation-theory diagrams which might yield this behavior is illustrated by Fig. 2. These diagrams all have their asymptotic behavior in the physical limit determined by the edge behavior, and it has been pointed out[12] that this does not give a cut in the complete amplitude. However, the discontinuity around the two-particle normal threshold given by putting the lines corresponding to $\alpha_1$ and $\alpha_2$ on the mass shell, does have a cut. Therefore if $t\to\infty$ on the *unphysical sheet* generated by this two-particle normal threshold, the asymptotic behavior corresponding to this cut will be obtained. Since this is a sheet-dependent behavior, it must correspond to a pinch contribution. In fact, it provides the simplest example of how pinch contributions can give Regge cuts. In the next section a more complicated example will be discussed in which the same mechanism generates a cut on the physical sheet.

In order to discuss the generation of cuts, a standard form slightly more complicated than (1) is required. It is given by

$$I=\int_{x_1}^{x_2}dx\int_{y_1}^{y_2}dy\int_0^{\beta_2}d\beta\,\frac{1}{[(xy+\beta)t+d]^{n+2}}. \tag{7}$$

After the $x$ and $y$ integrations have been performed,

$$I=\int_0^{\beta_2}d\beta\Bigg[\frac{1}{(n+1)t(\beta t+d)^{n+1}}\times\log\frac{[(x_1y_1+\beta)t+d][(x_2y_2+\beta)t+d]}{[(x_1y_2+\beta)t+d][(x_2y_1+\beta)t+d]}+R(\beta,t)\Bigg], \tag{8}$$

where $R(\beta, t)$ is a rational function. Whether the $\beta$ integration gives a different asymptotic behavior than that obtained by inspecting the integrand will depend on the behavior of the integrand near the end point $\beta=0$. Cancellations between the first and second terms of the integrand show that no change of asymptotic behavior results from the $\beta$ integration when the principal branch of the logarithm is chosen. However, when a branch is chosen on which $\log 1=2m\pi i$ ($m$ nonzero integer), then an extra term appears in the integrand which

$$\sim[2\pi mi/(n+1)t][1/(\beta t+d)^{n+1}],\quad\text{as}\quad\beta\to 0. \tag{9}$$

Such a term when integrated from $\beta=0$ gives an asymptotic behavior of $t^{-2}$. This asymptotic behavior is associated with the occurrence at $t=\infty$ of a singularity given by pinches in the $x$ and $y$ integrations, and an end point in the $\beta$ integration.

If $\beta$ is replaced by the product $\beta_1\cdots\beta_l$ and each $\beta_i$ is integrated from zero, the corresponding asymptotic behavior will be

$$[2\pi mi/n(n+1)d^n][(\log t)^{l-1}/(l-1)!]. \tag{10}$$

This standard result can now be used to analyze the asymptotic behavior of the Feynman integral associated with Fig. 2. The coefficient of $t$ in the denominator is given by[14]

$$g=\alpha_1\alpha_2C+\alpha_1P_1+\alpha_2P_2+Q, \tag{11}$$

where

$$C=C(L_1\cdots L_n), \tag{12}$$

$$P_1=\sum_{i=1}^{n}C(L_1\cdots L_{i-1})\gamma_i\prod_{k>i}\beta_k, \tag{13}$$

$$P_2=\sum_{j=1}^{n}\prod_{l\le j}\beta_l\gamma_jC(L_{j+1}\cdots L_n), \tag{14}$$

$$Q=\prod_{k=1}^{n+1}\beta_kC(L)+\sum_{j<i}\prod_{l\le j}\beta_l\gamma_jC(L_{j+1}\cdots L_{i-1})\gamma_i\prod_{k>i}\beta_k, \tag{15}$$

and $C(L_p\cdots L_q)$ represents the $C$ function associated with the graph composed of loops $L_p\cdots L_q$.[15]

On the unphysical sheet reached by crossing the normal threshold cut corresponding to the lines associated with $\alpha_1$ and $\alpha_2$ being on the mass shell, the $\alpha_1$ and $\alpha_2$ integrations are along contours which are bent back around the origin to negative values of $\alpha_1$ and $\alpha_2$. We may therefore expect that the new asymptotic behavior found on that sheet is associated with pinches in the $\alpha_1$ and $\alpha_2$ integrations and end points in the $\beta_i$ integrations. The expression for $g$ can be written in the form

[14] A convenient summary of results on the functions $C$ and $D$ is given in R. J. Eden, Phys. Rev. **119**, 1763 (1960).
[15] Interpreting $C(L_p\cdots L_q)=1$ if $q<p$.

$$C(\alpha_1 + P_2C^{-1})(\alpha_2 + P_1C^{-1}) + Q - P_1P_2C^{-1}, \quad (16)$$

and the $\alpha_1$ and $\alpha_2$ pinches occur at $-P_2C^{-1}$, and $-P_1C^{-1}$, respectively, corresponding to negative values of $\alpha_1$ and $\alpha_2$. In order that end points in the $\beta_i$ integrations should further increase the asymptotic behavior, it is necessary that the residual coefficient $Q - P_1P_2C^{-1}$ vanish when $\beta_m = 0$, for any $m$. This is trivially satisfied for the first term of $Q$ and for those terms of the sum in $Q$ for which $j \geq m$ or $i < m$. It is also trivially satisfied in $P_1P_2$ for those terms in the $P_1$ sum having $i < m$, and those terms in the $P_2$ sum having $j \geq m$. In both $Q$ and $-P_1P_2C^{-1}$ there remain terms with $j < m \leq i$. However, these cancel when the two terms are added together. This follows from the fact that, when $\beta_m = 0$,[15]

$$\begin{aligned} C(L_1 \cdots L_n) &= C(L_1 \cdots L_{m-1})C(L_m \cdots L_n), \\ C(L_1 \cdots L_{i-1}) &= C(L_1 \cdots L_{m-1})C(L_m \cdots L_{i-1}), \\ C(L_{j+1} \cdots L_n) &= C(L_{j+1} \cdots L_{m-1})C(L_m \cdots L_n), \\ C(L_{j+1} \cdots L_{i-1}) &= C(L_{j+1} \cdots L_{m-1})C(L_m \cdots L_{i-1}), \\ & \qquad j < m \leq i. \end{aligned} \quad (17)$$

Thus the residual coefficient vanishes when any $\beta_m$ is set equal to zero.

It is now necessary to evaluate the limit of $(Q - P_1P_2C^{-1})/\beta_1 \cdots \beta_{n+1}$ as all the $\beta_m \to 0$. This can be obtained from Eqs. (12)–(15) by use of the result that

$$\begin{aligned} C(\cdots L_mL_{m+1} \cdots) - C(\cdots L_m)C(L_{m+1} \cdots) \\ = O(\beta_m^2), \quad \text{as} \quad \beta_m \to 0. \end{aligned} \quad (18)$$

The answer is

$$C(LL_1 \cdots L_n)/C(L_1 \cdots L_n), \quad (19)$$

evaluated with $\beta_m = 0$ $(m = 1, \cdots, n + 1)$.

The combination of the results summarized in Eqs. (10), (16), and (19) enables the pinch contribution to the asymptotic behavior of Fig. 2 to be evaluated. The answer is

$$2\pi g^4 \left\{ i\left(\frac{-g^2}{16\pi^2}\right)^n \Gamma(n) \int_0^1 d\gamma_i \, d\delta_i \, d\delta \times \frac{[c(\gamma, \delta)]^{n-1} \, \delta(\sum \gamma + \sum \delta - 1)}{[d(\gamma, \delta; s)]^n} \right\} \frac{(\log t)^n}{t^2\Gamma(n+1)}. \quad (20)$$

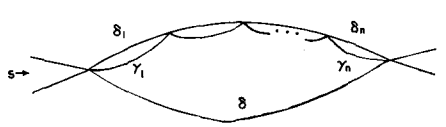


FIG. 3. The contracted diagram associated with Fig. 2.

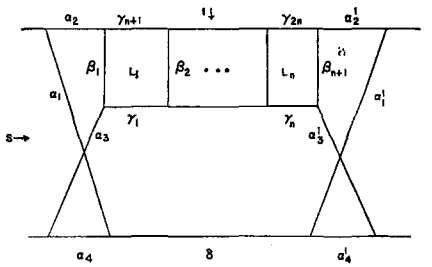


FIG. 4. A diagram contributing to a cut on the physical sheet.

$c(\gamma, \delta)$ and $d(\gamma, \delta; s)$ are the numerator and denominator functions associated with the contracted diagram Fig. 3. The expression in the curly brackets in (20) is the correct Feynman integral for Fig. 3 *evaluated in two dimensions*. It follows that this expression can be rewritten[16] as

$$\int_{\lambda \leq 0} \frac{ds_1 \, ds_2}{[\lambda(s, s_1, s_2)]^{\frac{1}{2}}} \frac{[K(s_1)]^n}{s_1 - m^2}, \quad (21)$$

where

$$\lambda(s, s_1, s_2) = s^2 + s_1^2 + s_2^2 - 2ss_1 - 2ss_2 - 2s_1s_2, \quad (22)$$

and

$$K(s_1) = \frac{-g^2}{16\pi^2} \int \frac{d\gamma \, d\delta \, \delta(\gamma + \delta - 1)}{[\gamma\delta s_1 - (\gamma + \delta)^2 m^2]}. \quad (23)$$

When the contributions from all possible ladder insertions in Fig. 2 are summed, the resulting asymptotic behavior is

$$2\pi g^4 \int_{\lambda \leq 0} \frac{ds_1 \, ds_2}{[\lambda(s, s_1, s_2)]^{\frac{1}{2}}} \frac{t^{\alpha(s_1)-1}}{s_2 - m^2}, \quad (24)$$

where

$$\alpha(s_1) = -1 + K_1(s_1), \quad (25)$$

and is the trajectory function associated with ladder diagrams. The expression (24) gives a Regge cut of the expected form.[8,9,12]

## 4. CUTS ON THE PHYSICAL SHEET

We now consider contributions from the set of diagrams of the form illustrated by Fig. 4. These diagrams have been studied by Mandelstam,[10] using a different technique.

The method used to evaluate the asymptotic form closely parallels that given in Secs. 2 and 3. The coefficient of $t$ is of the form

$$xyC(L_1 \cdots L_n) + P_1x + P_2y + Q, \quad (26)$$

where

$$\begin{aligned} x &= \alpha_1\alpha_3 - \alpha_2\alpha_4, \\ y &= \alpha_1'\alpha_3' - \alpha_2'\alpha_4', \end{aligned} \quad (27)$$

[16] I. T. Drummond, Nuovo Cimento 29, 720 (1963).

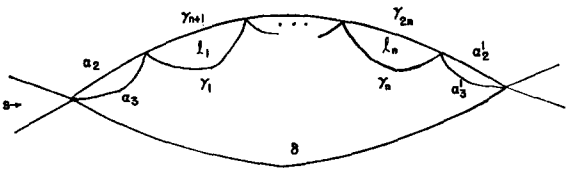


FIG. 5. The contracted diagram associated with Fig. 4.

and

$$Q = \beta_1 \cdots \beta_{n+1}[\alpha_1\alpha_1' C(L) + \alpha_4\alpha_4' C(L') + \alpha_1\alpha_4'\delta + \alpha_1'\alpha_4\delta] + \alpha_1\alpha_1' \sum_{i<i} \prod_{l\le i} \beta_l\gamma_i C(L_{i+1} \cdots L_{i-1})\gamma_i \prod_{k>i} \beta_k + \alpha_4\alpha_4' \sum_{i<i} \prod_{l\le i} \beta_l\gamma_{i+n} C(L_{i+1} \cdots L_{i-1})\gamma_{i+n} \prod_{k>i} \beta_k. \quad (28)$$

The loop $L$ is generated by $\alpha_4\alpha_3\gamma_1 \cdots \gamma_n\alpha_3'\alpha_4'\delta$, and the loop $L'$ is generated by $\alpha_1\alpha_2\gamma_{n+1} \cdots \gamma_{2n}\alpha_2'\alpha_1'\delta$.

Both $x$ and $y$ vanish in the physical region of integration. A corresponding pinch contribution is obtained with the factors $\delta(x+P_2C^{-1})$ and $\delta(y+P_1C^{-1})$ in the numerator of its integrand, and $C(L_1 \cdots L_n)$ in the denominator. The $\delta$ functions enable the $\alpha_4$ and $\alpha_4'$ integrations to be performed, resulting in the substitutions

$$\alpha_4 = \alpha_1\alpha_3\alpha_2^{-1} + O(\beta), \qquad \alpha_4' = \alpha_1'\alpha_3'\alpha_2'^{-1} + O(\beta), \quad \beta_m \to 0, \quad (29)$$

and the multiplication of the integrand by $(\alpha_2\alpha_2')^{-1} + O(\beta)$. The coefficient $\bar{g}$ of $t$ in the pinch contribution vanishes if $\alpha_1 = 0$, or $\alpha_1' = 0$, or $\beta_m = 0$ (any $m$). After performing the $\alpha_1$, $\alpha_1'$, and $\beta$ integrations, the resulting asymptotic behavior is given by

$$2\pi g^4\left\{i\left(\frac{-g^2}{16\pi^2}\right)^{n+2}\Gamma(n+2)\int_0^1 d\alpha_2\, d\alpha_3\, d\alpha_2'\, d\alpha_3'\, d\gamma_i\, d\delta \times \frac{\delta(\alpha_2 + \cdots + \alpha_3' + \delta + \sum\gamma - 1)[C(\alpha,\gamma,\delta)]^{n+2}}{f(\alpha,\gamma,\delta)[d(\alpha,\gamma,\delta;s]^{n+2}}\right\} \times \frac{(\log t)^{n+2}}{t^2\Gamma(n+3)}, \quad (30)$$

where $c$ and $d$ refer to the contracted diagram, Fig. 5. The function $f$ is given by

$$f = \operatorname*{Lim}_{\substack{\alpha_1\to 0\\ \alpha_1'\to 0\\ \beta_m\to 0}} \left(\frac{\alpha_2\alpha_2' C(L_1 \cdots L_n)\bar{g}}{\alpha_1\alpha_1'\beta_1 \cdots \beta_{n+1}}\right). \quad (31)$$

The evaluation of $f$ is the principal complication of the calculation.

There are terms in $f$ which arise from the combination of terms in $Q$ and $-P_1P_2C^{-1}$. These are of exactly the same form as those evaluated in Sec. 3 and yield

$$\alpha_2\alpha_2'[(\alpha_3 + \alpha_3' + \delta + \gamma_1 + \cdots + \gamma_n)C(l_1 \cdots l_n) - \sum_{i=1}^{n} C(l_1 \cdots l_{i-1})\gamma_i^2 C(l_{i+1} \cdots l_n)] + \alpha_3\alpha_3'[(\alpha_2 + \alpha_2' + \delta + \gamma_{n+1} \cdots + \gamma_{2n})C(l_1 \cdots l_n) - \sum_{i=1}^{n} C(l_1 \cdots l_{i-1})\gamma_{i+n}^2 C(l_{i+1} \cdots l_n). \quad (32)$$

There are also terms in $f$ arising solely from $Q$. These yield

$$(\alpha_2\alpha_3' + \alpha_3\alpha_2')\delta C(l_1 \cdots l_n). \quad (33)$$

Finally there are terms in $f$ arising solely from $-P_1P_2C^{-1}$ which yield

$$(\alpha_2\alpha_3' + \alpha_3\alpha_2') \sum_{i=1}^{n} C(l_1 \cdots l_{i-1})\gamma_i\gamma_{n+i} C(l_{i+1} \cdots l_n). \quad (34)$$

The combination of (32), (33), and (34) just gives

$$f = C(\alpha, \gamma, \delta). \quad (35)$$

When this is substituted into (30), the integral in the curly brackets is just the correct Feynman integral for Fig. 5 *evaluated in two dimensions.*

It now follows, just as in Sec. 3, that a summation of the contributions from diagrams of type Fig. 4 gives a Regge cut of the same form as Eq. (24). A somewhat curious feature is that the first two terms required in the sum are missing, since Eq. (30) starts with $n = 0$. The absence of the terms of order $t^{-2}$ and $t^{-2}\log t$ does not produce a new phenomenon since they can be absorbed in the G–P essential singularity at $l = -2$.

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# Behavior of the Scattering Amplitude for Large Angular Momentum*

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Langer's theory on the asymptotic behavior of the solutions of differential equations is applied to angular momentum, giving stronger results than were possible hitherto by Born approximation. It is shown that, for potentials $V(r)$ *analytic* in the right-hand $r$ plane satisfying $|r^2V(r)| < \infty$ at $r = 0$ and $|r| = \infty$, the phase shift has the asymptotic form ($\lambda = l + \frac{1}{2}$)

$$\delta \underset{\lambda\to\infty}{\to} -(2\lambda^{\frac{1}{2}})^{\frac{1}{2}} \frac{V(\lambda/k)}{2k^2} - \lambda^{-1} \int_{\lambda/k+\lambda^{-\frac{1}{2}}/k}^{\infty} \frac{V(r)r\,dr}{(k^2r^2/\lambda^2 - 1)^{\frac{1}{2}}}, \qquad \mathrm{Re}\,\lambda > 0,$$

in the $\lambda$ plane and for all complex $k$. Consequently, (a) all Regge trajectories are bounded for analytic potentials; there are no poles for $|\lambda| \to \infty$ in the right-half $\lambda$ plane, (b) stronger limits can be given for the feasibility of the Watson–Sommerfeld transformation. The pathological behavior of the cut off potentials (e.g., square-well) is attributed to the nonanalyticity of the potential.

## I. INTRODUCTION

THE analytical properties of the nonrelativistic scattering amplitude in the two complex variables, angular momentum $l$ and linear momentum $k$ (or energy), has been extensively studied for a large class of potentials. A large number of studies has been recently devoted to various aspects of this problem.[1-10] However, one of the most important ingredients of the theory, the knowledge of the asymptotic behavior of the amplitude for large complex $l$ which is needed in the Watson–Sommerfeld transformation, has not been studied in detail in the complex $l$ plane. Most authors refer to Born approximation results.[11] The primary purpose of this work is to present such a study. In particular we wish to answer the following questions:

(a) For which class of potentials do the Regge trajectories turn in the right-hand $l$ plane,[12] or why do the trajectories for the cutoff potentials extend to infinity in $l$ plane as $k \to \infty$?[9]

(b) For which class of potentials can one make the Watson–Sommerfeld transformation; or why this is not possible for cut-off potentials?[9]

These questions are answered by putting the Schrödinger equation into Langer's form[13] and applying his theory of the asymptotic form of the solution of differential equations as a function of analytic parameters. In our case the analyticity of the potential plays a dominant role and it is shown that the very different behavior, for large $l$, of the amplitude for cut-off potentials, such as square-well, is due to nonanalyticity of these potentials.

Coulomb potential does not satisfy the boundedness condition at infinity.

The general theory is developed in Secs. II, III, and IV. In Sec. V we evaluate the asymptotic form of the scattering amplitude and in Sec. VI we discuss the behavior of poles at infinity and the Watson–Sommerfeld transformation.

## II. THE METHOD OF LANGER

Our conclusions are due to an application of the Langer's results[13] on the asymptotic behavior of the solutions of a certain type of differential equation to the Schrödinger equation.

Langer has studied the asymptotic solutions of

* Supported in part by the Air Force Office of Scientific Research and the National Science Foundation.

[1] The boundedness of trajectories for Yukawa potentials was already shown by T. Regge, Nuovo Cimento **14**, 951 (1958).

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[7] R. G. Newton, J. Math. Phys. **3**, 867 (1962).

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[11] There is some information on asymptotic behavior for large $l$ in two recently announced papers: L. Brown, D. I. Fivel, B. W. Lee, and R. F. Sawyer, Ann Phys. (N. Y.), **23**, 187 (1963); and A. M. Jaffe and Y. S. Kim, Phys. Rev. **129**, 2818 (1963). See also F. Calogero, Nuovo Cimento **28**, 66 (1963); B. P. Desai and R. G. Newton, Phys. Rev. **129**, 1445 (1963).

[12] The turning of the trajectories in the right-hand $l$ plane for Yukawa potentials has been shown only *numerically*: A. Ahmadzadeh, P. Burke, and C. Tate, "Regge Trajectories for Yukawa potentials," UCRL-10216 (1962), and C. Lovelace and Mason, Proc. Intern. Conf. High Energy, CERN, Geneva, Switzerland, 1962.

[13] R. E. Langer, Trans. Am. Math. Soc. **34**, 449 (1932).

the equation

$$u''(z) + [\lambda^2\phi^2(z) - \chi(z)]u(z) = 0, \tag{1}$$

where $z$ and $\lambda$ are complex variables. The functions $\phi^2(z)$ and $\chi(z)$ are assumed to be holomorphic in some region $G$ of $z$ containing the origin, and $\phi^2(z)$ to have only a single zero of order $n \geq 0$ at the origin, i.e.,

$$\phi^2(z) = z^n\phi_1^2(z), \qquad n \geq 0, \qquad n \text{ real}, \tag{2}$$

and $\phi_1^2(z)$ is single-valued, holomorphic, and everywhere different from zero.

Under these conditions, the asymptotic form, for sufficiently large $|\lambda|$, of a pair of linearly independent solutions may always be written in the form

$$u^{\pm} \underset{|\lambda|\to\infty}{\longrightarrow} \exp(\pm i\xi)/\lambda^{\frac{1}{2}-\mu}\phi^{\frac{1}{2}}(z), \tag{3}$$

with derivatives

$$u^{\pm\prime} \underset{|\lambda|\to\infty}{\longrightarrow} \pm\exp(\pm i\xi)i\lambda^{-\mu+\frac{1}{2}}\Phi^{1-2\mu}(z)/\Psi^2(z)\phi^{\frac{1}{2}}(z) + u(z)\Psi'(z)/\Psi(z), \tag{4}$$

where

$$\Phi(z) = \int_0^z \phi(z')\,dz', \tag{5}$$

$$\xi = \lambda\Phi(z), \tag{6}$$

$$\Psi(z) = \Phi^{\frac{1}{2}-\mu}(z)/\phi^{\frac{1}{2}}(z), \tag{7}$$

and

$$\mu = 1/(2 + n). \tag{8}$$

The method gives not only the asymptotic form of the solutions but also that of their derivatives. This is one of its advantages over, for example, the Born approximation or the WKB method. Furthermore, the result includes the case of interest to us in which $\phi(z)$ vanishes at a finite point in the $z$ plane. This point corresponds to the turning point in the WKB method.

We also note that the above asymptotic forms are independent of $\chi(z)$ except that it has to be a holomorphic function.

Out of the two linearly independent solutions given by Eq. (3), the desired combination depending on the boundary condition will be constructed.

## III. LANGER'S FORM OF THE SCHRÖDINGER EQUATION

The radial Schrödinger equation

$$v''(r) + (k^2 - (\lambda^2 - \tfrac{1}{4})/r^2 - V(r))v(r) = 0, \tag{9}$$

where we have used

$$\lambda = l + \tfrac{1}{2} \quad \text{and} \quad \hbar^2/2m = 1,$$

can be transformed into the form of Eq. (1) by introducing the new variable $z$ defined by

$$r = \pm\lambda e^z, \tag{10}$$

and the new wavefunction

$$u(r) = r^{-\frac{1}{2}}v(r). \tag{11}$$

We obtain

$$u''(z) + \lambda^2\{[k^2 - V(\lambda e^z)]e^{2z} - 1\}u(z) = 0. \tag{12}$$

Thus, in our case

$$\chi(z) \equiv 0, \quad \text{and} \quad \phi^2(z, \lambda) = [k^2 - V(\lambda e^z)]e^{2z} - 1; \tag{13}$$

$\phi^2(z, \lambda)$ depends also on $\lambda$, but Langer's results are easily extended to this case if the conditions on $\phi$ are satisfied for each $\lambda$ as we discuss below.

In order to be able to use Langer's results we must consider potentials which may be continued analytically in $z$, $z = \ln(r/\lambda)$. Specifically, we consider potentials such that

(i) $r^2V(r)$ is bounded; (this condition will be used in Sec. IV).

(ii) $V(r)$ is analytically continuable into the region $-\theta_1 < \arg r \leq \theta_2$, $\theta_i \leq \frac{1}{2}\pi$, $|r| > 0$. (At $r = 0$ there could be a singularity such that $r^2V$ is finite).

(iii) $V(r)$ decreases monotonically when $|r|$ is sufficiently large within the region given in (ii).

Then, if we take the principal determination of the logarithm, $V(z)$ is holomorphic in a strip

$$-\theta_1 - \arg\lambda \leq \operatorname{Im} z \leq \theta_2 - \arg\lambda.$$

We now show that, in the region of complex $\lambda$ and $z$ where $|V(\pm\lambda e^z)|$ is monotonically decreasing, $\phi^2(z)$ defined by (13) has, for sufficiently large $|\lambda|$, one simple zero at $z_0$ such that

$$z_0 \underset{|\lambda|\to\infty}{\longrightarrow} \log(\pm 1/k) (\text{or at } r_0 \to \pm\lambda/k),$$

where the sign $\pm$ is chosen such that $r_0$ lies within the region of decreasing $V(r)$.

The quantity $z_0$ is given by [from (13)]

$$[k^2 - V(\pm\lambda e^{z_0})]e^{2z_0} - 1 = 0, \tag{14}$$

or

$$\operatorname{Re} z_0 = -\tfrac{1}{2}\log|k^2 - V(\pm\lambda e^{z_0})|. \tag{15}$$

Because $V(z)$ is bounded, $|k^2 - V(\pm\lambda e^{z_0})|$ is also bounded for fixed $k^2$; hence

$$\operatorname{Re} z_0 > -M, \quad \text{or} \quad |e^{z_0}| > e^{-M}, \tag{16}$$

where $M$ is some fixed constant. By choosing $|\lambda|$ sufficiently large we may make $|\lambda e^{z_0}|$ arbitrarily large and hence force it into the region where $|V|$ decreases monotonically and in that region we have $|V| \ll k^2$, so that for $k \neq 0$,

$$e^{z_0} \underset{|\lambda|\to\infty}{\to} \pm 1/k, \quad \text{or} \quad r_0 \underset{|\lambda|\to\infty}{\to} \pm(\lambda/k).$$

More precisely, expanding $\phi^2(r)$ around $r = \pm\lambda/k$, for fixed $k$,

$$\phi^2(r) = [k^2 - V(r)]\frac{r^2}{\lambda^2} - 1 = -\frac{1}{k^2}V(\pm\lambda/k) + \left[-\frac{1}{k^2}V'(\pm\lambda/k) \pm \frac{2}{\lambda k}[k^2 - V(\pm\lambda/k)]\right] \times (r \mp \lambda/k) + \cdots, \tag{17}$$

we get, for $r_0$ defined by $\phi^2(r_0) = 0$,

$$r_0 = \pm\lambda/k + V(\pm\lambda/k)/k^2 \times \left[\mp\frac{\lambda}{k}V'\left(\pm\frac{\lambda}{k}\right) \mp \frac{2(k^2 - V(\pm\lambda/k))}{\lambda k}\right] + \cdots = \pm\lambda/k + O(V(\pm\lambda/k)/k^2). \tag{18}$$

Thus, for $|\lambda| \to \infty$, $\phi^2(r)$ has a simple zero near $r_0 = \pm\lambda/k$ whenever either of the quantities lie in the region of decreasing $|V(r)|$, and Eq. (12) satisfies Langer's condition.

Formally, Langer's results are written with the zero of $\phi$ at the origin, $z_0 = 0$, and it is, of course, possible to write the Schrödinger equation in this form by making a translation $\eta = z - z_0$. It is completely equivalent, however, to retain the variables $z$ or $r$, and write, for example,

$$\Phi(z) = \int_{z_0}^{z}\phi(z')\,dz' \quad \text{or} \quad \Phi(r) = \int_{r_0}^{r}\phi(r')\frac{dr'}{r'}$$

in place of $\Phi(\eta) = \int_0^\eta \phi(\eta')\,d\eta''$. This we choose to do in the following.

Before proceeding further, it is important to see explicitly what regions of $\lambda$ and $k$ planes are covered by the present treatment.

(a) Potentials decreasing as a power $r^{-n}$, $n > 2$, as $r \to \infty$. An example would be the ratio of two polynomials such as $V(r) = (1 - r)/r(1 + r)^3$. Such potentials decrease asymptotically throughout the right-half $r$ plane so that if $-\frac{1}{2}\pi \leq \arg\lambda/k \leq \frac{1}{2}\pi$, $r_0 = \lambda/k$, and if $\arg\lambda/k \leq -\frac{1}{2}\pi$ or $\arg\lambda/k \geq \frac{1}{2}\pi$, $r_0 = -\lambda/k$ lie within the region of decreasing $V(r)$. Hence, excepting $k = 0$, our results will hold for all $\lambda$ and $k$ if $|\lambda|$ is taken to be sufficiently large.

(b) Exponential potential, $V(r) = e^{-\mu r}$. The potential decreases in the right-hand $r$ plane except along the imaginary axis where it oscillates. Therefore, all values of $\lambda$ and $k$ are permissible except when $\arg\lambda/k = \pm\frac{1}{2}\pi$. Thus, for example, for real $k$, the imaginary axis of $\lambda$ is excluded, and for imaginary $k$, the real $\lambda$ axis is excluded.

(c) Yukawa potential, $V(r) = e^{-\mu r}/r$. Due to the $1/r$ factor, the potential decreases throughout the right-half $r$ plane, including the imaginary axis, so that all $\lambda$ and $k$ are permissible. The same is clearly true for a superposition of Yukawa potentials or a modified Yukawa potential such as $V(r) = e^{-\mu r}/(1 + r^2)$.

(d) Gaussian potential, $V(r) = e^{-\mu r^2}$. Our asymptotic results may be proved within a region where $|\arg\lambda/k| < \frac{1}{4}\pi$. They may also hold for a larger domain but the method is inapplicable.

In the preceding reduction to Langer's form, $k$ has been assumed to have some fixed, finite, value, and hence we have used the fact that $|V(\lambda/k)| \ll k^2$ as $|\lambda| \to \infty$. Even if this fixed value of $k$ is made arbitrarily large, this result still holds for potentials less singular at the origin than $1/r^2$ even though now $|V(\lambda/k)| \not\to 0$ and may even become infinite. [See condition (i) on the potential.] In the following we shall generally consider, for simplicity, $k$ to be some fixed quantity. We consider $\lambda$ and $k$ as parameters, and $r$ an independent variable which, in the calculation of the scattering amplitude, tends to infinity independent of $\lambda$ and $k$. Furthermore, it is assumed for definiteness in the following, that $\lambda$ and $k$ are such that $r_0 \cong \lambda/k$, but the identical arguments hold for $r_0 = -\lambda/k$. For $\arg(\lambda/k) = \frac{1}{2}\pi$, either value $r_0 = \pm\lambda/k$ may be taken in the expression for $\Phi(r)$ which is independent of the lower limit $r_0$. Thus the two solutions obtained with $r_0 = \pm\lambda/k$ are identical on this line and therefore analytic continuation of each other.

## IV. ASYMPTOTIC FORM OF THE SOLUTIONS FOR LARGE $\lambda$

We can now apply the asymptotic formulas (3) and (4) for large $|\lambda|$ to Eq. (12). To illustrate the method we first consider a soluble example where the exact solution is known.

*Soluble Example:* $V(r) = -c/r^2$. From Eq. (13), written now in terms of $r$, we have

$$\phi(r) = [(k^2 + c/r^2)(r^2/\lambda^2) - 1]^{\frac{1}{2}}, \tag{19}$$

and, from (5), with $dr = rdz$ [Eq. (10)],

$$\Phi(r) = \int_{r_0}^{r}[(k^2 + c/r^2)(r^2/\lambda^2) + 1]^{\frac{1}{2}}\frac{dr}{r} = [k^2r^2/\lambda^2 - 1 + c/\lambda^2]^{\frac{1}{2}} - (1 - c/r^2)^{\frac{1}{2}}$$

$$\times \tan^{-1} [k^2r^2/\lambda^2 - 1 + c/\lambda^2]^{\frac{1}{2}}.$$

Furthermore, $\mu = \frac{1}{3}$ and the asymptotic form of the solutions for large $|\lambda|$ *but for all* $r$ is completely determined. We need, in particular, the form of the solution for large $r$ which is regular at $r = 0$. As we shall see later, this regular solution is given by the following combination of $u^*$ (Appendix II):

$$u = \tfrac{1}{2}(u^+ + u^-),$$

or

$$v = \tfrac{1}{2}(\lambda^{-\frac{1}{3}}kr)^{\frac{1}{2}}[e^{-i\frac{1}{2}\pi}u^+ + e^{i\frac{1}{2}\pi}u^-].$$

Using the expansion

$$\phi(r) \underset{r\to\infty}{\to} [k^2r^2/\lambda^2 - 1]^{\frac{1}{2}}(1 - c/2k^2r^2 + \cdots)$$

and

$$\Phi(r) \underset{r\to\infty}{\to} [k^2r^2/\lambda^2 - 1]^{\frac{1}{2}}(1 - c/2k^2r^2 + \cdots) - (1 - c/\lambda^2)^{\frac{1}{2}}(\tfrac{1}{2}\pi + \cdots),$$

we obtain

$$v(r) \underset{\substack{r\to\infty \\ |\lambda|\to\infty}}{\to} \cos(kr - \tfrac{1}{2}\pi\lambda(1 - c/\lambda^2)^{\frac{1}{2}} - \tfrac{1}{4}\pi) = \cos(kr - (\tfrac{1}{2}\pi)\tilde{\lambda} - \tfrac{1}{4}\pi), \qquad (20)$$

where

$$\tilde{\lambda} \equiv (\lambda^2 - c)^{\frac{1}{2}}.$$

In this simple case, one can of course obtain the solution directly. The asymptotic form of the exact solution $j_{\tilde{\lambda}}(kr) = (\frac{1}{2}\pi\ kr)^{\frac{1}{2}}J_{\tilde{\lambda}}(kr)$ when $|kr| \gg |\tilde{\lambda}|$ gives again Eq. (20).

We also evaluate the scattering amplitude for $|\lambda| \to \infty$ by two different methods. Anticipating Eq. (35), the scattering amplitude is given by

$$A(\lambda, k) = \sin(\lambda\Phi^0\delta\Phi)/i \exp(-i\lambda\Phi^0\delta\Phi),$$

where, from (34), $\Phi^0\ \delta\Phi = \Phi - \Phi^0$, and $\Phi^0$ is the value of $\Phi$ when $V(r) \equiv 0$, i.e., $c = 0$ in this example. We find

$$\Phi^0 = \left[\frac{k^2r^2}{\lambda^2} - 1\right]^{\frac{1}{2}} - \tan^{-1}\left[\frac{k^2r^2}{\lambda^2} - 1\right]^{\frac{1}{2}} \underset{|\lambda|\to\infty}{\to} \frac{k\pi}{\lambda} - \frac{\pi}{2},$$

and

$$\lambda\Phi^0\delta\Phi \underset{r\to\infty}{\to} \frac{\pi}{2}[\lambda^2 - (\lambda^2 - c)^{\frac{1}{2}}] \underset{|\lambda|\to\infty}{\to} -\frac{\pi}{4}\frac{c}{\lambda};$$

hence

$$A(\lambda, k) \to \frac{\pi i}{4}\frac{c}{\lambda}. \qquad (21)$$

On the other hand, we can evaluate the amplitude for our example directly from the Wronskian $W(j_{\tilde{\lambda}}(kr), j_\lambda(kr))$. From the differential equations

$$\left[\frac{d^2}{dr^2} - \frac{\lambda^2 - \frac{1}{4}}{r^2} + k^2\right]j_\lambda(kr) = 0,$$

$$\left[\frac{d^2}{dr^2} - \frac{\tilde{\lambda}^2 - \frac{1}{4}}{r^2} + k^2\right]j_{\tilde{\lambda}}(kr) = 0,$$

we obtain

$$W(j_{\tilde{\lambda}}(kr), j_\lambda(kr)) = (\tilde{\lambda}^2 - \lambda^2)\int_0^\infty \frac{j_\lambda(kr)j_{\tilde{\lambda}}(kr)\,dr}{r^2},$$

or[14]

$$W = (\tilde{\lambda}^2 - \lambda^2)\frac{\pi k}{2}\left[\frac{\Gamma(1)\Gamma(\lambda/2 + \tilde{\lambda}/2)}{2\Gamma(1 + \lambda/2 - \tilde{\lambda}/2)\Gamma(1 + \lambda/2 + \tilde{\lambda}/2)\Gamma(1 - \lambda/2 + \tilde{\lambda}/2)}\right]$$

$$= (\tilde{\lambda}^2 - \lambda^2)\frac{\pi k}{4\lambda}\frac{1}{\Gamma(1 + c/2\lambda)\Gamma(1 - c/2\lambda)} = (\tilde{\lambda}^2 - \lambda^2)\frac{k}{2c}\sin(\pi c/2\lambda) \underset{|\lambda|\to\infty}{\to} -\frac{\pi}{4}k\frac{c}{\lambda},$$

which is in agreement with (21) because

$$W(j_{\tilde{\lambda}}, j_\lambda) = k \sin \lambda\Phi^0\delta\Phi.$$

We turn now to the general case, and wish to show that for large $|\lambda|$, $\phi \to \phi^0$ and $\Phi \to \Phi^0$, where $\phi^0$ and $\Phi^0$ are the quantities corresponding to the unperturbed situation with $V(r) \equiv 0$:

$$\phi^0(r) = (k^2r^2/\lambda^2 - 1)^{\frac{1}{2}}, \qquad (22)$$

$$\Phi^0(r) = \int_{\lambda/k}^r (k^2r_1^2/\lambda^2 - 1)^{\frac{1}{2}}\,dr_1/r_1. \qquad (22')$$

Consider first $\phi(r)$ given by (13), i.e.,

$$\phi(r) = [(k^2 - V(r))r^2/\lambda^2 - 1]^{\frac{1}{2}}.$$

If $\arg(\lambda/k) = \theta \neq 0$, then $k^2r^2/\lambda^2 - 1$ cannot vanish on the real $r$ axis; in fact

$$|k^2r^2/\lambda^2 - 1|^2 \geq |e^{-2i\theta} - 1|^2 = 4\sin^2\theta.$$

Furthermore, if

$$r^2V(r) < \infty \quad \text{at} \quad r = 0 \quad \text{and} \quad r = \infty, \qquad (23)$$

$|V(r)r^2/\lambda^2|$ can be made arbitrarily small by taking $|\lambda|$ large enough. Thus,

[14] G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, London, England, 1944), p. 403.

$$\phi(r) = (k^2r^2/\lambda^2 - 1)^{\frac{1}{2}} \times [1 - V(r)r^2/\lambda^2/2(k^2r^2/\lambda^2 - 1) + \cdots],$$

or

$$|\phi(r) - \phi^0(r)| \approx \left|\frac{-V(r)r^2/\lambda^2}{2(k^2r^2/\lambda^2 - 1)}\right| \leq \left|\frac{V(r)r^2}{4\lambda^2 \sin\theta}\right| \leq \frac{a}{|\lambda|^2} \underset{|\lambda|\to\infty}{\to} 0. \quad (24)$$

For the case $\arg \lambda/k = \theta = 0$ which we had excluded, it is still true that $|k^2r^2/\lambda^2 - 1| \geq \epsilon$ where $\epsilon$ is a fixed nonzero number, except in a small neighborhood of $r = \lambda/k$. In that neighborhood both $\phi^2(r)$ and $\phi^{0*}(r)$ may be expanded in Taylor series, [Eq. (17) for $\phi^2(r)$] and

$$\phi^{0*}(r) = (1 + 2k/\lambda)(r - \lambda/k) + \cdots. \quad (25)$$

and we obtain

$$\phi^2(r) - \phi^{0*}(r) = -\frac{1}{k^2} V(\lambda/k) - \left[\frac{1}{k^2} V'(\lambda/k) + \frac{2V(\lambda/k)}{\lambda k}\right](r - \lambda/k) + \cdots \underset{|\lambda|\to\infty}{\to} 0$$

$$\text{for all } k \neq 0, \quad \text{for } \left|r - \frac{\lambda}{k}\right| < \epsilon. \quad (26)$$

This proves the assertion for $\phi(r)$. To study $\Phi(r)$,

$$\Phi(r) = \int_{r_0}^{r} [(k^2 - V(r_1))r_1^2/\lambda^2 - 1]^{\frac{1}{2}} \frac{dr_1}{r_1}, \quad (27)$$

one would like to expand the integrand as in (24) and (25). This cannot be done, however, in a neighborhood of the lower limit of the integral, because, by definition,

$$k^2r_0^2/\lambda^2 - 1 = (r_0^2/\lambda^2)V(r_0).$$

Therefore, we divide the integral into two parts, the first from $r_0$ to some point $R(\lambda)$, the other from $R(\lambda)$ to $r$, along which the expansions may be used. The point $R(\lambda)$ evidently must satisfy

$$|V(R)R^2/\lambda^2| \ll |k^2R^2/\lambda^2 - 1|. \quad (28)$$

A convenient choice is

$$R(\lambda) = r_0 + 1/(k\lambda^{\frac{1}{2}}), \quad (29)$$

in which case the left-hand side of (28) approaches $|V(\lambda/k)/k^2|$ for large $|\lambda|$, and the right-hand side becomes

$$|k^2R^2/\lambda^2 - 1| = \left|\frac{k^2}{\lambda^2}(r_0^2 + 2r_0/k\lambda^{\frac{1}{2}} + 1/k^2\lambda) - 1\right| \underset{|\lambda|\to\infty}{\to} |2\lambda^{-\frac{1}{2}}|.$$

Thus the inequality (28) is satisfied for large $|\lambda|$ and fixed $k$ if $V(\lambda/k)$ vanishes at least like $\lambda^{-(\frac{1}{2}+\epsilon)}$ as $|\lambda| \to \infty$. The inequality is obviously also satisfied for $k \to \infty$ as long as $V(r)$ is less singular than $r^{-2}$ at $r = 0$.

We have then

$$\Phi(r) - \Phi^0(r) = \int_{r_0}^{R} \left\{[k^2 - V(r)]\frac{r^2}{\lambda^2} - 1\right\}^{\frac{1}{2}} \frac{dr}{r} - \int_{\lambda/k}^{R} [k^2r^2/\lambda^2 - 1]^{\frac{1}{2}} \frac{dr}{r} - \int_{R}^{r} \frac{V(r)r^2/\lambda^2}{2[k^2r^2/\lambda^2 - 1]^{\frac{1}{2}}} \frac{dr}{r} + \int_{R}^{r} \frac{V^2(r)r^4/\lambda^4}{8[k^2r^2/\lambda^2 - 1]^{\frac{1}{2}}} \frac{dr}{r} + \cdots. \quad (30)$$

Because, for $|\lambda| \to \infty$, the region of integration for the first two integrals becomes infinitesimally small, we replace in these integrals $V(r)$ by $V(r_0)$; then the integrals may be performed:

$$I_1 = \int_{r_0}^{R} \left\{[k^2 - V(r_0)]\frac{r^2}{\lambda^2} - 1\right\}^{\frac{1}{2}} \frac{dr}{r} = \left\{[k^2 - V(r_0)]\frac{R^2}{\lambda^2} - 1\right\}^{\frac{1}{2}} - \tan^{-1}\left\{[k^2 - V(r_0)]\frac{R^2}{\lambda^2} - 1\right\}^{\frac{1}{2}},$$

or, expanding $\tan^{-1} x = x - \frac{1}{3}x^3 + \cdots$, because the argument is small,

$$I_1 = \tfrac{1}{3}[k^2R^2/\lambda^2 - 1]^{\frac{3}{2}}\left[1 - \frac{3}{2}\frac{V(r_0)R^2/\lambda^2}{k^2R^2/\lambda^2 - 1} + \cdots\right].$$

Similarly,

$$I_2 = \int_{\lambda/k}^{R} (k^2r^2/\lambda^2 - 1)^{\frac{1}{2}} \frac{dr}{r} = \tfrac{1}{3}(k^2R^2/\lambda^2 - 1)^{\frac{3}{2}} + O([k^2R^2/\lambda^2 - 1]^{5/2}).$$

The contribution from the first two integrals in (30) is therefore

$$-\tfrac{1}{2}[k^2R^2/\lambda^2 - 1]^{\frac{1}{2}}V(r_0)R^2/\lambda^2 \underset{|\lambda|\to\infty}{\to} -\sqrt{2}\,\lambda^{-\frac{1}{2}}\frac{V(\lambda/k)}{2k^2}.$$

In order that the last integral in (30) exist for all $r$, in particular for $r = 0$, the potential has to behave at the origin as

$$V(r) \underset{r\to 0}{\to} r^{-2+\epsilon}, \qquad \epsilon > 0. \quad (31)$$

The case $\epsilon = 0$ has been discussed as an example at the beginning of this section and represents indeed the first case in which $\Phi(r)$ does not approach $\Phi^0(r)$ in the limit.

Collecting the results, we have finally

$$\Phi(r) - \Phi^0(r) \underset{|\lambda|\to\infty}{\to} -\sqrt{2}\,\lambda^{-\frac{1}{2}} \times \frac{V(\lambda/k)}{2k^2} - \lambda^{-2}\int_{R}^{r} \frac{V(r)r\,dr}{2[k^2r^2/\lambda^2 - 1]^{\frac{1}{2}}}, \quad (32)$$

which approaches zero as $|\lambda| \to \infty$. Q.E.D. In the left half-plane we have to take the turning point $r_1' \approx -\lambda/k$; the argument of $V$ becomes $V(-\lambda/k)$.

## V. SCATTERING AMPLITUDE FOR LARGE $|\lambda|$

We write the partial wave amplitudes, in the usual manner, as the ratio of two Wronskians (Appendix I)

$$A(\lambda, k) = 2W(v(r), j_\lambda(kr))/W(v(r), h_\lambda^{(1)}(kr)), \tag{33}$$

where $j_\lambda = \frac{1}{2}[h_\lambda^{(1)} + h_\lambda^{(2)}]$ with $h_\lambda^{(1,2)}$ being the spherical Hankel functions. We write

$$\phi = \phi^0(1 + \delta\phi), \qquad \Phi = \Phi^0(1 + \delta\Phi), \tag{34}$$

and evaluate in a straightforward manner the above Wronskians (Appendix II). The result is, for $\mathrm{Re}\,\lambda > 0$,

$$A(\lambda, k) \underset{|\lambda|\to\infty}{\to} \frac{\sin(\lambda\Phi^0\delta\Phi)}{i\exp(-i\lambda\Phi^0\delta\Phi)}. \tag{35}$$

Thus the scattering amplitude is determined by the quantity $\Phi^0\delta\Phi$ alone which we have evaluated in the previous section, [Eq. (32)]:

$$\lambda\Phi^0\delta\Phi \underset{|\lambda|\to\infty}{\to} -\sqrt{2}\,\lambda^{\frac{1}{2}}\frac{V(\lambda/k)}{2k^2} - \frac{\lambda^{-1}}{2}\int_{r_0+k^{-1}\lambda^{-\frac{1}{2}}}^{\infty}\frac{V(r)r\,dr}{[k^2r^2/\lambda^2 - 1]^{\frac{1}{2}}}. \tag{36}$$

An upper bound may be placed on this expression by choosing a path of integration such that $|(k^2r^2/\lambda^2 - 1)^{\frac{1}{2}}|$ takes its minimum value at $r = R = r_0 + 1/k\lambda^{\frac{1}{2}}$. Hence,

$$|\lambda\Phi^0\delta\Phi| \underset{|\lambda|\to\infty}{\leq} \left|\frac{(2\lambda^{\frac{1}{2}})^{\frac{1}{2}}V(\lambda/k)}{2k^2}\right| + \tfrac{1}{2}\,|2\lambda^{\frac{1}{2}}|^{-\frac{1}{2}}\int_{r_0+k^{-1}\lambda^{-\frac{1}{2}}}^{\infty}|V(r)r|\,dr. \tag{37}$$

Under the stated restrictions placed upon the potential, $r^2V(r) = 0$ at $r = 0$ and $r = \infty$, each term in (37) vanishes for any value of $k$, finite or infinite. Thus, for sufficiently large $|\lambda|$,

$$\lambda\Phi^0\delta\Phi \underset{|\lambda|\to\infty}{\to} 0. \tag{38}$$

We then obtain, finally, the following asymptotic form of the scattering amplitude:

$$A(\lambda, k) \underset{|\lambda|\to\infty}{\to} i(2\lambda^{\frac{1}{2}})^{\frac{1}{2}}\frac{V(\lambda/k)}{2k^2} + i\lambda^{-1}\int_{\lambda/k+\lambda^{-\frac{1}{2}}/k}^{\infty}\frac{V(r)r\,dr}{(k^2r^2/\lambda^2 - 1)^{\frac{1}{2}}}, \quad \mathrm{Re}\,\lambda/k \geq 0. \tag{39}$$

In reference 2 it has been shown, under similar conditions, by means of generalized WKB method, that the wavefunction approaches the unperturbed one, a result which we have also noted. They then use the Born approximation limit for large $\lambda$,

$$A(\lambda, k) = 1 - e^{2i\delta} \approx -2i\delta = +\frac{2i}{k}\int_0^{\infty} j_\lambda^2(kr)V(r)\,dr. \tag{40}$$

Our result [Eq. (39)] is somewhat stronger than the Born approximation. Furthermore, the first term in (39) is explicit and suitable bounds may be placed on the second term, whereas in (40) conclusions are difficult to draw unless the integration from 0 to $\infty$ can be performed. The reason for this difference is that with Langer's method, the derivative of the wavefunctions is also known, a situation which enables one to consider the pertinent Wronskians directly, and consequently express the scattering amplitude in terms of an integral entirely in the asymptotic region of the potential instead of the region $0 \leq r \leq \infty$.

We can obtain the Born approximation (40) for a Yukawa potential, for example, from our result (39). We consider the dominant second term

$$I \cong \lambda^{-1}\int_{\lambda/k}^{\infty}\frac{e^{-\mu r}\,dr}{[k^2r^2/\lambda^2 - 1]^{\frac{1}{2}}},$$

or, with the change of variables, $\alpha = \mu/k$ and $\xi = \mu r/\lambda$,

$$I = \frac{\alpha}{\mu}\int_{\alpha}^{\infty}\frac{e^{-\lambda\xi}\,d\xi}{[\xi^2 - \alpha^2]^{\frac{1}{2}}}.$$

As $\lambda \to \infty$, the integrand is small except at $\xi^2 \approx \alpha^2$. Furthermore, for $k \gg \mu$ or $\alpha \ll 1$, $\xi^2 - \alpha^2 \cong 2[\cosh\xi - \cosh\alpha]$, and we get[15]

$$I \underset{\substack{|\lambda|\to\infty \\ k\gg\mu}}{\to} \frac{\alpha}{\mu\sqrt{2}}\int_{\alpha}^{\infty}\frac{e^{-\lambda\xi}\,d\xi}{[\cosh\xi - \cosh\alpha]^{\frac{1}{2}}} = \frac{1}{k}\,Q_{\lambda-\frac{1}{2}}\left(1 + \frac{\mu^2}{2k^2}\right), \qquad \alpha > 0, \qquad \mathrm{Re}\,\lambda > -\tfrac{1}{2},$$

which is the Born approximation result for the Yukawa potential.

## VI. APPLICATIONS

### A. Poles at Infinity

The poles in the angular-momentum plane are given by the zeros of the denominator of Eq. (35).

[15] Bateman Manuscript Project, *Higher Transcendental Functions*, edited by A. Erdelyi (McGraw-Hill Book Company, Inc., New York, 1953), Vol. I, p. 155.

But, because (38) holds, we conclude that under the restrictions of the potential there are no poles in the right-half $\lambda$ plane for large $|\lambda|$. This means of course that all Regge trajectories are bounded in the $\lambda$ plane, Re $\lambda \geq 0$, none extending to infinity.

Because, for example, a square-well potential which is analytically rounded off would show the same behavior, we must attribute the unbounded trajectories in cutoff potentials[9] to the nonanalyticity of the potential; all other requirements are satisfied.

### B. Watson–Sommerfeld Transformation

We now consider the representation of the total scattering amplitude

$$A(k^2, \cos\theta) = \frac{1}{2i}\int_c \frac{2\lambda A(\lambda, k) P_{\lambda-\frac{1}{2}}(-\cos\theta)\, d\lambda}{\sin\pi(\lambda - \frac{1}{2})}, \quad (41)$$

where $c$ is a contour enclosing the positive real axis, and ask for what class of potentials it is permissible to deform the contour $c$ such that

$$A(k^2, \cos\theta) = \frac{1}{2i}\int_{-i\infty}^{+i\infty} \frac{2\lambda A(\lambda, k) P_{\lambda-\frac{1}{2}}(-\cos\theta)\, d\lambda}{\sin\pi(\lambda - \frac{1}{2})} + \text{pole terms}. \quad (42)$$

Taking into account the behavior of

$$P_{\lambda-\frac{1}{2}}(-\cos\theta)/\sin\pi(\lambda - \tfrac{1}{2})$$

as $|\lambda| \to \infty$,[16] one can always choose a region of $\cos\theta$ such that even if $A(\lambda, k)$ behaves as a power along the imaginary axis, the transformation (42) is possible. One should make the Watson–Sommerfeld transformation for these suitable $\cos\theta$ values and then continue the result analytically.

From the estimate (37) we find that for a single Yukawa potential, $\delta \to_{|\lambda|\to\infty} O(|l|^{-\frac{1}{2}}) + O(|l|^{-\frac{3}{2}})$ except on the imaginary axis. For a superposition of Yukawa potential one can have $\delta \to O(|l|^{-\frac{3}{2}})$, in which case the transformation (42) is possible for all $\cos\theta$.

These are upper bounds. If we do the second integral in (39) for a superposition of Yukawa potential for $\lambda = iy$, we get,[17] with $\xi = kr/\lambda$,

$$\int_m^\infty \sigma(\mu)\, d\mu \int_1^\infty \frac{e^{-i\mu(y/k)}}{(\xi^2 - 1)^{\frac{1}{2}}}\, d\xi = \frac{\Gamma^2(\frac{1}{2})}{2i}\int_m^\infty H_0^{(2)}(\mu y/k)\sigma(\mu)\, d\mu \underset{y\to\infty}{\to} \frac{\pi}{4i} \times \int_m^\infty \sqrt{\frac{2k}{\pi\mu y}}\, e^{-i(\mu y/k - \frac{1}{4}\pi)}\sigma(\mu)\, d\mu.$$

Thus the amplitude actually goes as $O(|l|^{-\frac{1}{2}})$ along the imaginary axis. If the results of the present theory could be extended to a single Yukawa potential, then our limit above would give $O(|l|^{-\frac{1}{2}})$ along the imaginary axis.

### APPENDIX I

Two independent solutions of the unperturbed equation

$$h_\lambda^{(1),(2)}(kr) = (\tfrac{1}{2}\pi kr)^{\frac{1}{2}} H_1^{(1),(2)}(kr)$$

have the asymptotic forms

$$h_\lambda^{(1),(2)}(kr) \underset{r\to\infty}{\to} e^{\pm i(kr - \frac{1}{2}\pi\lambda - \frac{1}{4}\pi)}.$$

For $r \to \infty$, the radial wave equation can be written as a linear combination of these two solutions:

$$v_\lambda(r) \underset{r\to\infty}{\to} A h_\lambda^{(1)}(kr) + B h_\lambda^{(2)}(kr)$$

and

$$v_\lambda'(r) \underset{r\to\infty}{\to} A\frac{d}{dr}h_\lambda^{(1)}(kr) + B\frac{d}{dr}h_\lambda^{(2)}(kr).$$

Hence,

$$A = \frac{W(v_\lambda(r), h_\lambda^{(2)}(kr))}{W(h_\lambda^{(1)}(kr), h_\lambda^{(2)}(kr))} = -\frac{1}{2ik}W(v_\lambda(r), h_\lambda^{(2)}(kr)),$$

$$B = -\frac{W(v_\lambda(r), h_\lambda^{(1)}(kr))}{W(h_\lambda^{(1)}(kr), h_\lambda^{(2)}(kr))} = \frac{1}{2ik}W(v_\lambda(r), h_\lambda^{(1)}(kr)),$$

where $W(\phi_1, \phi_2)$ is the Wronskian $W(\phi_1, \phi_2) = \phi_1\phi_2' - \phi_2\phi_1'$. From the asymptotic form

$$v_\lambda(r) \to Be^{i(\pi\frac{1}{2}\lambda + \frac{1}{4}\pi)}[e^{-ikr} - e^{-i\pi l}(A/B)e^{ikr}],$$

the $S$ matrix is

$$S = \frac{A}{B} = -\frac{W(v_\lambda(r), h_\lambda^{(2)}(kr))}{W(v_\lambda(r), h_\lambda^{(1)}(kr))}.$$

Then Eq. (33) follows with $A(\lambda, k) = 1 - S$.

### APPENDIX II

From Eqs. (3) and (4),

$$u^{\pm}(z) \underset{|\lambda|\to\infty}{\to} \left(\frac{\lambda^{-\frac{1}{3}}}{\phi(z)}\right)^{\frac{1}{2}} e^{\pm i(\lambda\Phi(z))},$$

$$u_0^{\pm}(z) \to \left(\frac{1}{\phi_0(z)\lambda^{\frac{1}{3}}}\right)^{\frac{1}{2}} e^{\pm i\lambda\Phi_0(z)}.$$

Any solution may be expressed as a linear combination of these independent solutions. For the unperturbed case, the solutions are known to be the spherical Bessel functions and may be identified by well-known identities for these functions[18]:

[16] See, for example, reference 9, Appendix I.
[17] W. Gröbner and N. Hofreiter, *Integraltafeln* (Springer-Verlag, Vienna, 1957), Part II, p. 191.

$$h_\lambda^{(1)}(kr) \equiv (\tfrac{1}{2}\pi kr)^{\frac{1}{2}} H_\lambda^{(1)}(kr)$$
$$= (\lambda^{\frac{1}{2}} ke^z)^{\frac{1}{2}} e^{-\frac{1}{2}\pi i} u_0^+(z) \to (ke^z/\phi_0)^{\frac{1}{2}} e^{i(\lambda\Phi_0 - \frac{1}{4}\pi)},$$
$$h_\lambda^{(2)}(kr) \equiv (\tfrac{1}{2}\pi kr)^{\frac{1}{2}} H_\lambda^{(2)}(kr)$$
$$= (\lambda^{\frac{1}{2}} ke^z)^{\frac{1}{2}} e^{+\frac{1}{2}\pi i} u_0^-(z) \to (ke^z/\phi_0)^{\frac{1}{2}} e^{-(\lambda\Phi_0 - \frac{1}{4}\pi)},$$
$$j_\lambda(kr) \equiv \tfrac{1}{2}[h_\lambda^{(1)}(kr) + h_\lambda^{(2)}(kr)] \to (ke^z/\phi_0)^{\frac{1}{2}} \sin(\lambda\Phi_0 - \tfrac{1}{4}\pi).$$

The corresponding physical solution of the Schrödinger equation behaving as $r^{\lambda+\frac{1}{2}}$ at $r = 0$ is given by[13]

$$v_\lambda(r) = a(\lambda)u^+ + b(\lambda)u^-,$$
$$v_\lambda(r) \underset{|\lambda|\to\infty}{\to} \tfrac{1}{2}(\lambda^{\frac{1}{2}} ke^z)^{\frac{1}{2}}[e^{-\frac{1}{2}\pi i} u^+(z) + e^{+\frac{1}{2}\pi i} u^-(z)] \to \left(\frac{ke^z}{\phi}\right)^{\frac{1}{2}} \sin(\lambda\Phi - \tfrac{1}{4}\pi).$$

Although the asymptotic form of $u^*$ is known in the whole $\lambda$ plane, that of the physical wavefunction $v$ is known only for Re $\lambda > 0$. This result only holds in the right half-plane. We know only the asymptotic forms of $a(\lambda)$ and $b(\lambda)$. In order to continue $v_\lambda$ to Re $\lambda < 0$ we must know $a(\lambda)$ and $b(\lambda)$ completely.

With the above identification of the solutions, the evaluation of the Wronskians (33) is straightforward. One need merely to use, with $r \to \infty$, the forms (3) and (4), and the asymptotic evaluations

$$\phi^0 = [k^2e^{2z} - 1]^{\frac{1}{2}} \underset{|\lambda|\to\infty}{\to} ke^z,$$
$$\Phi^0 = [k^2e^{2z} - 1]^{\frac{1}{2}} - \tan^{-1}[k^2e^{2z} - 1]^{\frac{1}{2}} \to ke^z - \tfrac{1}{2}\pi.$$

Since $\phi \underset{|\lambda|\to\infty}{\to} \phi^0$, $\Phi \underset{|\lambda|\to\infty}{\to} \Phi^0$, it is convenient to write

$$\phi = \phi^0(1 + \phi), \qquad \Phi = \Phi^0(1 + \Phi).$$

The final results are found to be

$$W(v_\lambda(r), j_\lambda(kr)) \underset{\substack{r\to\infty \\ |\lambda|\to\infty}}{\to} k \sin\lambda\Phi^0 \delta\Phi,$$
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Hence we obtain Eq. (35).

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# Asymptotic Behavior of Schrödinger Scattering Amplitudes

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(Received 6 February 1963)

The behavior of the $S$-wave scattering amplitude for large $k$ is studied for potentials which vanish at infinity faster than any exponential, but are not cut off. The asymptotic behavior is very sensitive to the shape of the potential tail. If the potential decreases very rapidly, the growth of the Jost function resembles that with a cut-off potential. If $V(r)$ decreases only slightly more rapidly than an exponential, then $f(k)$ exhibits a very rapid growth in the vicinity of the positive imaginary axis. In this case also the zeros of $f(k)$ become very dense and are concentrated near the positive imaginary axis.

THE analytic properties of Schrödinger partial-wave scattering amplitudes have been the object of considerable study.[1] It is known[2] that if the potential behaves like $e^{-\alpha r}$ for large $r$, then the Jost function $f(k)$ is analytic in the region $-\infty < \text{Im } k < \frac{1}{2}\alpha$; if $V(r)$ decreases faster than any exponential, then $f(k)$ is an entire function. However, its detailed behavior has been studied only for potentials which vanish identically outside some finite radius. In such a case it was shown by Regge[3] and by Humblet[4] that $f(k)$ increases exponentially in the upper half-plane, and its large zeros are located just above the real axis, with approximately uniform spacing.

In this paper, the asymptotic behavior of $f(k)$ is studied for potentials which decrease more rapidly than any exponential, but are not cut off. Only the $S$-wave amplitude is considered, but it is to be ex-

* Present address: Massachusetts Institute of Technology, Cambridge, Massachusetts.

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$$h_\lambda^{(1)}(kr) \equiv (\tfrac{1}{2}\pi kr)^{\frac{1}{2}} H_\lambda^{(1)}(kr)$$
$$= (\lambda^{\frac{1}{2}} ke^z)^{\frac{1}{2}} e^{-\frac{1}{2}\pi i} u_0^+(z) \to (ke^z/\phi_0)^{\frac{1}{2}} e^{i(\lambda\Phi_0 - \frac{1}{4}\pi)},$$
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The corresponding physical solution of the Schrödinger equation behaving as $r^{\lambda+\frac{1}{2}}$ at $r = 0$ is given by[13]

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In this paper, the asymptotic behavior of $f(k)$ is studied for potentials which decrease more rapidly than any exponential, but are not cut off. Only the $S$-wave amplitude is considered, but it is to be ex-

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pected that the other partial waves will exhibit similar behavior.

It is, of course, not surprising to find that the form of the potential at very large distances, which must have a negligible effect on the physical scattering amplitude (real $k$), can radically alter the behavior of $f(k)$ elsewhere in the $k$ plane.

## I.

The solution of the $S$-wave Schrödinger equation with Jost-type boundary condition satisfies the integral equation

$$f(k, r) = e^{-ikr} + \frac{1}{k}\int_r^\infty \sin k(r' - r)\, V(r') f(k, r')\, dr'. \quad (1)$$

The Jost function $f(k) = f(k, 0)$ determines the $S$ matrix for the problem by

$$S(k) = f(k)/f(-k). \quad (2)$$

The analytic continuation of $f(k, r)$ to complex $k$ is defined by Eq. (1). When the potential vanishes faster at infinity than any exponential, the iterative solution

$$f(k, r) = \sum_n f^{(n)}(k, r), \quad (3)$$

$$f^{(0)}(k, r) = e^{-ikr};$$

$$f^{(n+1)}(k, r) = \frac{1}{k}\int_r^\infty \sin k(r' - r)\, V(r') f^{(n)}(k, r')\, dr' \quad (4)$$

converges absolutely in the entire $k$ plane.[2] Moreover, just as with cut-off potentials,[3] the solution for large $k$ is dominated by the first iteration (Born approximation). This assertion is proved in Appendix B. The Jost function is, therefore, given asymptotically by

$$f(k) \sim 1 + (1/2ik)[J - I(k)], \quad (5)$$

where[5]

$$J = \int_0^\infty V(r)\, dr, \quad (6a)$$

$$I(k) = \int_0^\infty V(r) e^{-2ikr}\, dr. \quad (6b)$$

The integral $J$ is independent of $k$ and requires no further consideration. We wish to examine the asymptotic behavior of $I(k)$, assuming at first that the potential follows a pure "exponential power law," i.e.,

$$V(r) = V_0 \exp[-(r/a)^p], \qquad p > 1. \quad (7)$$

With this potential the integral may be put into a standard form

$$I_p(\kappa) = V_0 a p^{-1/p} \int_0^\infty \exp\left(\kappa z - \frac{1}{p} z^p\right) dz, \quad (8)$$

where

$$z = p^{1/p}(r/a); \qquad \kappa = p^{-1/p}(-2ika). \quad (9)$$

We are interested in the behavior of (8) for large $\kappa$.

A power-series expansion for the integral is easily obtained. The result is

$$I_p(\kappa) = \frac{V_0 a}{p} \sum_{n=0}^\infty \frac{(p^{1/p}\kappa)^n}{n!}\, \Gamma\left(\frac{n+1}{p}\right). \quad (10)$$

The series (10) converges absolutely for all $\kappa$, as long as $p > 1$. It is, therefore, an entire function and constitutes a formal solution of the problem. The convergence is, of course, extremely slow for large values of $\kappa$, and the series appears to be useless for determining the asymptotic behavior. However, two theorems from the theory of entire functions may be employed to infer from (10) the maximum rate of growth of $I_p(\kappa)$. The first theorem[6] states that the order[7] is given in terms of the coefficients $a_n$ of the power series by the expression

$$\rho = \limsup_{n\to\infty} \frac{n \log n}{\log (1/|a_n|)}. \quad (11)$$

For the series (10), the limit in (11) is easily evaluated with the use of Stirling's formula for the $\Gamma$ function, and one obtains the result

$$\rho = p/(p - 1). \quad (12)$$

This result is valid for all $p > 1$. For large $p$, the order decreases toward unity. On the other hand, when $p = 1 + \epsilon$, the order is $1 + (1/\epsilon)$ and grows without limit as $\epsilon \to 0$. This was already pointed out by Regge,[3] although the estimate of the order given by him (the largest integer between 1 and $\frac{1}{2} + 3/2\epsilon$) appears to be incorrect.

A second theorem[8] states that the type[7] $\tau$ of the function is given by

[5] The separation of the Born approximation into two parts, of course, requires that each of these integrals exist, and this places some restriction on the potential. In addition to the requirement that $V(r)$ vanish faster than any exponential, it is certainly sufficient to assume that $\int |V(r)|\, dr < \infty$. Actually, as long as $\int r\, |V(r)|\, dr < \infty$, the neighborhood of the origin can cause no difficulty, since the combination $J - I$ must converge even though the separate terms may not. In such a case it would be necessary to combine the two integrals in the interval between 0 and some small $\delta$, but this interval does not contribute to the asymptotic behavior of $f(k)$.

[6] R. P. Boas, *Entire Functions* (Academic Press Inc., New York, 1954), p. 9.

[7] An entire function is of order $\rho$ if its maximum modulus $M(r)$ is $O(\exp r^{\rho+\epsilon})$ for all $\epsilon > 0$ but no $\epsilon < 0$. A function of finite order $\rho$ is of type $\tau$ if $M(r) = O(\exp(\tau + \epsilon) r^\rho)$ for all $\epsilon > 0$ but no $\epsilon < 0$.

[8] Reference 6, p. 11.

$$\tau = \nu/e\rho, \tag{13}$$

where

$$\nu = \limsup_{n\to\infty} n a_n^{\rho/n}. \tag{14}$$

For the series (10), the limit in (14) is just $e$. Therefore,

$$\tau = 1/\rho = (p-1)/p, \tag{15}$$

and the maximum modulus of $I_p(\kappa)$ must be

$$O\left(\exp\left\{\left[\epsilon + \frac{p-1}{p}\right]|\kappa|^{p/(p-1)}\right\}\right). \tag{16}$$

## II.

We next seek an actual asymptotic expansion for the integral (8). For a part of the $\kappa$ plane, such an expansion may be obtained from the following theorem[9]:

Let $F(t)$ be analytic in $\alpha < \arg t < \beta$, with

$$F(t) \approx \sum_\nu c_\nu t^{\lambda_\nu} \quad \text{for} \quad t \to 0,$$
$$-1 < \operatorname{Re}\lambda_0 < \operatorname{Re}\lambda_1 \cdots$$

and

$$|F(t)| < Ae^{a|t|} \quad \text{for} \quad |t| \geq R > 0, \qquad a \geq 0.$$

Then the integral

$$f(s) = \int_0^{\infty e^{i\phi}} e^{-st} F(t)\, dt$$

is analytic in $\operatorname{Re}(se^{i\phi}) > a$, $\alpha < \phi < \beta$, and possesses the asymptotic expansion

$$f(s) \sim \sum_\nu c_\nu \frac{\Gamma(\lambda_\nu + 1)}{s^{\lambda_\nu+1}} \tag{17}$$

for $s \to \infty$ on every ray with $-\beta - \frac{1}{2}\pi < \arg s < -\alpha + \frac{1}{2}\pi$, and uniformly in every interior sector.

In the present case the function

$$f(z) = \exp\left[-(1/p)z^p\right]$$

is bounded in $-\pi/2p < \arg z < \pi/2p$. (For non-integral $p$ there is a branch point at the origin, but this does not interfere with the validity of the theorem.) It follows that the asymptotic series

$$I_p(\kappa) \sim \sum_{n=0}^{\infty} \frac{\Gamma(np+1)}{(-p)^n n!(-\kappa)^{np+1}} \tag{18}$$

is valid in the interval

$$\tfrac{1}{2}\pi - \pi/2p < \arg\kappa < \pi/2p + \tfrac{3}{2}\pi, \tag{19}$$

and uniformly in any smaller interval. In particular, the interval always includes the positive imaginary axis (real axis in the $k$ plane).

According to (18), the leading term in the region (19) is always $\sim 1/\kappa$, regardless of the value of $p$. For our purposes only this leading term is significant, since the higher iterations in (2) will certainly contribute terms comparable to the higher terms in (18). Furthermore, when $I$ does have the asymptotic form (18), the Born approximation (5) is dominated by the other integral $J$, which is one order higher in $\kappa$. (This is always the case in $\operatorname{Re}\kappa < 0$, i.e., the lower half of the $k$ plane.)

Another approach to the asymptotic behavior, which is applicable also outside the region (19), is the method of steepest descents (Appendix A).[10] This method makes use of the fact that the important contributions to the integral come from regions where the exponent has its largest real part. By appropriate deformation of the path, these regions may be concentrated, for large $\kappa$, in the immediate vicinity of the end points or of saddle points. For the integral (8) under consideration, the end-point contribution reproduces the series (18), while the saddle-point integral is (Appendix A)

$$\left(\frac{2\pi}{p-1}\right)^{\frac{1}{2}} \exp\left(\frac{p-1}{p}\kappa^{p/(p-1)}\right) \Big/ \kappa^{(p-2)/(2p-2)}. \tag{20}$$

When $\arg\kappa$ is in the region (19), the contribution of (20) is vanishingly small for large $\kappa$, so the asymptotic behavior is given by (18). However, in the remainder of the $\kappa$ plane, i.e., for $-\frac{1}{2}\pi + \pi/2p < \arg\kappa < \frac{1}{2}\pi - \pi/2p$, the real part of the exponent is positive, and (20) is the dominant term in the asymptotic expansion. The result is in agreement with the estimate of the growth given by (16).

For the Jost function (5), the asymptotic behavior is then the following:

$$f(k) \sim \frac{[2\pi/(p-1)]^{\frac{1}{2}} V_0 a^2}{p^{1/(2p-2)}(-2ika)^{(3p-4)/(2p-2)}} \times \exp\left[(p-1)\left(\frac{-2ika}{p}\right)^{p/(p-1)}\right], \tag{21}$$

$$\pi/2p < \arg k < \pi - \pi/2p; \tag{22}$$

$$f(k) \sim 1 + \frac{1}{2ik}\int_0^\infty V(r)\, dr \quad \text{elsewhere.} \tag{23}$$

In (21) the argument of $-i$ must be taken as $-\frac{1}{2}\pi$.

When $p$ is large, i.e., when the potential goes very rapidly to zero, $f(k)$ approaches exponential type and the region in which (21) is the dominant be-

[9] G. Doetsch, *Handbuch der Laplace Transformation*.(Birkhauser Verlag, Basel, 1956), Vol. II, p. 48.

[10] H. Jeffreys and B. Jeffreys, *Methods of Mathematical Physics*, (Cambridge University Press, New York, 1956), p. 503.

havior comprises almost all of the upper half-plane. It is to be expected that if the potential vanishes more rapidly than does (7) for any value of $p$, then $f(k)$ is actually of order one and increases in the entire upper half-plane. This may be verified. For example, with the potential

$$V(r) = \exp(-e^r), \tag{24}$$

the integral $I(k)$ can be transformed to

$$\int_1^\infty u^{\kappa-1}e^{-u}\,du. \tag{25}$$

The asymptotic behavior is then given by Stirling's formula, since, for large $\kappa$, the integral from zero to one becomes vanishingly small. Hence, for potential (24),

$$I(\kappa) \sim \Gamma(\kappa) \sim \exp[(\kappa - \tfrac{1}{2})\log\kappa - \kappa], \quad \mathrm{Re}\,\kappa > 0. \tag{26}$$

The order of $f(k)$ in this case is unity, the type is infinite, and the growth is in the entire upper half of the $k$ plane.

For "slowly" decreasing potentials, ($p \approx 1$), the result (21) indicates that although the growth of $f(k)$ is extremely rapid, the region in which the function grows is confined to a very small sector enclosing the positive imaginary axis. Suppose the potential decreases still more slowly, e.g.,

$$V(r) = r^{-r}, \tag{27}$$

which vanishes more slowly than (7) for any $p$, although still more rapidly than any exponential. For such a potential, the saddle-point integration gives as the dominant term

$$I(\kappa) \sim \exp(e^\kappa), \tag{28}$$

which is of infinite order. However, (28) holds only within an infinitesimal neighborhood about the positive real axis (positive imaginary axis in the $k$ plane). The behavior of $f(k)$ is evidently quite pathological in this vicinity. It may be recalled that it is on the imaginary $k$ axis that the "redundant" poles and other singularities appear when the potential decreases so slowly that $f(k)$ ceases to be entire.

## III.

From the asymptotic expressions (21) and (23), it is clear that the large zeros of $f(k)$ must be located near the lines

$$\arg k = \pi/2p, \qquad \pi - \pi/2p. \tag{29}$$

The density of zeros can be estimated with the use of Jensen's theorem,[11] which gives the result

$$n(h) \sim (1/\pi)(p-1)(2ah/p)^{p/(p-1)}, \tag{30}$$

where $n(h)$ is the number of zeros with modulus $< h$. As is to be expected, the zeros are more dense, the greater the order of the function. [$n(h) = O(h^\rho)$.]

The location of the $n$th zero (counting only the ones in the first quadrant) may be roughly estimated from (21). Writing

$$k_n = h_n \exp i(\pi/2p + \delta_n), \tag{31}$$

and retaining only the leading terms, we obtain

$$2ah_n \sim p\left(\frac{2\pi n}{p-1}\right)^{(p-1)/p}, \tag{32}$$

$$\delta_n \sim p^{(p+1)/(p-1)}\left(\frac{3p-4}{2}\right)\frac{\log(2ah_n)}{2\pi n}. \tag{33}$$

The image point $h_n \exp i(\pi - \pi/2p - \delta_n)$ is also a zero; with this factor included the density as determined by (32) is in accord with the result (30).

When $p \to \infty$, Eqs. (31)–(33) show that the zeros approach the real axis, as well as the uniform spacing characteristic of cut-off potentials.[3] On the other hand, for $p$ close to unity, the large zeros are near the imaginary axis. In addition, the angle $\delta_n$, as given by (33), is negative: The zeros are just *outside* the region where (21) is the asymptotic behavior. The explanation is that the saddle-point integral is here of the form $\kappa^q \exp[-\epsilon\,|\kappa|^{p/(p-1)}]$, where $q > 0$ and the argument of the exponential has an infinitesimally negative real part. Such a term is large over a long distance, even though it eventually decreases exponentially and is overpowered by the term which decreases only as $1/\kappa$. The situation is quite delicate in such a boundary region, where one form of asymptotic behavior is disappearing and being replaced by another.

## IV.

We now wish to drop the assumption that the potential is purely of the form (7). Suppose, instead, that

$$V(r) = V_1(r), \qquad r < b, \tag{34a}$$

$$= V_0 \exp[-(r/a)^p], \qquad r > b, \tag{34b}$$

where $V_1$ is arbitrary, subject to the usual conditions of integrability.[5] Then the integral of Eq. (6b) is decomposed into two parts:

$$I(k) = \int_0^b V_1(r)e^{-2ikr}\,dr$$

[11] Reference 6, p. 2.

$$+ V_0 \int_b^\infty \exp\left[-2ikr - (r/a)^p\right] dr = I_a + I_b. \quad (35)$$

The first integral in (35) is just the one which occurs in the case of cut-off potentials. It is dominated by the vicinity of $r = b$, and can be treated by a straightforward extension of the theorem (17). Assuming that $V_1(r)$ can be expanded near $r = b$ in a series of the form

$$V_1(r) \approx \sum_\nu c_\nu (b - r)^{\lambda_\nu}, \quad -1 < \lambda_0 < \lambda_1 \cdots, \quad (36)$$

one gets for the asymptotic behavior of $I_a$

$$I_a \sim -e^{-2ikb} \sum_\nu c_\nu \frac{\Gamma(\lambda_\nu + 1)}{(2ik)^{\lambda_\nu + 1}}. \quad (37)$$

The first term of (37) is the result given by Regge[3] for cut-off potentials. If all the left derivatives $V_1^{(n)}$ exist at $r = b$, the result can also be written in the form

$$I_a \sim -e^{-2ikb} \sum_n \frac{V_1^{(n)}(b)}{(2ik)^{n+1}}. \quad (38)$$

The second integral in (35) differs from (8) only in having a finite end point and may be analyzed in the same manner. When $\arg k$ is between 0 and $\pi/2p$, the theorem of (17) holds and the result is of the form (38):

$$I_b \sim V_0 \exp\left[-2ikb - (b/a)^p\right]$$
$$\times \left[1/2ik - (p/a)(b/a)^{p-1}(1/2ik)^2 + O(1/k^3)\right]. \quad (39)$$

The contribution is comparable to that of $I_a$. If the potential happens to be continuous at $b$, the leading term in (39) cancels that of (37). If, in addition, (38) holds for $I_a$ and one or more derivatives are continuous at $b$, then further terms cancel, and the asymptotic behavior of $f(k)$ is

$$f(k) \sim (\text{const}) \exp\left[-2ikb - (b/a)^p\right]/(2ik)^{\alpha+2}, \quad (40)$$

where $\alpha$ is the first derivative which is discontinuous.[12] In any case $f(k)$ is of exponential growth instead of approaching unity, as does (23).

When $\arg k$ is in the region (22), $f(k)$ is once again dominated by the saddle-point integral. Since this integral is determined by the vicinity of the saddle point, removal of a distant portion of the path cannot have any effect, and the result is precisely the same as (21). A term (40) is of course also present, and if $b$ is large the factor $\exp(-ikb)$ causes such a term to be important over a long range of values of $k$. However, it must eventually be overtaken by the saddle-point contribution, which increases as $\exp(k^q)$ with $q > 0$. Hence, for any finite $b$, the asymptotic behavior in the region (22) is still given by (21).

Similar considerations apply to the location of the zeros. An estimate for the modulus $h_n$ is provided by the solution of the equation

$$[(p - 1)/p^{p/(p-1)}](2ah_n)^{p/(p-1)}$$
$$+ 2bh_n \sin\left[\tfrac{1}{2}\pi(p - 1)/p\right] = 2\pi n. \quad (41)$$

If $b$ is large, the location of many of the zeros will be appreciably shifted. Eventually, however, the first term in Eq. (39) becomes predominant and the solution reduces to (32). The angle $\delta_n$ is slightly changed: Instead of (33), it is given by

$$\delta_n \sim (\text{const})/(2\pi n)^{1/(p-1)}. \quad (42)$$

In addition, there will be another set of zeros, close to the real axis and with uniform spacing, determined solely by the behavior of the potential near $r = b$.

This discussion does not, by any means, exhaust the class of potentials which decrease faster than any exponential. It suffices, however, to demonstrate that the behavior of $f(k)$ near the positive imaginary axis (and, hence, also the order and type) depend quite sensitively on the shape of the potential tail. In the vicinity of the real axis, on the other hand, the asymptotic behavior is determined by the form of $V(r)$ at finite distances, as it must be on physical grounds. If the potential happens to be of the form (34) for some finite $b$, then the asymptotic form of $f(k)$ is given by Eqs. (21) and (23). In general, as long as a power-series expansion for $f(k)$ can be obtained, the order and type may be determined from Eqs. (11) and (13).

## APPENDIX A

The method of steepest descents[10] is applicable to integrals of the form

$$\int_a^b e^{f(z)}\, dz, \quad (A1)$$

in which $f(z)$ is analytic and depends linearly on some parameter $t$, and the integral is to be evaluated asymptotically for large $t$. The method consists of deforming the path of integration into segments along which the real and imaginary parts of $f(z)$ are, alternately, constant. On Im $f$ = const, the real part is monotonic, unless the path passes through a point where $f'(z) = 0$. At such a point, two paths Im $f$ = const cross; since Re $f$ is a solution of Laplace's equation, it must be a maximum along one of the

[12] There must be a derivative which is discontinuous, or else the form (34b) would extend to a smaller value of $r$.

paths, a minimum along the other (hence, the designation saddle point). The saddle point must be crossed along the former type of path, i.e., from valley to valley. Then, for large $t$, the integrand drops off rapidly on either side of the saddle point and the integral along this portion of the path is given asymptotically by

$$I \sim (2\pi)^{\frac{1}{2}} e^{f(z_0)} e^{i\alpha} / |f''(z_0)|^{\frac{1}{2}}, \tag{A2}$$

where $\alpha$ is the angle of the line of steepest descent at the saddle point $z_0$.

If the path is deformed properly, the only other relative maximum of Re $f$, in addition to the saddle points, must be at an end point. The leading term from this part of the path is [assuming for concreteness that Re $f(a) >$ Re f$(b)$]

$$I \sim -e^{f(a)}/f'(a). \tag{A3}$$

Formula (A3) provides the leading term in the asymptotic expansion of the integral whenever the path may be made to avoid all saddle points, or when Re $f(a)$ is greater than Re $f$ at whatever saddle points have to be traversed.

The integral (8) of the text is suited to treatment by this method. Consider first the case $p$ = integer. There are then $p - 1$ saddle points, the solutions of $z^{p-1} = \kappa$,

$$z_j = h^{1/(p-1)} \exp\,[i(\phi + 2\pi j)/(p-1)], \quad j = 0, 1, \cdots, p-2, \quad \kappa = he^{i\phi}. \tag{A4}$$

However, only the saddle point nearest the real axis ($j = 0$) will ever have to be traversed, and here formula (A2) leads to the result given in the text, Eq. (20). The end-point contribution comes from the origin, and gives a term $\sim 1/\kappa$, which is just the first term of the series (18). The higher terms of this series are also reproduced by the higher terms of (A3).

It remains to be established in what regions of arg $\kappa$ each of the contributions is dominant. We examine the first quadrant. Evidently, for

$$0 < \arg \kappa < \tfrac{1}{2}\pi(p-1)/p, \tag{A5}$$

the exponential in (20) has a positive real part and is large. Also, the path of steepest descents must pass through the saddle point, so the dominant term in the integral is of the form (20). In the sector

$$\tfrac{1}{2}\pi(p-1)/p < \arg \kappa < \tfrac{3}{2}\pi(p-1)/p, \tag{A6}$$

the saddle-point contribution is very small and the integral is dominated by the contribution from the origin. In the next sector,

$$\tfrac{3}{2}\pi(p-1)/p < \arg \kappa < \tfrac{5}{2}\pi(p-1)/p, \tag{A7}$$

the saddle-point integral is once again large. However, the path may be taken so as to go to infinity along lines of steepest descent without passing through any saddle point; the same is true for all the subsequent regions in which the saddle-point integral has a positive real part. Therefore, the integral (8) is large and given by (20) only within the central sector, (A5), and goes to zero as $1/\kappa$ elsewhere.

To examine the behavior of $f(k)$ when the potential goes to zero slowly, let

$$p = 1 + 1/n, \qquad n = \text{integer}. \tag{A8}$$

The function $f(z)$ has a branch point at the origin, but this causes no difficulty. We can draw a branch line along the negative real axis and proceed as before. There is only one saddle point, located at

$$z_0 = \kappa^n. \tag{A9}$$

For large $n$, the saddle point lies on one of the higher sheets of the Riemann surface, except when arg $\kappa$ is within an increasingly narrow range centered around zero. Outside this range, the steepest descents integral can proceed along the valley from the origin to infinity on the first sheet and always avoid the saddle point. Therefore, formula (21) holds also when $p$ is of the form (A1).

If $p$ is neither an integer nor of the form (A1), there are, in general, very many saddle points (an infinite number if $p$ is irrational.) However, almost all of them lie on distant sheets, and only the principal one $z_0 = h^{1/(p-1)} e^{i\phi/(p-1)}$ can affect the integral. The derivation proceeds as in the preceding cases, and the results (21) and (23) are, therefore, of general validity, for any $p > 1$.

## APPENDIX B

The statement that the Born approximation is adequate for large $k$ has to be proved. We first show that the order of $f(k)$ is given correctly by the lowest approximation. The $n$th iteration of (3) may be written

$$f^{(n)}(k, r) = \frac{e^{-ikr}}{(2ik)^n} \int_r^\infty dr_1\, V(r_1)(1 - e^{-2ik(r_1 - r)}) \int_{r_1}^\infty dr_2 \cdots \int_{r_{n-1}}^\infty dr_n\, V(r_n)(1 - e^{-2ik(r_n - r_{n-1})}). \tag{B1}$$

From this it follows, with $k = \mu + i\nu$, $\nu > 0$, and $h = |k|$, that

$$|f^{(n)}(k, r)| \leq \frac{e^{\nu r}}{h^n} \int_r^\infty dr_1\, |V(r_1)|\, e^{2\nu(r_1 - r)} \int_{r_1}^\infty dr_2$$

$$\cdots \int_{r_{n-1}}^{\infty} dr_n \, |V(r_n)| \, e^{2\nu(r_n - r_{n-1})},$$

$$\leq \frac{e^{-\nu r}}{h^n} \int_0^{\infty} dr_1 \, |V(r_1)| \int_0^{\infty} dr_2 \cdots \int_0^{\infty} dr_{n-1} \, |V(r_{n-1})| \int_0^{\infty} dr_n \, |V(r_n)| \, e^{2\nu r_n}$$

$$= e^{-\nu r}\left(\frac{c}{h}\right)^{n-1} \frac{g(\nu)}{n}, \tag{B2}$$

where

$$c = \int_0^{\infty} dr \, |V(r)|, \tag{B3}$$

$$g(\nu) = \int_0^{\infty} dr \, |V(r)| \, e^{2\nu r}. \tag{B4}$$

Inequality (B2) places an upper limit on the sum of all the higher iterations:

$$\left| \sum_{n=2}^{\infty} f^{(n)}(k) \right| \leq \frac{c/h}{1 - c/h} \frac{g(\nu)}{h}. \tag{B5}$$

Let $k$ be on the positive imaginary axis. Then, for potentials of the form (7), for which $g(\nu) = |I(k)|$, it follows directly that

$$\left| \sum_{2}^{\infty} f^{(n)}(k) \right| = O(f^{(1)}(k)/k), \tag{B6}$$

and the Born approximation is adequate for large imaginary $k$. Since the maximum growth of $f(k)$ takes place along the positive imaginary axis, the estimate of the order and type obtained from $f^{(1)}(k)$ must be correct. The same conclusion holds also when the potential is of the form (34), since in the region which contributes to the asymptotic behavior, the potential does not change sign.[13]

The preceding argument does not suffice to prove that $f^{(1)}(k)$ is everywhere the dominant term in the asymptotic behavior, since elsewhere than on the imaginary axis the first Born term $I(k)$ is not as large as $g(\nu)$. It is, therefore, necessary to study the behavior of the higher iterations in greater detail.

The second Born approximation for $f(k)$ has the form

$$f^{(2)}(k) = \frac{1}{(2ik)^2} \int_0^{\infty} dr_1 \, V(r_1) \int_{r_1}^{\infty} dr_2 \, V(r_2) \times [1 + e^{-2ikr_2} - e^{-2ikr_1} - e^{-2ik(r_2 - r_1)}]$$

$$= J_1 + J_2 + J_3 + J_4. \tag{B7}$$

We examine each of these integrals. The first is clearly, in absolute value, $\leq c^2/4h^2$. In order to estimate $J_2$, rewrite it as

$$J_2 = \frac{1}{(2ik)^2} \int_0^{\infty} dr_1 \, V(r_1) \times \left\{ \left( \int_0^{\infty} - \int_0^{r_1} \right) dr_2 \, V(r_2) e^{-2ikr_2} \right\}. \tag{B8}$$

In (B8) the first part is $(1/2ik)^2 JI(k)$. In the second part, the $r_2$ integral, over a finite range, is just of the form discussed in Sec. IV, and is described asymptotically by Eq. (37) or Eq. (38). Its contribution to $J_2$ is, therefore,

$$\frac{1}{(2ik)^3} \int_0^{\infty} dr_1 \, e^{-2ikr_1} \left\{ [V(r_1)]^2 + O\left(\frac{1}{2ik}\right) \right\}, \tag{B9}$$

which is sufficiently small. For example, if $V(r)$ is of the form (7), the dominant term in (B9) is

$$(\text{const}) \exp\left[ \frac{2(p-1)\left(-\frac{ika}{p}\right)^{p/(p-1)}}{(ika)^{(7p-8)/(2p-2)}} \right] \tag{B10}$$

in the region where the saddle-point integral is dominant, and $O(1/2ik)^4$ elsewhere.

The third term in (B7) becomes identical to the term just discussed if the order of integration is reversed, so its contribution is also given by (B9). Finally, for $J_4$ one has

$$J_4 = \frac{1}{(2ik)^2} \int_0^{\infty} dr_1 \, V(r_1) e^{2ikr_1} \times \left\{ \left( \int_0^{\infty} - \int_0^{r_1} \right) dr_2 \, V(r_2) e^{-2ikr_2} \right\}; \tag{B11}$$

$$|J_4| \leq \frac{1}{(2ik)^2} c \, |I(k)| + O(c^2/(2ik)^2).$$

All the terms which make up $f^{(2)}(k)$ are, therefore, at most $O(f^{(1)}(k)/2ik)$. The higher iterations can be similarly examined, and it is clear that each succeeding iteration introduces an additional power of $1/k$. Hence, the estimate (B6) is valid for all $k$.

[13] For a potential with an infinite number of changes of sign, this argument would have to be refined. The argument which follows would still apply, however.

# Coupled Schrödinger Equations and Statistical Boundary Conditions*

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The possibility of introducing distribution functions for the phase of a radial wavefunction at a boundary is studied for the case of elastic scattering. The properties of a simple class of distribution functions are discussed. The results are generalized to the solutions of an arbitrary number of coupled Schrödinger equations which satisfy time-reversal invariance, provided there are no closed channels.

## 1. INTRODUCTION

THE use of potentials for the description of nonrelativistic nucleon–nucleon interactions has always been very popular due to the concise way in which scattering data can be "stored" in the form of a phenomenological potential model and due to its transparency of interpretation. The long-range and intermediate-range nucleon–nucleon potentials, as they are known today, can be well interpreted as due to the exchange of one or two pions and are in agreement with a large amount of experimental information.[1] However, it is now clear that the hope of ever finding a nuclear potential which is defined up to very short distances cannot be realized without giving up certain desirable features as, for example, energy independence of the potential. The region of small distances (which plays an essential role in this paper and which will be called the core region) is, moreover, hard to explore. It is for that reason that one often tries to avoid an exact treatment of such a region, either by inserting an infinitely hard core with sharp boundary radius, suitably adjusted to give the proper binding energies of possible bound states, or by giving the boundary conditions of the wavefunctions at some finite distance $r_0$. Many of the (semi) phenomenological potential models[2–5] are of the first kind. The so-called boundary-condition model[6–9] is of the latter kind.

In the present paper an alternate approach is worked out, in which a core region ($r < r_0$) and a potential region ($r \geq r_0$) are distinguished under the assumption that the form of the potential is accurately known in the potential region and nothing is known with certainty in the core region. Instead of claiming exact knowledge of the boundary condition on the wavefunction and its derivative at the point $r_0$, the amount of knowledge is now represented by a distribution function of the phase angle at that point. So our approach is statistical in nature.

A distribution function for the *phase angles* at the boundary radius leads to a distribution function for the *phase shifts* in a quite natural way. In our case, where we possess no knowledge of the core region, we take a random phase distribution at the point $r_0$ and obtain phase-shift distributions of a particularly simple kind, depending on the form of the potential. It is true that the amount of information obtained in this way is less than in the boundary-condition model, but the advantage is its clear definition of the reliability of certain computed results. Moreover, it lends itself to generalizations, for example, when absorption has to be taken into account.

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[9] In the boundary-condition model, one originally made the same assumption about the exterior region as in the $R$-matrix theory of nuclear reactions, namely that the boundary radius is such that only nonpolarizing potentials (or no potentials at all) are present outside this boundary. [See for example J. M. Blatt and V. F. Weisskopf, *Theoretical Nuclear Physics* (John Wiley & Sons, Inc., New York, 1952) or A. M. Lane and R. G. Thomas, Rev. Mod. Phys. 30, 257 (1958)]. For nuclei, this is evidently a useful assumption since a nuclear boundary is fairly well defined. For nucleon–nucleon interactions, the determination of a suitable boundary radius is a more difficult task under the given conditions. No radius suggests itself *a priori*, and polarizing terms are already important in the one-pion exchange part of the potential. Also, with the present advance of high-speed computers, there is no longer any reason to avoid the numerical integration of coupled Schrödinger equations. The emphasis in this paper is completely placed on the exterior region which contains polarizing potentials as well. For a general method of solving coupled Schrödinger equations numerically, see J. J. de Swart and P. J. Eberlein, (Rochester NYO-9030, March, 1960) or J. J. de Swart and C. Dullemond, Ann. Phys. (N. Y.) 16, 263 (1961).

A few examples will illustrate the possible usefulness of the method. Let us depart from the radial wave equation and consider a one-dimensional scattering problem where $r$ is defined from $-\infty$ to $+\infty$ and where a potential barrier of finite but large height is present, so that particles scattering from the left or from the right cannot penetrate sufficiently to pass through the barrier. If one describes particles which scatter from the right, the wavefunction and its derivative, although small at the left of the barrier, will never vanish simultaneously and one is able to define a phase angle [$\cot^{-1}(k^{-1}\psi'/\psi)$, $k$ being the free-particle wavenumber] everywhere. But it is clear that large variations of the phase angle at a particular point left of the barrier will not noticeably influence the phase angle at a point right of the barrier. The exact boundary conditions at $-\infty$ are practically unimportant for the determination of the shape of the wavefunction of the particle coming from the right. So it seems that the barrier itself provides the proper boundary conditions to a large extent, and the boundary conditions are completely determined when the barrier is completely impenetrable (as in the case of an infinitely hard core). But this is not the whole story. Suppose that one varies the phase angle left of the barrier continuously. Then, for one very well defined value, it seems as if the particle is indeed able to penetrate the barrier, no matter how high. This is not surprising, because one now describes the scattering of a particle *coming from the left*; the roles of left and right side have been reversed. So there is always a critical phase angle for which penetration is possible, and a barrier will therefore define the boundary conditions, *provided* the conditions at the other side of the barrier are not critical. The chances that these critical conditions are met become increasingly small, the higher the barrier is, but they are nevertheless there. Coming back to the case of the radial wave equation, the conditions are the same except that only values of $r$ larger than zero are physical. Scattering can only take place from the "right," i.e., large positive values of $r$. If now a barrier is present, it will provide boundary conditions disregarding the conditions at $r = 0$ as long as the conditions at $r = 0$ are not critical. When they are indeed critical in the sense of the one-dimensional example given above, we have the conditions of a resonance. This is not exceptional, since merely varying the incoming particle energy will lead to such a situation, where suddenly the phase shifts show wild variations. To see what is happening becomes quite complicated in the case of coupled channels. The introduction of distribution functions of the phase angles and mixing parameters is a systematic way of obtaining insight into this kind of phenomena as we will see in subsequent sections.

The purpose of this paper is to discuss a class of distribution functions of practical importance and mathematical simplicity, and it is applied only to sufficiently simple examples to serve as illustrations of the method. After a mathematical introduction (Sec. 2), we introduce distribution functions for uncoupled equations (Sec. 3), coupled equations (Sec. 4), and finally the phase shifts are discussed (Sec. 5). A general discussion follows in Sec. 6.

Throughout this paper the symbols $k$ and $l$ are reserved for the $n \times n$ diagonal matrices of which the (positive) eigenvalues represent the free-particle wavenumbers, and the orbital-angular-momentum quantum numbers of coupled channels, respectively, while $r$ is always a distance between interacting particles. The symbol $S$ is reserved for the scattering matrix.

When no reference is made to a physical meaning of certain quantities, we will use Latin capitals for $n \times n$ matrices and script capitals for $2n \times 2n$ (or $2n \times n$) matrices. It is sometimes necessary to refer to the first or to the last $n$ columns for a $2n \times 2n$ matrix; in that case, subscripts $\alpha$ and $\beta$ are used to refer to the $2n \times n$ submatrices under consideration. Latin lower-case characters stand in general for $2n$-dimensional column matrices. The symbols $R$ and $\mathcal{R}$ are reserved for certain orthogonal matrices, $I$ and $\mathcal{I}$ stand for identity matrices, while $Q$ and $\mathcal{Q}$ are reserved for certain symmetric matrices. Primes indicate derivatives with respect to $r$ and the symbol $\sim$ stands for transposition.

Special symbols are introduced whenever certain quantities have a physical meaning. We call $\psi(r)$ (or just $\psi$) the $n \times n$ matrix representing $n$ arbitrary independent solutions of the wave equation; $\psi_i(r)$ is always a column matrix representing one particular solution, and $\tilde{\psi}_i(r)$ is the corresponding row matrix. The diagonal matrix of which the eigenvalues play a role as phases is denoted by $\varphi$, while the eigenvalues are indicated by $\varphi_i$ ($i = 1, \cdots, n$). Phase shifts are indicated by $\delta$ (the diagonal matrix) and $\delta_i$ (the eigenvalues). The symbol $\rho$ is reserved for the distribution function. Finally, the symbol det stands for the determinant of a matrix.

## 2. MATHEMATICAL PRELIMINARIES

In this section we set up a scheme for the description of $n$ coupled nonrelativistic channels suitable for the purposes of this paper. We only consider

the radial part of the wave equation and we assume that the reduced channel masses are not necessarily equal. Also we assume that no closed channels are present.

As a starting point we write down the radial wave equation for coupled channels:

$$k^{-1}\psi_i'' = \left[\left(\frac{k}{m}\right)^{-\frac{1}{2}} V(r)\left(\frac{k}{m}\right)^{-\frac{1}{2}} + k^{-1}\frac{l(l+1)}{r^2} - k\right]\psi_i \equiv W(r)\psi_i, \tag{2.1}$$

where $m$ is the diagonal matrix of the reduced channel masses and where the elements $\psi_{ij}$ $(j = 1, \cdots, n)$ of the column matrix $\psi_i$ are normalized such that, in the case of purely outgoing waves, $|\psi_{ij}|^2$ and $|\psi_{ik}|^2$ are equal if they represent waves of equal outgoing *flux*. The matrix $V(r)$ is proportional to the "potential" matrix and we assume that it is symmetric (as a consequence of time-reversal invariance) and real, although this last requirement is not strictly necessary for our method to be valid in principle. The matrix

$$\left(\frac{k}{m}\right)^{-\frac{1}{2}} V(r)\left(\frac{k}{m}\right)^{-\frac{1}{2}} + k^{-1}\frac{l(l+1)}{r^2}, \tag{2.2}$$

in which $l$ is an $n \times n$ diagonal matrix, is also real and symmetric and from now on we will refer to this as the "potential," since only in the discussion of phase shifts will it be necessary to make a distinction between the actual potential and the centrifugal barrier term.

If we make no distinction between regular and irregular solutions, Eq. (2.1) has $2n$ independent solutions which can be written in $n \times n$ matrix form, $\psi_\alpha$ and $\psi_\beta$. For the general solution we have

$$\begin{aligned} \psi &= \psi_\alpha M_\alpha + \psi_\beta M_\beta, \\ k^{-1}\psi' &= k^{-1}\psi_\alpha' M_\alpha + k^{-1}\psi_\beta' M_\beta, \end{aligned} \tag{2.3a}$$

or in matrix form,

$$\begin{Vmatrix} \psi \\ k^{-1}\psi' \end{Vmatrix} = \begin{Vmatrix} \psi_\alpha & \psi_\beta \\ k^{-1}\psi_\alpha' & k^{-1}\psi_\beta' \end{Vmatrix} \cdot \begin{Vmatrix} M_\alpha \\ M_\beta \end{Vmatrix}, \tag{2.3b}$$

where the $2n \times n$ matrix $\begin{Vmatrix} M_\alpha \\ M_\beta \end{Vmatrix}$ must be nonsingular when we want to have all columns of $\begin{Vmatrix} \psi \\ k^{-1}\psi' \end{Vmatrix}$ to be independent.

Without loss of generality and disregarding overall normalization, we may take, at an arbitrary point $r_1$,

$$\begin{aligned} \psi_\alpha(r_1) &= I, \qquad \psi_\beta(r_1) = 0, \\ k^{-1}\psi_\alpha'(r_1) &= 0, \qquad k^{-1}\psi_\beta'(r_1) = I. \end{aligned} \tag{2.4}$$

We then have, at another arbitrary point $r_2$,

$$\begin{Vmatrix} \psi(r_2) \\ k^{-1}\psi'(r_2) \end{Vmatrix} = \begin{Vmatrix} \psi_\alpha(r_2) & \psi_\beta(r_2) \\ k^{-1}\psi_\alpha'(r_2) & k^{-1}\psi_\beta'(r_2) \end{Vmatrix} \cdot \begin{Vmatrix} \psi(r_1) \\ k^{-1}\psi'(r_1) \end{Vmatrix}, \tag{2.5}$$

which means that if the boundary conditions at $r = r_1$ are known, the conditions at $r_2$ can be obtained by simple matrix multiplication. This demonstrates that

$$\Psi(r_2, r_1) = \begin{Vmatrix} \psi_\alpha(r_2) & \psi_\beta(r_2) \\ k^{-1}\psi_\alpha'(r_2) & k^{-1}\psi_\beta'(r_2) \end{Vmatrix} \tag{2.6}$$

contains all the information about the set of Eqs. (2.1) which is of interest for the construction of $\psi$ and $\psi'$. Notice that the matrix $\Psi_\beta(r_2, r_1)$ (for $r_2 \geq r_1$) consisting of the last $n$ columns of (2.6) actually represents the (unnormalized) wavefunction and its derivative at the point $r_2$ when an infinitely hard core is present at the point $r_1$.

The matrix $\Psi$ has several interesting properties which we will now discuss.

First of all one easily verifies that

$$\Psi(r_1, r_2)\Psi(r_2, r_3) = \Psi(r_1, r_3), \tag{2.7a}$$

and as a consequence, we have

$$\Psi(r_1, r_2) = \Psi^{-1}(r_2, r_1), \tag{2.7b}$$

$$\Psi(r, r) = \mathcal{I}. \tag{2.7c}$$

Secondly, the matrices are *symplectic*. Symplectic matrices are matrices of the form

$$\mathfrak{A} = \begin{Vmatrix} A_{\alpha 1} & A_{\beta 1} \\ A_{\alpha 2} & A_{\beta 2} \end{Vmatrix},$$

which have the property

$$\tilde{A}_{\alpha 1}A_{\alpha 2} - \tilde{A}_{\alpha 2}A_{\alpha 1} = 0, \tag{2.8a}$$

$$\tilde{A}_{\beta 1}A_{\beta 2} - \tilde{A}_{\beta 2}A_{\beta 1} = 0, \tag{2.8b}$$

$$\tilde{A}_{\alpha 1}A_{\beta 2} - \tilde{A}_{\alpha 2}A_{\beta 1} = I. \tag{2.8c}$$

The following identity follows easily:

$$\begin{Vmatrix} A_{\alpha 1} & A_{\beta 1} \\ A_{\alpha 2} & A_{\beta 2} \end{Vmatrix}^{-1} = \begin{Vmatrix} \tilde{A}_{\beta 2} & -\tilde{A}_{\beta 1} \\ -\tilde{A}_{\alpha 2} & \tilde{A}_{\alpha 1} \end{Vmatrix}. \tag{2.9}$$

It is also readily verified that when $\mathfrak{A}$ and $\mathfrak{B}$ are symplectic, also $\mathfrak{A}\mathfrak{B}$ is symplectic. The $2n \times 2n$

identity matrix is symplectic and so is the inverse of every symplectic matrix. So these matrices form a group, known as the *symplectic group*.[10] From Eq. (2.9) it follows that

$$\det \begin{Vmatrix} A_{\alpha 1} & A_{\beta 1} \\ A_{\alpha 2} & A_{\beta 2} \end{Vmatrix} = \pm 1,$$

but from reference 10 we learn that the group is simply connected and therefore only the + sign can hold, so

$$\det \mathfrak{A} = 1. \tag{2.10}$$

We will call the $2n \times n$ matrices $\mathfrak{A}_\alpha$ and $\mathfrak{A}_\beta$ also symplectic due to Eqs. (2.8a, b). The proof that $\Psi$ is symplectic is a consequence of the symmetry of $W$ in Eq. (2.1):

$$\begin{aligned} (d/dr)(\tilde{\psi}_\alpha k^{-1}\psi'_\alpha - \tilde{\psi}'_\alpha k^{-1}\psi_\alpha) &= \tilde{\psi}_\alpha(W - \tilde{W})\psi_\alpha = 0, \\ (d/dr)(\tilde{\psi}_\beta k^{-1}\psi'_\beta - \tilde{\psi}'_\beta k^{-1}\psi_\beta) &= 0, \qquad (2.10a) \\ (d/dr)(\tilde{\psi}_\alpha k^{-1}\psi'_\beta - \tilde{\psi}'_\alpha k^{-1}\psi_\beta) &= 0. \end{aligned}$$

Taking into account the conditions, Eq. (2.4), at the point $r_1$ we find that

$$\tilde{\psi}_\alpha k^{-1}\psi'_\alpha - \tilde{\psi}'_\alpha k^{-1}\psi_\alpha = 0, \tag{2.11a}$$

$$\tilde{\psi}_\beta k^{-1}\psi'_\beta - \tilde{\psi}'_\beta k^{-1}\psi_\beta = 0, \tag{2.11b}$$

$$\tilde{\psi}_\alpha k^{-1}\psi'_\beta - \tilde{\psi}'_\alpha k^{-1}\psi_\beta = I, \tag{2.11c}$$

which are exactly the conditions Eq. (2.8) for $\Psi$ to be a symplectic matrix.

The property Eq. (2.9) which is now also valid means that the generally laborious job of taking inverses of matrices is now reduced to a mere rearrangement of the same matrix elements. The properties Eqs. (2.7) and (2.9) together with Eq. (2.5) make it profitable to make the matrix $\Psi$ the first object to be computed numerically when a numerical integration of Schrödinger equations is desired. Since $\Psi$ tends to become very singular when $r_1$ and $r_2$ are taken far apart, it is advisable to compute a series of matrices $\Psi$, namely $\Psi(r, r_1)$ for $r_1 \leq r \leq r_2$, $\Psi(r, r_2)$ for $r_2 \leq r \leq r_3$, etc., where $r_1, r_2, \cdots$ are not too far apart. The property Eq. (2.7a) allows one to calculate the wavefunction and its derivative at any arbitrary point $r$ when arbitrary boundary conditions exist at any other arbitrary point $r_0$. Another example of the usefulness of $\Psi$ is, that one obtains a quick insight into the influence of variations in the hard-core radius on the wavefunction.

Let us now leave the matrix $\Psi$ for a while and study the properties of the symplectic matrices $\mathfrak{A}$ further, since they turn out to be important also in other aspects which are of use to us. First note that when $\mathfrak{A}$ is symplectic, $\tilde{\mathfrak{A}}$ is also symplectic, which gives a set of relations slightly different than those of the kind in Eq. (2.8). There is also the question of parameterization. From Eq. (2.8) it follows that $\mathfrak{A}$ can be rewritten in the form (provided $\det A \neq 0$)

$$\mathfrak{A} = \begin{Vmatrix} A & AQ_\beta \\ Q_\alpha A & \tilde{A}^{-1} + Q_\alpha A Q_\beta \end{Vmatrix}, \tag{2.12}$$

where $A$ is arbitrary nonsingular; $Q_\alpha$ and $Q_\beta$ are arbitrary symmetric. We see that if $\mathfrak{A}$ is real, it can be parameterized by $2n^2 + n$ real parameters and if complex then by twice as many.

We will now discuss some special classes of symplectic matrices of interest to us.

The orthogonal symplectic matrices not only satisfy Eq. (2.9), but also

$$\begin{Vmatrix} A_{\alpha 1} & A_{\beta 1} \\ A_{\alpha 2} & A_{\beta 2} \end{Vmatrix}^{-1} = \begin{Vmatrix} \tilde{A}_{\alpha 1} & \tilde{A}_{\alpha 2} \\ \tilde{A}_{\beta 1} & \tilde{A}_{\beta 2} \end{Vmatrix},$$

and we find that

$$A_{\alpha 1} = A_{\beta 2} \quad \text{and} \quad A_{\alpha 2} = -A_{\beta 1}.$$

The general form of the orthogonal symplectic matrices is therefore

$$\mathfrak{R} = \begin{Vmatrix} A_{\alpha 1} & -A_{\alpha 2} \\ A_{\alpha 2} & A_{\alpha 1} \end{Vmatrix}. \tag{2.13}$$

It follows that

$$\tilde{A}_{\alpha 1}A_{\alpha 2} = \tilde{A}_{\alpha 2}A_{\alpha 1}, \qquad A_{\alpha 1}\tilde{A}_{\alpha 2} = A_{\alpha 2}\tilde{A}_{\alpha 1}, \tag{2.14a}$$

$$\tilde{A}_{\alpha 1}A_{\alpha 1} + \tilde{A}_{\alpha 2}A_{\alpha 2} = A_{\alpha 1}\tilde{A}_{\alpha 1} + A_{\alpha 2}\tilde{A}_{\alpha 2} = I. \tag{2.14b}$$

In order to obtain a suitable parameterization, note that the matrices $\tilde{A}_{\alpha 1}A_{\alpha 1}$ and $A_{\alpha 1}\tilde{A}_{\alpha 1}$ are symmetric, can be diagonalized by orthogonal matrices, and have the same eigenvalues. Let $B^2$ be the matrix of the eigenvalues and let $\tilde{R}_2$ and $R_1$, respectively, be the diagonalizing matrices; then $B$ can always be chosen such that

$$A_{\alpha 1} = R_1 B R_2. \tag{2.15}$$

Adopting suitable conventions, one is able to eliminate ambiguities concerning the ordering of the eigenvalues in $B$ and minus or plus signs, and one can make an unique parameterization of $A_{\alpha 1}$ by giving the $\frac{1}{2}n(n-1)$ independent (real or complex) parameters of $R_1$, the $n$ (real or complex) parameters of $B$ and the $\frac{1}{2}n(n-1)$ parameters of $R_2$.

From Eq. (2.14b) we find

[10] H. Weyl, *The Classical Groups* (Princeton University Press, Princeton, New Jersey, 1947), 2nd ed.

$$A_{\alpha 2}\tilde{A}_{\alpha 2} = I - R_1 B^2 \tilde{R}_1 = R_1(I - B^2)\tilde{R}_1,$$
$$\tilde{A}_{\alpha 2}A_{\alpha 2} = I - \tilde{R}_2 B^2 R_2 = \tilde{R}_2(I - B^2)R_2,$$

and from this it follows that $R_1$ diagonalizes the matrix $A_{\alpha 2}\tilde{A}_{\alpha 2}$, and $\tilde{R}_2$ diagonalizes $\tilde{A}_{\alpha 2}A_{\alpha 2}$. The eigenvalues of both matrices are those of the diagonal matrix $I - B^2$. One can then adjust the signs of $(I - B^2)^{\frac{1}{2}}$ such that

$$A_{\alpha 2} = R_1(I - B^2)^{\frac{1}{2}}R_2.$$

The matrices $R_1$, $R_2$, $B$ and $(I - B^2)^{\frac{1}{2}}$ would have been real if $\mathfrak{R}$ were real, so we see that for real orthogonal symplectic matrices the eigenvalues of $B$ never exceed unity in absolute value. It follows that there exists a real diagonal matrix $\eta$ such that

$$\begin{aligned} A_{\alpha 1} &= R_1(\sin\eta)R_2, \\ A_{\alpha 2} &= R_1(\cos\eta)R_2, \end{aligned} \tag{2.16}$$

and one can restrict the eigenvalues $\eta_i$ to a region $+\frac{1}{2}\pi > \eta_i \geq -\frac{1}{2}\pi$. It follows that $\mathfrak{R}$ can be parameterized by $n^2$ real parameters if $\mathfrak{R}$ is real, and by $2n^2$ real parameters if $\mathfrak{R}$ is complex. For real $\mathfrak{R}$, the ordering convention $\eta_1 \geq \eta_2 \geq \cdots \geq \eta_n$ and proper sign conventions for $R_1$ and $R_2$ make the parameterization unique. Note that the vector $\mathfrak{R}_\alpha$ is always specified by exactly the same parameters as $\mathfrak{R}$ itself.

Another class of matrices is important for us, namely the symmetric symplectic matrices. They appear as coefficient matrices of quadratic equations (representing some kind of ellipsoids defined in a $2n$-dimensional space). The general form of these matrices is

$$\mathfrak{Q} = \begin{Vmatrix} A & C \\ \tilde{C} & B \end{Vmatrix}, \tag{2.17}$$

where $A = \tilde{A}$, $B = \tilde{B}$. If $A$ is nonsingular, one can write $\mathfrak{Q}$ in the form

$$\mathfrak{Q} = \begin{Vmatrix} A & AQ \\ QA & A^{-1} + QAQ \end{Vmatrix},$$

where $Q$ is symmetric. This follows again from Eq. (2.8). We find, therefore, that $\mathfrak{Q}$ can be parameterized by $n(n + 1)$ real (complex) parameters. Note that $AB = I + C^2$ so that one can find an arbitrary $\mathfrak{Q}$ by choosing $A$ and $B$ arbitrary symmetric. The matrix $\mathfrak{Q}$ being symmetric and symplectic, can be diagonalized by an orthogonal symplectic matrix $\mathfrak{R}$. (See Appendix I.) If all matrices involved are real, then the diagonal form of $\mathfrak{Q}$ is

$$\mathfrak{Q}_{\text{diag}} = \begin{Vmatrix} \Lambda^{-1} & 0 \\ 0 & \Lambda^{+1} \end{Vmatrix}, \tag{2.18}$$

where $\Lambda$ is an arbitrary real diagonal matrix. One can now order the eigenvalues of $\mathfrak{Q}_{\text{diag}}$ such that those $< 1$ are all in $\Lambda$, if all eigenvalues are positive (the only case of interest).

Note that the matrices $\mathfrak{R}$ do, but the matrices $\mathfrak{Q}$ do not form a group. It is easy to prove that *the group of all real orthogonal symplectic matrices is isomorphic with the group of unitary matrices.* (See Appendix I.) This was first noticed by S. Minakshisundaram.[11]

Finally there are the unitary symplectic matrices. We leave these out of the discussion here.

After this discussion of the different types of symplectic matrices, we return to Eq. (2.1) and the matrices $\Psi(r_1, r_2)$. Let us define a $2n$-dimensional vector space in every point $r > 0$ and let $\mathbf{v}$ be an arbitrary vector in that space. Now consider $\Psi(r_1, r_2)$ as the transformation matrix which maps the vector space at $r_2$ onto the vector space at $r_1$. We have, by definition

$$\mathbf{v}(r_1) = \Psi(r_1, r_2)\mathbf{v}(r_2), \tag{2.19a}$$

which can alternatively be written as

$$v(r_1) = \Psi(r_1, r_2)v(r_2), \tag{2.19b}$$

or

$$\tilde{v}(r_1) = \tilde{v}(r_2)\tilde{\Psi}(r_1, r_2), \tag{2.19c}$$

where $v$ and $\tilde{v}$ are just the equivalent column and row matrices. Property Eq. (2.10) now states that the Jacobian of the transformation is unity so that the volume of the parallelopiped spanned by $2n$ independent vectors $\mathbf{v}$ in that space is invariant under the transformation. Since the transformation Eq. (2.19) is linear we find that *quadratic expressions transform into quadratic expressions.* Since the transformation is real and unimodular, we conclude that ellipsoids transform into ellipsoids with the same volume.

The equation for the unit sphere is $\tilde{x}x = 1$ or equivalently $\mathbf{x}\cdot\mathbf{x} = 1$, or $|\mathbf{x}|^2 = 1$. The equation for an ellipsoid is

$$\tilde{x}\mathcal{G}x = 1,$$

where $\mathcal{G}$ is real and symmetric and has positive eigenvalues. The diagonalizing matrix is real orthogonal and specifies the direction vectors of the principal axes of the ellipsoid. The eigenvalues of $\mathcal{G}^{-1}$ are the squares of the lengths of the principal axes.

How does a unit sphere at $r_0$ transform into an

[11] S. Minakshisundaram, J. Ind. Math. Soc. **19**, 105 (1955).

ellipsoid at $r$? From Eq. (2.19) we have

$$1 = \mathfrak{x}(r_0)x(r_0)$$
$$= \mathfrak{x}(r)\tilde{\Psi}(r_0, r)\Psi(r_0, r)x(r) = \mathfrak{x}(r)\mathfrak{IC}(r_0, r)x(r), \quad (2.20)$$

where $\mathfrak{IC}$ is not only symmetric but also symplectic. From Eq. (2.18) we see that the principal axes then go in pairs such that the product of the lengths of the axes of each pair is just one.

It is also useful to introduce generalized 2-component vectors of the general form

$$\hat{\mathfrak{U}} = (U_1, U_2),$$

where $U_1$ and $U_2$ are $n \times n$ matrices.

Alternatively we use the matrix

$$\mathfrak{U} = \left\| \begin{matrix} U_1 \\ U_2 \end{matrix} \right\|,$$

or the matrix

$$\tilde{\mathfrak{U}} = \| \tilde{U}_1 \quad \tilde{U}_2 \|$$

as possible equivalent replacements of this vector. In every point $r$, instead of defining a $2n$-dimensional linear vector space, we could define a 2-dimensional vector space in which the vectors have matrix components. Again, let $\Psi(r_1, r_2)$ be the transformation matrix which transforms a vector at $r_2$ into a vector at $r_1$. The following notations are then equivalent:

$$\begin{aligned} \hat{\mathfrak{U}}(r_1) &= \Psi(r_1, r_2)\hat{\mathfrak{U}}(r_2), \\ \mathfrak{U}(r_1) &= \Psi(r_1, r_2)\mathfrak{U}(r_2), \\ \tilde{\mathfrak{U}}(r_1) &= \tilde{\mathfrak{U}}(r_2)\tilde{\Psi}(r_1, r_2). \end{aligned} \quad (2.21)$$

We say that the generalized vector $\mathfrak{F}$ satisfies the equation of the generalized ellipse if

$$\tilde{\mathfrak{X}}\mathfrak{IC}\mathfrak{X} = I,$$

where $\mathfrak{IC}$ is defined as in Eq. (2.20), i.e.,

$$\mathfrak{IC}(r_0, r) = \tilde{\Psi}(r_0, r)\Psi(r_0, r),$$

if the generalized ellipse is the transform of a generalized circle at $r_0$. Since $\mathfrak{s}$ is symplectic, a $2n$-dimensional unit sphere serves as generalized circle, but not every $2n$-dimensional ellipsoid serves as generalized ellipse in this picture.

We illustrate the contents of this section with an example.

Suppose that one has $n$ coupled channels and that for $r_0 \leq r \leq r_c$ a constant potential exists. For $r > r_c$, the potential is zero and no centrifugal barrier is present. We have for the wave equation, Eq. (2.1),

$$k^{-1}\psi_i'' = (-(k/m)^{-\frac{1}{2}}V_0(k/m)^{-\frac{1}{2}} - k)\psi_i \qquad (r_0 \leq r \leq r_c), \quad (2.22)$$

$$k^{-1}\psi_i'' = -k\psi_i \qquad (r > r_c),$$

where $V_0$ is a constant (i.e., independent of $r$), real, symmetric matrix with positive eigenvalues. Define the matrix $\kappa^2$:

$$\kappa^2 = (km)^{\frac{1}{2}}V_0(k/m)^{-\frac{1}{2}} + k^2,$$

and let $\kappa$ have all eigenvalues positive. One obtains the following set of equations:

$$\begin{aligned} \psi_i'' &= -\kappa^2\psi_i \qquad (r_0 \leq r \leq r_c), \\ \psi_i'' &= -k^2\psi_i \qquad (r > r_c). \end{aligned} \quad (2.23)$$

The matrix $\kappa^2$ has the property

$$\kappa^2 k = k\bar{\kappa}^2, \quad (2.24)$$

and if we assume that all eigenvalues of $\kappa^2$ are different, then we can find a similarity transformation $U$ which diagonalizes $\kappa^2$:

$$\kappa^2 = U\sigma^2U^{-1},$$

so that

$$\sigma^2(U^{-1}k\tilde{U}^{-1}) = (U^{-1}k\tilde{U}^{-1})\sigma^2.$$

Since $\sigma^2$ is diagonal and nondegenerate, it follows that $U^{-1}k\tilde{U}^{-1}$ is diagonal, so that this matrix commutes with any of the square roots $\sigma$ of $\sigma^2$, each of which must be diagonal. In fact, every function of $\sigma$ is diagonal and commutes with $U^{-1}k\tilde{U}^{-1}$, so we conclude that

$$\kappa k = k\bar{\kappa}, \quad (2.24a)$$

and generally

$$f(\kappa)k = kf(\bar{\kappa}). \quad (2.24b)$$

The matrix $\Psi(r, r_0)$ for $r_0 \leq r \leq r_c$ can now be constructed:

$$\Psi(r, r_0) = \left\| \begin{matrix} \cos \kappa(r - r_0) & \kappa^{-1} \sin \kappa(r - r_0)\cdot k \\ -k^{-1}\kappa \sin \kappa(r - r_0) & k^{-1} \cos \kappa(r - r_0)\cdot k \end{matrix} \right\|, \quad (2.25a)$$

or, equivalently, with (2.24b),

$$\Psi(r, r_0) = \left\| \begin{matrix} \cos \kappa(r - r_0) & k\bar{\kappa}^{-1} \sin \bar{\kappa}(r - r_0) \\ -k^{-1}\kappa \sin \kappa(r - r_0) & \cos \bar{\kappa}(r - r_0) \end{matrix} \right\|. \quad (2.25b)$$

One can now easily check that $\Psi$ is symplectic and that Eq. (2.7b) is valid. For $r \geq r_c$ we have simply

$$\Psi(r, r_c) = \left\| \begin{matrix} \cos k(r - r_c) & \sin k(r - r_c) \\ -\sin k(r - r_c) & \cos k(r - r_c) \end{matrix} \right\|. \quad (2.26)$$

The combination rule, Eq. (2.7a), gives for $r \geq r_c$

$$\Psi(r, r_0) = \Psi(r, r_c) \cdot \Psi(r_c, r_0)$$
$$= \begin{Vmatrix} \cos k(r - r_c) & \sin k(r - r_c) \\ -\sin k(r - r_c) & \cos k(r - r_c) \end{Vmatrix}$$
$$\times \begin{Vmatrix} \cos \kappa(r_c - r_0) & k\bar{\kappa}^{-1} \sin \bar{\kappa}(r_c - r_0) \\ -k^{-1}\kappa \sin (r_c - r_0) & \cos \bar{\kappa}(r_c - r_0) \end{Vmatrix}. \quad (2.27)$$

The last $n$ columns represent the solution for the case that there is an infinite hard core at $r = r_0$.

For the construction of $\mathfrak{K}(r_0, r)$ $(r_0 \leq r \leq r_c)$, one needs the inverse of Eq. (2.25) and its transpose. The eigenvalues and eigenvectors of $\mathfrak{K}$ characterize the shape and position of the ellipsoid corresponding to $\mathfrak{K}$. Even in this simple example these quantities are hard to obtain and we will not do this.

We close this section with the remark that although $\mathfrak{K}(r_0, r)$ is not the inverse of $\mathfrak{K}(r, r_0)$, their eigenvalues are each others inverses, and due to property Eq. (2.18), the eigenvalues are in fact the same. So $\mathfrak{K}(r_0, r)$ and $\mathfrak{K}(r, r_0)$ *represent ellipsoids of exactly the same shape and size, but different orientation.* In other words, a sphere at $r_0$ transforms into an ellipsoid at $r$, and a sphere at $r$ transforms in an ellipsoid at $r_0$ with the same shape and size, but different orientation.

### 3. DISTRIBUTION FUNCTIONS WHEN COUPLING IS ABSENT

In this section we discuss the case $n = 1$ (no coupling). In every point $r$ we define a two-dimensional vector space in which $\psi$ and $k^{-1}\psi'$ are the two components of each vector. The phase $\varphi = \cot^{-1}(k^{-1}\psi'/\psi)$ is just the angle which such a vector makes with the $k^{-1}\psi'$ axis.

Now consider a vector $\mathbf{v}(r_1)$ and its image $\mathbf{v}(r_2)$ at two different points $r_1$ and $r_2$. A linear unimodular transformation transforms $\mathbf{v}(r_1)$ into $\mathbf{v}(r_2)$, so when $\mathbf{v}(r_1)$ is rotated over an angle $d\varphi(r_1)$, then $\mathbf{v}(r_2)$ will be rotated over an angle $d\varphi(r_2)$ such that $|\mathbf{v}(r_1)|^2\, d\varphi(r_1) = |\mathbf{v}(r_2)|^2\, d\varphi(r_2)$, i.e., the area described by each vector is the same. Now when there is a certain probability that vector $\mathbf{v}(r_1)$ will be found within the interval $d\varphi(r_1)$, then this probability must be the same for vector $\mathbf{v}(r_2)$ to be found within the interval $d\varphi(r_2)$. So the probability densities for $\mathbf{v}(r_1)$ and $\mathbf{v}(r_2)$ have a ratio which is equal to that of $|\mathbf{v}(r_1)|^2$ and $|\mathbf{v}(r_2)|^2$. If one now defines a probability "amplitude" as the square root of the probability density, then this amplitude is proportional to $|\mathbf{v}|$. We see therefore, that *a radial plot of the probability amplitude in the two-dimensional space transforms as if every point on that plot were a vector.* Particularly, if that plot were an ellipse, it is an ellipse at every point $r$. The area under the allowed part of the ellipse must be one. We will call the probability density as function of $\varphi$ the distribution function.

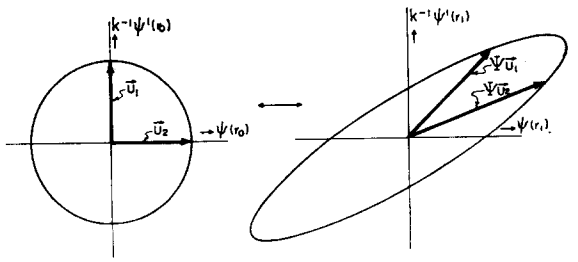


FIG. 1. Sketch of the way in which a random distribution at a point $r = r_0$ transforms into a distribution which favors certain phase angles at $r = r_1$, under influence of a potential or centrifugal barrier between $r_0$ and $r_1$. Uncoupled case.

What are the requirements for a distribution function which tells us that the boundary conditions at a particular point $r_0$ are unknown? If the potential (including the centrifugal barrier) is everywhere equal to that at infinity, i.e., zero, it is reasonable, that when one lacks information at a particular point, one lacks that information everywhere, so for this case the corresponding distribution function must be the same for all $r$. It must be an invariant under the transformations

$$\Psi_0(r, r_0) = \begin{Vmatrix} \cos k(r - r_0) & \sin k(r - r_0) \\ -\sin k(r - r_0) & \cos k(r - r_0) \end{Vmatrix},$$

where the index 0 of $\Psi$ indicates that there are no potentials. Since $\Psi_0$ is orthogonal, only circles stay invariant under the transformation. Therefore a circle is a suitable radial plot of the probability amplitude for this case. Now, if potentials are present, it is reasonable that our information varies from point to point; a circle still represents lack of information if one wants to make a mathematical definition of "lack of information" which is independent of the presence or absence of potentials. We discuss only those situations in which we indeed lack information about the phase at some point $r_0$; therefore we are only concerned with circles and ellipses as radial plots of the probability amplitude.

Suppose that for $r > r_0$ a repulsive potential exists, and that the phase at $r_0$ is unknown. A random phase distribution at $r_0$ represents this case. In Fig. 1 the screening effect of the potential is demonstrated, since at a point $r_1$ which lies outside the barrier, the distribution is not random any more, but there is a preference for certain phases, namely those which lie near the longest axes of the ellipse.

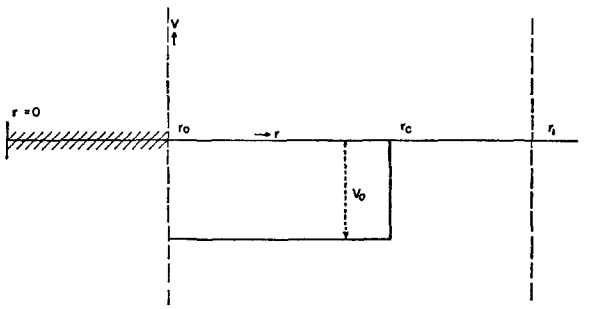


FIG. 2. Square-well potential with unknown core region or "black box."

The more screening occurs, the flatter the ellipse, which means that the barrier defines the boundary conditions on the wavefunction to a larger extent. For an impenetrable barrier, the ellipse would be infinitely long and flat and the phase is exactly known.

Suppose that one had a circle at the point $r_1$. This would then have been the transform of an ellipse at $r_0$. According to the discussion in Sec. 2, this ellipse has the same form and shape as the ellipse at $r_1$ due to a circle at $r_0$. This just means that the barrier is as impenetrable from one side as from the other. The direction of the longest axis of the ellipse at $r_0$ indicates the critical phase at which the phase at $r_1$ becomes uncertain. This has well-known consequences: Suppose that one varies the energy of the incident particles. Keeping the phase distribution at $r_0$ random, the elliptical phase distribution at $r_1$ changes its shape and orientation gradually and also the critical phase at $r_0$ changes continuously. At one particular energy, the critical phase coincides with the actual phase of the wavefunction at $r_0$. At that moment, the phase at $r = r_1$ varies wildly as a function of energy, and a resonance peak shows up in the cross section. But *a priori* we could not know where these peaks occur, because the behavior of the ellipse at that energy was strictly normal. We have here an instance of a resonance which is purely due to the conditions in the unknown region $r < r_0$ and which does not show up in this manner.

Resonances can also occur due to conditions in the known region of the potential and the following example illustrates that they then indeed show up. Suppose that outside the point $r_0$ we have a constant negative potential up to the point $r_c$, outside of which the potential is zero. The region $0 < r < r_0$ is unknown and we assume that the phase distribution at $r_0$ is random. (See Fig. 2.) Let $k_0$ be the wavenumber inside the well. A simple way of seeing what happens with the circular distribution is to change scales and consider the bottom of the well as the zero-potential level. Figure 3 shows how this change of scales transforms a circular distribution into an elliptical distribution which now just rotates in this new system when $r$ increases. At the point $r_c$ the rotation has taken place over a certain well-defined angle. Transforming back to the old system we see that the rotated ellipse stretches itself in the $\psi'$ direction so that certain phases close to 0° are favored, as is clear from the figure. The deeper the well, the flatter the ellipse and already a small rotation will cause the actual distribution to favor phases very close to 0°. However, when a rotation over a multiple of $\pi$ has taken place just as $r = r_c$, one has the original circular distribution back again. So, while in most of the cases one can be quite sure that the phase at $r_c$ is close to 0°, there are instances where the phase is unknown. This can occur in reality when the incident energy is varied. The sudden appearance of a circular distribution at $r_c$ when the energy is varied now indicates the possible appearance of a resonance. Why then does the position of this resonance depend so critically on the position of $r_0$? The answer is that the conditions for $r < r_0$ are only seldom so unknown that a completely random phase distribution at $r_0$ is warranted. In this case, the smallest amount of continuity of the potential at both sides of $r_0$ would have made a random distribution unrealistic. Nevertheless, one might have reasons to believe that the potential indeed changes radically at $r_0$, such that our information about the phase is lost. It is then indeed likely that a resonance occurs at the predicted energy.

## 4. DISTRIBUTION FUNCTIONS WHEN COUPLING IS PRESENT

We now generalize the ideas of Sec. 3 for the case of $n$ coupled channels.

The $2n \times n$ matrix

$$\begin{Vmatrix} \psi(r) \\ k^{-1}\psi'(r) \end{Vmatrix} \tag{4.1}$$

represents the complete solution of the set of $n$

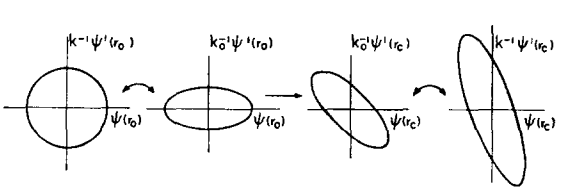


FIG. 3. Sketch of the way in which a random distribution changes under influence of a square-well potential.

coupled wave equations when the boundary conditions are specified. The matrix

$$\begin{Vmatrix} \psi(r)M \\ k^{-1}\psi'(r)M \end{Vmatrix} \qquad (\det M \neq 0)$$

is specified by exactly the same boundary conditions and represents exactly the same physical situation. In order to define phases and mixing parameters which are independent of $M$, we parameterize Eq. (4.1) as follows:

$$\begin{aligned} \psi &= \tau(\sin\varphi)\sigma, \\ k^{-1}\psi' &= \tau(\cos\varphi)\sigma, \end{aligned} \tag{4.2}$$

where $\tau$ is orthogonal, $\varphi$ real diagonal, and $\sigma$ arbitrary nonsingular. One can determine $\tau$ and $\varphi$ by noting that

$$(k^{-1}\psi')\psi^{-1} = \tau(\cot\varphi)\tilde{\tau},$$

then $\tau$ is just the diagonalizing matrix and cot $\varphi$ contains the eigenvalues. The symmetry of the left-hand side guarantees that this is possible. The $\sigma$ can be obtained immediately and can be called the "length" of the two-dimensional vector with matrix components. The parameters specifying $\tau$ will be called the mixing parameters, while the diagonal elements of $\varphi$ are called the phases. For the phases we set the limits $+\frac{1}{2}\pi > \varphi_1 \geq \cdots \geq \varphi_n \geq -\frac{1}{2}\pi$, which can always be satisfied by proper handling of $\tau$. In order to define distribution functions, we ask for the probability that the phases and mixing parameters be found within certain infinitesimal intervals of these parameters. It is useful to define a set of invariant intervals $d\xi_1, \cdots, d\xi_\nu\ [\nu = \frac{1}{2}n(n-1)]$ such that the probability for finding the actual mixing parameters within these intervals is always a constant for a random distribution of $\tau$ matrices. A more exact definition is given in Appendix III.

Suppose that the matrix

$$\begin{Vmatrix} \tau^0(\sin\varphi^0)\sigma^0 \\ \tau^0(\cos\varphi^0)\sigma^0 \end{Vmatrix}$$

at the point $r_0$ transforms into

$$\begin{Vmatrix} \tau(\sin\varphi)\sigma \\ \tau(\cos\varphi)\sigma \end{Vmatrix}$$

at the point $r$. Let a distribution function $\rho^0$ be given such that

$$\rho^0\, d\xi_1^0 \cdots d\xi_\nu^0\, d\varphi_1^0 \cdots d\varphi_n^0$$

is the probability for finding the phases and mixing parameters within the proper intervals. One can then calculate the corresponding distribution function $\rho$ at $r$. In Appendix II it is shown that

$$\rho = \rho^0 \left[\frac{\prod_{i<j}\sin(\varphi_i - \varphi_j)}{\prod_{i<j}\sin(\varphi_i^0 - \varphi_j^0)}\right] \cdot \left[\frac{\det\sigma}{\det\sigma^0}\right]^{n+1} \tag{4.3}$$

Here we see immediately, that if $\rho^0$ does not contain the factor $\prod_{i<j}\sin(\varphi_i^0 - \varphi_j^0)$, the $\rho$ has a series of unwanted poles. One concludes that every realistic distribution function must contain the factor

$$\prod_{i<j}\sin(\varphi_i - \varphi_j) \tag{4.3a}$$

if there is coupling between channels. Phases have therefore the tendency to avoid being close together.

Now let us find out whether it is possible to find a distribution function which corresponds to our lack of knowledge of the boundary conditions at a particular point. Again, if there are no potentials, this must imply that we lack that knowledge in every point. Let us consider that case. Our matrix $\Psi$ has then the form

$$\Psi_0(r_1, r_2) = \begin{Vmatrix} \cos k(r_1 - r_2) & \sin k(r_1 - r_2) \\ -\sin k(r_1 - r_2) & \cos k(r_1 - r_2) \end{Vmatrix}, \tag{4.4}$$

where all the submatrices are diagonal. This matrix is orthogonal and symplectic, but is a special case. The random distribution function must be invariant under this transformation, but that does not uniquely specify its form as it did in the case $n = 1$. We therefore approach this problem differently.

We have seen in Sec. 2 that $\mathfrak{R}_\beta$, representing the last $n$ columns of a real orthogonal and symplectic matrix $\mathfrak{R}$ is specified by just as many parameters as $\mathfrak{R}$ itself. Suppose that $\mathfrak{R}_\beta$ specifies the complete boundary conditions on the wavefunctions at the point $r_0$. Then the "length" $\sigma$ of $\mathfrak{R}_\beta$ has a determinant equal to 1, in fact $\sigma$ is orthogonal. In analogy to the case $n = 1$, where a circular distribution meant that the direction of a vector in the two-dimensional space is randomly chosen, *we now postulate that the distribution corresponding to a complete lack of knowledge of the phases and mixing parameters is a random distribution of the matrices* $\mathfrak{R}_\beta$.

One obtains a random distribution of $\mathfrak{R}_\beta$ if one has a random distribution of the matrices $\mathfrak{R}$ which form a group; randomness is quite naturally defined in group theory, and this is done in Appendix III where a distribution function for a random distribution is found:

$$\rho = \rho_0\left[\prod_{i<j}\sin(\varphi_i - \varphi_j)\right]. \tag{4.5}$$

One sees that the factor Eq. (4.3a) is present. Moreover it is invariant under the transformation Eq.

(4.4) since it is invariant under all real orthogonal and symplectic transformations.

What happens under general transformations $\Psi(r_1, r_2)$? From Eq. (4.3) one merely obtains

$$\rho = \rho_0[\prod_{i<j} \sin(\varphi_i - \varphi_j)]\cdot[\det \sigma]^{n+1}. \quad (4.6)$$

We will be concerned with distribution functions of this kind.

Now $\Psi(r, r_0)$ transforms a sphere at $r_0$ into an ellipsoid at $r$; in some way we can consider the sphere as representing our state of ignorance of the phases and mixing parameters, all "vectors" of the type Eq. (4.1) having unimodular "length," while the ellipsoid indicates that we possess some knowledge at the point $r$. Equation (4.6) suggests that the flatter the ellipsoid, the better the information we have. Ellipsoids therefore play an essential role, and knowledge of the directions and magnitudes of the principal axes is important. It is clear that det $\sigma$ is determined whenever such an ellipsoid is known and a particular set of phases and mixing parameters is given.

## 5. DISTRIBUTION FUNCTIONS FOR PHASE SHIFTS

So far we discussed phases and their associated mixing parameters. What one commonly calls mixing parameters are those which are associated with phase shifts. It is in this kind of parameters that we are interested. In order to be able to find them at all, the potential must approach zero sufficiently rapidly and we assume that this is the case.

Phase shifts are found by comparing the physical wavefunctions with the free wavefunctions which are of the Riccati–Bessel type. For sufficiently large values of $r$, the $2n \times n$ matrix representing the wavefunctions and their derivatives in the absence of a potential (but with centrifugal barriers still present) is

$$\left\| \begin{matrix} \sin(kr - \frac{1}{2}l\pi) \\ \cos(kr - \frac{1}{2}l\pi) \end{matrix} \right\|.$$

Now $\Psi_0(r, 0)$ as defined in Sec. 4 is just

$$\left\| \begin{matrix} \cos kr & \sin kr \\ -\sin kr & \cos kr \end{matrix} \right\|,$$

so when all $l_i$ are equal to zero, the last $n$ columns represent free particles for which all phase shifts must be zero. If one now defines

$$\Gamma_0(r_0) = \lim_{r\to\infty} \Psi_0(0, r)\Psi(r, r_0), \quad (5.1)$$

then the phases of

$$\Gamma_0(r_0)\cdot\left\| \begin{matrix} \psi(r_0) \\ k^{-1}\psi'(r_0) \end{matrix} \right\|$$

are just the phase shifts when all $l_i = 0$, and the boundary conditions at $r = r_0$ are as specified: The phase shifts should be zero when $r_0 = 0$, $\Psi = \Psi_0$, and when $\psi(0) = 0$.

When there are $l_i$ which are unequal to zero, a correction must be made for the extra shift of $-\frac{1}{2}l\pi$. The matrix

$$\left\| \begin{matrix} \cos(kr - \frac{1}{2}l\pi) & \sin(kr - \frac{1}{2}l\pi) \\ -\sin(kr - \frac{1}{2}l\pi) & \cos(kr - \frac{1}{2}l\pi) \end{matrix} \right\|$$

should replace $\Psi_0(r, 0)$. It is not proper to call this $\Psi_l(r, 0)$ since it does not satisfy $\Psi_l(0, 0) = \mathcal{I}$. Instead, we define a correction factor

$$\Omega_l = \left\| \begin{matrix} \cos\frac{1}{2}l\pi & -\sin\frac{1}{2}l\pi \\ \sin\frac{1}{2}l\pi & \cos\frac{1}{2}l\pi \end{matrix} \right\|, \quad (5.2)$$

which commutes with $\Psi_0$. Then $\Omega_l\Psi_0(r, 0)$ is the proper replacement of $\Psi_0(r, 0)$. Note that $\Omega_l$ is orthogonal, real, and symplectic.

The generalization of Eq. (5.1) becomes

$$\Gamma_l(r_0) = \lim_{r\to\infty} \tilde{\Omega}_l\Psi_0(0, r)\Psi(r, r_0), \quad (5.3)$$

and the phases of

$$\Gamma_l(r_0)\left\| \begin{matrix} \psi(r_0) \\ k^{-1}\psi'(r_0) \end{matrix} \right\| = \left\| \begin{matrix} \zeta_1 \\ \zeta_2 \end{matrix} \right\|$$

are the phase shifts in which we are interested. Here $\zeta_1$ and $\zeta_2$ are $n \times n$ matrices satisfying $\tilde{\zeta}_1\zeta_2 = \tilde{\zeta}_2\zeta_1$. Write

$$\zeta_1 = \epsilon(\sin\delta)\mu,$$

$$\zeta_2 = \epsilon(\cos\delta)\mu,$$

where $\epsilon$ is real orthogonal and represents the mixing parameters; $\delta$ is real and diagonal and represents the phase shifts, and $\mu$ is real and nonsingular. If then at $r = r_0$ the phases are unknown, and the $2n \times n$ matrix representing the wavefunctions and derivatives has an unimodular "length", the distribution function for the phase shifts and mixing parameters becomes

$$\rho = \rho_0[\prod_{i<j} \sin(\delta_i - \delta_j)](\det \mu)^{n+1}, \quad (5.4)$$

since $\Gamma_l$ is real and symplectic.

Once the phase shifts and mixing parameters are known, the scattering matrix $S$ is determined,

$$S = \epsilon e^{2i\delta}\tilde{\epsilon}, \quad (5.5)$$

which is symmetric as it should when time-reversal invariance holds.

Let us now write down more explicit forms for the phase-shift distribution functions. First we consider $n = 1$, where an ellipse with longest principal axis of length $\lambda^{-1}$ represents our distribution. Let $\delta_0$ be the phase shift belonging to the direction of this axis. The length $\sigma$ of a vector satisfying the equation of the ellipse is then

$$\sigma = [\lambda^2 \cos^2(\delta - \delta_0) + \lambda^{-2} \sin^2(\delta - \delta_0)]^{-\frac{1}{2}},$$

and the distribution function $\rho$ is proportional to the square of this,

$$\rho = \rho_0[\lambda^2 \cos^2(\delta - \delta_0) + \lambda^{-2} \sin^2(\delta - \delta_0)]^{-1}. \quad (5.6)$$

For $\delta = \delta_0$, this shows a peak which becomes sharper when $\lambda$ decreases. If we introduce $\delta_c$ by

$$\tan \delta_c = \lambda^2, \quad (5.7)$$

then it is equally likely that $\delta$ will be found between $\delta_0 - \delta_c$ and $\delta_0 + \delta_c$ than outside this range (when $\frac{1}{2}\pi > \delta \geq -\frac{1}{2}\pi$). When $\lambda$ is very small, then $\rho$ reduces to half its peak value at $\delta_0 \pm \delta_c$, which makes it justified to call $2\delta_c$ the half width of the peak. The analytic form of $\rho$ in that case is equal to that of a common resonance

$$\rho = \rho_0\lambda^2/[(\delta - \delta_0)^2 + \lambda^4]. \quad (5.8)$$

In this limit of small $\lambda$ it is perhaps useful to characterize the ellipse by the location of a simple pole in the complex $\delta$ plane, namely $\rho$ becomes singular when $\delta = \delta_0 \pm i\lambda^2$, which contains just all the parameters of interest.

The case $n \neq 1$ is more complex. Let

$$\tilde{\mathfrak{X}}\mathfrak{IC}\mathfrak{X} = I \quad (5.9)$$

be the equation of the generalized ellipse representing the phase shift distribution. Here $\mathfrak{X}$ is defined by

$$\mathfrak{X} = \begin{Vmatrix} \epsilon(\sin\delta)\mu \\ \epsilon(\cos\delta)\mu \end{Vmatrix}, \quad (5.10)$$

where $\epsilon$ is orthogonal and represents the mixing parameters; $\delta$ is the matrix of the phase shifts, and $\mu$ is the length of the generalized vector. We are interested in det $\mu$ and we find

$$(\det\mu)^2 = \left[\det\left\{||(\sin\delta)\tilde{\epsilon}\ \ (\cos\delta)\tilde{\epsilon}||\cdot\mathfrak{IC}\cdot\begin{Vmatrix}\epsilon\sin\delta \\ \epsilon\cos\delta\end{Vmatrix}\right\}\right]^{-1}. \quad (5.11)$$

Parameterize $\mathfrak{IC}$ as follows:

$$\mathfrak{IC} = \begin{Vmatrix} U_1 & U_2 \\ -U_2 & U_1 \end{Vmatrix}\cdot\begin{Vmatrix}\Lambda^{-2} & 0 \\ 0 & \Lambda^2\end{Vmatrix}\cdot\begin{Vmatrix}\tilde{U}_1 & -\tilde{U}_2 \\ \tilde{U}_2 & U_1\end{Vmatrix}, \quad (5.12)$$

where $\Lambda^{-1}$ represents the lengths of the $n$ largest principal axes, and

$$U_1 = \epsilon_0(\cos\delta_0)\nu_0,$$
$$U_2 = \epsilon_0(\sin\delta_0)\nu_0,$$

where again $\epsilon_0$ and $\nu_0$ are real and orthogonal, and $\delta_0$ real diagonal. Inserting Eq. (5.12) into Eq. (5.11), one sees that the expression between braces can be factorized into two complex matrices which are each other's Hermitian adjoint. Call this product $HH^\dagger$, then $|\det H|^2 = \det(HH^\dagger)$ and $H$ is sufficient for finding det $\mu$. One finds for $H$:

$$H = \{(\sin\delta)\tilde{\epsilon}\epsilon_0(\cos\delta_0) - (\cos\delta)\tilde{\epsilon}\epsilon_0(\sin\delta_0)\}\nu_0\Lambda^{-1}$$
$$+ i\{(\sin\delta)\tilde{\epsilon}\epsilon_0(\sin\delta_0) + (\cos\delta)\tilde{\epsilon}\epsilon_0(\cos\delta_0)\}\nu_0\Lambda. \quad (5.13)$$

This form can be simplified even further if one introduces the real symmetric matrix

$$\Delta = \epsilon\delta\tilde{\epsilon}.$$

If one then tries to solve the set of $n^2$ equations

$$H = 0$$

for $\Delta$, then one finds a complex and generally asymmetric solution $\Delta_s$, namely

$$\tan\Delta_s = \epsilon_0\{\sin\delta_0 - i\cos\delta_0(\nu_0\Lambda^2\tilde{\nu}_0)\}$$
$$\times\{\cos\delta_0 + i\sin\delta_0(\nu_0\Lambda^2\tilde{\nu}_0)\}^{-1}\tilde{\epsilon}_0. \quad (5.14)$$

In terms of $\tan\Delta_s$, the matrix $H$ has a simple form:

$$H = \tilde{\epsilon}\cos\Delta(\tan\Delta - \tan\Delta_s)\epsilon_0$$
$$\times\{(\cos\delta_0)\nu_0\Lambda^{-1} + i(\sin\delta_0)\nu_0\Lambda\}. \quad (5.15)$$

Here $\det\tilde{\epsilon} = \det\epsilon_0 = 1$, and the factor between braces is independent of $\Delta$, so its determinant can be absorbed into the constant $\rho_0$ in the expression for $\rho$ and we find from Eqs. (5.4), (5.11), (5.12), and (5.15),

$$\rho = \rho_0[\prod_{i<j}\sin(\delta_i - \delta_j)]$$
$$\times[\det(\cos\Delta)\cdot|\det(\tan\Delta - \tan\Delta_s)|]^{-(n+1)}. \quad (5.16)$$

If $\nu_0\Lambda^2\tilde{\nu}_0$ is very small, which occurs in the case of barriers which are hard to penetrate, Eq. (5.14) can be simplified by omitting higher-order terms in $\Lambda^2$, and we obtain

$$\tan\Delta_s = \epsilon_0\{\tan\delta_0 - i(\cos\delta_0)^{-1}(\nu_0\Lambda^2\tilde{\nu}_0)(\cos\delta_0)^{-1}\}\tilde{\epsilon}_0, \quad (5.17)$$

which is a symmetric matrix. Introducing

$$\Delta_0 = \epsilon_0\delta_0\tilde{\epsilon}_0,$$

we obtain from Eq. (5.17)

$$\tan \Delta_s = \tan \Delta_0 - i(\cos \Delta_0)^{-1}(\epsilon_0 \nu_0 \Lambda^2 \bar{\nu}_0 \bar{\epsilon}_0)(\cos \Delta_0)^{-1}. \quad (5.18)$$

Here Eq. (5.18) expresses that the highest-order singularity in $\rho$ occurs near the directions of the largest principal axes of the ellipsoid. From Eqs. (5.16) and (5.18) we obtain a good idea of how $\rho$ depends on $\Delta$.

We close here the discussion of the distribution functions.

We demonstrate the contents of the first half of this section with an example similar to the one in Sec. 2, except that we now include higher $l$ waves. We will assume that all channels have the same $l$ value. Instead of Eq. (2.22), we use

$$\begin{aligned} k^{-1}\psi_i'' &= [-(k/m)^{-\frac{1}{2}} V_0 (k/m)^{-\frac{1}{2}} \\ &\quad + k^{-1} l(l+1)/r^2 - k]\psi_i \quad (r_0 \le r \le r_c), \quad (5.19) \\ k^{-1}\psi_i'' &= [k^{-1} l(l+1)/r^2 - k]\psi_i, \quad (r > r_c), \end{aligned}$$

where $V_0$ is again independent of $r$ and real symmetric with positive eigenvalues. Define again a matrix $\kappa^2$:

$$\kappa^2 = (km)^{\frac{1}{2}} V_0 (k/m)^{-\frac{1}{2}} + k^2, \quad (5.20)$$

where $\kappa$ is that square root of $\kappa^2$ which has positive eigenvalues. One then obtains the set of equations

$$\begin{aligned} \psi_i'' &= [l(l+1)/r^2 - \kappa^2]\psi_i \quad (r_0 \le r \le r_c), \\ \psi_i'' &= [l(l+1)/r^2 - k^2]\psi_i \quad (r > r_c). \end{aligned} \quad (5.21)$$

Assuming again $\kappa^2$ to be nondegenerate, $\kappa$ can be found uniquely, and again,

$$f(\kappa)k = kf(\bar{\kappa})$$

for a function $f$ of $\kappa$.

We can find $\Psi(r, r_0)$ for $r_0 \le r < r_c$ by defining some hypothetical point $\bar{r}$ such that

$$\lim_{r\to\infty} \Psi(r, \bar{r}) = \begin{Vmatrix} \cos(\kappa r - \frac{1}{2}l\pi) & k\bar{\kappa}^{-1} \sin(\bar{\kappa} r - \frac{1}{2}l\pi) \\ -k^{-1}\kappa \sin(\kappa r - \frac{1}{2}l\pi) & \cos(\bar{\kappa} r - \frac{1}{2}l\pi) \end{Vmatrix},$$

which is symplectic. In that case, $\Psi(r, \bar{r})$ itself becomes

$$\begin{Vmatrix} -\kappa r n_l(\kappa r) & k r j_l(\bar{\kappa} r) \\ -k^{-1}[\kappa r n_l(\kappa r)]' & [r j_l(\bar{\kappa} r)]' \end{Vmatrix}, \quad (5.22)$$

where $n_l$ and $j_l$ are the spherical Neumann and Bessel functions. We have

$$\begin{aligned} \Psi(r, r_0) &= \Psi(r, \bar{r})\Psi(\bar{r}, r_0) = \Psi(r, \bar{r})\Psi^{-1}(r_0, \bar{r}) \\ &= \begin{Vmatrix} -\kappa r n_l(\kappa r) & k r j_l(\bar{\kappa} r) \\ -k^{-1}[\kappa r n_l(\kappa r)]' & [r j_l(\bar{\kappa} r)]' \end{Vmatrix} \\ &\quad \times \begin{Vmatrix} [r_0 j_l(\kappa r_0)]' & -k r_0 j_l(\bar{\kappa} r_0) \\ k^{-1}[\kappa r_0 n_l(\kappa r_0)]' & -\bar{\kappa} r_0 n_l(\bar{\kappa} r_0) \end{Vmatrix}, \quad (5.23) \end{aligned}$$

with the help of Eqs. (2.7a), (2.7b), (2.9), and (2.24b).

For $r > r_c$, one has

$$\begin{aligned} \Psi(r, r_c) &= \begin{Vmatrix} -k r n_l(kr) & k r j_l(kr) \\ -[r n_l(kr)]' & [r j_l(kr)]' \end{Vmatrix} \\ &\quad \times \begin{Vmatrix} [r_c j_l(kr_c)]' & -k r_c j_l(kr_c) \\ [r_c n_l(kr_c)]' & -k r_c n_l(kr_c) \end{Vmatrix}. \quad (5.24) \end{aligned}$$

The expression for $\Gamma_l(r_0)$ as defined in Eq. (5.3) becomes

$$\Gamma_l(r_0) = \lim_{r\to\infty} \tilde{\Omega}_l \Psi_0(0, r)\Psi(r, r_c)\Psi(r_c, r_0). \quad (5.25)$$

Due to cancellation of some factors, one obtains

$$\begin{aligned} \Gamma_l(r_0) &= \begin{Vmatrix} [r_c j_l(kr_c)]' & -k r_c j_l(kr_c) \\ [r_c n_l(kr_c)]' & -k r_c n_l(kr_c) \end{Vmatrix} \\ &\quad \times \begin{Vmatrix} -\kappa r_c n_l(\kappa r_c) & k r_c j_l(\bar{\kappa} r_c) \\ -k^{-1}[\kappa r_c n_l(\kappa r_c)]' & [r_c j_l(\bar{\kappa} r_c)]' \end{Vmatrix} \\ &\quad \times \begin{Vmatrix} [r_0 j_l(\kappa r_0)]' & -k r_0 j_l(\bar{\kappa} r_0) \\ k^{-1}[\kappa r_0 n_l(\kappa r_0)]' & -\bar{\kappa} r_0 n_l(\bar{\kappa} r_0) \end{Vmatrix}, \quad (5.26) \end{aligned}$$

which returns to an expression not involving $r_c$ when $\kappa = k$, as it should. One sees also the different stages of matching wavefunctions and derivatives at different points where the potential makes a jump. We have now that

$$\mathcal{K} = \tilde{\Gamma}_l^{-1}(r_0)\Gamma_l^{-1}(r_0)$$

characterizes the phase-shift distribution due to a random distribution at the point $r_0$. The screening effect of the centrifugal barrier is also demonstrated in $\Gamma_l(r_0)$. If one varies $r_0$ to very small values, the last factor of Eq. (5.26) will contain very large numbers due to $n_l$ and very small numbers due to $j_l$. The resulting ellipsoid is therefore very flat and very much stretched, which shows the screening effect.

The second part of this section can be demonstrated for $n = 2$ with the following example. If $\Lambda^2$ is sufficiently small, then in Eq. (5.16), $\cos \Delta$ can be replaced by $\cos \Delta_0$ and also the factor $\prod \sin(\delta_i - \delta_j)$ does not change. Therefore, only the following factor is important:

$$|\det(\tan \Delta_s - \tan \Delta)|^{-(n+1)}.$$

For a given $\Delta_s$ we can now plot curves of constant

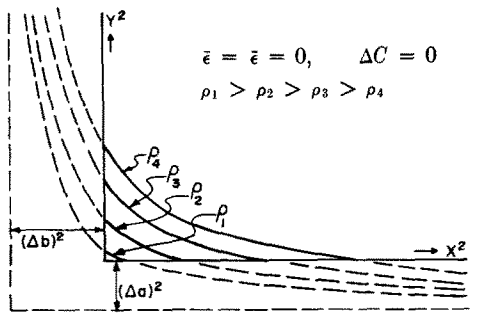


FIG. 4. Contour diagram of $y^2 = (\tan \delta_2 - \tan \delta_{02})^2$ vs $x^2 = (\tan \delta_1 - \tan \delta_{01})^2$ for different values of $\rho$.

$\rho$ in a $(\tan \delta_1, \tan \delta_2)$ diagram if $\epsilon$ is taken equal to $\epsilon_0$. These curves are the same as those of constant $|\det(\tan \Delta_s - \tan \Delta)|^2$.

From Eq. (5.18), let $\tan \Delta_0$ be diagonal and let $\tan \Delta_s$ be

$$\tan \Delta_s = \begin{Vmatrix} \tan \delta_{01} - i\Delta a & -i\Delta c \\ -i\Delta c & \tan \delta_{02} - i\Delta b \end{Vmatrix},$$

where $\Delta a$, $\Delta b$, and $\Delta c$ are small numbers such that $\Delta a$ and $\Delta b > 0$, and $(\Delta a)(\Delta b) - (\Delta c)^2 = \mathfrak{D} > 0$.

Define

$$x = \tan \delta_1 - \tan \delta_{01},$$

$$y = \tan \delta_2 - \tan \delta_{02}.$$

Then we have

$$|\det(\tan \Delta_s - \tan \Delta)|^2 = x^2y^2 + (\Delta b)^2x^2 + (\Delta a)^2y^2 + 2(\Delta c)^2xy + \mathfrak{D}^2.$$

In the case that $\Delta c = 0$, this is a quadratic function of $x^2$ and $y^2$, and in fact it represents a hyperbola with its center at the point $(-(\Delta b)^2, -(\Delta a)^2)$. Details are shown in Fig. 4. Figure 5 shows a plot of $x$ against $y$ which follows from Fig. 4. If we consider small $x$ and $y$, then the term $x^2y^2$ does not appear, and so near the origin we have ellipses. When $\Delta c \neq 0$, these ellipses are rotated, which is shown in Fig. 6.

Finally let us see how $\rho$ depends on $\epsilon$ for the case that $\delta_1 = \delta_{01}$, $\delta_2 = \delta_{02}$ and $\epsilon_0 = I$. Let $\epsilon$ be parameterized as follows:

$$\epsilon = \begin{Vmatrix} \cos \bar{\epsilon} & -\sin \bar{\epsilon} \\ \sin \bar{\epsilon} & \cos \bar{\epsilon} \end{Vmatrix}.$$

Then we obtain

$$\tan \Delta - \tan \Delta_s = \begin{Vmatrix} -\sin^2 \bar{\epsilon} & \cos \bar{\epsilon} \sin \bar{\epsilon} \\ \cos \bar{\epsilon} \sin \bar{\epsilon} & \sin^2 \bar{\epsilon} \end{Vmatrix} (\tan \delta_{01} - \tan \delta_{02}) + i \begin{Vmatrix} \Delta a & \Delta c \\ \Delta c & \Delta b \end{Vmatrix}.$$

We find for the determinant

$$-(\tan \delta_{01} - \tan \delta_{02})^2 \sin^2 \bar{\epsilon} - \mathfrak{D} + i(\tan \delta_{01} - \tan \delta_{02}) \times [\sin^2 \bar{\epsilon}(\Delta a - \Delta b) - 2 \cos \bar{\epsilon} \sin \bar{\epsilon}(\Delta c)].$$

Then if $\tan \delta_{01}$ is sufficiently different from $\tan \delta_{02}$, then for small $\Delta a$, $\Delta b$, and $\Delta c$, we can replace $\sin \bar{\epsilon}$ by $\bar{\epsilon}$, and $\cos \bar{\epsilon}$ by 1. Calling $\tan \delta_{01} - \tan \delta_{02} = t$, we get

$$-t^2\bar{\epsilon}^2 - \mathfrak{D} + it[(\Delta a - \Delta b)\bar{\epsilon}^2 - 2(\Delta c)\bar{\epsilon}],$$

and we find the distribution function proportional to

$$[(t^2\bar{\epsilon}^2 + \mathfrak{D})^2 + t^2\bar{\epsilon}^2\{(\Delta a - \Delta b)\bar{\epsilon} - 2\Delta c\}^2]^{-\frac{1}{2}}.$$

We see here how $\Delta c$ causes the function to be asymmetric under the substitution $\bar{\epsilon} \to -\bar{\epsilon}$. From this expression it becomes clear under which conditions $\bar{\epsilon}$ is accurately known.

## 6. DISCUSSION

In the foregoing sections it is made clear that, in the case of uncoupled or coupled Schrödinger equations, certain predictions of phase shifts and mixing parameters can be made even if the potential is only partially known. The accuracy of the results

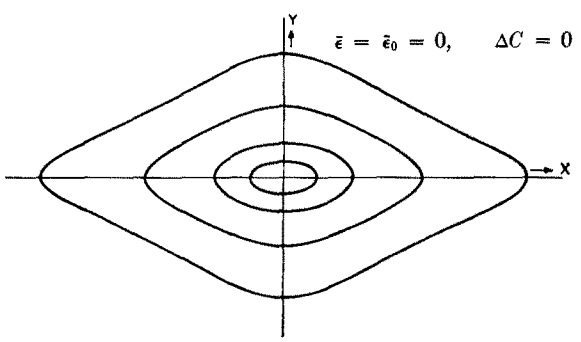


FIG. 5. Contour diagram of $y = \tan \delta_2 - \tan \delta_{02}$ vs $x = \tan \delta_1 - \tan \delta_{01}$ for different $\rho$-values; $\Delta c = 0$.

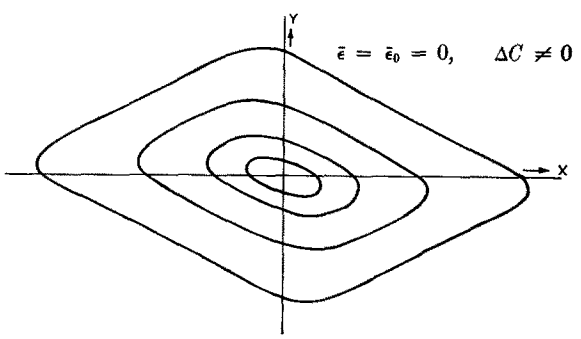


FIG. 6. Contour diagram of $y = \tan \delta_2 - \tan \delta_{02}$ vs $x = \tan \delta_1 - \tan \delta_{01}$ for different $\rho$ values; $\Delta c \neq 0$.

is well defined and this is important when a comparison with empirical phase shifts and mixing parameters is made. These phase shifts should be where $\rho$ is very large, or otherwise one has a resonance; in any case, the phase shifts should return to the values indicated by large $\rho$ when the energy of the incident particles is changed in order to move out of the resonance region. If the phase shifts are persistently different from the expected ones, one has an indication that the potential model is wrong. Then, by moving $r_0$ farther outward, the calculated accuracy of the results may become sufficiently low to account for the differences with experiment. If the experimental values are better known than the theoretical values, one might try to make $r_0$ smaller, thereby assuming some suitable form of the potential between the old and the new $r_0$. Or if one has reasons that this cannot be done satisfactorily, one could assume instead a phase distribution at $r_0$ which favors certain phases above others and leave it that way.

Then the assumption has been made that all channels are open. If there are closed channels it is not possible to define a phase distribution which is independent of $r$, when all potentials and centrifugal barriers are equal to zero, and which does not contain singularities. It is not clear whether our approach can be suitably modified to treat this case also.

Finally, when there is absorption but no closed channels, a modification of what has been described in this paper will be possible and estimates about the most likely amount of absorption under given circumstances can be made. This allows one to obtain elastic scattering cross sections for low-energy $p - \bar{p}$ scattering if the potential is known for $r \geq r_0$ and is real there, while an unknown potential with absorptive part exists for $r < r_0$.


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## APPENDIX I. SOME THEOREMS ABOUT DIAGONALIZABLE $2n \times 2n$ SYMPLETIC MATRICES

Let

$$\mathfrak{a} = \begin{Vmatrix} A & C \\ B & D \end{Vmatrix}$$

be an arbitrary $2n \times 2n$ symplectic matrix. If $\mathfrak{a}$ can be diagonalized, its eigenvectors span a $2n$-dimensional space. We assume that $\mathfrak{a}$ satisfies this condition.

*Theorem 1.* The eigenvectors of $\mathfrak{a}$ go in pairs such that the products of the two corresponding eigenvalues are 1.

*Proof*: The eigenvalues of $\mathfrak{a}$ are the solutions of the characteristic equation

$$\det(\mathfrak{a} - \lambda \mathfrak{g}) = 0. \tag{I.1}$$

The eigenvectors of an $m$-times degenerate eigenvalue span an $m$-dimensional space. If one expands Eq. (I.1) as a power series in $\lambda$, one obtains

$$\lambda^{2n} - \lambda^{2n-1} \operatorname{Tr}^{(1)}[\mathfrak{a}] + \lambda^{2n-2} \operatorname{Tr}^{(2)}[\mathfrak{a}] - \cdots + \operatorname{Tr}^{(2n)}[\mathfrak{a}] = 0, \tag{I.2}$$

where $\operatorname{Tr}^{(p)}[\mathfrak{a}]$ is the sum of all $p \times p$ principal minors (determinants of submatrices of $\mathfrak{a}$ of which the row and column indices are the same). There is a theorem which says that[12]

$$\operatorname{Tr}^{(p)}[\mathfrak{a}] = (\det \mathfrak{a}) \operatorname{Tr}^{(2n-p)}[\mathfrak{a}^{-1}] \quad (1 \leq p \leq 2n-1). \tag{I.3}$$

Let a bar indicate an operation which transforms $\mathfrak{a}$ into

$$\bar{\mathfrak{a}} = \begin{Vmatrix} \tilde{D} & -\tilde{C} \\ -\tilde{B} & \tilde{A} \end{Vmatrix},$$

regardless of $\mathfrak{a}$ being symplectic. Then by inspection one finds

$$\operatorname{Tr}^{(p)}[\mathfrak{a}] = \operatorname{Tr}^{(p)}[\bar{\mathfrak{a}}],$$

and the symplectic property gives [with Eq. (2.9)]

$$\operatorname{Tr}^{(p)}[\mathfrak{a}] = \operatorname{Tr}^{(p)}[\mathfrak{a}^{-1}]; \tag{I.4}$$

so from Eq. (I.3),

$$\operatorname{Tr}^{(p)}[\mathfrak{a}] = (\det \mathfrak{a}) \operatorname{Tr}^{(2n-p)}[\mathfrak{a}] = \operatorname{Tr}^{(2n-p)}[\mathfrak{a}], \tag{I.5}$$

with the help of Eq. (2.10). Moreover, $\operatorname{Tr}^{(2n)}[\mathfrak{a}] = \det \mathfrak{a} = 1$.

Rewriting Eq. (1.2) in the form

$$\lambda^n - \lambda^{n-1} \operatorname{Tr}^{(1)}[\mathfrak{a}] + \lambda^{n-2} \operatorname{Tr}^{(2)}[\mathfrak{a}] - \cdots + \lambda^{-n} \operatorname{Tr}^{(2n)}[\mathfrak{a}] = 0,$$

one sees that this equation stays invariant when $\lambda$ is replaced by $\lambda^{-1}$ and as a result we have that if $\lambda_i$ is an $m$-times degenerate root, then $\lambda_i^{-1}$ is also an $m$-times degenerate root, while $\lambda = \pm 1$ is always

[12] See, for example, G. Kowalewski, *Einführung in die Determinantentheorie* (Walter de Gruyter & Co., 1954) p. 80.

degenerate with even $m$. One can therefore always form $n$ pairs of eigenvectors with the property of Theorem 1.

Note that the bar operation satisfies the property

$$\overline{\mathfrak{A}\mathfrak{B}} = \bar{\mathfrak{B}}\,\bar{\mathfrak{A}}, \tag{I.6a}$$

$$\overline{\mathfrak{A}^{-1}} = \bar{\mathfrak{A}}^{-1}, \tag{I.6b}$$

and

$$\bar{\bar{\mathfrak{A}}} = \mathfrak{A}. \tag{I.6c}$$

*Theorem 2.* If a symplectic matrix can be diagonalized, one can always find a symplectic diagonalizing matrix.

*Proof:* Let $\mathfrak{z}$ be a matrix which diagonalizes $\mathfrak{A}$:

$$\mathfrak{z}^{-1}\mathfrak{A}\mathfrak{z} = \mathfrak{A}_d,$$

$\mathfrak{A}_d$ being diagonal, and the ordering of the eigenvalues can always be done such that $\mathfrak{A}_d$ is symplectic, according to Theorem 1. We have

$$\bar{\mathfrak{z}}\,\bar{\mathfrak{A}}\,\overline{\mathfrak{z}^{-1}} = \bar{\mathfrak{A}}_d,$$

or

$$\bar{\mathfrak{z}}\,\mathfrak{A}\,\overline{\mathfrak{z}^{-1}} = \mathfrak{A}_d;$$

thus $\mathfrak{z}$ and $\overline{\mathfrak{z}^{-1}}$ both diagonalize $\mathfrak{A}$ in the same way. Then the space spanned by the $m$ independent columns of $\mathfrak{z}$ belonging to the same ($m$-times degenerate) eigenvalue $\lambda$ is the same as the space spanned by the $m$ independent columns of $\overline{\mathfrak{z}^{-1}}$ belonging to that eigenvalue; in particular when $m = 1$, the corresponding columns of $\mathfrak{z}$ and $\overline{\mathfrak{z}^{-1}}$ are proportional. There must also be a set of $m$ independent columns of $\mathfrak{z}$ belonging to the eigenvalue $\lambda^{-1}$ (if $\neq\lambda$), and similarly for $\overline{\mathfrak{z}^{-1}}$. If one now chooses $m$ arbitrary independent vectors in the $\mathfrak{z}$ space associated with $\lambda$, then the corresponding $m$ independent vectors in the $\overline{\mathfrak{z}^{-1}}$ space associated with $\lambda^{-1}$ are fixed. One is now free to choose the vectors corresponding to $\lambda$, equal for $\mathfrak{z}$ as for $\overline{\mathfrak{z}^{-1}}$. If $\lambda = \pm 1$, the spaces associate with $\lambda$ and $\lambda^{-1}$ coincide but are of even dimension. One can still choose $\frac{1}{2}m$ independent vectors such that they, together with the remaining $\frac{1}{2}m$ vectors in that space (which are now fixed) span the whole of $m$-dimensional space. As a result we have

$$\mathfrak{z} = \overline{\mathfrak{z}^{-1}},$$

i.e., $\mathfrak{z}$ is symplectic. There is still a considerable amount of arbitrariness in the choice of $\mathfrak{z}$.

*Theorem 3.* The matrix which diagonalizes a symmetric and symplectic matrix can be chosen orthogonal and symplectic.

*Proof:* Any symmetric matrix $\mathfrak{A}$ can be diagonalized by an orthogonal matrix $\mathfrak{R}$, and if $\mathfrak{A}$ is symplectic, there exists a symplectic matrix $\mathfrak{z}$ which diagonalizes $\mathfrak{A}$:

$$\mathfrak{z}^{-1}\mathfrak{A}\mathfrak{z} = \mathfrak{A}_d.$$

Let $\mathfrak{z}$ be

$$\mathfrak{z} = \begin{Vmatrix} T_1 & T_3 \\ T_2 & T_4 \end{Vmatrix},$$

and let

$$\mathfrak{A}\begin{Vmatrix} T_1 \\ T_2 \end{Vmatrix} = \begin{Vmatrix} T_1 \\ T_2 \end{Vmatrix}\Lambda,$$

where $\Lambda$ is a nonsingular diagonal $n \times n$ matrix. We have, respectively,

$$\bar{\mathfrak{A}}\begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix} = \begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix}\Lambda \rightarrow \bar{\mathfrak{A}}\begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix} = \begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix}\Lambda$$

$$\rightarrow \mathfrak{A}^{-1}\begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix} = \begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix}\Lambda,$$

and consequently,

$$\mathfrak{A}\begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix} = \begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix}\Lambda^{-1}.$$

So if there are $n$ independent eigenvectors corresponding to the columns of $\begin{Vmatrix} T_1 \\ T_2 \end{Vmatrix}$ and belonging to the eigenvalues $\Lambda$, then there are $n$ independent eigenvectors corresponding to the columns of $\begin{Vmatrix} -T_2 \\ T_1 \end{Vmatrix}$ belonging to the eigenvalues $\Lambda^{-1}$. Now if one chooses the columns of $\begin{Vmatrix} T_1 \\ T_2 \end{Vmatrix}$ orthonormal, as one is able to do in the case of symmetric matrices, one has

$$\tilde{T}_1 T_1 + \tilde{T}_2 T_2 = I,$$

so the matrix

$$\begin{Vmatrix} T_1 & -T_2 \\ T_2 & T_1 \end{Vmatrix}$$

is symplectic and therefore orthogonal, from Eq. (2.9).

Finally, some theorems about the group properties of symplectic matrices are presented.

*Theorem 4.* The group of real orthogonal symplectic $2n \times 2n$ matrices is isomorphic with the $n \times n$ unitary group.

*Proof:* Let

$$\mathfrak{A} = \begin{Vmatrix} A & -B \\ B & A \end{Vmatrix}$$

be real orthogonal and symplectic. Introduce $\mathfrak{I}$ defined by

$$\mathfrak{I} = \frac{1}{\sqrt{2}} \begin{Vmatrix} I & iI \\ iI & I \end{Vmatrix};$$

then

$$\mathfrak{I}^{-1}\mathfrak{A}\mathfrak{I} = \frac{1}{2} \begin{Vmatrix} I & -iI \\ -iI & I \end{Vmatrix} \cdot \begin{Vmatrix} A & -B \\ B & A \end{Vmatrix} \cdot \begin{Vmatrix} I & iI \\ iI & I \end{Vmatrix} = \begin{Vmatrix} A - iB & 0 \\ 0 & A + iB \end{Vmatrix}.$$

We have

$$(A - iB)^{\dagger}(A - iB) = (\tilde{A} + i\tilde{B})(A - iB) = (\tilde{A}A + \tilde{B}B) - i(\tilde{A}B - \tilde{B}A) = I,$$

so $A - iB$ is unitary and so is $A + iB$. A one-to-one mapping of the real orthogonal symplectic group onto the unitary group has been established which preserves the group properties. This proves the theorem.[11]

*Theorem 5.* The group of orthogonal symplectic matrices of $2n$ dimensions is isomorphic with the full linear group of $n$ dimensions.

*Proof:* Let $M$ be arbitrary nonsingular. Then one can uniquely construct an orthogonal symplectic matrix by defining $A = (M + \tilde{M}^{-1})/2$ and $B = (M - \tilde{M}^{-1})/2i$ which satisfy $\tilde{A}A + \tilde{B}B = I$ and $\tilde{A}B = \tilde{B}A$. This leads to the wanted result.

## APPENDIX II. TRANSFORMATION PROPERTIES OF DISTRIBUTION FUNCTIONS

In this Appendix we use the symbols $i, j, k, l, p, q$ to indicate positive-integer indices, and we reserve $n$ for the number of coupled channels. Suppose that, at the points $r_0$ and $r$, the generalized symplectic vectors $(A_0, B_0)$ and $(A, B)$ are given such that $(A, B)$ is the transform of $(A_0, B_0)$ under a symplectic transformation $\Psi(r, r_0)$. We have $\tilde{A}_0B_0 = \tilde{B}_0A_0$ and $\tilde{A}B = \tilde{B}A$, but also

$$\tilde{A}_0\, dB_0 - \tilde{B}_0\, dA_0 = \tilde{A}\, dB - \tilde{B}\, dA, \qquad \text{(II.1)}$$

which follows from Eq. (2.10a) if the vector $(A_0 + dA_0, B_0 + dB_0)$ and its transform $(A + dA, B + dB)$ are again symplectic. Here $dA_0$, $dB_0$, $dA$, and $dB$ are small variations. For simplicity we take the length of $(A_0, B_0)$ equal to $I$ and the length of $(A, B)$ equal to $M$ (det $M \neq 0$). We have

$$\begin{aligned} A_0 &= R_0 \sin \eta_0, \\ B_0 &= R_0 \cos \eta_0, \\ A &= R(\sin \eta)M, \\ B &= R(\cos \eta)M, \end{aligned} \qquad \text{(II.2)}$$

where $R_0$ and $R$ are real orthogonal, $\eta_0$ and $\eta$ real diagonal such that

$$\tfrac{1}{2}\pi > \eta_{01} \geq \cdots \geq \eta_{0n} \geq -\tfrac{1}{2}\pi,$$
$$\tfrac{1}{2}\pi > \eta_1 \geq \cdots \geq \eta_n \geq -\tfrac{1}{2}\pi.$$

From Eq. (II.1) we have, with the help of (II.2),

$$\begin{aligned} (\sin \eta_0)\tilde{R}_0 d[R_0 \cos \eta_0] - (\cos \eta_0)\tilde{R}_0 d[R_0 \sin \eta_0] \\ = \tilde{M}\{(\sin \eta)\tilde{R} d[R \cos \eta] \\ - (\cos \eta)\tilde{R} d[R \sin \eta]\}M. \end{aligned} \qquad \text{(II.3)}$$

Call $\tilde{R}_0 dR_0 = dT_0$ and $\tilde{R}dR = dT$; then $d\tilde{T}_0 = -dT_0$, and $d\tilde{T} = -dT$. Then from Eq. (II.3) we obtain

$$\begin{aligned} (\sin \eta_0)(dT_0) \cos \eta_0 - (\cos \eta_0)(dT_0) \sin \eta_0 - d\eta_0 \\ = \tilde{M}\{(\sin \eta)(dT) \cos \eta \\ - (\cos \eta)(dT) \sin \eta - d\eta\}M. \end{aligned} \qquad \text{(II.4)}$$

We now introduce the matrices $T_{ij}$ such that

$$(T_{ij})_{kl} = \delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl}. \qquad \text{(II.5)}$$

Since $dT$ and $dT_0$ are antisymmetric, it is now possible to define sets of $\frac{1}{2}n(n-1)$ *invariant infinitesimal intervals* $d\xi^0_{ij}$ and $d\xi_{ij}$ such that

$$\begin{aligned} dT_0 &= \sum_{i<j} T_{ij}\, d\xi^0_{ij}, \\ dT &= \sum_{i<j} T_{ij}\, d\xi_{ij}. \end{aligned} \qquad \text{(II.6)}$$

For $n > 2$, the intervals $d\xi_{ij}$ are not integrable, i.e., whatever parameterization one adopts for the matrices $R$, the condition Eq. (II.6) can only be satisfied locally. As is shown in Appendix III, the intervals $d\xi_{ij}$ are quite natural to use for a local parameterization of $R$, and they are often preferable above any integrable set of infinitesimal intervals.

Inserting Eq. (II.6) into Eq. (II.4) we find by considering the diagonal elements,

$$d\eta_{0k} = 2 \sum_{p<q} M_{pk}M_{qk} \sin(\eta_p - \eta_q)\, d\xi_{pq} + \sum_p M_{pk}M_{pk}\, d\eta_p, \qquad \text{(II.7)}$$

and the $(k, l)$ elements $(k < l)$ give

$$\sin(\eta_{0k} - \eta_{0l})\, d\xi^0_{kl} = \sum_{p<q} \sin(\eta_p - \eta_q)(M_{pk}M_{ql} + M_{qk}M_{pl})\, d\xi_{pq} + \sum_p M_{pk}M_{pl}\, d\eta_p. \quad \text{(II.8)}$$

Introduce new variables for $k < l$:

$$d\zeta^2_{kl} = \sin(\eta_{0k} - \eta_{0l})\, d\xi^0_{kl}, \qquad d\zeta_{kl} = \sin(\eta_k - \eta_l)\, d\xi_{kl}. \quad \text{(II.9)}$$

The Jacobians of the transformations to the new sets of variables are

$$\text{and} \quad \prod_{p<q} \sin(\eta_{0p} - \eta_{0q}), \quad \prod_{p<q} \sin(\eta_p - \eta_q), \quad \text{(II.10)}$$

respectively. Substituting Eq. (II.9) into Eq. (II.7) and Eq. (II.8), one obtains

$$d\eta_{0k} = \sum_p M_{pk}M_{pk}\, d\eta_p + 2\sum_{p<q} M_{pk}M_{qk}\, d\zeta_{pq},$$
$$d\zeta^0_{kl\ (k<l)} = \sum_p M_{pk}M_{pl}\, d\eta_p + \sum_{p<q} (M_{pk}M_{ql} + M_{qk}M_{pl})\, d\zeta_{pq}. \quad \text{(II.11)}$$

We need also the Jacobian of this transformation. This can be found by considering the following. If we define

$$d\eta_p = d\zeta_{pp}, \qquad d\eta_{0p} = d\zeta^0_{pp},$$
$$d\zeta_{pq} = d\zeta_{qp}, \qquad d\zeta^0_{pq} = d\zeta^0_{qp},$$

we obtain

$$d\zeta^0_{kl} = \sum_{p,q} M_{pk}M_{ql}\, d\zeta_{pq},$$

which is just the transformation of a symmetric tensor in an $n$-dimensional space. The Jacobian of this transformation is det $M$, which is of $n$th degree as function of the elements of $M$. If we consider the elements of the symmetric tensor as components of a vector in a $\frac{1}{2}n(n+1)$-dimensional space, the transformation is again linear and its Jacobian is of degree $n(n+1)$ as function of the elements of $M$. Moreover, since the Jacobian must be a scalar density, and since the only scalar densities available are powers of det $M$, the Jacobian is a power of det $M$. By inspection we find for the exponent $n(n+1)/n = (n+1)$. We can now relate volume elements spanned on the infinitesimal intervals at $r_0$ and at $r$. From the result we just obtained and from Eqs. (II.9) and (II.10), we find

$$d\xi^0_{12}\, d\xi^0_{13} \cdots d\xi^0_{n-1\,n}\, d\eta_{01} \cdots d\eta_{0n} = \frac{\prod_{p<q} \sin(\eta_p - \eta_q)}{\prod_{p<q} \sin(\eta_{0p} - \eta_{0q})} \times (\det M)^{n+1}\, d\xi_{12} \cdots d\xi_{n-1\,n}\, d\eta_1 \cdots d\eta_n, \quad \text{(II.12)}$$

but since it is equally likely to find an event in a volume element at $r_0$ as in the transformed volume element at $r$, we conclude that for the densities $\rho^0$ at $r_0$ and $\rho$ at $r$, we have the relation

$$\rho = \rho^0 \frac{\prod_{p<q} \sin(\eta_p - \eta_q)}{\prod_{p<q} \sin(\eta_{0p} - \eta_{0q})} (\det M)^{n+1}, \quad \text{(II.13)}$$

and we can make this general by taking the length of the vector at $r_0$ not as $I$ but $M_0$, in which case one obtains

$$\rho = \rho^0 \frac{\prod_{p<q} \sin(\eta_p - \eta_q)}{\prod_{p<q} \sin(\eta_{0p} - \eta_{0q})} \cdot \left(\frac{\det M}{\det M_0}\right)^{n+1}. \quad \text{(II.14)}$$

For $n = 1$, this reduces to a relation between density "amplitudes" as discussed in Sec. 3.

## APPENDIX III. DERIVATION OF DISTRIBUTION FUNCTIONS FOR ENSEMBLES OF RANDOMLY CHOSEN TRANSFORMATIONS OF A GIVEN GROUP

Let $U$ be an arbitrary element and $\delta U$ an infinitesimal element of a given group. Then, if we define $dX = \delta U - I$, we have

$$U + dU = U\delta U, \qquad dU = U(\delta U - I) = U dX, \qquad dX = U^{-1}dU. \quad \text{(III.1)}$$

Suppose now that $U$ depends on $\nu$ independent real parameters $\alpha_i$ and $dX$ on $\nu$ independent real parameters $d\chi_i$. We have then

$$dU = \sum_{i=1}^{\nu} \frac{\partial U}{\partial \alpha_i} d\alpha_i, \qquad dX = \sum_{i=1}^{\nu} \frac{\partial X}{\partial \chi_i} d\chi_i. \quad \text{(III.2)}$$

The $\partial U/\partial\alpha_i$ are then still functions of $\alpha_i$, but the $\partial X/\partial\chi_i$ are constant. From the definition of $dX$, it follows that it is independent of $U$, since $\delta U$ is independent of $U$; therefore we call the set of infinitesimal intervals $d\chi_i$ an invariant set of intervals. From Eq. (III.1) we obtain

$$\sum_{i=1}^{\nu_i} \frac{\partial U}{\partial \alpha_i} d\alpha_i = \sum_{i=1}^{\nu_i} U \frac{\partial X}{\partial \chi_i} d\chi_i. \quad \text{(III.3)}$$

If $U$ is a matrix, then Eq. (III.3) just yields $\nu$ linear equations which can be chosen to be independent, and a transformation $d\chi_i \to d\alpha_i$ is established in a $\nu$-dimensional space.

An ensemble of randomly chosen transformations $U$ has the property that the number of transformations $U + dU$ for which the set $d\chi_i$ lies within a

volume element $d\chi_1 \cdots d\chi_r$ is independent of $U$. The distribution function of the ensemble is then proportional to the Jacobian of the transformation equation (III.3).

The following is a simple illustration. Consider the group of rotations in three dimensions. Let $R$ be equal to $R_1(\varphi)\, R_2(\vartheta)\, R_1(\psi)$, where

$$R_1(\varphi) = \begin{Vmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{Vmatrix},$$

$$R_2(\vartheta) = \begin{Vmatrix} 1 & 0 & 0 \\ 0 & \cos\vartheta & \sin\vartheta \\ 0 & -\sin\vartheta & \cos\vartheta \end{Vmatrix}.$$

Then

$$dX = \begin{Vmatrix} 0 & d\chi_{12} & d\chi_{13} \\ -d\chi_{12} & 0 & d\chi_{23} \\ -d\chi_{13} & -d\chi_{23} & 0 \end{Vmatrix}.$$

We have

$$(dR_1(\varphi)/d\varphi) = T_1 R_1(\varphi) = R_1(\varphi) T_1,$$

and

$$(dR_2(\vartheta)/d\vartheta) = T_2 R_2(\vartheta) = R_2(\vartheta) T_2,$$

where

$$T_1 = \begin{Vmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{Vmatrix}, \quad \text{and} \quad T_2 = \begin{Vmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{Vmatrix}.$$

From Eq. (III.3) we have

$$R_1(\varphi)R_2(\vartheta)R_1(\psi)\, dX = T_1 R_1(\varphi)R_2(\vartheta)R_1(\psi)\, d\varphi + R_1(\varphi)T_2 R_2(\vartheta)R_1(\psi)\, d\vartheta + R_1(\varphi)R_2(\vartheta)T_1 R_1(\psi)\, d\psi.$$

From this we obtain

$$dX = (\tilde{R}_2 T_1 R_2)\, d\varphi + T_2\, d\vartheta + T_1\, d\psi,$$

and it follows that

$$\begin{Vmatrix} d\chi_{12} \\ d\chi_{13} \\ d\chi_{23} \end{Vmatrix} = \begin{Vmatrix} \cos\vartheta & 0 & 1 \\ -\sin\vartheta & 0 & 0 \\ 0 & 1 & 0 \end{Vmatrix} \cdot \begin{Vmatrix} d\varphi \\ d\vartheta \\ d\psi \end{Vmatrix}.$$

The Jacobian of this transformation is $-\sin\vartheta$, and as a result, we find the distribution function for a random distribution,

$$\rho = \rho_0 \sin\vartheta.$$

One possible way to parametrize an $n \times n$ (non-exceptional) orthogonal matrix $R$ is by defining an antisymmetric matrix $A$ such that

$$A = (I - R)/(I + R).$$

If the $\frac{1}{2}n(n-1)$-independent parameters of $A$ are given, the matrix

$$R = (I - A)/(I + A) \qquad [\det(I + A) \neq 0]$$

is determined. Writing

$$A = \sum_{i<j} T_{ij}\alpha_{ij},$$

where $T_{ij}$ is defined by Eq. (II.5), and using $\alpha_{ij}$ as parameters, the distribution function for a random distribution of matrices $R$ turns out to be

$$\rho = \rho_0[\det(I + A)]^{1-n} = \rho_0[\det(I - A)]^{1-n}.$$

The application to the real orthogonal and symplectic group is rather trivial. We demand that the distribution function be invariant under transformation, and from the discussion of Appendix II it follows immediately that

$$\rho = \rho_0[\prod_{i<j} \sin(\eta_i - \eta_j)],$$

where $\rho_0$ is constant. The group members $\mathfrak{R}$ are here parametrized in the standard way,

$$\mathfrak{R} = \begin{Vmatrix} R_1 & 0 \\ 0 & R_1 \end{Vmatrix} \cdot \begin{Vmatrix} \cos\eta & \sin\eta \\ -\sin\eta & \cos\eta \end{Vmatrix} \cdot \begin{Vmatrix} R_2 & 0 \\ 0 & R_2 \end{Vmatrix},$$

where $R_1$ and $R_2$ are real orthogonal, $\eta$ real diagonal;

$$\tfrac{1}{2}\pi > \eta_1 \geq \cdots \geq \eta_n \geq -\tfrac{1}{2}\pi.$$

Since $\rho$ does not depend on $R_1$ and $R_2$, we see that when the matrices $\mathfrak{R}$ are randomly distributed, also the $R_1$ and $R_2$ are randomly distributed. Due to isomorphy with the unitary group, the distribution function is the same for this group.

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# Canonical Variables for the Interacting Gravitational and Dirac Fields*

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The problem of reducing the Lagrangian for the interacting gravitational and Dirac fields to canonical form is discussed, using the vierbein formalism. The arbitrary gauge variables corresponding to local Lorentz transformations of the vierbein are removed by imposing Schwinger's "time-guage" condition, and a further condition that the spatial part of the vierbein be symmetric. It is shown that in this guage the Lagrangian can be expressed in a canonical form involving essentially the same gravitational-field variables as in the absence of matter, and that the generators of spatial translations and rotations have the expected form.

## 1. INTRODUCTION

IN order to discuss the quantization of the gravitational field it is necessary to eliminate the arbitrary variables corresponding to the arbitrary gauge variables of the electromagnetic field. The reduction of the gravitational Lagrangian to a canonical form in which only four dynamical variables appear was performed by Arnowitt, Deser, and Misner,[1] starting with the Palitini form of the Lagrangian in which the independent variables are the contravariant metric tensor density $\mathfrak{g}^{\mu\nu}$ and the affinity $\Gamma^{\lambda}{}_{\mu\nu}$. An alternative, but equivalent, formulation may be obtained, following Weyl,[2] by using as independent variables the vierbein $e_{\alpha}{}^{\mu}$ and the local analog of the affinity, $\omega^{\alpha}{}_{\beta\mu}$. Recently, Schwinger[3] has shown that this form of the Lagrangian can readily be reduced to a canonical form involving essentially the same dynamical variables, and also that the same reduction can be performed for the gravitational field interacting with a scalar field. The purpose of the present paper is to discuss the analogous problem for the interacting gravitational and spinor fields.

The formulation in terms of the metric tensor is, at first sight, the more natural one for the gravitational field in the absence of matter, and even perhaps for the gravitational field interacting with other tensor fields. However, when spinor fields are introduced, the vierbein formalism becomes much the simplest. Moreover, this form of the gravitational equations is the one which arises most naturally if the gravitational field is introduced into a Lorentz-invariant theory to obtain a more general invariance.[4] We shall, therefore, employ this formalism here.

The existence of spin introduces additional complications which do not appear in the scalar case. It would not be hard to extend the discussion to fields of higher spin, but since the essential features already appear in the case of a Dirac field, we shall restrict our attention to this case. Moreover, for simplicity, we consider only a real (Majorana) field. It is clear, however, that any number of internal degrees of freedom for the Dirac field can be introduced without in any way affecting the discussion.

## 2. THE LAGRANGIAN

Instead of describing the gravitational field directly through a metric tensor, one may introduce at every point of space–time a vierbein, or set of four vectors $e_{\alpha}{}^{\mu}$, related to the metric by[2]

$$e_{\alpha}{}^{\mu}e^{\alpha\nu} \equiv \eta^{\alpha\beta}e_{\alpha}{}^{\mu}e_{\beta}{}^{\nu} = g^{\mu\nu},$$

where $\eta^{\alpha\beta}$ is the flat-space metric[5]

$$\eta^{\alpha\beta} = \delta^{\alpha\beta} - 2\delta^{\alpha 0}\delta^{\beta 0}.$$

Any tensor may be specified by its components either with respect to the over-all coordinate system, or in the local Lorentz frame defined by the $e_{\alpha}{}^{\mu}$. For instance, for a vector the two forms are related by

$$v^{\mu} = e_{\alpha}{}^{\mu}v^{\alpha}.$$

Thus, we have to distinguish two kinds of tensor indexes, "world tensor" and "local tensor" indexes. The notation is as follows: Greek indices run from 0 to 3, and Latin indices from 1 to 3. In both cases,

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[1] R. Arnowitt, S. Deser, and C. W. Misner, Phys. Rev. **116**, 1322 (1959) and **117**, 1595 (1960).

[2] H. Weyl, Z. Physik **56**, 330 (1929).

[3] J. Schwinger, Phys. Rev. **130**, 1253 (1963).

[4] T. W. B. Kibble, J. Math. Phys. **2**, 212 (1961).

[5] The signature of the metric is opposite to that of reference 4. The quantities $h_i{}^{\mu}$, $A^i{}_{j\mu}$, $c_{ij}{}^k$ of that paper are here denoted by $e_{\alpha}{}^{\mu}$, $\omega^{\alpha}{}_{\beta\mu}$, $\Omega_{\alpha\beta}{}^{\gamma}$. The corresponding quantities in reference 3 are $e^{\mu}{}_{\alpha}$, $-\omega_{\mu}{}^{\alpha}{}_{\beta}$, $\Omega^k{}_{ij}$.

we use letters from the early part of the alphabet for local-tensor indices, and those from the middle of the alphabet for world-tensor indices. We define also the inverse $\tilde{e}^{\alpha}{}_{\mu}$ of $e_{\alpha}{}^{\mu}$:

$$\tilde{e}^{\alpha}{}_{\mu}e_{\alpha}{}^{\nu} = \delta_{\mu}{}^{\nu}, \qquad \tilde{e}^{\alpha}{}_{\mu}e_{\beta}{}^{\mu} = \delta^{\alpha}{}_{\beta}.$$

It is related to the covariant metric tensor by

$$\tilde{e}^{\alpha}{}_{\mu}\tilde{e}_{\alpha\nu} = g_{\mu\nu}.$$

Since at a later stage in this paper the distinction between the two kinds of indices will be removed, we only allow raising and lowering of indices with the flat-space metric $\eta^{\alpha\beta}$. We therefore use a tilde to avoid possible confusion; $e_{\alpha}{}^{\mu}$ and $\tilde{e}^{\alpha}{}_{\mu}$ are here to be regarded as different (inverse) quantities, rather than as contravariant and covariant components of the same set of vectors.

The basic gravitational-field variables are the sixteen variables, $e_{\alpha}{}^{\mu}$, and the twenty-four variables $\omega^{\alpha\beta}{}_{\mu} = -\omega^{\beta\alpha}{}_{\mu}$ which serve to define covariant derivatives of local tensors just as the affinity $\Gamma^{\mu}{}_{\nu\rho}$ does for world tensors. It is often convenient to use instead the variables

$$\tilde{\omega}^{\alpha}{}_{\beta\gamma} = e_{\gamma}{}^{\mu}\omega^{\alpha}{}_{\beta\mu}.$$

We define also

$${}^{4}e = \det \tilde{e}^{\alpha}{}_{\mu}$$

and

$${}^{4}R^{\alpha}{}_{\beta\mu\nu} = \omega^{\alpha}{}_{\beta\mu,\nu} - \omega^{\alpha}{}_{\beta\nu,\mu} - \omega^{\alpha}{}_{\gamma\mu}\omega^{\gamma}{}_{\beta\nu} + \omega^{\alpha}{}_{\gamma\nu}\omega^{\gamma}{}_{\beta\mu}.$$

Here, and in the sequel, a comma denotes ordinary differentiation. The superscript 4 indicates that these are four-dimensional quantities.

In terms of these variables, the Lagrangian for the gravitation field alone may be written as[6]

$$\mathfrak{L}_{G} = -\tfrac{1}{2}\,{}^{4}e\,{}^{4}R = -\tfrac{1}{2}\,{}^{4}ee_{\alpha}{}^{\mu}e^{\beta\nu}R^{\alpha}{}_{\beta\mu\nu}.$$

In the quantized theory, we should of course consider the problem of ordering of operators, and the Lagrangian should be written in an appropriately symmetrized form. However, we shall not indicate this symmetrization explicitly, and we shall ignore the noncommutativity of the variables, (except of course that two Dirac fields are required to anticommute). The Lagrangian may also be written in terms of $\tilde{\omega}^{\alpha}{}_{\beta\gamma}$ rather than $\omega^{\alpha}{}_{\beta\mu}$, in the form

$$\mathfrak{L}_{G} = ({}^{4}ee_{\alpha}{}^{\mu}\tilde{\omega}^{\alpha\beta}{}_{\beta})_{,\mu} - \tfrac{1}{2}\,{}^{4}e\Omega_{\alpha\beta}{}^{\gamma}\tilde{\omega}^{\alpha\beta}{}_{\gamma} + {}^{4}e\Omega_{\alpha\beta}{}^{\beta}\tilde{\omega}^{\alpha\gamma}{}_{\gamma} + \tfrac{1}{2}\,{}^{4}e(\tilde{\omega}^{\alpha}{}_{\gamma\alpha}\tilde{\omega}^{\gamma\beta}{}_{\beta} - \tilde{\omega}^{\alpha}{}_{\gamma\beta}\tilde{\omega}^{\gamma\beta}{}_{\alpha}),$$

where

$$\Omega_{\alpha\beta}{}^{\gamma} = (e_{\alpha}{}^{\mu}e_{\beta}{}^{\nu} - e_{\alpha}{}^{\nu}e_{\beta}{}^{\mu})\tilde{e}^{\gamma}{}_{\mu,\nu}.$$

Note that

$$\Omega_{\alpha\beta}{}^{\alpha} = ({}^{4}e)^{-1}({}^{4}ee_{\beta}{}^{\mu})_{,\mu}.$$

The Lagrangian for the Majorana–Dirac field including gravitational interaction may be taken to be

$$\mathfrak{L}_{D}{}^{(0)} = \tfrac{1}{2}\,{}^{4}e(ie_{\alpha}{}^{\mu}\psi\alpha^{\alpha}\psi_{;\mu} - m\psi\beta\psi),$$

where the matrices $\alpha^{\alpha} = \beta\gamma^{\alpha}$ and $\beta = \gamma^{0}$ satisfy the conditions

$$\alpha_{\alpha}^{\dagger} = \alpha_{\alpha} = \alpha_{\alpha}{}^{*},$$

$$\beta^{\dagger} = \beta = -\beta^{*},$$

$$\{\gamma^{\alpha}, \gamma^{\beta}\} = -2\eta^{\alpha\beta},$$

and the covariant derivative $\psi_{;\mu}$ is defined by

$$\psi_{;\mu} = \psi_{,\mu} + \tfrac{1}{4}\omega^{\alpha\beta}{}_{\mu}\gamma_{\alpha\beta}\psi,$$

$$\gamma_{\alpha\beta} = \tfrac{1}{2}[\gamma_{\alpha}, \gamma_{\beta}].$$

An alternative form is

$$\mathfrak{L}_{D}{}^{(0)} = \tfrac{1}{2}\,{}^{4}e(ie_{\alpha}{}^{\mu}\psi\alpha^{\alpha}\psi_{,\mu} - m\psi\beta\psi - \tilde{\omega}^{\beta\gamma}{}_{\alpha}S^{\alpha}{}_{\beta\gamma}),$$

where the spin tensor $S^{\alpha}{}_{\beta\gamma}$ is given by

$$S^{\alpha}{}_{\beta\gamma} = -\tfrac{1}{4}i\psi\beta\gamma^{\alpha}{}_{\beta\gamma}\psi,$$

$$\gamma_{\alpha\beta\gamma} = \tfrac{1}{2}\{\gamma_{\alpha}, \gamma_{\beta\gamma}\} = \epsilon_{\alpha\beta\gamma\delta}\gamma^{\delta}\gamma^{5},$$

$$\gamma^{5} = \gamma_{0}\gamma_{1}\gamma_{2}\gamma_{3}.$$

It was pointed out by Weyl[7] that the Lagrangian $\mathfrak{L}_{G} + \mathfrak{L}_{D}{}^{(0)}$ is not equivalent to the Lagrangian one would most naturally write down in terms of the metric tensor. The difference arises because the equations of motion for $\tilde{\omega}^{\alpha}{}_{\beta\gamma}$ involve the spin tensor $S^{\alpha}{}_{\beta\gamma}$. It can be made equivalent by adding extra terms representing a direct spin–spin interaction similar to the Fermi interaction, namely[8]

$$\mathfrak{L}_{D}{}^{(1)} = -\tfrac{1}{8}\,{}^{4}eS^{\alpha}{}_{\beta\gamma}S^{\beta\gamma}{}_{\alpha}.$$

For the purposes of this paper, it is immaterial whether these are included or not. The reduction to canonical form can be carried out equally well in either case. One might perhaps expect that the choice is not in fact arbitrary. It is interesting to conjecture that one might be able to distinguish between these two forms by using consistency conditions of the kind discussed by Schwinger.[9] It may turn out, in fact, that in the quantized theory Lorentz covariance actually requires a particular choice. For definiteness, and for reasons of simplicity of the final expressions, we shall include the extra

[6] We use natural units in which $c = \hbar = 1$ and $\kappa = 8\pi G = 1$.

[7] H. Weyl, Phys. Rev. **77**, 699 (1950).

[8] See reference 4. Note however that the sign of $\mathfrak{L}^{(1)}$ given in Eq. (7.1) of that paper is incorrect.

[9] J. Schwinger, Phys. Rev. **130**, 406, 800 (1963).

terms. Thus, our final Lagrangian is

$$\mathfrak{L} = \mathfrak{L}_G + \mathfrak{L}_D^{(0)} + \mathfrak{L}_D^{(1)}.$$

It would be easy, however, to subtract $\mathfrak{L}_D^{(1)}$ from the final expression if desired.

The Lagrangian $\mathfrak{L}$ has two quite distinct invariances, under general coordinate transformations (with $\psi$ transforming as a scalar) and under local Lorentz transformations among the $e_\alpha{}^\mu$. The reduction of $\mathfrak{L}$ to canonical form involves, as in the electromagnetic case, the choice of a particular "gauge". Like the radiation gauge, this gauge is appropriate only to a particular choice of the time coordinate, and manifest Lorentz invariance is necessarily lost, though in principle one can check this invariance at the end by examining the energy density commutator.[9] In the following sections, the arbitrary gauge variables will be eliminated successively in three sets, corresponding to local pure Lorentz transformations, to local spatial rotations, and to coordinate transformation, respectively.

### 3. TIME GAUGE

The invariance under local Lorentz transformations implies the existence of six arbitrary gauge functions, which may be eliminated by tying the local axes $e_\alpha{}^\mu$ in some way to the overall coordinate system. Three of these may be eliminated by imposing the condition

$$e_a{}^0 = 0,$$

which Schwinger[3] has called the "time gauge". This condition may also be expressed in terms of the inverse $\tilde{e}^\alpha{}_\mu$; it then takes the form

$$\tilde{e}^0{}_i = 0.$$

It also follows that $\tilde{e}^a{}_i$ is the inverse of $e_a{}^i$:

$$\tilde{e}^a{}_i e_a{}^j = \delta_i{}^j, \qquad \tilde{e}^a{}_i e_b{}^i = \delta^a{}_b,$$

and that

$$\tilde{e}^0{}_0 e_0{}^0 = 1.$$

Moreover, defining

$${}^3e = \det \tilde{e}^a{}_i,$$

we have

$${}^3e = {}^4e e_0{}^0.$$

The time-gauge condition presupposes that

$$g^{00} = e_a{}^0 e^{a0} = e_0{}^0 e^{00} < 0,$$

or, equivalently, that the three-dimensional metric,

$$g_{ij} = \tilde{e}^a{}_i \tilde{e}_{aj},$$

is positive-definite. This means that the choice of time coordinate must be such that the constant-time surfaces are genuine spacelike surfaces. It is clear that this is a necessary prerequisite for a canonical formalism of the usual kind.

The field equations for the variables $\tilde{\omega}^\alpha{}_{\beta\gamma}$ can be written in the form

$$\tilde{\omega}_{\alpha\beta\gamma} = \tfrac{1}{2}(\Omega_{\alpha\beta\gamma} - \Omega_{\beta\gamma\alpha} - \Omega_{\gamma\alpha\beta}) - \tfrac{1}{2}S_{\alpha\beta\gamma}.$$

We first examine the equations containing an even number of indices zero. In the time gauge these become

$$\tilde{\omega}_{0a0} = \Omega_{0a0} = e_0{}^0 e_a{}^i \tilde{e}_{00,i},$$

$$\tilde{\omega}_{abc} = \tfrac{1}{2}(\Omega_{abc} - \Omega_{bca} - \Omega_{cab}) - \tfrac{1}{2}S_{eab},$$

which also imply

$$\tilde{\omega}^b{}_{ab} = \Omega_{ba}{}^b = ({}^3e)^{-1}({}^3e e_a{}^i)_{,i}.$$

It follows from the time-gauge condition that $\Omega_{abc}$ contains no time derivatives. Therefore, $\tilde{\omega}_{0a0}$ and $\tilde{\omega}_{abc}$ are purely constraint variables, and may be eliminated from the Lagrangian.

Next we consider the components with an odd number of indices zero. It is convenient to introduce a notation for the symmetric and antisymmetric parts of a tensor:

$$T_{(ab)} = \tfrac{1}{2}(T_{ab} + T_{ba}),$$

$$T_{[ab]} = \tfrac{1}{2}(T_{ab} - T_{ba}).$$

In the time gauge, $\Omega_{ab0} = 0$; thus, the remaining equations are

$$\tilde{\omega}_{ab0} = -\Omega_{0[ab]} - \tfrac{1}{2}S_{0ab},$$

$$\tilde{\omega}_{0ab} = \Omega_{0(ab)} - \tfrac{1}{2}S_{0ab}.$$

It follows that the antisymmetric components $\tilde{\omega}_{0[ab]}$ are also constraint variables and may be eliminated from the Lagrangian. When this is done, the variables $\tilde{\omega}_{ab0}$ also drop out, and we are left with a Lagrangian containing only the symmetric components $\tilde{\omega}_{0(ab)}$. Omitting explicit divergence terms,[10] it is

$$\begin{aligned}\mathfrak{L} = {}^4e[&-(\Omega_0{}^{ab}\tilde{\omega}^0{}_{(ab)} - \Omega_{0a}{}^a\tilde{\omega}^{0b}{}_b)\\ &+ \tfrac{1}{2}(\tilde{\omega}_{0(ab)}\tilde{\omega}^{0(ab)} - \tilde{\omega}_{0a}{}^a\tilde{\omega}^{0b}{}_b)\\ &- \tfrac{1}{2}{}^3R + \tfrac{1}{4}\Omega_{ab}{}^c S^{ab}{}_c + \tfrac{1}{2}\Omega_{0a}{}^b S^{0a}{}_b\\ &+ \tfrac{1}{2}i(e_0{}^0\psi\psi_{,0} + e_0{}^i\psi\psi_{,i} + e_a{}^i\psi\alpha^a\psi_{,i}) - \tfrac{1}{2}m\psi\beta\psi],\end{aligned}$$

[10] For the gravitational field, one must be more cautious about doing this than is usually necessary, because some of the field variables do not go rapidly to zero at spatial infinity. The asymptotic behavior of the field variables is discussed in detail by R. Arnowitt, S. Deser, and C. W. Misner, Phys. Rev. **121**, 1556 (1961).

where ${}^3R$ is the three-dimensional curvature scalar formed out of the $e_a{}^i$, namely,

$$ {}^3R = 2({}^3e)^{-1}[{}^3ee^{ai}\Omega_{ba}{}^b]_{,i} - \Omega_{ab}{}^b\Omega^{ac}{}_c + \tfrac{1}{4}\Omega_{ab}{}^c\Omega^{ab}{}_c - \tfrac{1}{2}\Omega_{ab}{}^c\Omega_c{}^{ab}. $$

The dynamical variables whose time derivatives still appear in the Lagrangian are $\psi$, $e_a{}^i$, $\bar{\omega}^0{}_{(ab)}$. In order to cast the Lagrangian into canonical form, it is convenient to absorb appropriate factors of ${}^3e$ into these variables. We define

$$ \Psi = ({}^3e)^{\frac{1}{2}}\psi, $$
$$ f_a{}^i = {}^3ee_a{}^i, $$
$$ \varpi_{ab} = {}^3e\bar{\omega}^0{}_{(ab)}, $$

and, correspondingly,

$$ \mathcal{S}^\alpha{}_{\beta\gamma} = {}^3eS^\alpha{}_{\beta\gamma} = -\tfrac{1}{4}i\Psi\beta\gamma^\alpha{}_{\beta\gamma}\Psi, $$
$$ \bar{f}^a{}_i = ({}^3e)^{-1}\bar{e}^a{}_i. $$

We note that

$$ \det f_a{}^i = ({}^3e)^2 = {}^3g. $$

The quantity $\Omega_{ab}{}^c$ may be expressed in terms of $f_a{}^i$ in the form

$$ {}^3e\Omega_{ab}{}^c = \Delta_{ab}{}^c = (f_a{}^if_b{}^j - f_a{}^jf_b{}^i)\bar{f}^c{}_{i,j} - \tfrac{1}{2}(\delta_a{}^cf_b{}^j - \delta_b{}^cf_a{}^j)f_d{}^i\bar{f}^d{}_{i,j}. $$

The remaining variables $e_0{}^0$, $e_0{}^i$ are not true dynamical variables. Their time derivatives are not determined by the equations of motion; instead, the corresponding equations impose constraints on the dynamical variables. It is convenient to define the variables

$$ n_0 = ({}^3e)^{-1}\bar{e}^0{}_0, $$
$$ n^i = \bar{e}^0{}_0e_0{}^i, $$

which then appear linearly in the Lagrangian and play the role of Lagrange multipliers. The quantities $\Omega_{0a}{}^b$, which contain the only time derivatives of $f_a{}^i$ are expressible in terms of these variables in the form

$$ {}^4e(\Omega_{0a}{}^b - \delta_a{}^b\Omega_{0c}{}^c) = {}^3e\bar{f}^b{}_i[f_a{}^i{}_{,0} - f_a{}^jn^i{}_{,j} + (n^jf_a{}^i)_{,j}]. $$

Omitting some further divergence terms, the Lagrangian then reduces to

$$ \mathcal{L} = \tfrac{1}{2}i\Psi\Psi_{,0} - f^b{}_if_a{}^i{}_{,0}(\varpi_{ab} - \tfrac{1}{2}\mathcal{S}^0{}_{ab}) - n_\mu T^\mu, $$

where

$$ T^0 = \tfrac{1}{2}\,{}^3\mathcal{R} - \tfrac{1}{4}\Delta_{ab}{}^c\mathcal{S}^{ab}{}_c - \tfrac{1}{2}if_a{}^i\Psi\alpha^a\Psi_{,i} + \tfrac{1}{2}m^2e\Psi\beta\Psi + \tfrac{1}{2}(\varpi_{ab}\varpi^{ab} - \varpi_a{}^a\varpi_b{}^b), $$

$$ T_i = -\tfrac{1}{2}i\Psi\Psi_{,i} + \bar{f}^b{}_jf^{aj}(\varpi_{ab} - \tfrac{1}{2}\mathcal{S}^0{}_{ab})_{,i} - f^{aj}[\bar{f}^b{}_j(\varpi_{ab} - \tfrac{1}{2}\mathcal{S}^0{}_{ab})]_{,i} $$

in which

$$ {}^3\mathcal{R} = {}^3g\,{}^3R = 2{}^3e[({}^3e)^{-1}f^{ai}\Delta_{ba}{}^b]_{,i} - \Delta_{ab}{}^b\Delta^{ac}{}_c + \tfrac{1}{4}\Delta_{ab}{}^c\Delta^{ab}{}_c - \tfrac{1}{2}\Delta_{ab}{}^c\Delta_c{}^{ab}. $$

## 4. SPATIALLY SYMMETRIC TIME GAUGE

The Lagrangian obtained in the previous section still possesses an invariance under spatial rotations of the local axes. To eliminate the corresponding arbitrariness, we have to tie the local quantities $f_a{}^i$ in some way to the three-dimensional coordinate system. We define

$$ q^{ij} = f_a{}^if^{aj} = {}^3g\,{}^3g^{ij}, $$

where ${}^3g^{ij}$ is the inverse of the three-dimensional metric tensor $g_{ij}$. Then the problem is to reexpress the Lagrangian in terms of the six variables $q^{ij}$ instead of the nine variables $f_a{}^i$. If $\mathcal{S}^0{}_{ab}$ were zero, the terms involving time derivatives would automatically be expressible in terms of $q^{ij}{}_{,0}$ alone. However, the presence of spin introduces a complication at this point which forces us to choose a specific gauge condition such that the $f_a{}^i$ become explicit functions of the $q^{ij}$. That such a condition is necessary may also be seen by considering the fact that the dynamical variable $\Psi$ is not determined until we specify the gauge. The simplest choice is to impose the symmetry condition

$$ f^{[ai]} = 0, $$

so that

$$ f^{ai} = (q^{\frac{1}{2}})^{ai}, $$

in the sense of the matrix square root. (Recall that $q^{ij}$ is a positive-definite matrix). This may be called the spatially symmetric time gauge. Note that this condition removes the distinction between local indices and world indices, as indeed it must. We continue to raise and lower all three-dimensional tensor indices with the flat-space metric $\delta_{ij}$.

In order to obtain a canonical form in this gauge, we have to transform from the variables $\varpi_{ab}$ to a new set $\pi_{ij}$ conjugate to $q^{ij}$. This means that we have to find a symmetric $\pi_{ij}$ such that

$$ (\varpi_{ab} - \tfrac{1}{2}\mathcal{S}^0{}_{ab})\bar{f}^b{}_j = f_a{}^i\pi_{ij} + \sigma_{aj}, \qquad \sigma_{(aj)} = 0, $$

for then the time-derivative term may be written

$$ -f^{aj}{}_{,0}(\varpi_{ab} - \tfrac{1}{2}\mathcal{S}^0{}_{ab})\bar{f}^b{}_j = -f^{aj}{}_{,0}f_a{}^i\pi_{ij} = -\tfrac{1}{2}q^{ij}{}_{,0}\pi_{ij}. $$

It is easy to solve this equation for $\sigma_{aj}$; we find

$$\sigma_{ab} = k^c{}_a \mathcal{S}^0{}_{bc} + k^c{}_b \mathcal{S}^0{}_{ca} + k^c{}_c \mathcal{S}^0{}_{ab},$$

where $k^a{}_b$ is defined by

$$(k^{-1})_a{}^b = \hat{f}_a{}^b = f_a{}^b - \delta_a{}^b f_c{}^c.$$

We then find that the equation for $\pi_{ij}$ may be written

$$f_a{}^i \pi_{ij} f_b{}^j = \varpi_{ab} - \Sigma_{ab},$$

where $\Sigma_{ab}$ is a symmetric quantity constructed out of the spin tensor, namely

$$\Sigma_{ab} = \hat{k}^c{}_{(a} \hat{f}_{b)}{}^d \mathcal{S}^0{}_{cd},$$

$$\hat{k}^a{}_b = k^a{}_b - \delta^a{}_b k^c{}_c.$$

Reexpressing the Lagrangian in terms of $q^{ij}$ and $\pi_{ij}$ we obtain

$$\mathfrak{L} = \tfrac{1}{2} i \Psi \Psi_{,0} - \tfrac{1}{2} q^{ij}{}_{,0} \pi_{ij} - n_\mu T^\mu,$$

where

$$T^0 = \tfrac{1}{2}\, {}^3\mathcal{R} - \tfrac{1}{4} \Delta_{ab}{}^c \mathcal{S}^{ab}{}_c - \tfrac{1}{2} i f_a{}^i \Psi \alpha^a \Psi_{,i} + \tfrac{1}{2} m^3 e \Psi \beta \Psi + \tfrac{1}{2} q^{ik} q^{jl} (\pi_{ik} \pi_{jl} - \pi_{il} \pi_{jk}) - \pi_{ij} f_a{}^i f_b{}^j \Sigma^{ab} + \tfrac{1}{2} \Sigma_{ab} \Sigma^{ab},$$

and

$$T_i = -\tfrac{1}{2} i \Psi \Psi_{,i} + \tfrac{1}{2} q^{jk}{}_{,i} \pi_{jk} + (q^{jk} \pi_{ki})_{,j} - (q^{jk} \pi_{jk})_{,i} - \Sigma_i{}^j{}_{,j} - \tfrac{1}{2} \mathcal{S}^{0j}{}_{i,j}.$$

In these expressions, $f_a{}^i$ is of course to be regarded as a function (namely the matrix square-root) of $q^{ij}$.

The expression ${}^3\mathcal{R}$ can also be expressed explicitly in terms of $q^{ij}$ and its inverse $\tilde{q}_{ij}$ in the form[11]

$${}^3\mathcal{R} = q^{ij}{}_{,ij} - \tfrac{1}{2} \tilde{q}_{ij} q^{ik}{}_{,l} q^{jl}{}_{,k} + \tfrac{1}{4} q^{ij} \tilde{q}_{kl} \tilde{q}_{mn} q^{km}{}_{,i} q^{ln}{}_{,j} - \tfrac{1}{8} q^{ij} \tilde{q}_{kl} \tilde{q}_{mn} q^{kl}{}_{,i} q^{mn}{}_{,j}.$$

For completeness, we note that if we had retained the divergence terms throughout the additional terms would be $D^\mu{}_{,\mu}$ where

$$D^0 = q^{ij} \pi_{ij},$$

$$D^i = (q^{ik} \pi_{kj} - \Sigma^i{}_j - \tfrac{1}{2} \mathcal{S}^{0i}{}_j) n^j - ({}^3e)^{-1} q^{ij} ({}^3e n_0)_{,j}.$$

## 5. FINAL REDUCTION TO CANONICAL FORM

This Lagrangian is now in precisely the same form as that for the gravitational field in the absence of matter, and the remaining reduction follows the same procedure. We shall, therefore, merely summarize the discussion, omitting the details.[12] We make the orthogonal decomposition of $\pi_{ij}$,

$$\pi_{ij} = \pi_{ij}{}^T + \tfrac{1}{2}(\pi_{i,j} + \pi_{j,i}) - \delta_{ij} \pi_{k,k} + \pi_{,ij},$$

$$\pi_{ij}{}^T{}_{,j} = 0, \qquad \pi_{ii}{}^T = 0,$$

and a similar decomposition of $q^{ij}$. Then the true dynamical variables are $\Psi$, $q^{ijT}$, and $\pi_{ij}{}^T$. The constraint equations have the form

$$T^0 = \tfrac{1}{2} q^{ij}{}_{,ij} + \vartheta^0 = 0,$$

$$T_i = (\pi_{ij,j} - \pi_{jj,i}) + \vartheta_i = 0,$$

and serve to determine $q$ and $\pi_i$ implicitly in terms of the remaining variables. The undetermined variables $q^i$ and $\pi$ may be identified in an appropriate way with the coordinates, by imposing "gauge" conditions which remove the remaining arbitrariness corresponding to general coordinate transformations. One possible choice is to write the coordinates as explicit functions of $q^i$ and $\pi$:

$$x^0 = \pi, \qquad x^i = -\tfrac{1}{2} q^i.$$

In this gauge, the generators of rigid Lorentz transformations are simply

$$P^\mu = \int d_3x\, \vartheta^\mu,$$

$$J^{\mu\nu} = \int d_3x\, (x^\mu \vartheta^\nu - x^\nu \vartheta^\mu).$$

In particular, the generators of spatial translations and rotations are explicit functions of the dynamical variables alone:

$$P_i = \int d_3x\, (-\tfrac{1}{2} i \Psi \Psi_{,i} + \tfrac{1}{2} q^{ikT}{}_{,i} \pi_{ik}{}^T),$$

$$J_{ij} = \int d_3x\, [(-x_{[i} \Psi \Psi_{,j]} + \mathcal{S}^0{}_{ij}) + (\pi_{kl}{}^T x_{[i} q^{klT}{}_{,j]} - 2 q_{[i}{}^{kT} \pi_{j]k}{}^T)].$$

As expected, these expressions are just the sums of the corresponding expressions for the Dirac and gravitational-field variables separately. It is easy to verify that they do correctly generate translations and rotations of the dynamical variables. On the other hand, $P^0$ and $J^{0i}$ involve integrals of $\vartheta^0$, which is a complicated implicit function of the dynamical variables.

## ACKNOWLEDGMENTS

The author is indebted to Dr. Lowell Brown and Dr. S. Deser for helpful discussions.

[11] Compare reference 3.

[12] See references 1 and 3. Here we follow essentially the treatment of reference 3. Note that $\Pi_{ij}$ there corresponds to our $-\tfrac{1}{2}\pi_{ij}$.

# Cluster Development in an $N$-Body Problem*

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The procedure for generating useful cluster development in problems dealing with the Jastrow wavefunction, as proposed by Wu and Feenberg, is discussed in detail. The existence of the expansion is proved to all orders; also a simple rule is given for computing the expansion coefficients. The result can be considered as a generalization of the Ursell–Mayer formulas.

## I. INTRODUCTION

In the statistical and quantum mechanical treatment of an $N$-body system, one often needs the technique of the Ursell–Mayer-type cluster expansion[1-3] in evaluating physical quantities of interest. In the general case the quantity considered may be a function of $N$ distinct indices. For example, in case of fermions, when a trial wavefunction involving $N$ single-particle orbitals is used to describe the system, all quantities calculated for this system depend on the $N$ orbitals explicitly. This kind of problem was first taken up by Jastrow[4] who introduced a correlated wavefunction containing a factor describing the correlation among particles in addition to a Slater determinant composed of plane-wave orbitals. The mathematics of the cluster expansion in problems involving such wavefunction has been discussed exhaustively by Hartogh and Tolhoek[5] in a series of papers in which general expansion theorems are fully developed. On the other hand, a much simpler formalism which is more general, in the sense that the problem of Jastrow wavefunction appears as a special case of its application, was introduced by Iwamoto and Yamada.[6] Considering the complicated notation and the large quantity of combinatorial algebra involved in the discussion of Hartogh and Tolhoek, an alternative rigorous treatment along the more general lines indicated by Iwamoto and Yamada seems desirable. However it is rather difficult to demonstrate the general character of the cluster expansion by the method of Iwamoto and Yamada; also the existence of the expansion for arbitrary order is not easily proved. An alternative procedure which retains the essential simplicity and directness of the Iwamoto–Yamada approach has been found by Wu and Feenberg and used by them to compute numerical results in a study of the fermion liquid.[7] It is therefore the purpose of this note to present a further detailed discussion of the latter procedure. The existence of the expansion is proved to all orders; also a simple rule is given for computing the expansion coefficients. The result reduces to the Ursell–Mayer formulas if one neglects the difference between all indices and, therefore, our formula is, in a sense, a generalization of the Ursell–Mayer formalism.

## II. PROCEDURE OF CLUSTER DEVELOPMENT

As is well-known, the cluster-expansion procedure is usually used in evaluating the logarithm of quantity which behaves like exponential function of $N$. In applications, the quantity of the order of $e^{\alpha N}$ often has an integral form

$$K_{12\cdots N} = \int W_{12\cdots N}(\tau_1, \tau_2, \cdots, \tau_N)\, d\tau_1\, d\tau_2 \cdots d\tau_N, \tag{1}$$

in which the indices $1, 2, \cdots, N$ refer to, e.g., the $N$ different single-particle orbitals involved in the trial wavefunction. The function $W$ is symmetric in all coordinates $\tau_1, \tau_2, \cdots, \tau_N$, of the $N$ particles and the subscripts $1, 2, \cdots, N$. A systematic way to handle the problem, i.e., to evaluate $\ln K_{12\cdots N}$ is as follows.[5,7]

First one defines the reduced $K$ quantities by specifying certain rules by which one generates the $K$ quantities of one index, two indices, etc. For example if $K_{12\cdots N}$ is given by Eq. (1), one way to define the reduced $K$'s is[5]

$$K_1 = \int W_1(\tau_1)\, d\tau_1, \tag{2}$$

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$$K_{mn} = \int W_{mn}(\tau_1, \tau_2)\, d\tau_1\, d\tau_2, \text{ etc.}, \tag{3}$$

with $l, m, n \cdots$ referring to different indices in the set $1, 2, \cdots, N$. The range of integration is the same in all these integrals. Then the following relations generate a set of $X$ quantities, or a set of cluster integrals:

$$K_l = X_l,$$

$$K_{lm} = X_l X_m + X_{lm},$$

$$K_{lmn} = X_l X_m X_n + X_l X_{mn} + X_m X_{nl} + X_n X_{lm} + X_{lmn}, \cdots, \tag{4}$$

until finally one reaches

$$K_{12\cdots N} = \sum_{\sum_s m_s = N}^{*} \{\cdots \underset{m_1 \text{ factors}}{X_i \cdots X_j} \cdots\} \times \{\cdots \underset{m_2 \text{ factors}}{X_{kl} \cdots X_{mn}} \cdots\} \cdots, \tag{5}$$

in which the summation extends over all possible products subject to conditions (i) no repeated indices; (ii) permutation within a bracket not distinguishable. Each $K$, hence $X$, is symmetric with respect to its indices.

As stated earlier, in application we are interested only in the cases

$$\ln K_{12\cdots N} \sim O(N). \tag{6}$$

In fact if the rule that specifies the reduced $K$'s is taken properly, one always has

$$X_{(m \text{ indices})} \sim O(N^{1-m}), \tag{7}$$

and Eq. (6) follows as a result of Eq. (7), as we shall see. Both Eqs. (6) and (7) are checked easily in the special case of Mayer's cluster expansion for a classical imperfect gas for which all $X$'s having the same number of indices are identical.

It is convenient to write

$$K_{12\cdots N} = X_1 X_2 \cdots X_N I, \tag{8}$$

$$x_{lm\cdots n} = X_{lm\cdots n}/X_l X_m \cdots X_n, \tag{9}$$

$$I = 1 + \sum_{m<n} x_{mn} + \sum_{l<m<n} x_{lmn} + \sum_{h<l<m<n} (x_{hl}x_{mn} + x_{hm}x_{nl} + x_{hn}x_{lm} + x_{hlmn}) + \cdots; \tag{10}$$

then

$$\ln K_{12\cdots N} = \sum_{l=1}^{N} \ln X_l + \ln I. \tag{11}$$

The problem is now reduced to the evaluation of $\ln I$. At this stage, Iwamoto and Yamada[5] write down a set of differential equations and solve the problem by constructing successive approximate solutions. The extension of their method to arbitrary order is difficult to carry out. In particular, the differential equations must be written down with great care in order to not overcount many terms.[8] In the following, we shall first outline the alternative procedures suggested by Wu and Freenberg[7] and then extend the discussion to all orders.

Let $I_{lm\cdots n}$ denote the function generated by omitting all terms in Eq. (10) containing indices in the set $l, m, \cdots, n$. Then it is easy to see that in Eq. (10) the coefficient of the factor $x_{qm}$ is exactly $I_{qm}$, of $x_{qmn}$ is $I_{qmn}$, etc. It follows that Eq. (10) can be rewritten as

$$I = I_q + \sum_m x_{qm} I_{qm} + \sum_{m<n} x_{qmn} I_{qmn} \cdots + \sum_{m<n<\cdots<l} x_{qmn\cdots l} I_{qmn\cdots l} \cdots + x_{12\cdots N}. \tag{12}$$

Now we write

$$\ln I = G,$$

$$\ln I_q = G_q = G - H_q, \tag{13}$$

$$\ln I_{qm} = G_{qm} = (G - H_q - H_m)[1 + O(1/N)], \text{ etc.},$$

where $G_{lm\cdots n}$ denotes the function generated by omitting all terms in $G$ containing indices in the set $l, m, \cdots, n$. Retaining only the leading terms in the exponentials, we transform Eq. (12) into

$$e^{H_q} = 1 + \sum_m x_{qm} e^{-H_m} + \frac{1}{2!} \sum_{mn} x_{qmn} e^{-(H_m + H_n)} + \cdots. \tag{14}$$

Here the convention that any $x$ with repeated indices vanishes, i.e. $x_{\cdots i \cdots i \cdots} = 0$, is introduced. We emphasize that the substitutions Eq. (13) will be justified by actually determining $G$.

Both sides of Eq. (14) and also each multiple sum are now independent of $N$ so that a formal expansion of the exponentials is permissible. Taking the logarithms of the left- and right-hand members of Eq. (14), one obtains

$$H_q = W - \tfrac{1}{2}W^2 + \tfrac{1}{3}W^3 - \cdots, \tag{15a}$$

$$W = \sum_m x_{qm}\left[1 - H_m + \frac{1}{2!}H_m^2 - \cdots\right] + \frac{1}{2!}\sum_{mn} x_{qmn} \times \left[1 - (H_m + H_n) + \frac{1}{2!}(H_m + H_n)^2 - \cdots\right] + \cdots. \tag{15b}$$

As the equation stands, $H_q$ can be generated by an

[8] We are indebted to Dr. Iwamoto for this remark.

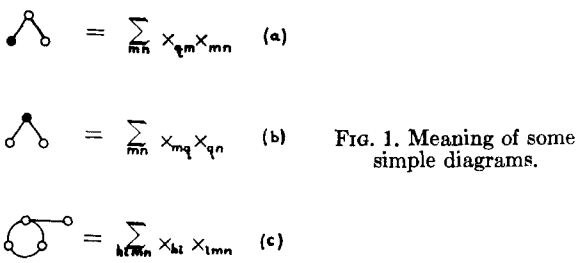

FIG. 1. Meaning of some simple diagrams.

obvious iteration procedure. Indeed, we get for the first few terms

$$H_q = \sum_m x_{qm} + \sum_{mn}\left(\frac{1}{2!}x_{qmn} - \frac{1}{2}x_{mq}x_{qn} - x_{qm}x_{mn}\right) + \cdots, \quad (16)$$

which, in turn, produces

$$G = \frac{1}{2!}\sum_{mn} x_{mn} + \sum_{lmn}\left(\frac{1}{3!}x_{lmn} - \frac{1}{2}x_{lm}x_{mn}\right) + \cdots, \quad (17)$$

as observed from the relation

$$H_q = G - G_q. \quad (18)$$

This observation is best demonstrated if one starts from the expression of $G$ given by Eq. (17) and uses Eq. (18) to compute $H_q$; then

$$\begin{aligned} H_q = {} & \frac{1}{2!}\sum_{mn} x_{mn} + \sum_{lmn}\left(\frac{1}{3!}x_{lmn} - \frac{1}{2}x_{lm}x_{mn}\right) + \cdots \\ & - \left[\frac{1}{2!}\sum_{mn\neq q} x_{mn} + \sum_{lmn\neq q}\left(\frac{1}{3!}x_{lmn} - \frac{1}{2}x_{lm}x_{mn}\right) + \cdots\right] = \frac{1}{2!}\sum_m (x_{qm} + x_{mq}) \\ & + \sum_{mn}\left[\frac{1}{3!}(x_{qmn} + x_{mqn} + x_{mnq}) - \frac{1}{2}(x_{qm}x_{mn} + x_{mq}x_{qn} + x_{mn}x_{nq})\right] + \cdots, \end{aligned} \quad (16')$$

which is identically Eq. (16) on taking account of the symmetry of the $x$'s in the indices. Clearly the ratio between the coefficients of $\sum_{mn} x_{mq}\, x_{qn}$ and $\sum_{mn} x_{qm}\, x_{mn}$ in Eq. (16) must be 1 : 2 in order to generate the term $\sum_{lmn} x_{lm}\, x_{mn}$ in $G$. The necessity of such correlation between the coefficients in the expansion of $H_q$ persists to all orders. The explicit statement of such correlation will be made after we introduce the diagrammatical representation below. Also one easily checks, with the help of Eqs. (7) and (9), that the first three terms of Eq. (17) are of the order $O(N)$. This linear dependence on $N$ also persists to all terms of $G$. This fact follows from the structure of Eq. (15b) which tells us that the inclusion of each $m$ index $x \sim O(N^{1-m})$ brings in exactly $m - 1$ free summations, and hence a factor $N^{1-m}\cdot N^{m-1} \sim O(1)$.

A diagrammatical representation which will facilitate our discussion is now introduced. In the following, the $x$'s are called elements. An $m$-index element is imagined as a rigid frame with $m$ holes (or vertices) attached to it: open holes represent the dummy indices of a summation, and a black or solid hole (indexed by $q$) is not summed over. No meaning is attached to the order of holes in an element (symmetry of an element in all indices). A collection of elements (i.e., a product of $x$'s) is called a diagram. The meaning of some simple diagrams are given by Fig. 1. A diagram is singly connected if all elements of the diagram are connected without forming any closed path; i.e., each hole common to two or more elements is an articulation which, if omitted, would dissociate the diagram into disconnected parts or branches. The degeneracy $S$ of a hole with respect to a diagram is the number of holes equivalent to it because of the symmetry of the elements in the indices. In counting the degeneracy, we make no distinction between the black and white holes. Thus $S = 2, 1$ for the black holes of the diagrams of Figs. 1(a) and 1(b), respectively. Also $S = m$ for the holes of a single $m$-vertex element. It is also convenient to define the symmetry number[9] $T$ of a diagram as the number of ways one can permute a definite set of distinct numbers attached to the open holes of the diagram without changing the topology of the diagram. For example, $T = 1, 2, 2$ for the diagrams of Figs. 1(a), 1(b), 1(c), respectively. Also $T = m!$ for a single $m$-vertex element with no black hole, and $T = (m-1)!$ for the same element when one of the holes is black. It is clear that if in a diagram a black hole is replaced by an open hole, the symmetry number is changed from $T$ to $ST$ where $S$ is the degeneracy of the hole under consideration.

With this diagrammatical notation, it is readily observed from the structure of Eq. (15) that each term in the expression of $H_q$ can be represented by a singly connected diagram with one black hole. In fact one can always find terms in Eq. (16) corresponding to an arbitrary diagram. Therefore we write

$$H_q = \sum h_\alpha \left[\begin{matrix}\text{all distinct singly connected}\\ \text{diagrams with one black hole}\end{matrix}\right], \quad (19)$$

with appropriate coefficient $h_\alpha$ for each diagram. The correlation among the coefficients $h_\alpha$ to ensure the existence of $G$ is now clear: consider two diagrams

composed of the same collection of elements which differ only by the different positions taken by the black holes [e.g., Figs. 1(a) and 1(b)], the criterion is simply to require the ratio of their $h$ coefficients be [see Eqs. (16) and (16′)]

$$h_a/h_b = S_a/S_b = T_b/T_a, \tag{20}$$

with $S_a$, $T_a$; $S_b$, $T_b$ referring to, respectively, the corresponding degeneracies of the black holes and the symmetry numbers. In the last step of Eq. (20) we have used the relation

$$S_aT_a = \begin{bmatrix}\text{the symmetry number of the diagram if}\\ \text{the black hole is replaced by an open hole}\end{bmatrix} = S_bT_b. \tag{21}$$

Once Eq. (20) is established, one has immediately

$$G = g\begin{bmatrix}\text{all distinct singly connected}\\ \text{diagrams with no black holes}\end{bmatrix}, \tag{22}$$

in which the coefficient $g$ of an arbitrary diagram is given by the following procedure. First one changes (any) one of the holes in this diagram into a black one and looks for the coefficient $h_a$ of this new diagram in Eq. (19). If the degeneracy of the black hole is denoted by $S_a$, then

$$g = h_a/S_a. \tag{23}$$

Therefore our problem is to show the validity of Eq. (20) and to obtain an explicit expression for $h_a$. To this end we state the following Lemmas to be proved in the Appendix.

*Lemma A.* In the expansion of $H_a$, let $h_1$, $h_2$, $\cdots$ denote the coefficients of diagrams in which the black hole is not an articulation, and $h_a$ the coefficient of a diagram in which the black hole is an articulation having $n_1$, $n_2$, $\cdots$ identical branches with coefficients $h_1$, $h_2$, $\cdots$, respectively. Then

$$h_a = (-1)^{n-1}(n-1)!\prod_i h_i^{n_i}/n_i!, \tag{24}$$

where $n = \sum_i n_i$ is the total number of branches at the articulation.

*Lemma B.* The coefficient $h_a$ of an arbitrary diagram in Eq. (19) is given by

$$h_a = \frac{1}{T_a}\prod_{\begin{bmatrix}\text{all holes of}\\ \text{the diagram}\end{bmatrix}}(-1)^{n_i-1}(n_i-1)!, \tag{25}$$

in which $T_a$ is the symmetry number of this diagram and $n_i$ the number of elements connected by the $i$th hole ($n_i = 1$ if the hole is not an articulation).

An immediate consequence of Lemma B is Eq. (20). Therefore we have completed the proof that the expansion of $G$ exists. Finally upon combining

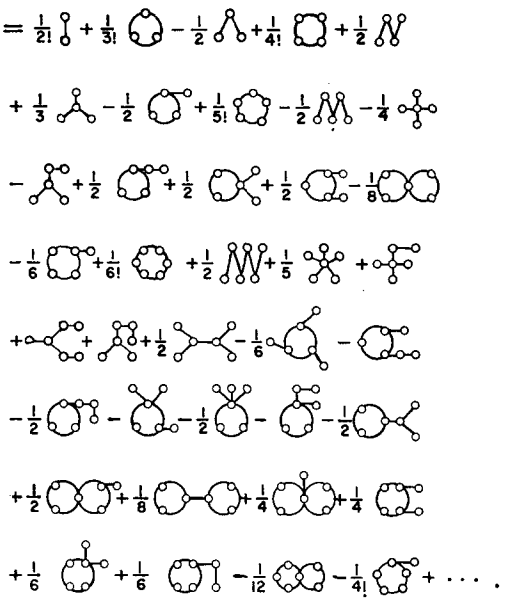

FIG. 2. Diagrammatical equation for $G$ up to terms involving six indices.

Eqs. (23), (25), and (21), the coefficient $g$ belonging to an arbitrary diagram in Eq. (22) has the explicit form

$$g = \left(\frac{1}{\text{symmetry number of the diagram}}\right) \times \prod_{\begin{bmatrix}\text{all holes of}\\ \text{the diagram}\end{bmatrix}}(-1)^{n_i-1}(n_i-1)!. \tag{26}$$

This concludes the derivation of the expansion formula for $G = \ln I$. We give in Fig. 2 the explicit expression for $G$ up to terms involving six indices. As checked easily, this result reduces to the Ursell–Mayer expansion if the cluster integrals involving the same number of indices are all identical.

## III. CONCLUSION

We have shown that the logarithm of the quantity $I$ of Eq. (10) can be expanded into a sum of terms represented by singly connected diagrams in the form of Eq. (22), with Eq. (26) furnishing an easy way to determine the expansion coefficients. We must note that terms down by a factor $1/N$ are neglected in the result. Also, the expansion is useful only when it converges fast enough so that the leading terms produce a good approximation. This seems, indeed, to be the cases in application.[5,7]

## ACKNOWLEDGMENTS

The author wishes to express his thanks to Professor Eugene Feenberg for suggesting this problem, as well as for a critical reading of the manuscript.

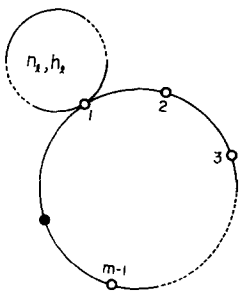


FIG. 3. Schematical diagram of an $m$-hole element with only one hole attaching branches.

He is also indebted to Dr. Tohru Morita for illuminating comments and for calling attention to the resemblance of this expansion to the fugacity expansion formula for the classical fluids under the presence of external field.[9] The expansion formulas obtained here, as pointed out by Dr. Morita, can also be derived on the basis of the technique developed in references 9 and 10. Helpful discussions with C. T. Chen–Tsai is also appreciated.

## APPENDIX

*Proof of Lemma A:* The diagram with the black hole having $n$ branches clearly comes from the term $(-W)^n/n$ of Eq. (15a). The multiplicity for occurence of such a diagram in the expansion of $W^n$ is $n!/\prod n_l!$, with coefficient $\prod h_l^{n_l}$. Upon combining these with the factor $(-)^n/n$, Eq. (24) is derived. Q.E.D.

*Proof of Lemma B:* Lemma B will be proved by induction. First, it is obvious from Eq. (15) that Lemma B holds for a single $m$-vertex element for which

$$h_\alpha = 1/(m-1)! = 1/T_\alpha. \tag{27}$$

Therefore it remains only to show that Lemma B holds for any diagram if it applies to arbitrary diagram composed of fewer elements.

First let us consider diagrams having articulation black holes. Let the branches of the diagram be specified by the set $\{n_l, h_l\}$ as stated in Lemma A; then the symmetry number of the diagram is given by

$$T_\alpha = \prod_l T_l^{n_l} n_l!, \tag{28}$$

where $T_l$ denote the symmetry numbers of the branches. Now, by assumption, Lemma B applies to diagrams composed of fewer elements so that the coefficient $h_l$ of each branch is given by

$$h_l = \frac{1}{T_l} \prod_{\left[\begin{smallmatrix}\text{all holes of}\\ \text{the branch}\end{smallmatrix}\right]} (-1)^{n_i-1}(n_i-1)!. \tag{29}$$

The substitution of Eqs. (29) and (28) into Eq. (24) now yields

$$h_\alpha = \frac{1}{T_\alpha} \prod_{\left[\begin{smallmatrix}\text{all holes of}\\ \text{the diagram}\end{smallmatrix}\right]} (-1)^{n_i-1}(n_i-1)!.$$

Q.E.D.

Next consider the diagram in which the black hole is not an articulation. In the most general case, the black hole sits on an $m$-hole element, with $p$ of the $m$ holes attaching branches. In order to illustrate the essential points of the proof, we shall consider the case of $p = 1$ only. The proof for the general case can be constructed in a completely similar fashion.[11]

Consider the diagram shown schematically in Fig. 3 in which the black hole sits on an $m$-hole element with one open hole attaching $n$ branches denoted again by the set $\{n_l, h_l, T_l\}$. The symmetry number of the diagram is now given by

$$T_\alpha = (m-2)! \prod_l T_l^{n_l} n_l!, \tag{30}$$

with the symmetry numbers $T_l$ of the individual branches related to $h_l$ through Eq. (29). The coefficient $h_\alpha$ of this diagram comes from the term $W$ of Eq. (15a). More specifically it comes from the following terms:

$$\frac{1}{(m-1)!} \sum_{12\cdots m-1} x_{q12\cdots m-1} \sum_{i=1}^{m-1} \sum_{k=1}^{n} \frac{(-H_i)^k}{k!}$$

$$= \frac{1}{(m-2)!} \sum_{12\cdots m-1} x_{q12\cdots m-1} \sum_{k=1}^{n} \frac{(-H_1)^k}{k!}. \tag{31}$$

Comparison of Eq. (31) with Fig. 3 indicates that we need to collect terms represented by the set of branches $\{n_l, h_l, T_l\}$ in the expansion of $H_1^k$. The first term $H_1$ contains only one such term. The second term $H_1^2$ contains more than one contribution. In fact, for each distinct way that the $n$ branches are divided into two groups, there corresponds a contribution with one factor of $H_1$ contributing to one group of branches, and another $H_1$ to the other group. The multiplicity for occurence of such terms in the expansion of $H_1^2$ is 1 if the two groups are identical, and 2 otherwise. In general for the term $H_1^k$ we consider all the distinct ways that the $n$ branches are divided into $k$ groups of which $\beta_1, \beta_2, \cdots, \beta_r$ are identical. Let the $h$ coefficients of these groups be denoted by $\bar{h}_1, \bar{h}_2, \cdots, \bar{h}_r$, respectively. Then for each distinct way that the

[9] T. Morita and K. Hiroike, Progr. Theoret. Phys. (Kyoto) **25**, 537 (1961).

[10] T. Morita, Progr. Theoret. Phys. (Kyoto) **21**, 501 (1959).

[11] F. Y. Wu, Dissertation, Washington University (1963).

$n$ branches are divided, there corresponds, in the expansion of $H_1^k$, a contribution to the coefficient $h_\alpha$ with multiplicity $k!/\beta_1!\beta_2! \cdots \beta_r!$. It follows then from Eq. (31)

$$h_\alpha = \frac{1}{(m-2)!} \sum_{k=1}^{n} \frac{(-1)^k}{k!} \times \sum_{(\beta_1\beta_2\cdots\beta_r)} \frac{k!}{\beta_1!\,\beta_2! \cdots \beta_r!} \bar{h}_1^{\beta_1} \cdots \bar{h}_r^{\beta_r}, \quad (32)$$

in which $(\beta_1\beta_2 \cdots \beta_r)$ denotes the summation taken under the restriction $\beta_1 + \beta_2 + \cdots + \beta_r = k$. Now the coefficients $\bar{h}_1, \bar{h}_2, \cdots \bar{h}_r$ can be obtained by Lemma A. However it proves useful at this point to note that the factor $(n-1)!/\prod n_l!$ appearing in Eq. (24) is just the number of distinct ways to perform cyclic permutations on the group of $n$ branches (among which $n_1, n_2, \cdots$ are identical). Using this interpretation of Lemma A for the expressions of $\bar{h}_1, \bar{h}_2, \cdots, \bar{h}_r$, we get

$$\bar{h}_1^{\beta_1}\bar{h}_2^{\beta_2} \cdots \bar{h}_r^{\beta_r} = (-1)^{n-k} \left[\begin{array}{l}\text{product of the number of}\\ \text{distinct cyclic paramutations}\\ \text{of the branches in each group}\end{array}\right] \prod_l h_l^{n_l}. \quad (33)$$

Substituting Eq. (33) into Eq. (32), we have

$$h_\alpha = \frac{1}{(m-2)!}(-1)^n M \prod_l h_l^{n_l}, \quad (34)$$

where

$$M = \sum_{k=1}^{n} \sum_{(\beta_1\beta_2\cdots\beta_r)} \frac{1}{\beta_1!\,\beta_2! \cdots \beta_r!} \left[\begin{array}{l}\text{product of the number of distinct cyclic}\\ \text{permutations of the branches in each}\\ \text{group}\end{array}\right]$$

$$= \sum_{k=1}^{n} \sum_{(\beta_1\beta_2\cdots\beta_r)} \left[\begin{array}{l}\text{the number of distinct ways one can}\\ \text{permute the } n \text{ branches under the}\\ \text{particular grouping by performing}\\ \text{cyclic permutations within each}\\ \text{group while the groups are un-}\\ \text{numbered}\end{array}\right]$$

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It is well-known that each permutation of a collection of objects can be analyzed into groups of cyclic permutations in an unique way. Therefore also

$$M = \left[\begin{array}{l}\text{the number of distinct permutations of}\\ \text{the } n \text{ branches}\end{array}\right] = n!/\prod n_l!. \quad (35)$$

The substitution of Eqs. (29) and (35) into Eq. (34) and the introduction of Eq. (30) now yields Eq. (25). Q.E.D.

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# Strict Localization

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(Received 24 June 1963)

A complete characterization for a general quantum field theory is given of the strictly localized states introduced by J. Knight. It is shown that each such state can be generated from the vacuum by a partially isometric operator. Necessary and sufficient conditions are given for the superposition of such states to be also strictly localized. Finally, it is shown that there is a connection between the von Neumann type of the ring generated by the field operator in a finite region and the possibility of constructing strictly localized states.

## I. INTRODUCTION

THE notion of strictly localized states has recently been introduced by Knight.[1] Let $\varphi(x)$ be a complete, local, scalar Hermitian field. Let $\Omega$ denote the vacuum state. Then a state $\Psi$ is said to be strictly localized in a region $G$ of Minkowski space if for any $n$,

$$\langle \Psi, \varphi(x_1) \cdots \varphi(x_n)\Psi \rangle = \langle \Omega, \varphi(x_1) \cdots \varphi(x_n)\Omega \rangle,$$

when all the $x_1 \cdots x_n$ are outside $G$.

Knight has shown, for the case of the free field, that such states cannot contain a finite number of particles. He has also shown that states of the form

$$e^{iA}\Omega,$$

where $A$ is a smoothed polynomial in the field in a

[1] J. M. Knight, J. Math. Phys. 2, 459 (1961).

$n$ branches are divided, there corresponds, in the expansion of $H_1^k$, a contribution to the coefficient $h_\alpha$ with multiplicity $k!/\beta_1!\beta_2! \cdots \beta_r!$. It follows then from Eq. (31)

$$h_\alpha = \frac{1}{(m-2)!} \sum_{k=1}^{n} \frac{(-1)^k}{k!} \times \sum_{(\beta_1\beta_2\cdots\beta_r)} \frac{k!}{\beta_1!\,\beta_2! \cdots \beta_r!} \bar{h}_1^{\beta_1} \cdots \bar{h}_r^{\beta_r}, \quad (32)$$

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[1] J. M. Knight, J. Math. Phys. 2, 459 (1961).

region $G$, are strictly localized in the union of the forward and backward light cones subtended by $G$.

In the following we will investigate strict localization in a general quantum field theory using the language of operator rings.[2,3] In Sec. II it will be shown that each strictly localized state can be generated from the vacuum by a certain partially isometric operator. In Sec. III, necessary and sufficient conditions are given for the superposition of such states to be also strictly localized. In Sec. IV, we show that there is a connection between the von Neumann type of the operator rings and the possibility of constructing strictly localized states.

## II. STRICTLY LOCALIZED STATES

For any open region $G$ in Minkowski space, we will denote by $R(G)$ the weakly closed symmetric ring of bounded operators generated by the projectors associated with the field $\varphi(x)$ in $G$.[4] The symbol $G'$ will denote the spacelike complement of $G$. The commutant of the ring $R(G)$ will be denoted by $R'(G)$. The Hilbert space of physical states will be denoted by $H$.

In this notation, we have found it convenient to define strictly localized states as follows:

*Definition 1.* The state $\Psi$ is said to be strictly localized *outside* the open region $G$, if for any $A \in R(G)$,

$$\langle \Psi, A\Psi \rangle = \langle \Omega, A\Omega \rangle. \tag{1}$$

A class of strictly localized states is given in the following theorem.

*Theorem I.* If $W$ is any partially isometric operator in $R'(G)$ such that

$$W^\dagger W = 1, \tag{2}$$

then the state

$$\Psi = W\Omega \tag{3}$$

is strictly localized outside $G$.

*Proof:* Let $A \in R(G)$; consider

$$\langle \Psi, A\Psi \rangle = \langle \Omega, W^\dagger A W \Omega \rangle,$$

since $W \in R'(G)$,

$$\langle \Psi, A\Psi \rangle = \langle \Omega, A W^\dagger W \Omega \rangle,$$

by (2),

$$\langle \Psi, A\Psi \rangle = \langle \Omega, A\Omega \rangle.$$

If $W W^\dagger = 1$, then $W$ is unitary, and we have the class of states considered by Knight. However, in general, $W W^\dagger = P \neq 1$, where $P$ is some projector in $R'(G)$, as by (2),

$$P^2 = W W^\dagger W W^\dagger = P.$$

The operators $W$ of Theorem I have a rather interesting property. If $\Phi_1$, $\Phi_2$ are any two states in $H$, and if $A$ is any operator in $R(G)$, then

$$\langle W\Phi_1, AW\Phi_2 \rangle = \langle \Phi_1, A\Phi_2 \rangle. \tag{4}$$

The proof is the same as in Theorem I. This leads us to make the following definition.

*Definition 2.* A bounded operator $W$ is said to be strictly localized outside the region $G$, if Eq. (4) holds for all $\Phi_1, \Phi_2 \in H$, and all $A \in R(G)$.

*Theorem II.* The bounded operator $W$ is strictly localized outside the region $G$, if and only if

$$W^\dagger W = 1,$$

and

$$W \in R'(G).$$

*Proof:* The sufficiency is immediate. We will prove the necessity. Equation (4), since it holds for any $\Phi_1, \Phi_2, \in H$, implies that

$$W^\dagger A W = A, \tag{5}$$

for all $A \in R(G)$. In particular, for $A = 1$,

$$W^\dagger W = 1. \tag{6}$$

However, for any $A \in R(G)$,

$$W^\dagger A W = W^\dagger [A, W] + W^\dagger W A = W^\dagger [A, W] + A,$$

by (6). Thus

$$W^\dagger [A, W] = 0. \tag{7}$$

Similarly, we find that

$$[W^\dagger, A] W = 0. \tag{8}$$

Now, since $A \in R(G)$, then $A^\dagger$ and $A^\dagger A \in R(G)$, and by (5),

$$W^\dagger A^\dagger A W = A^\dagger A = [W^\dagger, A^\dagger][A, W] + [W^\dagger, A^\dagger] W A + A^\dagger W^\dagger [W, A] + A^\dagger W^\dagger W A.$$

Using Eqs. (6), (7), and (8), we get

$$([A, W])^\dagger [A, W] = 0.$$

Let $\Phi \in H$. This implies that

$$|[A, W]\Phi|^2 = 0, \quad \text{and} \quad [A, W]\Phi = 0,$$

which implies, since $\Phi$ is arbitrary,

$$[A, W] = 0.$$

Thus, $W \in R'(G)$.

Theorems I and II together imply that if $W$ is an

[2] R. Haag and B. Schroer, J. Math. Phys. 3, 248 (1962).
[3] M. A. Naimark, *Normed Rings*, translated from the 1st Russian edition by L. F. Boron (P. Noordhoff, Ltd., Groningen, The Netherlands, 1959).
[4] H. Reeh and S. Schlieder (to be published).

operator strictly localized outside a region $G$, then the state $W\Omega$ is strictly localized outside $G$. The next theorem will show that all strictly localized states are of this form.

*Theorem III.* To every state $\Psi$, strictly localized outside an open region $G$, there corresponds an operator $W$, strictly localized outside $G$, such that

$$W\Omega = \Psi.$$

*Proof:* To prove this theorem we will need the following Lemma.

*Lemma.* If $G$ is an open region in Minkowski space, then

$$\text{closure } (R(G)\Omega) = H.$$

*Proof:* Let $\mathfrak{A}(G)$ denote the operator algebra generated by finite polynomials in the field $\varphi(x)$, smoothed by testing functions with support in $G$. Reeh and Schlieder[5] have shown that

$$\text{closure } (\mathfrak{A}(G)\Omega) = H. \tag{9}$$

They have also shown[4] that

$$\mathfrak{A}''(G) = R(G),$$

and that this with (9) implies the above Lemma.

Now let $\Phi$ be any element of $H$. By the Lemma, there exists a sequence $\{A_n, A_n \in R(G), n=1, 2\cdots\}$, such that

$$A_n\Omega \to \Phi, \tag{10}$$

i.e.,

$$|A_n\Omega - \Phi| \to 0.$$

Consider the expression

$$\Psi(\Phi) = \lim_{n\to\infty} A_n\Psi. \tag{11}$$

This limit exists, for

$$|A_n\Psi - A_m\Psi| = |(A_n - A_m)\Psi|,$$

Since $\Psi$ is localized outside $G$,

$$\Psi(\Phi) = |(A_n - A_m)\Omega| \to 0,$$

by Eq. (9). The space $H$ is complete. Thus $\Psi(\Phi)$ exists and is unique. The limit (11) is also independent of the particular sequence $\{A_n\}$. For if $\{A_n'\}$ is another such sequence,

$$|A_n\Psi - A_n'\Psi| = |(A_n - A_n')\Psi| = |(A_n - A_n')\Omega| \le |(A_n\Omega - \Phi)| + |(A_n'\Omega - \Phi)| \to 0.$$

[5] H. Reeh and S. Schlieder, Nuovo Cimento **22**, 1051 (1961).

Thus $\Psi(\Phi)$ depends only on the states $\Psi$ and $\Phi$. We claim that it is linear in $\Phi$. For if $\{A_n^1\}$ and $\{A_n^2\}$ are two sequences in $R(G)$ such that

$$A_n^i\Omega \to \Phi^i, \qquad i = 1, 2,$$

then clearly, for any complex numbers $\alpha, \beta$,

$$(\alpha A_n^1 + \beta A_n^2)\Omega \to \alpha\Phi^1 + \beta\Phi^2,$$

and

$$\Psi(\alpha\Phi^1 + \beta\Phi^2) = \lim_{n\to\infty} ((\alpha A_n^1 + \beta A_n^2)\Psi) = \alpha \lim_{n\to\infty} A_n^1\Psi + \beta \lim_{n\to\infty} A_n^2\Psi = \alpha\Psi(\Phi^1) + \beta\Psi(\Phi^2).$$

The correspondence

$$\Phi \to \Psi(\Phi)$$

thus defines a unique linear operator $W$, depending only on $\Psi$, such that

$$\Psi(\Phi) = W\Phi.$$

This operator is bounded, for

$$|W\Phi| = \lim_{n\to\infty} |A_n\Psi| = \lim_{n\to\infty} |A_n\Omega| = |\Phi|.$$

We claim that

$$W\Omega = \Psi.$$

For, the sequence $\{A_n = 1\}$ is such that

$$A_n\Omega \to \Omega,$$

but now

$$W\Omega = \lim_{n\to\infty} A_n\Psi = \Psi.$$

The operator $W$ is strictly localized outside $G$. For let $\Phi_1, \Phi_2 \in H$, $A \in R(G)$. Then there exist sequences $\{A_n^i\} \subset R(G)$, $i = 1, 2$, such that

$$A_n^i\Omega \to \Phi^i, \qquad i = 1, 2.$$

Consider

$$\langle W\Phi^1, AW\Phi^2\rangle = \lim_{n,m\to\infty} \langle A_n^1\Psi, AA_m^2\Psi\rangle = \lim_{n,m\to\infty} \langle \Psi, A_n^{1\dagger}AA_m^2\Psi\rangle,$$

since $\Psi$ is strictly localized outside $G$,

$$\langle W\Phi^1, AW\Phi^2\rangle = \lim_{n,m\to\infty} \langle \Omega, A_n^{1\dagger}AA_m^2\Omega\rangle = \langle \Phi^1, A\Phi^2\rangle.$$

*Corollary 1.* Let $\Psi$ be strictly localized outside $G$.

The operator $W$ constructed above is unique in the sense that it is the only operator in $R'(G)$ such that $W\Omega = \Psi$. It is not, however, the only operator which can create $\Psi$ from the vacuum.

*Proof:* Suppose $V \in R'(G)$ and $V\Omega = \Psi$. Then for any $A \in R(G)$,

$$A(W - V)\Omega = 0 = (W - V)A\Omega.$$

Since states of the form $A\Omega$ are dense in $H$, this implies that

$$W = V.$$

Now the operator $WP_\Omega$, where $P_\Omega$ is the projector onto the vacuum, certainly generates $\Psi$ from the vacuum. We cannot, however, have

$$WP_\Omega = W,$$

for then, premultiplying both sides of this equation by $W^\dagger$, we would obtain

$$P_\Omega = 1,$$

a contradiction.

Given a state $\Psi$ strictly localized outside $G$, the problem now arises as to whether there exists some region $F$ such that the associated operator $W$ is in $R(F)$. The solution rests on the validity of the duality theorem, which has been partially proved by Haag and Schroer.[2] This theorem states that for any open region $G$,

$$R'(G) = R(G'),$$

from which it immediately follows that $F = G'$.

### III. SUPERPOSITION OF STRICTLY LOCALIZED STATES

With the aid of the associated localized operators, it is now possible to give the conditions under which it is possible to superimpose localized states.

*Theorem IV.* Let $\Psi_1$, $\Psi_2$ be two states strictly localized outside an open region $G$. Let $W_1$, $W_2$ be the corresponding strictly localized operators. Then the states

$$\Psi(\alpha, \beta) = N[\alpha\Psi_1 + \beta\Psi_2], \tag{12}$$

where $\alpha$ and $\beta$ are any complex numbers and

$$N = |\alpha\Psi_1 + \beta\Psi_2|^{-1},$$

will be strictly localized outside $G$ if and only if

$$W_2^\dagger W_1 = (\Omega, W_2^\dagger W_1 \Omega) = r, \quad \text{say.} \tag{13}$$

*Proof:* We will prove the sufficiency first. Suppose (13) holds. Then the operator

$$W = N(\alpha W_1 + \beta W_2)$$

is in $R'(G)$, and is such that

$$\begin{aligned} W^\dagger W = (|\alpha|^2 + |\beta|^2 + \alpha\beta^* r + \alpha^*\beta r^*)^{-1} \\ \times [|\alpha|^2 W_1^\dagger W_1 + |\beta|^2 W_2^\dagger W_2 \\ + \alpha\beta^* W_2^\dagger W_1 + \alpha^*\beta W_1^\dagger W_2] \\ = 1. \end{aligned}$$

By Theorem I, the state

$$\Psi(\alpha, \beta) = W\Omega$$

is strictly localized outside $G$.

We will prove now the necessity. Suppose that $\Psi(\alpha, \beta)$ is strictly localized outside $G$. Then for any $A \in R(G)$,

$$\langle \Psi(\alpha, \beta), A\Psi(\alpha, \beta)\rangle = \langle \Omega, A\Omega\rangle.$$

Using the expression (12), and the strict locality of the states $\Psi_1$ and $\Psi_2$, we find that

$$\begin{aligned} \alpha^*\beta\langle \Omega, W_1^\dagger A W_2 \Omega\rangle + \alpha\beta^*\langle \Omega, W_2^\dagger A W_1 \Omega\rangle \\ = (\alpha^*\beta r^* + \beta^*\alpha r)\langle \Omega, A\Omega\rangle. \end{aligned}$$

Since this must hold for all $\alpha$, $\beta$, we conclude that

$$\langle \Omega, W_2^\dagger A W_1 \Omega\rangle = r\langle \Omega, A\Omega\rangle.$$

Now suppose $A = A_1^\dagger A_2$, for arbitrary $A_i \in R(G)$, $i = 1, 2$. Since $W_i \in R'(G)$,

$$\langle A_1\Omega, W_2^\dagger W_1 A_2 \Omega\rangle = r\langle A_1\Omega, A_2\Omega\rangle.$$

But by the Reeh–Schlieder Lemma, states of the form $A\Omega$, $A \in R(G)$ are dense in $H$. This implies, by continuity,

$$\langle \Phi_1, W_1^\dagger W_1 \Phi_2\rangle = r\langle \Phi_1, \Phi_2\rangle$$

for all $\Phi_1, \Phi_2 \in H$. Thus,

$$W_2^\dagger W_1 = r.$$

*Corollary.* If the states $\Psi(\alpha, \beta)$ are strictly localized outside $G$, then we may express one of the operators $W_i$, $W_2$ say, in the form

$$W_2 = r^* W_1 + (1 - |r|^2)^{\frac{1}{2}} U. \tag{14}$$

where the operator $U$ is strictly localized outside $G$, and takes $H$ into a subspace orthogonal to the subspace $W_1 H$.

*Proof:* The number $r$ is in magnitude less than 1, as

$$|r| = |\langle \Omega, W_2^\dagger W_1 \Omega\rangle| \leq |\Omega|^2 \, |W_2^\dagger| \, |W_1| = 1.$$

Thus the root in (14) is real. The operator $U$ is clearly in $R'(G)$. By Eq. (13),

$$U^\dagger W_1 = 0. \tag{15}$$

Since $W_2^\dagger W_2 = 1$, we get

$$U^\dagger U = 1, \text{ i.e., } U \text{ is partially isometric.}$$

Thus $U$ is strictly localized outside $G$. Consider the projectors

$$P_1 = W_1 W_1^\dagger, \qquad P = UU^\dagger.$$

From (15) it follows that

$$PP_1 = 0.$$

Thus $W_1$ and $U$ take $H$ into mutually orthogonal subspaces.

## IV. VON NEUMANN TYPES

There has been some interest expressed recently[2] in determining the von Neumann factor types of the rings $R(G)$. The following theorem has a physical interpretation which makes factor type III seem most reasonable.

*Theorem V.* Suppose that

(a) The Hilbert space $H$ is separable.

(b) For any open region $G$, the ring $R(G)$ is a factor, i.e., $R(G) \cap R'(G) = (\alpha 1)$.

Then to each projector $P \in R(G)$ there corresponds a partially isometric operator $W \in R(G)$, such that $W^\dagger W = 1$, $P = WW^\dagger$, if and only if the factor $R(G)$ is of von Neumann type III.

*Proof:* Assumption (a) has generally been assumed to be true.[2] A partial proof of assumption (b) based on primitive causality has been given by Haag and Schroer.[2]

Let us suppose that the factor $R(G)$ is of type III. Then the relative dimension function $D$, defined on projectors in $R(G)$, takes on only the values $0, \infty$.[6] It is 0 only for the null projector. This implies that all nonnull projectors in $R(G)$ project onto infinite subspaces. The separability of $H$ then implies that all such projectors are equivalent,[7] in particular, equivalent to 1, i.e., that $P \in R(G)$, $P = 0$ implies the existence of a $W \in R(G)$ such that

$$P = WW^\dagger, \qquad W^\dagger W = 1.$$

Thus we have proven the sufficiency of the above condition.

Consider now the necessity. If to every nonnull projector $P \in R(G)$ there corresponds an operator $W \in R(G)$ such that

$$W^\dagger W = 1, \qquad WW^\dagger = P,$$

then each such projector is equivalent to the unit operator. This implies that for $P \neq 0$,[8]

$$D(P) = D(1).$$

There are only two von Neumann types compatible with this condition—type $I_1$, or type III. The type $I_1$ must however be ruled out, as it would imply that $R(G)$ consisted of only multiples of the identity.[9]

This theorem may be interpreted as follows: To each proposition $q$ concerning a measurement made by an apparatus located in the region $G$, there is associated a projector $P \in R(G)$,[10] such that for any state $\Phi \in H$, $P\Phi = \Phi$ if $q$ is true in $\Phi$, but $P\Phi = 0$ if it is false. A partially isometric operator $W \in R(G)$ such that $W^\dagger W = 1$, $WW^\dagger = P$, we interpret as representing an apparatus in $G$, which alters any state such that the proposition corresponding to $P$ is true, i.e.,

$$PW\Phi = WW^\dagger W\Phi = W\Phi.$$

Moreover, by Theorem II, the state $W\Phi$ will not differ from $\Phi$ as far as measurements made in $G'$ are concerned.

With this interpretation, Theorem V is equivalent to the statement that the ring $R(G)$ will be of von Neumann type III if and only if for every proposition $q$ in $G$, there is an apparatus in $G$ which can alter any state such that $q$ is true, without affecting any measurement made in the region $G'$.

*Note added in proof.* The author is indebted to Professor H. Araki for the following comments.

(1) The notion of strict localization is a special case of the notion of "equivalence". Two states are said to be "equivalent in a region $G$", if their expectation values are the same for all operators in $R(G)$. A state equivalent to the vacuum in $G$ is then strictly localized outside $G$.

(2) Theorem III can be proven more directly by defining an operator $V$ by

$$VA\Omega = A\Psi$$

for all $A \in R(G)$. The closure of this operator can be shown to exist, and to have the required properties.

(3) Theorem V can also be interpreted as saying that $R(G)$ is of type III if and only if for any projector $P \in R(G)$, and any state $\Psi \in H$, there is an eigenstate of $P$ that is equivalent to $\Psi$ in $G'$.

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[6] Reference 3, p. 469, Theorem 2.
[7] Reference 3, p. 457, Proposition VI.
[8] Reference 3, p. 465, Eq. (3**).
[9] Reference 3, p. 483, Theorem 2.
[10] J. von Neumann, *Mathematische Grundlagen der Quantenmechanik* (Springer-Verlag, Berlin, 1932) [English edition: Princeton University Press, Princeton, New Jersey, 1955].