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# Studies in the $C^*$-Algebraic Theory of Nonequilibrium Statistical Mechanics: Dynamics of Open and of Mechanically Driven Systems

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We construct a $C^*$-algebraic formulation of the dynamics of a pair of mutually interacting quantum-mechanical systems $\tilde{S}$ and $\hat{S}$, the former being finite and the latter infinite. Our basic assumptions are that: (i) $\hat{S}$, when isolated, satisfies the Dubin–Sewell dynamical axioms; (ii) the coupling between $\tilde{S}$ and $\hat{S}$ is energetically bounded and spatially localized; and (iii) the initial states of $\tilde{S}$ and $\hat{S}$ are mutually uncorrelated, with $\tilde{S}$ in an arbitrary normal state and $\hat{S}$ in a Gibbs state. Our formulation leads to a rigorous theory of (a) the dynamics of a finite open system, i.e., of a finite system ($\tilde{S}$) coupled to an "infinite reservoir" ($\hat{S}$), and of (b) the dynamics of an infinite system ($\hat{S}$), driven from equilibrium by a "signal generator" ($\tilde{S}$). As regards (a), we show that the state of $\tilde{S}$ always remains normal, and we derive a generalized master equation (in an appropriate Banach space) governing its temporal evolution. As regards (b), we show that the state of $\hat{S}$ always corresponds to a (time-dependent) density matrix in the representation space of the algebra of observables for $\hat{S}$, induced by the initial Gibbs state. By formulating the linear part (appropriately defined) of the response of $\hat{S}$ to $\tilde{S}$, we generalize the fluctuation–dissipation theorem to infinite systems. Further, we show that the total effect of $\tilde{S}$ on $\hat{S}$ reduces to that of a "classical" time-dependent external force in cases where the initial state of $\tilde{S}$ possesses certain coherence properties similar to those of the Glauber type.

## 1. INTRODUCTION

The algebraic formulation of statistical mechanics provides a rigorous mathematical basis for the study of both finite and infinite systems (cf. Haag, Hugenholtz, and Winnink[1] (HHW), and Ruelle[2]). In this formulation, the bounded observables of a physical system correspond to self-adjoint elements of an appropriate $C^*$-algebra $\mathfrak{A}$, and the states of the system correspond to positive normalized linear functionals on $\mathfrak{A}$. By the Gel'fand–Naimark–Segal (GNS) construction, each state $\phi$ determines a cyclical $^*$-representation $\pi_\phi$ of $\mathfrak{A}$ in a Hilbert space $\mathcal{H}_\phi$. Thus, $\phi$ is canonically associated with an "island" of states $\mathcal{I}_\phi = \{\Phi \circ \pi_\phi | \Phi \text{ is a normal state on } \pi_\phi(\mathfrak{A})\}$. Of particular importance in statistical mechanics are the Gibbs states (cf. Ref. 1) and their associated islands.

The dynamics of an infinite quantum-mechanical system may be formulated in terms of the dynamical laws for finite systems, subject to supplementary assumptions concerning the existence of certain "infinite volume limits." Thus, HHW have proposed a set of "axioms" which lead to a description of time translations in an infinite system as automorphisms of its $C^*$-algebra $\mathfrak{A}$ of observables. More recently, Dubin and Sewell[3] (DS) have proposed a weaker set of "axioms", leading to the result that if $\phi$ is a Gibbs state, then temporal evolution in the island $\mathcal{I}_\phi$ corresponds to automorphisms of the weak closure of $\pi_\phi(\mathfrak{A})$, though not necessarily of $\mathfrak{A}$ itself. The advantages, from a physical standpoint, of the latter axioms were discussed in Ref. 3.

The present article will be concerned, for motives that will be described below, with the study of the dynamics of a composite quantum-mechanical system S, formed by two mutually interacting systems $\tilde{S}$ and $\hat{S}$, the former being finite and the latter infinite. It is assumed that:

(i) $\hat{S}$ satisfies the DS axioms, when uncoupled from $\tilde{S}$;

(ii) the interaction between $\tilde{S}$ and $\hat{S}$ is energetically bounded and spatially localized, in a sense made precise in Sec. 3 (the class of interactions considered is wide enough to cover the cases where $\tilde{S}$ and $\hat{S}$ interact via forces between hard-core particles confined to finite regions of space); and

(iii) the initial states of $\tilde{S}$ and $\hat{S}$ are mutually uncorrelated, with $\tilde{S}$ in an arbitrary normal state and $\hat{S}$ in a Gibbs state.

We have two principal motives for studying the dynamics of the composite system S. First, it leads to a theory of the dynamics of a finite open system, i.e., of a finite system ($\tilde{S}$) coupled to an "infinite reservoir" ($\hat{S}$). Secondly, it enables us to formulate the dynamics of an infinite system ($\hat{S}$), driven from equilibrium by the action of a "signal generator" ($\tilde{S}$).

The material of this article will be presented as follows. In Sec. 2, we shall introduce our mathematical notation and shall derive three pertinent lemmas concerning tensor products of $W^*$-algebras. In Sec. 3, we shall formulate our mathematical descriptions of the systems $\tilde{S}, \hat{S}$, and S: This will include a statement of the DS axioms, as applied to $\hat{S}$.

In Sec. 4, we shall formulate the time-dependence of the state of S, subject to the above assumptions (i)–(iii). It will be shown (Corollary to Theorem 4.1) that the state of $\tilde{S}$ (induced by that of S) always remains normal, and that the state of $\hat{S}$ always remains in the island of the initial Gibbs state.

In Sec. 5, we shall adapt Zwanzig's[4] projective technique so as to derive a generalized master equation (GME) governing the evolution of the state of $\tilde{S}$. This GME is actually similar to that obtained by Emch and Sewell,[5] by traditional methods that required a number of additional mathematical assumptions.

In Sec. 6, we shall formulate the response of $\hat{S}$ to the "driving force" generated by $\tilde{S}$, in the case where the interaction between $\tilde{S}$, and $\hat{S}$ corresponds to a (tensor) product of observables for the two systems. By extracting the linear part (appropriately defined) of this response, we generalize the fluctuation–dissipation theorem to infinite systems. Further, we show that the *total* effect of $\tilde{S}$ on $\hat{S}$ reduces to that of a "classical" time-dependent external force in cases where the initial state of $\tilde{S}$ possesses certain coherence properties similar to those of the Glauber type.[6]

In Section 7, we shall summarize our conclusions.

In the Appendix, we shall explicitly formulate a class of states of $\tilde{S}$ possessing the above-mentioned coherence properties.

## 2. MATHEMATICAL PRELIMINARIES

In this section, we shall present our mathematical notation, and then derive three lemmas concerning tensor products of $W^*$-algebras.

### A. Notation

We employ the standard symbols $\mathbf{C}, \mathbf{R}, \mathbf{R}_+, \mathbf{Z}, \mathbf{Z}_+$ to denote the complex plane, the real line, the positive reals, the integers, and the positive integers, respectively. If $f$ is an $\mathcal{S}$ (or $\mathcal{S}'$)-class function on $\mathbf{R}$, in the sense of Schwartz, we denote its Fourier transform by $\bar{f}$:

$$\bar{f}(\omega) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dt\, e^{-i\omega t} f(t). \tag{2.1}$$

Let $\mathfrak{B}$ be a Banach space or algebra. We denote the set of all bounded linear transformations of $\mathfrak{B}$ by $\mathcal{L}(\mathfrak{B})$.

Let $\mathfrak{A}$ be a $C^*$-algebra[7] in a Hilbert space $\mathcal{H}$. We denote the set of all (resp. normal, i.e., ultraweakly continuous) functionals on $\mathfrak{A}$ by $\mathfrak{A}^*$ (resp. $\mathfrak{A}_*$). The set of all positive elements of $\mathfrak{A}^*$ (resp. $\mathfrak{A}_*$) is denoted by $\mathfrak{A}_+^*$ (resp. $\mathfrak{A}_*^+$). For arbitrary $A \in \mathfrak{A}$ and $\psi \in \mathfrak{A}^*$, we shall sometimes denote $\psi(A)$ by $\langle \psi; A \rangle$.

*Note*[8]: $\mathfrak{A}_*$ is a closed subspace of the Banach space $\mathfrak{A}^*$.

*Definition 2.1:* For $x \in \mathcal{H}$, we define the vector functional $\omega_x$ on $\mathfrak{A}$ by the formula $\omega_x(A) = (x, Ax)$, $\forall\ t \in \mathfrak{A}$.

*Definition 2.2:* Let $\sigma$ be a map from a set $K$ into $\mathcal{L}(\mathfrak{A})$. We define the dual map $\sigma^*: K \to \mathcal{L}(\mathfrak{A}^*)$ by

$$\langle \sigma^*(k)\psi; A \rangle = \langle \psi; \sigma(k)A \rangle, \quad \forall A \in \mathfrak{A},\ \psi \in \mathfrak{A}^*,\ k \in K.$$

We recall now that the Kubo–Martin–Schwinger (KMS) conditions may be defined as follows (cf. Ref. 1).

*Definition 2.3:* Let $\psi \in \mathfrak{A}_+^*, \beta \in \mathbf{R}$, and let $\tau$ be a homomorphism of $\mathbf{R}$ into Aut$\mathfrak{A}$. For arbitrary $A, B \in \mathfrak{A}$, let $F_{AB}^{(1)}, F_{AB}^{(2)}$ be the functions of $\mathbf{R}$ defined by

$$F_{AB}^{(1)}(t) = \psi(B\tau(t)A) \text{ and } F_{AB}^{(2)}(t) = \psi((\tau(t)A)B), \ \forall t \in \mathbf{R}.$$

Then we say that $\psi$ satisfies the KMS conditions with respect to $(\tau, \beta)$ if, for any $A, B \in \mathfrak{A}$, (i) $F_{AB}^{(1)}, F_{AB}^{(2)}$ are continuous functions on $\mathbf{R}$, and (ii) the Fourier transforms of these functions, considered as elements of $\mathcal{S}'$, satisfy the relation

$$\bar{F}_{AB}^{(1)}(\omega) = \bar{F}_{AB}^{(2)}(\omega) e^{\beta\omega}, \quad \forall\ \omega \in \mathbf{R}.$$

*Note:* It follows[9] from this definition that if $\psi$ satisfies the KMS conditions with respect to $(\tau, \beta)$, then $\psi$ is invariant under $\tau_\beta^*(\mathbf{R})$.

*Definition 2.4:* Let $\Sigma$ be a physical system, characterized by a $C^*$-algebra $\mathfrak{A}$ (of bounded observables), together with the states and automorphisms of $\mathfrak{A}$. We term $\Sigma$ to be finite if it satisfies the following three conditions:

(i) $\mathfrak{A}$ is a type-I factor;

(ii) $\mathfrak{A}$ is equipped with a one-parameter group $\{\sigma(t) \mid t \in \mathbf{R}\}$ of inner automorphisms of $\mathfrak{A}$, corresponding to time translations; and

(iii) for arbitrary $\beta \in \mathbf{R}_+$, there exists a unique normal state on $\mathfrak{A}$, which satisfies the KMS conditions with respect to $(\sigma, \beta)$.

*Note:* This definition may be seen to accord with the usual requirements[10] of finiteness.

*Note:* We shall use the term "infinite system" in the special sense of Ref. 1. Thus, we use the term to signify more than a "system which is not finite, in the sense of Def. 2.4."

*Definition 2.5:* Let $\mathfrak{A}_1, \mathfrak{A}_2$ be $W^*$-algebras[11] in Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$, respectively. We denote by $\mathfrak{A}_1 \otimes \mathfrak{A}_2$ (resp. $\mathfrak{A}_1 \bar{\otimes} \mathfrak{A}_2$) the smallest $W^*$ (resp. $C^*$)-algebra generated by $\{A_1 \otimes A_2 \mid A_1 \in \mathfrak{A}_1, A_2 \in \mathfrak{A}_2\}$ in the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$.

*Definition 2.6:* Let $\psi_1, \psi_2$ be normal linear functionals on the $W^*$-algebras $\mathfrak{A}_1, \mathfrak{A}_2$, respectively. Then

there is a unique[12] element $\psi$ of $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)_*$ for which $\psi(A_1 \otimes A_2) = \psi_1(A_1)\psi_2(A_2)$, $\forall A_1 \in \mathfrak{A}_1$, $A_2 \in \mathfrak{A}_2$ We denote this functional $\psi$ by $\psi_1 \otimes \psi_2$.

*Definition 2.7:* Let $\sigma_1, \sigma_2$ be normal (i.e., ultraweakly continuous) homomorphisms of the $W^*$-algebras $\mathfrak{A}_1, \mathfrak{A}_2$ onto $W^*$-algebras $\mathfrak{B}_1, \mathfrak{B}_2$, respectively. Then there exists a unique[13] normal homomorphism $\sigma$ of $\mathfrak{A}_1 \otimes \mathfrak{A}_2$ onto $\mathfrak{B}_1 \otimes \mathfrak{B}_2$, such that $\sigma(A_1 \otimes A_2) = \sigma_1(A_1) \otimes \sigma_2(A_2), \forall A_1 \in \mathfrak{A}_1$, $A_2 \in \mathfrak{A}_2$. We denote this element $\sigma$ by $\sigma_1 \otimes \sigma_2$.

*Definition 2.8:* Let $\mathfrak{A}_1, \mathfrak{A}_2$ be $W^*$-algebras. We denote by $\mathfrak{A}_{1*} \otimes \mathfrak{A}_{2*}$ the closure, in the norm topology of $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)^*$, of the linear manifold

$$\{\sum_1^N \psi_1^{(n)} \otimes \psi_2^{(n)} \mid \psi_1^{(n)} \in \mathfrak{A}_{1*},\ \psi_2 \in \mathfrak{A}_{2*}, N < \infty\}.$$

## B. Lemmas Concerning Tensor Products

*Lemma 2.1:* Let $\mathfrak{A}_1, \mathfrak{A}_2$ be $W^*$-algebras in Hilbert spaces $\mathfrak{K}_1, \mathfrak{K}_2$, respectively. Then $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)_* = \mathfrak{A}_{1*} \otimes \mathfrak{A}_{2*}$.

*Proof:* Since $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)_*$ is a closed subspace of $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)^*$ (cf. Note preceding Def. 2.1), it follows from Def. 2.8 that $\mathfrak{A}_{1*} \otimes \mathfrak{A}_{2*} \subset (\mathfrak{A}_1 \otimes \mathfrak{A}_2)_*$.

On the other hand, $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)_*$ is the strong closure,[14] in $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)^*$, of the linear manifold generated by the vector functionals on $\mathfrak{A}_1 \otimes \mathfrak{A}_2$. Hence, in order to show that $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)_* \subset \mathfrak{A}_{1*} \otimes \mathfrak{A}_{2*}$, and thus to prove the lemma, it suffices for us to show that the vector functionals on $\mathfrak{A}_1 \otimes \mathfrak{A}_2$ all belong to $\mathfrak{A}_{1*} \otimes \mathfrak{A}_{2*}$.

Let $x \in \mathfrak{K}_1 \otimes \mathfrak{K}_2$. Then $x$ is the strong limit of a sequence $\{x_n\}$, each element of which is a finite linear combination of terms $f \otimes g$, with $f \in \mathfrak{K}_1$, $g \in \mathfrak{K}_2$. It follows from Defs. 2.1, 2.6, and 2.8 that the vector states $\{\omega_{x_n}\}$ all belong to $\mathfrak{A}_{1*} \otimes \mathfrak{A}_{2*}$. Further, by Def. 2.1,

$$|\omega_{x_n}(A) - \omega_x(A)| < \|A\|\,\|x_n - x\|(\|x_n\| + \|x\|), \quad \forall A \in \mathfrak{A}_1 \otimes \mathfrak{A}_2.$$

Hence $\omega_{x_n}$ converges strongly to $\omega_x$ in $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)^*$. Thus, since $\{\omega_{x_n}\} \in \mathfrak{A}_{1*} \otimes \mathfrak{A}_{2*}$, and since this latter set is a closed subspace of $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)^*$, it follows that $\omega_x \in \mathfrak{A}_{1*} \otimes \mathfrak{A}_{2*}$. QED

*Lemma 2.2:* Let $\mathfrak{A}_1, \mathfrak{A}_2$ be $W^*$-algebras and let $\mathfrak{A} = \mathfrak{A}_1 \otimes \mathfrak{A}_2$. Let $a_1: \mathfrak{A}^* \to \mathfrak{A}_1^*$ and $a_2: \mathfrak{A}^* \to \mathfrak{A}_2^*$ be defined by

$$\langle a_1\psi; A_1\rangle = \langle \psi; A_1 \otimes I_2\rangle, \quad \forall \psi \in \mathfrak{A}^*,\ A_1 \in \mathfrak{A}_1 \qquad (2.2)$$

and

$$\langle a_2\psi; A_2\rangle = \langle \psi; I_1 \otimes A_2\rangle, \quad \forall \psi \in \mathfrak{A}^*,\ A_2 \in \mathfrak{A}_2, \qquad (2.3)$$

where $I_1, I_2$ are the unit elements of $\mathfrak{A}_1\mathfrak{A}_2$, respectively. Then $a_1$ (resp. $a_2$) maps $\mathfrak{A}_*$ onto $\mathfrak{A}_{1*}$ (resp. $\mathfrak{A}_{2*}$).

*Proof:* We first note that the homomorphism of $\mathfrak{A}_1$ into $\mathfrak{A}$, given by $A_1 \to A_1 \otimes I_2$, is normal. Hence by Eq. (2.2), the image of $\mathfrak{A}_*$ under $a_1$ lies in $\mathfrak{A}_{1*}$. In order to show that the map $a_1$ is surjective, let $\psi_1$ be an arbitrary element of $\mathfrak{A}_{1*}$, and let $\psi_2 (\in \mathfrak{A}_{2*})$ have the property that $\psi_2(I_2) = 1$. Then $\psi_1 \otimes \psi_2 \in \mathfrak{A}_*$, and, by Eq. (2.2), $a_1(\psi_1 \otimes \psi_2) = \psi_1$. Since $\psi_1$ is an arbitrary element of $\mathfrak{A}_{1*}$, it follows immediately that $a_1$ maps $\mathfrak{A}_*$ *onto* $\mathfrak{A}_{1*}$. Likewise, $a_2$ maps $\mathfrak{A}_*$ onto $\mathfrak{A}_{2*}$.

*Lemma 2.3:* Let $\mathfrak{A}_1, \mathfrak{A}_2$ be type-$I$ factors. Let $\psi$, $\{\psi^{(n)}\}$ be elements of $(\mathfrak{A}_1 \otimes \mathfrak{A}_2)_*^+$ such that $\lim \psi^{(n)}(A) = \psi(A)$, $\forall A \in \mathfrak{A}_1 \otimes \mathfrak{A}_2$ as $n \to \infty$. Then $\psi^{(n)}$ converges uniformly to $\psi$, on $\mathfrak{A}_1 \otimes \mathfrak{A}_2$, as $n \to \infty$.

*Proof:* We first note that, if $\psi$ were known to be the $w^*$-limit of $\psi^{(n)}$ on $\mathfrak{A}_1 \otimes \mathfrak{A}_2$, then the required result would follow immediately from a lemma due to Dell'Antonio.[15] In fact, we shall show that Dell'Antonio's demonstration of his lemma may be adapted so as to yield a proof of the present lemma.

Since $\mathfrak{A}_1, \mathfrak{A}_2$ are type-$I$ factors, it follows[16] that there exist Hilbert spaces $\mathfrak{K}_1, \mathfrak{K}_2$ such that $\mathfrak{A}_1, \mathfrak{A}_2, \mathfrak{A}_1 \otimes \mathfrak{A}_2, \mathfrak{A}_1 \bar{\otimes} \mathfrak{A}_2$ are algebraically isomorphic with $\mathfrak{L}(\mathfrak{K}_1)$, $\mathfrak{L}(\mathfrak{K}_2)$, $\mathfrak{L}(\mathfrak{K}_1) \otimes \mathfrak{L}(\mathfrak{K}_2)$, $\mathfrak{L}(\mathfrak{K}_1) \bar{\otimes} \mathfrak{L}(\mathfrak{K}_2)$, respectively. Thus, it suffices to show that if $\phi, \{\phi^{(n)}\}$ are elements of $(\mathfrak{L}(\mathfrak{K}_1) \otimes \mathfrak{L}(\mathfrak{K}_2))_*^+$, such that $\phi$ is the $w^*$-limit, as $n \to \infty$, of $\phi^{(n)}$ on $\mathfrak{L}(\mathfrak{K}_1) \otimes \mathfrak{L}(\mathfrak{K}_2)$, then $\phi^{(n)}$ converges uniformly to $\phi$ on $\mathfrak{L}(\mathfrak{K}_1) \otimes \mathfrak{L}(\mathfrak{K}_2)$. Further, on consulting the proof of Dell'Antonio's lemma, one sees that it may be extended so as to prove the required uniform convergence of $\phi^{(n)}$, provided that the following proposition[17] is established: If $f$ is an arbitrary vector in $\mathfrak{K}_1 \otimes \mathfrak{K}_2$, then the corresponding one-dimensional projection operator $E_f$ lies in $\mathfrak{L}(\mathfrak{K}_1) \bar{\otimes} \mathfrak{L}(\mathfrak{K}_2)$.

Now any vector $f$ in $\mathfrak{K}_1 \otimes \mathfrak{K}_2$ is the strong limit of a sequence $\{f_n\}$, each element of which is a finite linear combination of terms $g \otimes h$, with $g \in \mathfrak{K}_1$, and $h \in \mathfrak{K}_2$. Thus, $E_{f_n} \in \mathfrak{L}(\mathfrak{K}_1) \bar{\otimes} (\mathfrak{K}_2)$. Further,

$$\|(E_{f_n} - E_f)x\| \le \|x\|(\|f_n\| + \|f\|)\,\|f_n - f\|, \quad \forall x \in \mathfrak{K}_1 \otimes \mathfrak{K}_2.$$

Hence $E_f$ is the norm limit of a sequence of elements $\{E_{f_n}\}$ of the $C^*$-algebra $\mathfrak{L}(\mathfrak{K}_1) \bar{\otimes} \mathfrak{L}(\mathfrak{K}_2)$; and therefore $E_f$ belongs to this algebra. QED

## 3. THE MODEL

In this Section, we shall present our mathematical description of the systems $\tilde{\mathbf{S}}, \hat{\mathbf{S}}$, and $\mathbf{S}$.

## A. The System $\tilde{\mathbf{S}}$

We assume that $\tilde{\mathbf{S}}$ is a finite system, in the sense of Def. 2.4. Thus, we assume that the algebra of (bounded) observables $\tilde{\mathfrak{A}}$ of this system is a type-$I$ factor in a Hilbert space $\tilde{\mathfrak{K}}$. Time translations in $\tilde{\mathbf{S}}$, when isolated, are taken to correspond to a one-parameter group $\{\tilde{\tau}(t) \mid t \in \mathbf{R}\}$ of inner automorphism of $\tilde{\mathfrak{A}}$, unitarily implemented in $\tilde{\mathfrak{K}}$ by a strongly continuous representation $\tilde{U}$ of $\mathbf{R}$:

$$\tilde{\tau}(t)\tilde{A} = \tilde{U}(t)\tilde{A}\tilde{U}(-t) \equiv \tilde{A}(t), \quad \forall \tilde{A} \in \tilde{\mathfrak{A}},\ t \in \mathbf{R} \qquad (3.1)$$

*Note:* Although we refer to $\tilde{\mathbf{S}}$ as a finite system, we never actually use the assumption that this system satisfies condition (iii) of Def. 2.4.

## B. The System $\hat{\mathbf{S}}$

We assume that $\hat{\mathbf{S}}$ is an infinite system in the sense of Ref. 1. Thus, we assume that $\hat{\mathbf{S}}$ may be specified in terms of a sequence $\{\hat{\mathbf{S}}^{(n)}\}$ of finite systems, in the sense of Def. 2.4, such that:

(i) For each $n \in \mathbf{Z}_+$, the algebra of observables $\hat{\mathfrak{A}}^{(n)}$, for $\hat{\mathbf{S}}^{(n)}$, is a type-$I$ factor in a Hilbert space $\hat{\mathfrak{K}}$, this latter space being independent of $n$.

(ii) Each $\hat{\mathfrak{A}}^{(n)}$ is equipped with a one-parameter group

of inner automorphisms $\{\hat{\tau}^{(n)}(t) \mid t \in \mathbf{R}\}$, corresponding to time translations in $\hat{\mathbf{S}}^{(n)}$. It is assumed that this group is unitarily implemented in $\hat{\mathcal{H}}$ by a strongly continuous representation $\hat{U}^{(n)}$ of $\mathbf{R}$;

$$\hat{\tau}^{(n)}(t)\hat{A} = \hat{U}^{(n)}(t)\hat{A}\hat{U}^{(n)}(-t) \equiv \hat{A}^{(n)}(t), \quad \forall\, \hat{A} \in \hat{\mathfrak{A}}^{(n)}, t \in \mathbf{R}. \tag{3.2}$$

(iii) For each $\beta \in \mathbf{R}_+$ and $n \in \mathbf{Z}_+$, there exists a unique normal state $\hat{\phi}_\beta^{(n)}$ on $\hat{\mathfrak{A}}^{(n)}$ which satisfies the KMS conditions with respect to $(\hat{\tau}^{(n)}, \beta)$. This state corresponds to the Gibbs state for $\hat{\mathbf{S}}^{(n)}$ at the inverse temperature $\beta$.

(iv) $\mathfrak{A}^{(n)}$ is isotonic with respect to $n$ (i.e., $\hat{\mathfrak{A}}^{(n)} \supset \hat{\mathfrak{A}}^{(m)}$ if $n > m$).

Having thus specified $\{\hat{\mathbf{S}}^{(n)}\}$, we define $\hat{\mathfrak{A}}_L$ to be $\cup_{n \in \mathbf{Z}_+} \hat{\mathfrak{A}}^{(n)}$; and we define $\hat{\mathfrak{A}}$ to be the norm closure of $\hat{\mathfrak{A}}_L$. The $C^*$-algebra $\hat{\mathfrak{A}}$ is taken to be the algebra of observables for $\hat{\mathbf{S}}$. The subalgebras $\hat{\mathfrak{A}}^{(n)}$ of $\hat{\mathfrak{A}}$ may be regarded as algebras of observables for systems $\hat{\mathbf{S}}^{(n)}$ occupying finite regions of "physical" space (cf. Ref. 1).

We shall employ the DS scheme to formulate the Gibbs states for $\hat{\mathbf{S}}$, and the dynamics of $\hat{\mathbf{S}}$ in the associated islands of states. The DS axioms are

(i) $\lim_{n\to\infty} \hat{\phi}_\beta^{(n)}(\hat{A}_1^{(n)}(t_k)\cdots\hat{A}_k^{(n)}(t_k))$ exists $\forall\, \hat{A}_1, \ldots, \hat{A}_k \in \hat{\mathfrak{A}}_L, t_1, \ldots, t_k \in \mathbf{R}, k < \infty$,

and

(ii) $$\lim_{m\to\infty}\lim_{n\to\infty} \hat{\phi}_\beta^{(n)}(\hat{A}_1^{(n)}(t_1)\cdots\hat{A}_k^{(n)}(t_k) \times \hat{A}_{k+1}^{(m)}(t_{k+l})\cdots\hat{A}_{k+l}^{(m)}(t_{k+l})) = \lim_{n\to\infty} \hat{\phi}_\beta^{(n)}(\hat{A}_1^{(n)}(t_1)\cdots\hat{A}_k^{(n)}(t_k)\hat{A}_{k+1}^{(n)}(t_{k+1})\cdots\hat{A}_{k+l}^{(n)}(t_{k+l})),$$

$$\forall\, \hat{A}_1\ldots,\hat{A}_{k+l} \in \hat{\mathfrak{A}}_L, \quad t_1, \ldots, t_{k+l} \in \mathbf{R}, \quad k + l < \infty.$$

The principle consequences of these axioms may be summarized as follows.

(a) There exists a unique state $\hat{\phi}_\beta$ on $\hat{\mathfrak{A}}$ such that

$$\hat{\phi}_\beta(\hat{A}) = \lim_{n\to\infty} \hat{\phi}_\beta^{(n)}(\hat{A}), \quad \forall\, \hat{A} \in \hat{\mathfrak{A}}_L. \tag{3.3}$$

Thus, $\hat{\phi}_\beta$ is the Gibbs state for $\hat{\mathbf{S}}$ at the inverse temperature $\beta$. By the GNS construction, this state induces a $^*$-representation $\hat{\pi}_\beta$ of $\hat{\mathfrak{A}}$ in a Hilbert space $\hat{\mathcal{H}}_\beta$ with cyclical vector $\hat{\Omega}_\beta$, such that $\hat{\phi}_\beta(\cdot) \equiv (\hat{\Omega}_\beta, \hat{\pi}_\beta(\cdot)\hat{\Omega}_\beta)$. We shall denote the images of $\hat{A}(\in \hat{A})$ and $\hat{A}$ under $\pi_\beta$ by $\hat{A}_\beta$, $\hat{\mathfrak{A}}_\beta$, respectively. We shall also denote the island of states associated with $\hat{\phi}_\beta$ by $\hat{\mathfrak{I}}_\beta$, i.e.,

$$\hat{\mathfrak{I}}_\beta = \{\Psi \circ \hat{\pi}_\beta \mid \Psi \in (\hat{\mathfrak{A}}_\beta)_*^+, \|\Psi\| = 1\}.$$

(b) Let $\hat{\Phi}_\beta$ be the state on $\mathfrak{A}_\beta''$ defined by

$$\hat{\Phi}_\beta(\hat{Q}) = (\hat{\Omega}_\beta, \hat{Q}\hat{\Omega}_\beta), \quad \forall\, \hat{Q} \in \hat{\mathfrak{A}}_\beta''. \tag{3.4}$$

Then there exists a homomorphism $\hat{\tau}_\beta$ of $\mathbf{R}$ into Aut $\hat{\mathfrak{A}}_\beta''$, unitarily implemented in $\hat{\mathcal{H}}_\beta$ by a strongly continuous representation $\hat{U}_\beta$ of $\mathbf{R}$, such that $\hat{\Omega}_\beta$ is invariant under $U_\beta(\mathbf{R})$ and

$$\lim_{n\to\infty} \hat{\phi}_\beta^{(n)}(\hat{A}_1^{(n)}(t_1)\cdots\hat{A}_k^{(n)}(t_k)) = \hat{\Phi}_\beta(\hat{A}_{1,\beta}(t_1)\cdots\hat{A}_{k,\beta}(t_k)),$$

$$\forall\, \hat{A}_1, \ldots, \hat{A}_k \in \hat{\mathfrak{A}}_L, \quad t_1, \ldots, t_k \in \mathbf{R}, \quad k < \infty, \tag{3.5}$$

where

$$\hat{A}_\beta(t) = \hat{\tau}_\beta(t)\hat{A}_\beta(\equiv \hat{\tau}_\beta(t)\hat{\pi}_\beta(\hat{A})) = \hat{U}_\beta(t)\hat{A}_\beta U_\beta(-t), \quad \forall\, \hat{A} \in \hat{\mathfrak{A}}, \quad t \in \mathbf{R}. \tag{3.6}$$

(c) $\hat{\Phi}_\beta$ satisfies the KMS conditions with respect to $(\hat{\tau}_\beta, \beta)$.

In particular, we interpret (b) as signifying that time translations in the island $\hat{\mathfrak{I}}_\beta$ correspond to the group $\hat{\tau}_\beta(\mathbf{R})$ of automorphisms of $\hat{\mathfrak{A}}_\beta''$.

*Lemma 3.1:* Let $\hat{\pi}_{\beta|n}$ be the restriction of $\hat{\pi}_\beta$ to $\hat{\mathfrak{A}}^{(n)}$. Then $\pi_{\beta|n}$ is a normal representation of $\hat{\mathfrak{A}}^{(n)}$ in $\hat{\mathcal{H}}_\beta$.

*Proof:* Let $\hat{\phi}_{\beta|n}$ (resp. $\hat{\phi}_{\beta|n}^{(m)}$, with $m > n$) denote the restriction of $\hat{\phi}_\beta$ (resp. $\hat{\phi}_\beta^{(m)}$) to $\hat{\mathfrak{A}}^{(n)}$. Then it follows from Eq. (3.3) that $\hat{\phi}_{\beta|n} = w^*\text{-}\lim \hat{\phi}_{\beta|n}^{(m)}$ as $m \to \infty$. Hence, since $\hat{\mathfrak{A}}^{(n)}$ is a $W^*$-algebra and since $\hat{\phi}_\beta^{(m)}$ is normal, it follows from a theorem due to Sakai[18] that $\hat{\phi}_{\beta|n}$ is normal.

Let $\{\hat{A}_\gamma\}$ be a sequence of elements of the unit ball of $\hat{\mathfrak{A}}^{(n)}$, which converges weakly to $\hat{A}$. Let $\hat{B}_1, \hat{B}_2 \in \mathfrak{A}_L$. Then, for $m$ sufficiently large, $\{A_\gamma\}, \hat{A}, \hat{B}_1$, and $\hat{B}_2 \in \hat{\mathfrak{A}}^{(m)}$. Hence, it follows from the definitions of $\pi_{\beta|n}$ $\hat{\phi}_{\beta|m}$, and $\hat{\Omega}_\beta$ that

$$\hat{\phi}_{\beta|m}(\hat{B}_1^*(\hat{A}_\gamma - \hat{A})\hat{B}_2) = (\hat{\pi}_\beta(\hat{B}_1)\hat{\Omega}_\beta, \hat{\pi}_{\beta|n}(\hat{A}_\gamma - \hat{A})\hat{\pi}_\beta(\hat{B}_2)\hat{\Omega}_\beta), \quad \forall\, \hat{B}_1, \hat{B}_2 \in \hat{\mathfrak{A}}_L. \tag{3.7}$$

As proved above, $\hat{\phi}_{\beta|m}$ is normal, for all $m \in \mathbf{Z}_+$. Hence, since $\hat{A}_\gamma$ tends weakly to $\hat{A}$ in the unit ball of $\hat{\mathfrak{A}}^{(n)}$, it follows that the left-hand side of Eq. (3.7) tends to zero as $\gamma \to \infty$. Therefore, since $\hat{\pi}_\beta(\hat{\mathfrak{A}}_L)\hat{\Omega}_\beta$ is dense in $\hat{\mathcal{H}}_\beta$, it follows from Eq. (3.7) that $\hat{\pi}_{\beta|n}(\hat{A}_\gamma - \hat{A})$ tends weakly to zero as $\gamma \to \infty$. Thus, we have shown that $\hat{\pi}_{\beta|n}$ is weakly continuous in the unit ball of $\hat{\mathfrak{A}}^{(n)}$ and, therefore,[19] is ultraweakly continuous, i.e., normal, in $\hat{\mathfrak{A}}^{(n)}$. QED

*Lemma 3.2:* Let $\hat{B}, \hat{\dot{B}}$ be elements of $\hat{\mathfrak{A}}_L$, such that, for all $n$ greater than some fixed $n_0 (\in \mathbf{Z}_+)$, $w - (d/dt)\hat{B}^{(n)}(t) = \hat{\dot{B}}^{(n)}(t)$, $\forall\, t \in \mathbf{R}$. Then $w - (d/dt)\hat{B}_\beta(t) = \hat{\dot{B}}_\beta(t)$, $\forall\, t \in \mathbf{R}$.

*Proof:* Let $\hat{A}_1, \hat{A}_2 \in \hat{\mathfrak{A}}_L$. Thus, $\hat{A}_1, \hat{A}_2 \in \hat{\mathfrak{A}}^{(m)}$ for $m$ sufficiently large. Hence it follows from the given equation of motion for $\hat{B}^{(n)}(t)$ and from the normality of $\phi_\beta^{(n)}$ that

$$\frac{d}{dt}\hat{\phi}_\beta^{(n)}(\hat{A}_1^*\hat{B}^{(n)}(t)\hat{A}_2) = \hat{\phi}_\beta^{(n)}(\hat{A}_1^*\hat{\dot{B}}^{(n)}(t)\hat{A}_2), \quad \forall\, n > (m, n_0).$$

Thus,

$$\hat{\phi}_\beta^{(n)}(\hat{A}_1^*\hat{B}^{(n)}(t)\hat{A}_2) - \hat{\phi}_\beta^{(n)}(\hat{A}_1^*\hat{B}\hat{A}_2) = \int_0^t dt_1 \hat{\phi}_\beta^{(n)}(\hat{A}_1^*\hat{\dot{B}}^{(n)}(t_1)\hat{A}_2), \quad \forall\, n > (m, n_0).$$

Hence, by Eqs. (3.4) and (3.5),

$$(\hat{A}_{1,\beta}\hat{\Omega}_\beta, (\hat{B}_\beta(t) - \hat{B}_\beta)\hat{A}_{2,\beta}\hat{\Omega}_\beta) = \int_0^t dt_1 (\hat{A}_{1,\beta}\Omega_\beta, \hat{\dot{B}}_\beta(t_1)\hat{A}_{2,\beta}\Omega_\beta).$$

Since this last equation is valid for all $\hat{A}_1, \hat{A}_2 \in \mathfrak{A}_L$, and since $\hat{\pi}_\beta(\hat{\mathfrak{A}}_L)\hat{\Omega}_\beta$ is dense in $\hat{\mathcal{H}}_\beta$, it follows that

$$(f, (\hat{B}_\beta(t) - \hat{B}_\beta)g) = \int_0^t dt_1 (f, \hat{\dot{B}}_\beta(t_1)g), \quad \forall\, f, g \in \hat{\mathcal{H}}_\beta.$$

The required result follows directly from this equation and the fact that the strong continuity of $U_\beta(t)$ guarantees that of $\hat{B}_\beta(t)$. QED

### C. The System S

We specify the composite system S in terms of a sequence $\{S^{(n)} = (\tilde{S} + \hat{S}^{(n)})\}$ of finite systems, by a procedure similar to that employed for $\hat{S}$.

Let $\mathcal{K}$ be the completed tensor product $\tilde{\mathcal{K}} \otimes \hat{\mathcal{K}}$, and let $\mathfrak{A}^{(n)}, \mathfrak{A}_L, \mathfrak{A}$ be the algebras in $\mathcal{K}$ defined by $\mathfrak{A}^{(n)} = \tilde{\mathfrak{A}} \otimes \hat{\mathfrak{A}}^{(n)}$, $\mathfrak{A}_L = \cup_{n \in \mathbf{Z}_+} \mathfrak{A}^{(n)}$, and $\mathfrak{A}$ = the norm closure of $\mathfrak{A}_L$.

We take $\mathfrak{A}, \mathfrak{A}^{(n)}$ to be the algebras of observables for $S, S^{(n)}$, respectively. If follows that the observables for $\tilde{S}$ (resp. $\hat{S}$) may be represented as elements of S by the injective mappings $\tilde{A} \to \tilde{A} \otimes \hat{I}$ (resp. $\hat{A} \to \tilde{I} \otimes \hat{A}$) of $\tilde{\mathfrak{A}}$ (resp. $\hat{\mathfrak{A}}$) into $\mathfrak{A}$.

We assume that, for all $n$ greater than some fixed $n_0$, time translations of $S^{(n)}$ correspond to a one-parameter group $\{\tau^{(n)}(t) \mid t \in \mathbf{R}\}$ of inner automorphisms of $\mathfrak{A}^{(n)}$, of the form

$$\tau^{(n)}(t)A = \exp[i(H^{(n)} + V)t] \cdot A \exp[-i(H^{(n)} + V)t], \quad \forall A \in \mathfrak{A}^{(n)}, t \in \mathbf{R}, \tag{3.8}$$

where $V$ is a self-adjoint element of $\mathfrak{A}^{(n)}$ and $H^{(n)}$ is defined by

$$\tilde{U}(t) \otimes \hat{U}^{(n)}(t) = \exp(iH^{(n)}t), \quad \forall t \in \mathbf{R}. \tag{3.9}$$

*Note:* The strong continuity of $\tilde{U}(t)$ and $\hat{U}^{(n)}(t)$ ensures that $\tilde{U}(t) \otimes \hat{U}^{(n)}(t)$ has an infinitesimal generator, and thus that Eq. (3.9) provides a definition of $H^{(n)}$. Further, $\tau^{(n)}(t)$, as defined by Eq. (3.8), is indeed an inner automorphism of $\mathfrak{A}^{(n)}$, for the following reason. Since $\tilde{\tau}(t)$, $\hat{\tau}^{(n)}(t)$ are inner automorphisms of $\tilde{\mathfrak{A}}, \hat{\mathfrak{A}}^{(n)}$, respectively, it follows that $\tilde{U}(t) \in \tilde{\mathfrak{A}}$ and $\hat{U}^{(n)}(t) \in \hat{\mathfrak{A}}^{(n)}$. Hence, by Eq. (3.9), $e^{iH^{(n)}t} \in \mathfrak{A}^{(n)}$, and therefore the operator $H^{(n)}$ is affiliated to $\mathfrak{A}^{(n)}$ [i.e., it commutes with the elements of $(\mathfrak{A}^{(n)})'$]. Consequently, $(H^{(n)} + V)$ is also affiliated to $\mathfrak{A}^{(n)}$ and therefore $\exp i(H^{(n)} + V)t \in \mathfrak{A}^{(n)}$. Thus, by eq. (3.8), $\tau^{(n)}(t)$ is an inner automorphism of $\mathfrak{A}^{(n)}$.

The dynamics of S will be formulated in Sec. 4, subject to prescribed initial conditions, as an appropriate limit of that of $S^{(n)}$. For the moment, we note that the interaction $V$ may be any self-adjoint element of $\mathfrak{A}_L$. Thus, the model is sufficiently general to include, for example, local interactions between systems of particles with hard cores, as formulated by Robinson.[20]

### D. The Representation $\pi_\beta$

Let $\mathcal{K}_\beta$ be the completed tensor product $\tilde{\mathcal{K}} \otimes \hat{\mathcal{K}}_\beta$. By Def. 2.7 and Lemma 3.1, there exists a normal *-representation $\pi_{\beta|n} \equiv \tilde{I} \otimes \hat{\pi}_{\beta|n}$ of $\mathfrak{A}$ in $\mathcal{K}_\beta$, where $\tilde{I}$ is the identity map of $\tilde{\mathfrak{A}}$ onto $\tilde{\mathfrak{A}}$. Since $\mathfrak{A}^{(n)}$ is isotonic with respect to $n$ and since $\mathfrak{A}_L$ is norm-dense in $\mathfrak{A}$, it follows that there exists a unique *-representation of $\mathfrak{A}$ in $\mathcal{K}_\beta$, whose restriction to $\mathfrak{A}^{(n)}$ is $\pi_{\beta|n}$, $\forall n \in \mathbf{Z}_+$. We denote this representation of $\mathfrak{A}$ by $\pi_\beta$. The images of $A (\in \mathfrak{A})$ and $\mathfrak{A}$ under $\pi_\beta$ will be denoted by $\mathfrak{A}_\beta, A_\beta$, respectively. Thus,

$$\mathfrak{A}''_\beta = \tilde{\mathfrak{A}} \otimes \mathfrak{A}''_\beta = \{\sum_{r=1}^{n} \tilde{A}_r \otimes \hat{\pi}_\beta(\hat{A}_r) \mid \tilde{A}_r \in \tilde{\mathfrak{A}}, \hat{A}_r \in \hat{\mathfrak{A}}_L, N < \infty\}''.$$

Finally, we define $\mathcal{J}_\beta$ to be the island of states of S associated with $\pi_\beta$, i.e.,

$$\mathcal{J}_\beta = \{\Psi \circ \pi_\beta \mid \Psi \in (\mathfrak{A}''_\beta)^+_*, \|\Psi\| = 1\}.$$

## 4. DYNAMICS OF S

We shall define the dynamics of S in terms of that of $\{S^{(n)}\}$ as follows. Let $S^{(n)}$ evolve from an initial state $\phi^{(n)}$ in which $\tilde{S}$ and $\hat{S}^{(n)}$ are mutually uncorrelated, with $\tilde{S}$ in an arbitrary normal state and $\hat{S}^{(n)}$ in the (normal) Gibbs state $\hat{\phi}_\beta^{(n)}$, i.e., $\phi^{(n)} = \tilde{\phi} \otimes \hat{\phi}_\beta^{(n)}$. Since time translations in $S^{(n)}$ correspond to the automorphisms $\tau^{(n)}(\mathbf{R})$ of $\mathfrak{A}^{(n)}$, or equivalently (cf. Def. 2.2) to the dual group $\tau^{(n)*}(\mathbf{R})$ of transformations of $\mathfrak{A}^{(n)*}$, it follows that the state of $S^{(n)}$ at time $t$ is $\tau^{(n)*}(t)(\tilde{\phi} \otimes \hat{\phi}_\beta^{(n)})$. Now it will be shown (Theorem 4.1) that the assumptions of Sec. 3 imply that, for fixed $\tilde{\phi}, \beta$ and $t$, there exists a unique state $\phi(t)$ on $\mathfrak{A}$ such that

$$\langle \phi(t); A \rangle = \lim_{n \to \infty} \langle \tau^{(n)*}(t)(\tilde{\phi} \otimes \hat{\phi}_\beta^{(n)}); A \rangle, \quad \forall A \in \mathfrak{A}_L, t \in \mathbf{R}. \tag{4.1}$$

Thus, we shall refer to $\phi(t)$ as the state of S at time $t$, corresponding to the evolution of that system from an initial state in which $\tilde{S}$ and $\hat{S}$ are mutually uncorrelated with $\tilde{S}$ in the state $\tilde{\phi}$ and $\hat{S}$ in the state $\hat{\phi}_\beta$.

*Theorem 4.1:* With the above definitions and assumptions, there exists a group $\{\tau_\beta(t) \mid t \in \mathbf{R}\}$ of spatial automorphisms of $\mathfrak{A}''_\beta$ such that Eq. (4.1) is satisfied when

$$\phi(t) = (\tau_\beta^*(t)(\phi \otimes \Phi_\beta)) \circ \pi_\beta, \tag{4.2}$$

where $\tau_\beta^*(t)$ is the transformation of $(\mathfrak{A}''_\beta)^*$, dual to $\tau_\beta(t)$. Further, $\tau_\beta(\mathbf{R})$ is given explicitly by the formula

$$\tau_\beta(t)Q = \exp[i(H_\beta + V_\beta)t] \cdot Q \exp[-i(H_\beta + V_\beta)t], \quad \forall Q \in \mathfrak{A}''_\beta, \quad t \in \mathbf{R}, \tag{4.3}$$

where $V_\beta = \pi_\beta(V)$ (in the notation specified in Sec. 3) and $H_\beta$ is defined by

$$\tilde{U}(t) \otimes \hat{U}_\beta(t) = \exp(iH_\beta t), \quad \forall t \in \mathbf{R}. \tag{4.4}$$

Before proving this theorem, we note that the following corollary follows directly from the statement of the theorem, together with Lemma 2.2, and the definitions of the islands $\mathcal{J}_\beta, \hat{\mathcal{J}}_\beta$.

*Corollary:* Let $\tilde{\phi}(t), \hat{\phi}(t)$ be the states induced in $\tilde{S}, \hat{S}$, respectively, by $\phi(t)$, i.e.,

$$\langle \tilde{\phi}(t); \tilde{A} \rangle = \langle \phi(t); \tilde{A} \otimes \hat{I} \rangle, \quad \forall \tilde{A} \in \tilde{\mathfrak{A}}, t \in \mathbf{R} \tag{4.5}$$

and

$$\langle \hat{\phi}(t); \hat{A} \rangle = \langle \phi(t); \tilde{I} \otimes \hat{A} \rangle, \quad \forall \hat{A} \in \hat{\mathfrak{A}}, \quad t \in \mathbf{R} \tag{4.5'}$$

*Then* $\phi(t) \in \mathcal{J}_\beta$, $\hat{\phi}(t) \in \hat{\mathcal{J}}_\beta$, and $\tilde{\phi}(t)$ is normal for all $t \in \mathbf{R}$.

Our proof of Theorem 4.1 will be based on the next three lemmas. Before presenting those lemmas, we first introduce the following definition.

*Definition 4.1:* (i) For $n \in \mathbf{Z}_+$, we define $\tau_0^{(n)}$ to be the homomorphism of $\mathbf{R}$ into aut $\mathfrak{A}^{(n)}$ specified by

$$\tau_0^{(n)}(t) = \tilde{\tau}(t) \otimes \hat{\tau}^{(n)}(t), \quad \forall t \in \mathbf{R}, \quad n \in \mathbf{Z}_+. \tag{4.6}$$

The image of $A (\in \mathfrak{A}^{(n)})$ under $\tau_0^{(n)}(t)$ will be denoted by $A^{(n)}(t)$, i.e., [using Eqs. (3.1), (3.2), and (3.9)].

$$A^{(n)}(t) = \tau_0^{(n)}(t)A = \exp(iH^{(n)}t)A \cdot \exp(-iH^{(n)}t), \quad \forall A \in \mathfrak{A}^{(n)}, \quad t \in \mathbf{R}. \tag{4.7}$$

(ii) We define $\tau_{0\beta}$ to be the homomorphism of $\mathbf{R}$ into aut $\mathfrak{A}''_\beta$ ( $\equiv$ aut $\tilde{\mathfrak{A}} \otimes \hat{\mathfrak{A}}''_\beta$ ) specified by

$$\tau_{0\beta}(t) = \tilde{\tau}(t) \otimes \hat{\tau}_\beta(t), \qquad \forall\, t \in \mathbf{R}. \tag{4.8}$$

For $A \in \mathfrak{A}$, the image of $A_\beta$ under $\tau_{0\beta}(t)$ will be denoted by $A_\beta(t)$, i.e., [using Eqs. (3.1), (3.6), and (4.4)]

$$A_\beta(t) = \tau_{0\beta}(t)A_\beta = \exp(iH_\beta t)\,A_\beta \exp(-iH_\beta t), \qquad \forall\, A \in \mathfrak{A},\ t \in \mathbf{R}. \tag{4.9}$$

*Lemma 4.1:* With the above definitions and assumptions,

$$\lim_{n\to\infty} \langle \tilde{\psi} \otimes \phi_\beta; A_k^{(n)}(t_k) \ldots A_1^{(n)}(t_1)\rangle = \langle \tilde{\psi} \otimes \hat{\Phi}_\beta; A_{k,\beta}(t_k) \ldots A_{1,\beta}(t_1)\rangle,$$
$$\forall\, \tilde{\psi} \in \tilde{\mathfrak{A}}_*;\ A_1, \ldots, \quad A_k \in \bigcup_{n\in\mathbf{Z}_+} \tilde{\mathfrak{A}} \bar{\otimes} \hat{\mathfrak{A}}^{(n)},$$
$$t_1, \ldots, t_k \in \mathbf{R},\ k < \infty. \tag{4.10}$$

*Proof:* Let $A_1, \ldots, A_k \in \bigcup_{n\in\mathbf{Z}_+} \tilde{\mathfrak{A}} \bar{\otimes} \hat{\mathfrak{A}}^{(n)}$. Then, by choosing $m$ sufficiently large, we can ensure that $A_1, \ldots, A_k \in \tilde{\mathfrak{A}} \bar{\otimes} \hat{\mathfrak{A}}^{(m)}$. Let $\mathfrak{A}_0^{(m)} = \left\{ \sum_{r=1}^{n} \tilde{A}_r \otimes \hat{A}_r \,|\, \tilde{A}_r \in \tilde{\mathfrak{A}}, \hat{A}_r \in \hat{\mathfrak{A}}^{(m)}, N < \infty \right\}$. Then it follows from Eqs. (3.5), (3.6), and (4.6)–(4.9) that Eq. (4.10) is valid when $A_1, \ldots, A_k \in \mathfrak{A}_0^{(m)}$. Since this latter algebra is norm dense in $\mathfrak{A} \bar{\otimes} \hat{\mathfrak{A}}^{(m)}$, the required result follows by continuity. QED

*Lemma 4.2:* Let $m$ be a fixed element of $\mathbf{Z}_+$, and let $\{A_r\}, \{t_r\}$ be arbitrary sequences of elements of $\mathfrak{A}^{(m)}, \mathbf{R}$, respectively. For each $n \in \mathbf{Z}_+$, let $\{\psi_r^{(n)}\}, \{\Psi_r\}$ be the sequences in $\mathfrak{A}_*^{(n)+}, (\mathfrak{A}''_\beta)_*^+$, respectively, defined by the following formulas:

$$\psi_0^{(n)} = (\tilde{\tau}^*(t_0)\tilde{\psi}) \otimes \hat{\phi}_\beta^{(n)};$$
$$\psi_r^{(n)}(\cdot) = \psi_{r-1}^{(n)}(A_r^{*(n)}(t_r)(\cdot)A_r^{(n)}(t_r)), \qquad \text{for } r > 0; \tag{4.11}$$
$$\Psi_0 = (\tilde{\tau}^*(t_0)\tilde{\psi}) \otimes \hat{\Phi}_\beta; \Psi_r(\cdot) = \Psi_{r-1}(A_{r,\beta}^*(t_r)(\cdot)A_{r,\beta}(t_r)), \qquad \text{for } r > 0, \tag{4.12}$$

with $\tilde{\psi} \in \tilde{\mathfrak{A}}_*^+$. Then for each fixed $r \in \mathbf{Z}_+$, $\psi_r^{(n)}$ tends uniformly to $\Psi_r \circ \pi_\beta$, on $\mathfrak{A}^{(m)}$, as $n \to \infty$.

*Proof:* It follows from the normality of the functionals $\psi_r^{(n)}, \Psi_r$, and of the representation $\pi_{\beta|m}$ of $\mathfrak{A}^{(m)}$ (defined in Sec. 3 D) that the restrictions of $\psi_r^{(n)}$ (for $n > m$) and $\Psi_r \circ \pi_\beta$ to $\mathfrak{A}^{(m)}$ are normal. Hence, in view of Lemma 2.3, it suffices for us to prove that, for arbitrary choices of the sequences $\{A_r\}, \{t_r\}$ required for the definitions of $\{\psi_r^{(n)}\}$ and $\{\Psi_r\}$,

$$\lim_{n\to\infty} \langle \psi_r^{(n)}; A\rangle = \langle \Psi_r; A_\beta\rangle, \qquad \forall\, A \in \tilde{\mathfrak{A}} \bar{\otimes} \hat{\mathfrak{A}}^{(m)}. \tag{4.13}$$

We shall establish this result by induction. For this purpose we note that, in view of Lemma 4.1 and Eqs. (4.11) and (4.12), Eq. (4.13) is valid for $r = 0$; and, in cases where $A_1 \in \tilde{\mathfrak{A}} \otimes \hat{\mathfrak{A}}^{(m)}$, it is also valid for $r = 1$. Hence, in order to prove the present lemma by induction, it suffices to establish the following proposition. If, for arbitrary $l \in \mathbf{Z}_+ \cup 0$ and arbitrary choice of the sequences $\{A_r\}, \{t_r\}$ used for the definitions of $\{\psi^{(n)}\}$ and $\{\Psi_r\}$,

(i) $$\lim_{n\to\infty} \langle \psi_l^{(n)}; A\rangle = \langle \Psi_l; A_\beta\rangle, \qquad \forall\, A \in \tilde{\mathfrak{A}} \bar{\otimes} \hat{\mathfrak{A}}^{(m)} \tag{4.14}$$

and

(ii) $$\lim_{n\to\infty} \langle \psi_l^{(n)}; B^{*(n)}(t)AB^{(n)}(t)\rangle = \langle \Psi_l; B_\beta^*(t)A_\beta B_\beta(t)\rangle,$$
$$\forall\, A, B \in \tilde{\mathfrak{A}} \bar{\otimes} \hat{\mathfrak{A}}^{(m)},\ t \in \mathbf{R}, \tag{4.15}$$

then

$$\lim_{n\to\infty} \langle \psi_l^{(n)}; K^{*(n)}(t)AK^{(n)}(t)\rangle = \langle \Psi_l; K_\beta^*(t)A_\beta K_\beta(t)\rangle,$$
$$\forall\, A \in \tilde{\mathfrak{A}} \bar{\otimes} \hat{\mathfrak{A}}^{(m)}, \quad K \in \mathfrak{A}^{(m)},\ t \in \mathbf{R}. \tag{4.16}$$

Now it follows from Lemma 2.3 and the above assumption (i) that $\psi_l^{(n)}$ tends uniformly and hence weakly to $\Psi_l \circ \pi_\beta$ on $\mathfrak{A}^{(m)}$, for all choices of the sequences $\{t_r\}$, $\{A_r\}$. Further, it follows from Eqs. (4.11), (4.12), and the invariance[21] of $\tilde{\phi}_\beta^{(n)}, \Phi_\beta$ under $\tilde{\tau}^{(n)*}(\mathbf{R}), \tilde{\tau}_\beta^*(\mathbf{R})$, respectively, that $\langle \psi_r^{(n)}; A\rangle$ is invariant under the transformation $t_0 \to t_0 - t$, $t_j \to t_j + 2t$ (for $j > 0$), $A \to A^{(n)}(t)$; and that $\langle \Psi_r; A_\beta\rangle$ is invariant under $t_0 \to t_0 - t, t_j \to t_j + 2t$ (for $j > 0$), and $A_\beta \to A_\beta(t)$. Hence (i) implies that

$$\lim_{n\to\infty} \langle \psi_l^{(n)}; A^{(n)}(t)\rangle = \langle \Psi_l; A_\beta(t)\rangle, \qquad \forall\, A \in \mathfrak{A}^{(m)},\ t \in \mathbf{R}. \tag{4.17}$$

In order to derive Eq. (4.16) from (i) and (ii), we choose an arbitrary element $K$ of $\mathfrak{A}^{(m)}$ and introduce a sequence $\{K_s\}$ of normwise uniformly bounded elements of $\tilde{\mathfrak{A}} \bar{\otimes} \hat{\mathfrak{A}}^{(m)}$, which converges strongly to $K$ as $s \to \infty$: The existence of such a sequence is guaranteed by Kaplansky's density theorem. We then use the inequality

$$|\langle \psi_l^{(n)}; K^{*(n)}(t)AK^{(n)}(t)\rangle - \langle \Psi_l; K_\beta^*(t)A_\beta K_\beta(t)\rangle| \tag{4.18}$$
$$\leq |\langle \Psi_l; K_\beta^*(t)A_\beta K_\beta(t) - K_{s,\beta}^*(t)A_\beta K_{s,\beta}(t)\rangle| \tag{4.18a}$$
$$+ |\langle \psi_l^{(n)}; K_s^{*(n)}(t)AK_s^{(n)}t)\rangle - \langle \Psi_l; K_{s,\beta}^*(t)A_\beta K_{s,\beta}(t)\rangle| \tag{4.18b}$$
$$+ |\langle \psi_l^{(n)}; K_s^{*(n)}(t)A(K - K_s)^{(n)}(t)\rangle| + |\langle \psi_l^{(n)}; (K^* - K_l^*)^{(n)}(t)AK^{(n)}(t)\rangle|. \tag{4.18c}$$

Since $K_s$ tends strongly to $K$, it follows from the normality of $\pi_{\beta|m}$, the uniform boundedness of $\{\|K_s\|\}$, and the unitary implementation in $\mathfrak{K}_\beta$ of the automorphism $\tau_{0\beta}(t)$ that w-lim $K_{s,\beta}^*(t)A_\beta K_{s,\beta}(t) = K_\beta^*(t)A_\beta K_\beta(t)$ as $s \to \infty$. Hence, it follows from the normality of $\Psi_l$ and the uniform boundedness of $\{\|K_s\|\}$ that

$$\lim_{s\to\infty} \text{term}(4.18\text{a}) = 0. \tag{4.19}$$

Further, it follows from Eq. (4.16) that

$$\lim_{n\to\infty} \text{term } (4.18\text{b}) = 0. \tag{4.20}$$

Next we note that, since $\psi_l^{(n)}$ is a positive element of $\mathfrak{A}_*^{(n)}$, we may use the Schwarz inequality $|\langle \psi_l^{(n)}; A_1A_2\rangle| \leq \langle \psi_l^{(n)}; A_1A_1^*\rangle^{1/2} \langle \psi_l^{(n)}; A_2A_2\rangle^{1/2}$, $\forall\, A_1, A_2 \in \mathfrak{A}^{(n)}$.

Thus,

$$\text{term } (4.18\text{c}) \leq \langle \psi_l^{(n)}; [(K^* - K_s^*)(K - K_s)]^{(n)}(t)\rangle^{1/2} \times [\langle \psi_l^{(n)}; K_s^{*(n)}(t)AA^*K_s^{(n)}(t)\rangle^{1/2} + \langle \psi_l^{(n)}; K^{*(n)}(t)AA^*K^{(n)}(t)\rangle^{1/2}].$$

Consequently, in view of the uniform boundedness of

$\{\|K_s\|\}$ we can easily find a finite quality $D$, independent of $l, s$, and $n$, such that

$$\text{term (4.18c)} \le D\,\langle \psi_l^{(n)}; [(K^* - K_s^*)(K - K_s)]^{(n)}(t)\rangle^{1/2}. \tag{4.21}$$

Moreover, it follows from Eq. (4.17), Def. 4.1 (ii), and the definition of $\pi_{\beta|m}$ that

$$\lim_{n\to\infty} \langle \psi_l^{(n)}; ((K^* - K_s^*)(K - K_s))^{(n)}(t)\rangle = \langle \Psi_l; \tau_{0\beta}(t)\pi_{\beta|m}((K^* - K_s^*)(K - K_s))\rangle. \tag{4.22}$$

In view of the normality of $\Psi_l$ and $\pi_{\beta|m}$, the uniform boundedness of $\{\|K_s\|\}$ and the strong convergence of $K_s$ to $K$, it follows that the right-hand side of Eq. (4.22) tends to zero as $s\to\infty$. Hence Eqs. (4.21) and (4.22) imply that

$$\lim_{s\to\infty}\lim_{n\to\infty} \text{term (4.18c)} = 0. \tag{4.23}$$

Since term (4.18a) is independent of $n$, it follows from Eqs. (4.18)–(4.20) and (4.23) that

$$\lim_{s\to\infty}\lim_{n\to\infty} \text{term (4.18)} = 0.$$

Since term (4.18) is independent of $s$, it follows that it tends to zero as $n\to\infty$. Hence, assumptions (i) and (ii) imply Eq. (4.16). QED

*Lemma 4.3:* With the above definitions and assumptions,

$$\lim_{n\to\infty} \langle \tilde\psi \otimes \hat\phi_\beta^{(n)}; A_k^{(n)}(t_k)\cdots A_1^{(n)}(t_1)\rangle = \langle \tilde\psi \otimes \hat\Phi_\beta; A_{k,\beta}(t_k)\cdots A_{1,\beta}(t_1)\rangle,$$
$$\forall\, \tilde\psi \in \tilde{\mathfrak{A}}_*^\dagger, \quad A_1,\ldots,A_k \in \mathfrak{A}_L, \quad t_1,\ldots,t_k \in \mathbf{R}, \quad k < \infty.$$

*Proof:* Let $A_1,\ldots,A_k \in \mathfrak{A}_L$. Then, for sufficiently large $m(\in \mathbf{Z}_+)$, these elements of $\mathfrak{A}$ all belong to $\mathfrak{A}^{(m)}$. For each $A_j, j = 1,\ldots,k$, we introduce a sequence $\{A_{j,s}\}$ of normwise uniformly bounded elements of $\tilde{\mathfrak{A}} \otimes \hat{\mathfrak{A}}^{(m)}$ which converges strongly to $A_j$ as $s\to\infty$. We then use the inequality

$$|\langle \tilde\psi \otimes \hat\phi_\beta^{(n)}; A_k^{(n)}(t_k)\cdots A_1^{(n)}(t_1)\rangle - \langle \tilde\psi \otimes \hat\Phi_\beta; A_{k,\beta}(t_k)\cdots A_{1,\beta}(t_1)\rangle| \tag{4.24}$$
$$\le |\langle \tilde\psi \otimes \hat\phi_\beta^{(n)}; A_k^{(n)}(t_k)\cdots A_1^{(n)}(t_1)\rangle - \langle \tilde\psi \otimes \hat\Phi_\beta; A_{k,s,\beta}(t_k)\cdots A_{1,s,\beta}(t_1)\rangle| \tag{4.24a}$$
$$+ |\langle \tilde\psi \otimes \hat\Phi_\beta; A_{k,\beta}(t_k)\cdots A_{1,\beta}(t_1) - A_{k,s,\beta}(t_k)\cdots A_{1,s,\beta}(t_1)\rangle| \tag{4.24b}$$
$$+ \sum_{j=1}^{k} |\langle \tilde\psi \otimes \hat\phi_\beta^{(n)}; A_{k,s}^{(n)}(t_k)\cdots A_{j+1,s}^{(n)}(t_{j+1}) (A_j - A_{j,s})^{(n)}(t_j) A_{j-1}^{(n)}(t_{j-1})\cdots A_1^{(n)}(t_1)\rangle|. \tag{4.24c}$$

Now, since $\{A_{j,s}\} \in \tilde{\mathfrak{A}} \otimes \hat{\mathfrak{A}}^{(m)}$, it follows from Lemma 4.1 that

$$\lim_{n\to\infty} \text{term (4.24a)} = 0. \tag{4.25}$$

Further, it follows from the normality of $\pi_{\beta|m}$ and $\tilde\psi \otimes \hat\Phi_\beta$, together with the strong convergence of $A_{j,s}$ to $A_j$ and the uniform boundedness of $\{\|A_{j,s}\|\}$, that

$$\lim_{s\to\infty} \text{term (4.24b)} = 0. \tag{4.26}$$

In order to treat term (4.24c), we invoke the Schwartz inequality

$$|\langle \tilde\psi \otimes \hat\phi_\beta^{(n)}; B_1 B_2 B_3\rangle| \le \langle \tilde\psi \otimes \hat\phi_\beta^{(n)}; B_1 B_1^*\rangle^{1/2} \times \langle \tilde\psi \otimes \hat\phi_\beta^{(n)}; B_3^* B_2^* B_2 B_3\rangle^{1/2}.$$

Applying this inequality to the case where $B_1 = A_{k,s}^{(n)}(t_k)\cdots A_{j+1,s}^{(n)}(t_{j+1})$, $B_2 = (A_j - A_{j,s})^{(n)}(t_j)$, and $B_3 = A_{j-1}^{(n)}(t_{j-1})\cdots A_1^{(n)}(t_1)$, and using the definition of $\psi_j^{(n)}$ given by Eq. (4.11), we see that (for $t_0 = 0$)

summand in (4.24c)
$$\le \langle \psi_{j-1}^{(n)}; ((A_j^* - A_{j,s}^*)(A - A_{j,s}))^{(n)}(t_j)\rangle^{1/2} \times \langle \tilde\psi \otimes \hat\phi_\beta^{(n)}; A_{k,s}^{(n)}(t_k)\cdots A_{j+1,s}^{(n)}(t_{j+1}) \times A_{j+1,s}^{*(n)}(t_{j+1})\cdots A_{k,s}^{*(n)}(t_k)\rangle^{1/2}$$

Hence, in view of the uniform boundedness of $\{\|A_{j,s}\|\}$, we can easily find a finite positive quantity $L$, independent of $n, j$, and $s$, such that

$$\text{summand in (4.24c)} < L\langle \psi_{j-1}^{(n)}; ((A_j^* - A_{j,s}^*) \times (A_j - A_{j,s}))^{(n)}(t_j)\rangle^{1/2}. \tag{4.27}$$

By Lemma 4.2, we are now justified in assuming Eq. (4.15) and thus in treating the inequality (4.27) by the method applied earlier to the inequality (4.21). Hence,

$$\lim_{s\to\infty}\lim_{n\to\infty} \text{term (4.24c)} = 0. \tag{4.28}$$

Since term (4.24b) is independent of $n$, it follows from the inequalities (4.20)–(4.26) and (4.28) that

$$\lim_{s\to\infty}\lim_{n\to\infty} \text{term (4.24)} = 0.$$

Thus, since term (4.24) is independent of $s$, it tends to zero as $n\to\infty$. QED

*Proof of Theorem 4.1:* Our proof of this theorem will consist of two stages. First, we shall show that $\tau_\beta(t)$, defined by Eq. (4.3) as a map from $\mathfrak{A}_\beta''$ into $\mathfrak{L}(\mathfrak{K}_\beta)$, is indeed an automorphism of $\mathfrak{A}_\beta''$. Secondly, we shall show that $\phi(t)$, defined by Eq. (4.2) in terms of this automorphism, does satisfy Eq. (4.1).

Thus, we start by noting that, since $V_\beta \in \mathfrak{L}(\mathfrak{K}_\beta)$, it follows from Eqs. (4.3) and (4.9) that $\tau_\beta(t)$ may be expressed in terms of $\tau_{0\beta}(t)$ by the following interaction-representational formula (cf. Guenin[22]):

$$\tau_\beta(t)A_\beta = A_\beta(t) + \sum_{r=1}^{\infty} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \times \int_0^{t_{r-1}} dt_r \eta_\beta(t_r)\eta_\beta(t_{r-1})\cdots\eta_\beta(t_1)A_\beta(t), \quad \forall\, A \in \mathfrak{A}, \quad t \in \mathbf{R}, \tag{4.29}$$

where $\eta_\beta$ is the map from $\mathbf{R}$ into $\mathfrak{L}(\mathfrak{A}_\beta'')$ defined by

$$\eta_\beta(t)Q = i\,[V_\beta(t), Q]_-, \quad \forall\, Q \in \mathfrak{A}_\beta'', \quad t \in \mathbf{R}, \tag{4.30}$$

and where the integrals in Eq. (4.29) are strong limits of Riemann sums. It follows from Eq. (4.30) that the norm of the summand in Eq. (4.29) is majorized by $\|A\|(2\|V\|\|t\|)^r/r!$ Thus Eq. (4.29) expresses $\tau_\beta(t)$ as the strong limit of a sequence of elements of $\mathfrak{A}_\beta''$ whose

norms are uniformly bounded by $\|A\| \exp(2\|V\|\,|t|)$. Since $\mathfrak{A}''_\beta$ is a $W^*$-algebra and is therefore strongly closed, it follows that $\tau_\beta(t)$ maps $\mathfrak{A}_\beta$ into $\mathfrak{A}''_\beta$. Further, since this mapping is unitarily implemented in $\mathfrak{K}_\beta$, it follows that $\tau_\beta(t) \in \mathrm{Aut}\,\mathfrak{A}''_\beta$.

It remains for us to show that $\phi(t)$, as defined by Eq. (4.2), satisfies Eq. (4.1). For this purpose, we note that $\tilde{\phi} \otimes \hat{\Phi}_\beta \in (\mathfrak{A}''_\beta)_*$ and, therefore, is strongly continuous in any bounded region of $\mathfrak{A}''_\beta$. Thus, since Eq. (4.29) expresses $\tau_\beta(t)A_\beta$ as a strong limit of elements in such a region, it follows from that formula together with Def. 2.2 and Eq. (4.2) that

$$\langle \phi(t);A\rangle = \langle \tilde{\phi} \otimes \hat{\Phi}_\beta; A_\beta(t)\rangle + \sum_{r=1}^{\infty} \int_0^t dt_1 \cdots \times \int_0^{t_{r-1}} dt_r \langle \tilde{\phi} \otimes \hat{\Phi}_\beta; \eta_\beta(t_r)\cdots\eta_\beta(t_1)A_\beta(t)\rangle, \quad \forall A \in \mathfrak{A},\ t \in \mathbf{R}. \tag{4.31}$$

Similarly, it follows from Eqs. (3.8) and (4.7) that

$$\langle \tau^{(n)*}(t)(\tilde{\phi} \otimes \hat{\phi}_\beta^{(n)});A\rangle = \langle \tilde{\phi} \otimes \hat{\phi}_\beta^{(n)}; A^{(n)}(t)\rangle + \sum_{r=1}^{\infty} \int_0^t dt_1 \cdots \int_0^{t_{r-1}} dt_r \langle \tilde{\phi} \otimes \hat{\phi}_\beta^{(n)}; \eta^{(n)}(t_r)\cdots \times \eta^{(n)}(t_1)A^{(n)}(t)\rangle, \quad \forall A \in \mathfrak{A}^{(n)},\ t \in \mathbf{R}. \tag{4.32}$$

where $\eta^{(n)}$ is the map from $\mathbf{R}$ into $\mathfrak{A}^{(n)}$ defined by

$$\eta^{(n)}(t)A = i[V^{(n)}(t), A]_-, \quad \forall A \in \mathfrak{A}^{(n)},\ t \in \mathbf{R}. \tag{4.33}$$

Now by Lemma 4.3 and Eqs. (4.30), (4.33),

$$\lim_{n\to\infty} \langle \tilde{\phi} \otimes \hat{\phi}_\beta^{(n)}; \eta_\beta^{(n)}(t_r)\cdots\eta^{(n)}(t_1)A^{(n)}(t)\rangle = \langle \tilde{\phi} \otimes \hat{\Phi}_\beta; \eta_\beta(t_r)\cdots\eta_\beta(t_1)A_\beta(t)\rangle, \quad \forall A \in \mathfrak{A}_L,\ t_1,\ldots,t_r, t \in \mathbf{R},\ r < \infty. \tag{4.34}$$

Further, it follows from Eq. (4.33) that the modulus of the summand in Eq. (4.32) is majorized by $\|A\| \times \|V\|^r |2t|^r/r!$ and, therefore, the sum in that equation converges uniformly with respect to $n$. Hence, Eq. (4.1) follows directly from Eqs. (4.31), (4.32), and (4.34). QED

## 5. GENERALIZED MASTER EQUATION FOR $\tilde{\mathbf{S}}$

In this Section, we shall derive a generalized master equation (GME) governing the evolution of the state of $\tilde{\mathbf{S}}$, subject to the conditions of Sec. 4. Under these conditions, the time-dependent state $\tilde{\phi}(t)$ of $\tilde{\mathbf{S}}$ will always lie in $\tilde{\mathfrak{A}}_*$ (by the Corollary to Theorem 4.1). Our GME, which will be formulated in Theorem 5.1, is an integro-differential equation, in $\tilde{\mathfrak{A}}_*$, for $\tilde{\phi}(t)$.

*Definition 5.1:* (i) We define a map $a$ (which exists by virtue of Lemma 2.2) of $(\mathfrak{A}''_\beta)_*$ onto $\tilde{\mathfrak{A}}_*$, by the formula

$$\langle a\Psi;\tilde{A}\rangle = \langle \Psi;\tilde{A} \otimes \hat{I}_\beta\rangle, \quad \forall \tilde{A} \in \tilde{\mathfrak{A}},\ \Psi \in (\mathfrak{A}''_\beta)_*. \tag{5.1}$$

(ii) We define a map $\gamma$ of $\tilde{\mathfrak{A}}_*$ into $(\mathfrak{A}''_\beta)_*$ by the formula

$$\gamma\tilde{\psi} = \tilde{\psi} \otimes \hat{\Phi}_\beta, \quad \forall \psi \in \tilde{\mathfrak{A}}_*. \tag{5.2}$$

(iii) We define $\theta_{\beta*} (\in \mathfrak{L}((\mathfrak{A}''_\beta)_*))$ by the formula

$$\theta_{\beta*} = I_{\beta*} - \gamma \circ a, \tag{5.3}$$

where $I_{\beta*}$ is the unit operator in $(\mathfrak{A}''_\beta)_*$.

*Note:* It follows from these definitions that

$$a \circ \theta_{\beta*} = 0, \tag{5.4}$$

$$\theta_{\beta*} \circ \gamma = 0, \tag{5.5}$$

and $\theta_{\beta*}$ is a parallel projector, i.e., $\theta_{\beta*}^2 = \theta_{\beta*}$. This latter property enables us to adapt Zwanzig's[5] techniques to the present situation.

Next we note that, since $\tilde{\tau}(\mathbf{R})$ is a group of spatial automorphisms of $\tilde{\mathfrak{A}}$ in $\tilde{\mathfrak{K}}$, it follows that the dual group $\tilde{\tau}^*(\mathbf{R})$ maps $\tilde{\mathfrak{A}}_*$ onto $\tilde{\mathfrak{A}}_*$. Likewise the group $\tau^*_\beta(\mathbf{R})$ (resp. $\tau^*_{0\beta}(\mathbf{R})$, $\hat{\tau}^*_\beta(\mathbf{R})$) maps $(\mathfrak{A}''_\beta)_*$ [resp. $(\mathfrak{A}''_\beta)_*$, $(\hat{\mathfrak{A}}''_\beta)_*$] onto itself. Further, it follows from Eq. (4.30) that, fixed $t \in \mathbf{R}$, $\eta_\beta(t)$ is an ultraweakly continuous linear transformation of $\mathfrak{A}''_\beta$; and, consequently, the dual transformation $\eta^*_\beta(t)$ maps $(\mathfrak{A}''_\beta)_*$ into $(\mathfrak{A}''_\beta)_*$. These considerations permit one to make the following definitions.

*Definition 5.2:* (i) We define $\tilde{\tau}_*(\mathbf{R})$ to be the group in $\mathfrak{L}(\tilde{\mathfrak{A}}_*)$ given by the restriction to $\tilde{\tau}^*(\mathbf{R})$ to $\tilde{\mathfrak{A}}_*$.

(ii) We define $\hat{\tau}_{\beta*}(\mathbf{R})$ to be the group in $\mathfrak{L}((\hat{\mathfrak{A}}''_\beta)_*)$ given by the restriction of $\hat{\tau}^*_\beta(\mathbf{R})$ to $(\hat{\mathfrak{A}}''_\beta)_*$.

(iii) We define $\tau_{\beta*}(\mathbf{R})$ [resp. $\tau_{0\beta*}(\mathbf{R})$] to be the group in $\mathfrak{L}((\mathfrak{A}''_\beta)_*)$ given by the restriction of $\tau^*_\beta(\mathbf{R})$ [resp. $\tau^*_{0\beta}(\mathbf{R})$] to $\mathfrak{L}((\mathfrak{A}''_\beta)_*)$.

(iv) We define $\eta_{\beta*}$ to be the map from $\mathbf{R}$ into $\mathfrak{L}((\mathfrak{A}''_\beta)_*)$ such that, for $t \in \mathbf{R}$, $\eta_{\beta*}(t)$ is the restriction of $\eta^*_\beta(t)$ to $(\mathfrak{A}''_\beta)_*$.

(v) We define the map $\tilde{\sigma}_*$ of $\mathbf{R}$ into $\mathfrak{L}(\tilde{\mathfrak{A}}_*)$ by the formula.

$$\tilde{\sigma}_*(t) = a \circ \tau_{\beta*}(t) \circ \gamma, \quad \forall t \in \mathbf{R}. \tag{5.6}$$

Thus, it follows from Eqs. (4.2), (4.4), and (5.6), together with Def. 5.1, that $\tilde{\phi}(t)$ may be expressed in the form

$$\tilde{\phi}(t) = \tilde{\sigma}_*(t)\tilde{\phi}, \quad \forall t \in \mathbf{R}. \tag{5.7}$$

*Lemma 5.1:* (i) $\tilde{\tau}_*(t)$ is strongly continuous with respect to $t$ in $\mathfrak{L}(\tilde{\mathfrak{A}}_*)$; and (ii) $\tau_{\beta*}(t)$, $\tau_{0\beta*}(t)$, and $\eta_{\beta*}(t)$ are strongly continuous with respect to $t$ in $\mathfrak{L}((\mathfrak{A}''_\beta)_*)$.

*Proof:* (i) In view of the group property of $\tilde{\tau}_*(\mathbf{R})$, it suffices for us to prove strong continuity at $t = 0$. Further, since $\tilde{\mathfrak{A}}_*$ is the norm closure of linear combinations of vector functionals[14] on $\mathfrak{A}$, it suffices to prove continuity of $\tilde{\tau}_*(t)$ (at $t = 0$) on these latter functionals.

Let $\tilde{\omega}_x$ be the vector functional on $\tilde{\mathfrak{A}}$ corresponding to $x \in \mathfrak{K}$. Then it follows from Eq. (3.1) and Defs. (2.1), 5.2 (i) that

$$\|\langle \tilde{\tau}_*(t)\tilde{\omega}_x - \tilde{\omega}_x;\tilde{A}\rangle\| \le 2\,\|\tilde{A}\|\,\|x\|\,\|\tilde{U}(t)x - x\|, \quad \forall \tilde{A} \in \tilde{\mathfrak{A}},\ t \in \mathbf{R}.$$

Hence, in view of the strong continuity of $\tilde{U}(t)$, it follows that $\tilde{\tau}_*(t)\tilde{\omega}_x$ tends strongly to $\tilde{\omega}_x$ (in $\tilde{\mathfrak{A}}_*$) as $t \to 0$. Thus, $\tilde{\tau}_*(\mathbf{R})$ is a strongly continuous group in $\mathfrak{L}(\tilde{\mathfrak{A}}_*)$. (ii) The strong continuity of $\tau_{\beta*}(\mathbf{R})$ and $\tau_{0\beta*}(\mathbf{R})$ likewise follows from the fact that these groups are unitarily implemented by strongly-con-

tinuous groups in $\mathcal{K}_\beta$. Further, it follows from Def. 5.2 (i) and Eqs. (4.9) and (4.30) that $\eta_{\beta*}(t) = \tau_{0\beta*}(-t) \times \eta_{\beta*}(0)\tau_{0\beta*}(t)$, $\forall\, t \in \mathbf{R}$. Thus, the uniform boundedness of $\|\tau_{0\beta*}(t)\|\,(=1)$ and the strong continuity of $\tau_{0\beta*}(t)$ ensure the strong continuity of $\eta_{\beta*}(t)$. QED

It follows[23] from this Lemma that the groups $\tilde{\tau}_*(\mathbf{R})$, $\tau_{0\beta*}(\mathbf{R})$, and $\tau_{\beta*}(\mathbf{R})$ are generated by closed, densely defined linear transformations of $\tilde{\mathfrak{A}}_*$, $(\mathfrak{A}''_\beta)_*$, and $(\mathfrak{A}''_\beta)_*$, respectively.

*Definition 5.3:* We denote the infinitesimal generators of $\tilde{\tau}_*(\mathbf{R})$, $\tau_{\beta*}(\mathbf{R})$, $\tau_{0\beta*}(\mathbf{R})$ (i.e., the strong derivatives of $\tilde{\tau}_*(t)$, $\tau_{\beta*}(t)\tau_{0\beta*}(t)$ at $t = 0$) by $\xi_*$, $\xi_{\beta*}$, $\xi_{0\beta*}$; and the domains of these generators by $\mathfrak{D}_*\mathfrak{D}_{\beta*}$, $\mathfrak{D}_{0\beta*}$, respectively.

*Lemma 5.2:* With the above definitions and assumptions, $\mathfrak{D}_{\beta*} = \mathfrak{D}_{0\beta*}$ and

$$\xi_{\beta*} = \xi_{0\beta*} + \eta_{\beta*}(0).$$

*Proof:* Let $Q \in \mathfrak{A}''_\beta$ and $\Psi \in (\mathfrak{A}''_\beta)_*$. Then, following the procedure used to derive Eq. (4.31), we obtain the formula

$$\langle \tau^*_\beta(t)\Psi; Q\rangle = \langle \tau^*_{0\beta}(t)\Psi; Q\rangle + \sum_{r=1}^{\infty} \int_0^t dt_1 \cdots \int_0^{t_{r-1}} dt_r \times \langle \Psi; \eta_\beta(t_r)\cdots\eta_\beta(t_1)(\tau_{0\beta}(t)Q)\rangle.$$

Hence, using Defs. 5.2 (iii), 5.2 (iv) and Eq. (4.30), we obtain the inequality

$$\left\| \left\langle \frac{(\tau_{\beta*}(t) - I_{\beta*})}{t}\Psi - \frac{(\tau_{0\beta*}(t) - I_{\beta*})}{t}\Psi - \eta_{\beta*}(0)\Psi; Q\right\rangle \right\| \le \left( \left| t^{-1}\int_0^t dt_1 \| \eta_{\beta*}(t_1) - \eta_{\beta*}(0)\| \right| + \sum_{r=2}^{\infty} 2^r |t|^{r-1}\|V\|^r/r! \right)\|Q\|.$$

Consequently, in view of the strong continuity of $\eta_{\beta*}(t)$ [Lemma 5.1 (ii)],

$$(s, (\mathfrak{A}''_\beta)_*) - \lim_{t\to 0} \left( \frac{(\tau_{\beta*}(t) - I_{\beta*})}{t} - \frac{(\tau_{0\beta*}(t) - I_{\beta*}}{t} - \eta_{\beta*}(0) \right)\Psi = 0, \quad \forall\, \Psi \in (\mathfrak{A}''_\beta)_*. \tag{5.8}$$

Since $\eta_{\beta*}(0)$ is bounded, and since $\mathfrak{D}_{\beta*}, \mathfrak{D}_{0\beta*}$ are the domains[23] on which $t^{-1}(\tau_{\beta*}(t) - I_{\beta*}), t^{-1}(\tau_{0\beta*}(t) - I_{\beta*})$, respectively, converge strongly as $t \to 0$, the required result follows from Eq. (5.8) and Def. 5.3. QED

*Corollary:*

(i) $\gamma$ maps $\tilde{\mathfrak{D}}_*$ into $\mathfrak{D}_{\beta*}$;

(ii) $a$ maps $\mathfrak{D}_{\beta*}$ into $\tilde{\mathfrak{D}}_*$;

(iii) $\theta_{\beta*}$ maps $\mathfrak{D}_{\beta*}$ into $\mathfrak{D}_{\beta*}$;

(iv) $\tilde{\sigma}_t(t)$ maps $\tilde{\mathfrak{D}}_*$ into $\tilde{\mathfrak{D}}_*$, $\forall\, t \in \mathbf{R}$;

(v) $a \circ \xi_{0\beta*} \circ \gamma = \tilde{\xi}_*$ on $\tilde{\mathfrak{D}}_*$;

(vi) $\theta_{\beta*}\xi_{0\beta*} = \xi_{0\beta*}\theta_{\beta*} = \theta_{\beta*}\xi_{0\beta*}\theta_{\beta*}$ on $\mathfrak{D}_{\beta*}$; and

(vii) $a \circ \xi_{0\beta*}\theta_{\beta*} = 0$ on $\mathfrak{D}_{\beta*}$.

*Proof:* (i) By Defs. 4.1 (ii), 5.1 (ii), 5.2 (i), and 5.2 (iii), together with the invariance of $\hat{\Phi}_\beta$ under $\hat{\tau}_{\beta*}(\mathbf{R})$,

$$\tau_{0\beta*}(t)\gamma\tilde{\Psi} = (\tilde{\tau}_*(t)\tilde{\Psi}) \otimes \hat{\Phi}_\beta, \quad \forall\, \tilde{\Psi} \in \tilde{\mathfrak{A}}_*,\ \tau \in \mathbf{R}. \tag{5.9}$$

Since $\tilde{\mathfrak{D}}_*$, $\mathfrak{D}_{0\beta*}$ are the domains in which $\tau_*(t)$, $\tau_{0\beta*}(t)$ are strongly differentiable, it follows from Eq. (5.9) that, if $\tilde{\Psi} \in \tilde{\mathfrak{D}}_*$ then $\gamma\tilde{\Psi} \in \mathfrak{D}_{0\beta*}$ ($\equiv \mathfrak{D}_{\beta*}$, by the Lemma). Hence $\gamma$: $\mathfrak{D}_* \to \mathfrak{D}_{\beta*}$.

(ii) By Defs. 4.1 (ii), 5.1 (i), 5.2 (i), and 5.2 (ii),

$$\langle \tilde{\tau}_*(t)a\Psi; A\rangle = \langle \tau_{0\beta*}(t)\Psi; \tilde{A} \otimes \hat{I}_\beta\rangle, \quad \forall\, \tilde{A} \in \hat{\mathfrak{A}},\ t \in \mathbf{R}, \Psi \in (\mathfrak{A}''_\beta)_*. \tag{5.10}$$

Let $\Psi \in \mathfrak{D}_{\beta*}$ ($\equiv \mathfrak{D}_{0\beta*}$). Then $s - (d/dt)\tau_{0\beta*}(t)\Psi = \xi_{0\beta*}\Psi$ at $t = 0$, and hence, using Eq. (5.10),

$$\lim_{t\to 0} \sup_{\|\tilde{A}\| \le 1} \left| \left\langle \frac{(\tilde{\tau}_*(t) - \tilde{I}_*)}{t} a\Psi - a\xi_{0\beta*}\Psi; A\right\rangle \right| \equiv \lim_{t\to 0} \sup_{\|\tilde{A}\| \le 1} \left| \left\langle \left(\frac{\tau_{0\beta*}(t) - I_{\beta*}}{t}\right)\Psi - \xi_{0\beta*}\Psi; \tilde{A} \otimes \hat{I}_\beta\right\rangle \right| = 0. \tag{5.11}$$

Thus $\tilde{\tau}_*(t)a\Psi$ has a strong derivative ($= a\xi_{0\beta*}\Psi$) at $t = 0$, if $\Psi \in \mathfrak{D}_{\beta*}$. Hence $a$ maps $\mathfrak{D}_{\beta*}$ into $\tilde{\mathfrak{D}}_*$.

(iii) follows from (i), (ii), and Eq. (5.3).

(iv) follows from (i) and (ii) together with Def. 5.2 (iii) and the stability[23] of $\mathfrak{D}_{\beta*}$ under $\tau_{\beta*}(\mathbf{R})$.

(v) It follows from Defs. 4.1 (ii), 5.1 (i), 5.1 (ii), 5.2 (i)–(iii) and the invariance of $\hat{\Phi}_\beta$ under $\hat{\tau}_{\beta*}(\mathbf{R})$ that

$$a \circ \tau_{0\beta*}(t) \circ \gamma = \tilde{\tau}_*(t), \quad \forall\, t \in \mathbf{R}. \tag{5.12}$$

Hence by part (i) of this Corollary we may take the strong derivative of Eq. (5.12) on $\tilde{\mathfrak{D}}_*$ with the result that, using Def. 5.3, $a \circ \xi_{0\beta*} \circ \gamma = \tilde{\xi}_*$ on $\tilde{\mathfrak{D}}_*$, as required.

(vi) By Defs. 4.1 (ii), 5.1 (iii), and 5.2 (iii),

$$\theta_{\beta*}\tau_{0\beta*}(t) = \tau_{0\beta*}(t)\theta_{\beta*} = \tau_{0\beta*}(t)\theta_{\beta*}\tau_{0\beta*}(t)\theta_{\beta*}, \quad \forall\, t \in \mathbf{R}.$$

By part (iii) of this Corollary, we may differentiate this equation with respect to $t$ on $\mathfrak{D}_{0\beta*}$ ($\equiv \mathfrak{D}_{\beta*}$). Hence, by Def. 5.3,

$$\theta_{\beta*}\xi_{0\beta*} = \xi_{0\beta*}\theta_{\beta*} = \theta_{\beta*}\xi_{0\beta*}\theta_{\beta*} \text{ on } \mathfrak{D}_{\beta*}, \text{ as required.}$$

(vii) It follows from (vi) and Eq. (5.4) that, on $\mathfrak{D}_{\beta*}$,

$$a \circ \xi_{0\beta*}\theta_{\beta*} = a \circ \theta_{\beta*} = 0. \quad \text{QED}$$

*Lemma 5.3:* Let

$$\xi_{1\beta*} = \xi_{0\beta*} + \theta_{\beta*}\eta_{\beta*}(0)\theta_{\beta*}. \tag{5.13}$$

Then there exists a unique one-parameter group $\{\tau_{1\beta*}(t) \mid t \in \mathbf{R}\}$ ($\in \mathcal{L}(\mathfrak{A}''_\beta)$), whose infinitesimal generator is $\xi_{1\beta*}$.

*Proof:* Let $R(z; \xi_{r\beta*})$ be the resolvent operator for $\xi_{r\beta*}(r = 0, 1)$, with $z \in \mathbf{C}$, i.e.,

$$R(z; \xi_{r\beta*}) = (zI_{\beta*} - \xi_{r\beta*})^{-1}, \quad \text{for } r = 0 \text{ or } 1, \tag{5.14}$$

both sides of this equation being defined in the resolvent set of $\xi_{r\beta*}$.

Since $\|\tau_{0\beta*}(t)\| = 1$, $\forall\, t \in \mathbf{R}$, it follows[24] that

$$\|R(x; \xi_{0\beta})\| \le x^{-1}, \quad \forall\, x \in \mathbf{R}_+. \tag{5.15}$$

Let $x_0$ be an element of $\mathbf{R}_+$ which exceeds $\|\theta_{\beta*}\eta_{\beta*}(0) \times$

$\theta_{\beta*}\|$, this latter norm being finite since $\theta_{\beta*}$ and $\eta_{\beta*}(0)$ both belong to $\mathfrak{L}((\mathfrak{A}''_\beta)_*)$. Then it follows from Eqs. (5.13)–(5.15) that

$$\|R(x+x_0;\xi_{1\beta*})\| < \sum_{n=0}^{\infty} \|\theta_{\beta*}\eta_{\beta*}(0)\theta_{\beta*}\|^n (x+x_0)^{-(n+1)} = (x+x_0-\|\theta_{\beta*}\eta_{\beta*}(0)\theta_{\beta*}\|)^{-1} \le x^{-1}, \quad \forall\, x \in \mathbf{R}_+. \tag{5.16}$$

Moreover, it follows from Eq. (5.14) that $R(z+z_0;\xi_{1\beta*}) \equiv R(z;\xi_{1\beta*} - x_0 I_{\beta*})$, the resolvent operator for $\xi_{1\beta*} - x_0 I_{\beta*}$. Thus, by Eqs. (5.15) and (5.16),

$$\|R(x;\xi_{1\beta*} - x_0 I_{\beta*})\| \le x^{-1}, \quad \forall\, x \in \mathbf{R}_+.$$

By a classical theorem on semigroups,[24] it follows from this last inequality that $(\xi_{1\beta*} - x_0 I_{\beta*})$ is the generator of a uniquely defined one-parameter semigroup $\{\tau_{2\beta*}(t) \mid t \in \mathbf{R}_+\}$, with s-lim $\tau_{2\beta*}(t) = I_{\beta*}$ as $t \to +0$. Hence, defining $\tau^{(+)}_{1\beta*}(t) = \tau_{2\beta*}(t)e^{x_0 t}$, we see that $\xi_{1\beta*}$ is the infinitesimal generator of the semigroup $\{\tau^{(+)}_{1\beta*}(t) \mid t \in \mathbf{R}\}$, with s-lim $\tau^{(+)}_{1\beta*}(t) = I_{\beta*}$ as $t \to +0$.

It remains for us to extend this semigroup into a group. For this purpose, we note that our result concerning the generation of $\tau^{(+)}_{1\beta*}(\mathbf{R}_+)$ by $\xi_{1\beta*}$ followed from Eq. (5.13) together with the facts that (i) $\xi_{0\beta*}$ is the generator of the group $\tau_{0\beta*}(\mathbf{R})$, (ii) $\|\tau_{0\beta*}(t)\| = 1$, and (iii) $\theta_{\beta*}\eta_{\beta*}(0)\theta_{\beta*}$ is bounded. Now it follows from (i)–(iii) that (i)′ $-\xi_{0\beta*}$ is the generator of the group $\{\tau^{(-)}_{0\beta*}(t) \mid t \in \mathbf{R}\}$ defined by the formula $\tau^{(-)}_{0\beta*}(t) \equiv \tau_{0\beta*}(-t)$, (ii)′ $\|\tau^{(-)}_{0\beta*}(t)\| \equiv 1$, and (iii)′ $(-\theta_{\beta*}\eta_{\beta*}(0)\theta_{\beta*})$ is bounded. Hence, by (i)′–(iii)′ and Eq. (5.13), we may apply to $-\xi_{1\beta*}$ precisely the same treatment we used for $\xi_{1\beta*}$. In this way we obtain the result that $-\xi_{1\beta*}$ is the generator of a unique one-parameter semigroup $\{\tau^{(-)}_{1\beta*}(t) \mid t \in \mathbf{R}_+\}$, with s-lim $\tau^{(-)}_{1\beta*}(t) = I_{\beta*}$ as $t \to +0$.

We now note that it follows from Eq. (5.13) and the boundedness of $\theta_{\beta*}\eta_{\beta*}(0)\theta_{\beta*}$ that the domain of $\pm\xi_{1\beta*}$ is $\mathfrak{D}_{\beta*}$. Hence $\tau^{(\pm)}_{1\beta*}(t)$ is strongly differentiable on $\mathfrak{D}_{\beta*}(\equiv \mathfrak{D}_{0\beta*})$ for $t > 0$. Therefore, since $\xi^{(+)}_{1\beta*}$ is the generator of $\tau^{(\pm)}_1(\mathbf{R})$, it follows that

$$s - \frac{d}{dt}(\tau^{(+)}_{1\beta*}(t)\tau^{(-)}_{1\beta*}(t)) = \frac{d}{dt}(\tau^{(-)}_{1\beta*}(t)\tau^{(+)}_{1\beta*}(t)) = 0, \quad \forall\, t \in \mathbf{R}_+.$$

It follows from this equation that, since $\mathfrak{D}_{\beta*}$ is dense in $(\mathfrak{A}''_\beta)_*$ and since $\tau^{(\pm)}_{1\beta*}(t)$ tends strongly to $I_{\beta*}$ as $t \to \pm 0$, then

$$\tau^{(+)}_{1\beta*}(t)\tau^{(-)}_{1\beta*}(t) = \tau^{(-)}_{1\beta*}(t)\tau^{(+)}_{1\beta*}(t) = I_{\beta*}, \quad \forall\, t \in \mathbf{R}.$$

Hence we may construct a one-parameter group $\{\tau_{1\beta*}(t) \mid t \in \mathbf{R}\}$ according to the definition

$$\tau_{1\beta*}(t) = \begin{cases} \tau^{(+)}_{1\beta*}(t), & \text{for } t > 0 \\ I_{\beta*}, & \text{for } t = 0 \\ \tau^{(-)}_{1\beta*}(-t), & \text{for } t < 0 \end{cases}$$

It follows from this construction and from our definition of $\tau^{(\pm)}_{1\beta*}(\mathbf{R}_+)$ that $\xi_{1\beta*}$ is the generator of the group $\tau_{1\beta*}(\mathbf{R})$. QED

*Theorem 5.1:* With the above definitions and assumptions, let $\tilde{\phi} \in \tilde{\mathfrak{D}}_*$. Then $\tilde{\phi}(t)$ lies in $\tilde{\mathfrak{D}}_*$ for all $t \in \mathbf{R}$, and satisfies the GME:

$$(s, \tilde{\mathfrak{A}}_*) - \frac{d}{dt}\phi(t) = \tilde{\xi}_*\tilde{\phi}(t) + \int_0^t dt_1 \tilde{\kappa}(t-t_1)\tilde{\phi}(t_1), \tag{5.17}$$

where

$$\tilde{\xi}_* = \tilde{\xi}_* + a \circ \eta_{\beta*}(0) \circ \gamma \tag{5.18}$$

and

$$\tilde{\kappa}(t) = a \circ \eta_{\beta*}(0)\tau_{1\beta*}(t)\theta_{\beta*}\eta_{\beta*}(0) \circ \gamma, \quad \forall\, t \in \mathbf{R}. \tag{5.19}$$

*Proof:* Assume that $\tilde{\phi} \in \tilde{\mathfrak{D}}_*$. Then it follows from Eq. (5.7), Lemma 5.2, and Corollary (iv) that $\tilde{\phi}(t) \in \tilde{\mathfrak{D}}_*$, $\forall\, t \in \mathbf{R}$.

In order to derive a GME for $\tilde{\phi}(t)$, we define $\Psi(t), \Psi_1(t)$ $[\in (\mathfrak{A}''_\beta)_*]$ by the formulas

$$\Psi(t) = \tau_{\beta*}(t)\gamma\tilde{\phi}, \quad \forall\, t \in \mathbf{R} \tag{5.20}$$

and

$$\Psi_1(t) = \theta_{\beta*}\Psi(t), \quad \forall\, t \in \mathbf{R}. \tag{5.21}$$

Hence, by Eqs. (5.3), (5.6), (5.7), (5.20), and (5.21),

$$\tilde{\phi}(t) = a\Psi(t), \quad \forall\, t \in \mathbf{R} \tag{5.22}$$

and

$$\Psi(t) = \Psi_1(t) + \gamma\tilde{\phi}(t), \quad \forall\, t \in \mathbf{R}. \tag{5.23}$$

Since $\tilde{\phi} \in \tilde{\mathfrak{D}}_*$, it follows from Eqs. (5.20)–(5.22) and Lemma 5.2, Corollary (i) that $\Psi(t), \Psi_1(t)$, and $\tilde{\phi}(t)$ are strongly differentiable with respect to $t$, for all $t \in \mathbf{R}$. Thus, by Eq. (5.20) and Def. 5.3,

$$(s, (\mathfrak{A}''_\beta)_*) - \frac{d}{dt}\Psi(t) = \xi_{\beta*}\Psi(t).$$

We convert this equation into a pair of simultaneous differential equations for $\tilde{\phi}(t)$ and $\Psi_1(t)$ by operating on it with $a$ and $\theta_{\beta*}$, respectively. Thus, using Eqs. (5.21)–(5.23),

$$(s, \tilde{\mathfrak{A}}_*) - \frac{d}{dt}\tilde{\phi}(t) = a\xi_{\beta*}\gamma\tilde{\phi}(t) + a\xi_{\beta*}\Psi_1(t) \tag{5.24}$$

and

$$(s, (\mathfrak{A}''_\beta)) - \frac{d}{dt}\Psi_1(t) = \theta_{\beta*}\xi_{\beta*}\Psi_1(t) + \theta_{\beta*}\xi_{\beta*}\gamma\tilde{\theta}(t). \tag{5.25}$$

Further, it follows from Lemma 5.2, its Corollaries (v)–(vii), and Eqs. (5.3)–(5.5), (5.13), (5.18), and (5.21) that

$$a\xi_{\beta*}{}_\gamma = \tilde{\xi}_*, \quad a\xi_{\beta*}\Psi_1(t) = a\eta_{\beta*}(0)\Psi_1(t),$$

$$\theta_{\beta*}\xi_{\beta*}\Psi_1(t) = \xi_{1\beta*}\Psi_1(t),$$

and

$$\theta_{\beta*}\xi_{\beta*}{}_\gamma\tilde{\phi}(t) = \theta_{\beta*}\eta_{\beta*}(0)\gamma\tilde{\phi}(t).$$

In view of these relations, Eqs. (5.24) and (5.25) may be re-expressed in the forms

$$(s, \tilde{\mathfrak{A}}_*) - \frac{d}{dt}\tilde{\phi}(t) = \tilde{\xi}_*\tilde{\phi}(t) + a\eta_{\beta*}(0)\Psi_1(t) \tag{5.26}$$

and

$$(s, (\mathfrak{A}''_\beta)_*) - \frac{d}{dt}\Psi_1(t) - \xi_{1\beta*}\Psi_1(t) = \theta_{\beta*}\eta_{\beta*}(0)\gamma\tilde{\phi}(t).$$

Operating with $\tau_{1\beta*}(-t)$ on this last equation and using Lemma 5.3, we obtain

$$(s, (\mathfrak{A}''_\beta)_*) - \frac{d}{dt}(\tau_{1\beta*}(-t)\Psi_1(t)) = \tau_{1\beta*}(-t)\theta_{\beta*}\eta_{\beta*}(0)\gamma\tilde{\phi}(t). \tag{5.27}$$

Further, since $\tau_{\beta*}(0) = I_{\beta*}$, it follows from Eqs. (5.4), (5.20), and (5.21) that $\Psi_1(0) = 0$. Hence, using the group property of $\tau_{1\beta*}(\mathbf{R})$, we may integrate Eq. (5.27) in the form

$$\Psi_1(t) = (s, (\mathfrak{A}''_\beta)_*) - \int_0^t dt_1 \tau_{1\beta *}(t - t_1)\theta_{\beta *}\eta_{\beta *}(0)\gamma\tilde{\phi}(t_1).$$

On substituting this formula for $\Psi_1(t)$ into Eq. (5.26), we obtain the required GME, as given by Eq. (5.17).

QED

## 6. RESPONSE OF $\tilde{\mathbf{S}}$ TO A MECHANICAL DRIVING FORCE

### A. The Response Functional $\mathfrak{F}$

Since $\hat{\mathbf{S}}$ is coupled to $\tilde{\mathbf{S}}$, one may regard $\tilde{\mathbf{S}}$ as the source of a "driving force" which acts on $\hat{\mathbf{S}}$. The time-dependent response to $\hat{\mathbf{S}}$ to this force is given by the state $\phi(t)$, defined by Eq. (4.5). We shall formulate certain basic properties of this response for cases where $V$ is of the form

$$V = \lambda \tilde{B} \otimes \hat{B}, \tag{6.1}$$

where $\lambda \in \mathbf{R}$ and $\tilde{B}, \hat{B}$ are self-adjoint elements of $\tilde{\mathfrak{A}}$, $\hat{\mathfrak{A}}_L$, respectively. This form of $V$ covers a considerable number of cases of physical interest.

Let $\mathfrak{F}$ be the map from $\mathbf{R} \times \mathbf{R} \times \hat{\mathfrak{A}}$ into $\mathbf{C}$ defined by

$$\mathfrak{F}(\lambda, t; \hat{A}) \equiv \langle \hat{\phi}(t); \hat{A} \rangle_{V = \lambda \tilde{B} \otimes \hat{B}}. \tag{6.2}$$

Then $\mathfrak{F}$ represents the response of $\hat{\mathbf{S}}$ to the driving force generated by $\tilde{\mathbf{S}}$. In order to formulate the properties of $\mathfrak{F}$ we introduce the following definitions.

*Definition 6.1:* (i) For $s = \pm 1$, we define $\tilde{\eta}_s$ to be the map from $\mathbf{R}$ into $\mathcal{L}(\tilde{\mathfrak{A}})$ given by

$$\tilde{\eta}_{-1}(t)\tilde{A} = i\,[\tilde{B}(t), \tilde{A}]_-, \quad \tilde{\eta}_1(t)\tilde{A} = [\tilde{B}(t), \tilde{A}]_+, \quad \forall\, \tilde{A} \in \tilde{\mathfrak{A}},\ t \in \mathbf{R}, \tag{6.3}$$

where $\tilde{B}(t) \equiv \tilde{\tau}(t)\tilde{B}$, as in Eq. (3.1). (ii) For $s = \pm 1$, we define $\hat{\eta}_{\beta,s}$ to be the map from $\mathbf{R}$ into $\mathcal{L}(\hat{\mathfrak{A}}''_\beta)$ given by

$$\hat{\eta}_{\beta,-1}(t)\hat{Q} = i[\hat{B}_\beta(t), \hat{Q}]_-, \quad \hat{\eta}_{\beta,1}(t)\hat{Q} = [\hat{B}_\beta(t), \hat{Q}]_+, \quad \forall\ \hat{Q} \in \hat{\mathfrak{A}}''_\beta,\ t \in \mathbf{R}, \tag{6.4}$$

where $\hat{B}_\beta(t) = \tau_\beta(t)\,\hat{B}_\beta$, as in Eq. (3.6).

*Note:* It follows from Defs. 4.1 (ii), 6.1, together with Eqs. (4.30) and (6.1), that

$$\eta_\beta(t)(\tilde{A} \otimes \hat{Q}) = \tfrac{1}{2}\lambda \sum_{s=\pm 1} \tilde{\eta}_{-s}(t)\tilde{A} \otimes \hat{\eta}_{\beta,s}(t)\hat{Q}, \quad \forall\, \tilde{A} \in \tilde{\mathfrak{A}},\ \hat{Q} \in \hat{\mathfrak{A}}''_\beta,\ t \in \mathbf{R}. \tag{6.5}$$

In particular,

$$\eta_\beta(t)(\tilde{I} \otimes \hat{Q}) = \lambda \tilde{B}(t) \otimes \hat{\eta}_{\beta,-1}(t)\hat{Q}, \quad \forall\ \hat{Q} \in \hat{\mathfrak{A}}''_\beta,\ t \in \mathbf{R}. \tag{6.6}$$

*Definition 6.2:* For $\tilde{\phi} \in \tilde{\mathfrak{A}}^\dagger_*$ and $n \in \mathbf{Z}_+$, we define the map $F_n$ from $\{-1, 1\}^{n-1} \times \mathbf{R}^n$ into $\mathbf{C}$ by the formulas

$$F_1(t) = \tilde{\phi}(\tilde{B}(t)), \quad \forall\, t \in \mathbf{R} \tag{6.7}$$

and, for $n > 1$,

$$F_n(s_2, \ldots, s_n; t_1, \ldots, t_n) = 2^{1-n}\tilde{\phi}(\eta_{-s_n}(t_n) \cdots \tilde{\eta}_{-s_2}(t_2)\tilde{B}(t_1)),$$
$$\forall\, s_2, \ldots, s_n \in \{-1, 1\}, \quad t_1, \ldots, t_n \in \mathbf{R}. \tag{6.8}$$

It will be seen from Eq. (6.9) (below) that the $F_n$ may be regarded as "driving forces."

It follows now from Eqs. (4.5), (4.31), (6.2), and (6.5)–(6.8) that the response functional $\mathfrak{F}$ may be expressed in the following form:

$$\mathfrak{F}(\lambda, t; \tilde{A}) = \hat{\phi}_\beta(\hat{A}) + \lambda \int_0^t dt_1 F_1(t_1)\langle \hat{\Phi}_\beta; \hat{\eta}_{\beta,-1}(t_1)\hat{A}_\beta(t)\rangle + \sum_{r=2}^{\infty} \lambda^r \sum_{s_2=\pm 1} \cdots \sum_{s_r=\pm 1} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \times \int_0^{t_{r-1}} dt_r F_r(s_2, \cdots, s_r; t_1, \cdots, t_r) \times \langle \hat{\Phi}_\beta; \hat{\eta}_{\beta,s_r}(t_r) \ldots \hat{\eta}_{\beta,s_2}(t_2)\hat{\eta}_{\beta,-1}(t_1)\hat{A}_\beta(t)\rangle,$$
$$\forall\, \hat{A} \in \hat{\mathfrak{A}},\ t \in \mathbf{R},\ \lambda \in \mathbf{R}. \tag{6.9}$$

### B. The Fluctuation–Dissipation Theorem

We shall now generalize the fluctuation-dissipation theorem[25] to infinite systems. This theorem will serve to express $(\partial/\partial\lambda)\mathfrak{F}(\lambda, t; \hat{A})_{\lambda=0}$ (i.e., the linear part of the response of $\hat{\mathbf{S}}$ to $\tilde{\mathbf{S}}$) in terms of spontaneous fluctuations of $\mathbf{S}$ about its equilibrium states.

*Definition 6.3:* We define the functions $K_\beta, G_\beta$, from $\hat{\mathfrak{A}} \times \hat{\mathfrak{A}} \times \mathbf{R}$ into $\mathbf{C}$ by the formulas

$$K_\beta(\hat{A}, \hat{B}; t) = -i\,\hat{\Phi}_\beta([\hat{A}_\beta(t), \hat{B}_\beta]_-), \quad \forall\, \hat{A}, \hat{B} \in \hat{\mathfrak{A}},\ t \in \mathbf{R} \tag{6.10}$$

and

$$G_\beta(\hat{A}, \hat{B}; t) = \hat{\Phi}_\beta([\hat{A}_\beta(t), \hat{B}_\beta]_+). \tag{6.11}$$

We also define $\overline{K}_\beta(A, B; \cdot), \overline{G}_\beta(A, B; \cdot)$ to be the Fourier transforms of $K_\beta(A, B; \cdot), G_\beta(A, B; \cdot)$, in the notation of Eq. (2.1); these functions on $\mathbf{R}$ all being $\mathcal{S}'$-class.

*Theorem 6.1:* With the above definitions and notations,

(a) $$\frac{\partial}{\partial\lambda}\,\mathfrak{F}(\lambda, t; \hat{A})_{\lambda=0} = \int_0^t dt_1 K_\beta(\hat{A}, \hat{B}; t - t_1)F_1(t_1); \tag{6.12}$$

(b) $$\overline{K}_\beta(\hat{A}, \hat{B}; \omega) = i\tanh(\tfrac{1}{2}\beta\omega)\overline{G}_\beta(\hat{A}, \hat{B}; \omega), \quad \forall\, A, B \in \hat{\mathfrak{A}},\ \omega \in \mathbf{R}; \tag{6.13}$$

(c) if $\hat{A}$ (like $\hat{B}$) is self-adjoint and if $\hat{B}$ satisfies the assumptions of Lemma 3.2, then

$$\mathrm{Im}\overline{K}_\beta(\hat{A}, \hat{B}; \omega) = f_\beta(\omega)\mathrm{Im}\overline{G}_\beta(\hat{A}, \hat{B}; \omega), \quad \forall\, \hat{A} \in \hat{\mathfrak{A}},\ \omega \in \mathbf{R}, \tag{6.14}$$

where

$$f_\beta(\omega) = \begin{cases} \omega^{-1}\tanh\tfrac{1}{2}\beta\omega, & \text{for } \omega \neq 0 \\ \tfrac{1}{2}\beta, & \text{for } \omega = 0 \end{cases}. \tag{6.15}$$

(d) If further $(\hat{E}_\beta(0)\hat{\mathfrak{A}}''_\beta\hat{E}_\beta(0))''$ is Abelian, where $\hat{E}_\beta(0)$ is the projector for the maximal subspace of $\hat{\mathfrak{K}}_\beta$ that is invariant under $\hat{U}_\beta(\mathbf{R})$, then

$$\overline{K}_\beta(\hat{A}, \hat{B}; \omega) = f_\beta(\omega)\overline{G}_\beta(\hat{A}, \hat{B}; \omega), \quad \forall\, \hat{A} \in \hat{\mathfrak{A}},\ \omega \in \mathbf{R}. \tag{6.16}$$

*Note:* (a), (b), (c) constitute a generalized fluctuation-dissipation theorem, as applied to $\hat{\mathbf{S}}$. As regards the supplementary assumption required for (d), one sees that it is satisfied in either of the following important cases:

(i) $\hat{\Omega}_\beta$ is the only vector in $\hat{\mathcal{H}}_\beta$ that is invariant under $U_\beta(\mathbf{R})$ (i.e., $\hat{\Phi}_\beta$ is $\mathbf{R}$-ergodic);

(ii) $\hat{\mathfrak{A}}_\beta''$ is $\mathbf{R}$-Abelian, in the sense of Lanford and Ruelle.[26]

*Proof of Theorem 6.1:* (a) It follows from Eqs. (6.3)–(6.5) and (6.8) that the modulus of the coefficient of $\lambda^r$ in Eq. (6.9) is majorized by $\|\hat{A}\|(2|t|\times\|\tilde{B}\|\,\|\hat{B}\|)^r/r!$ Thus, we may differentiate Eq. (6.9) term by term with respect to $\lambda$. Hence, using Eq. (6.4),

$$\frac{\partial}{\partial\lambda}\mathfrak{F}(\lambda,t;\hat{A})_{\lambda=0} = -i\int_0^t dt_1\hat{\Phi}_\beta([\hat{A}_\beta(t),\hat{B}_\beta(t_1)]-)F_1(t_1). \tag{6.17}$$

Since $\hat{\Phi}_\beta$ is invariant under $\hat{\tau}_\beta^*(\mathbf{R})$, it follows from Eq. (6.10) that Eq. (6.17) is equivalent to the required formula (6.12).

(b) Equation (6.13) follows directly from the application of the KMS conditions for $\Phi_\beta$ (cf. Def. 2.3) to our Def. 6.3 for $\overline{K}_\beta, \overline{G}_\beta$.

(c) It follows from (b), together with Eq. (6.15), Def. 6.3 and Lemma 3.2 that

$$i\omega[\overline{K}_\beta(\hat{A},\hat{B};\omega) - f_\beta(\omega)\,\overline{G}_\beta(\hat{A},\hat{\tilde{B}};\omega)] = 0, \quad \forall\,\omega\in\mathbf{R}.$$

Since $K_\beta(\hat{A},\hat{B};\cdot)$ and $G_\beta(\hat{A},\hat{\tilde{B}};\cdot)$ are bounded functions of $t$, it follows from this last equation that

$$\overline{K}_\beta(\hat{A},\hat{B};\omega) = f_\beta(\omega)\overline{G}_\beta(\hat{A},\hat{\tilde{B}};\omega) + g\delta(\omega), \quad \forall\,\omega\in\mathbf{R}, \tag{6.18}$$

where $g$ is a constant with respect to $\omega$.

Let $\hat{A},\hat{B}$ be self-adjoint. Then it follows from Def. 6.3 that $\overline{K}_\beta(\hat{A},\hat{B};\omega)$, $\overline{G}_\beta(\hat{A},\hat{\tilde{B}};\omega)$ are the complex conjugates of $\overline{K}_\beta(\hat{A},\hat{B};-\omega)$, $\overline{G}_\beta(\hat{A},\hat{\tilde{B}};-\omega)$, respectively. Hence by Eq. (6.18) and the fact that $f_\beta$ is an even real-valued function on $\mathbf{R}$, it follows that $g$ is real and, therefore,

$$\mathrm{Im}\overline{K}_\beta(\hat{A},\hat{B};\omega) = f_\beta(\omega)\,\mathrm{Im}\overline{G}_\beta(\hat{A},\hat{\tilde{B}};\omega), \quad \forall\,\omega\in\mathbf{R},$$

as required.

(d) Let $\{h_n\}$ be a sequence of $\mathcal{S}$-class functions on $\mathbf{R}$, whose Fourier transforms $\{\bar{h}_n\}$ possess the following properties:

$$\text{(i)}\quad \bar{h}_n(0) = 1, \quad \forall n\in\mathbf{Z}_+, \tag{6.19}$$

$$\text{(ii)}\quad \lim_{n\to\infty}\bar{h}_n(\omega) = 0, \quad \forall\,\omega\in\mathbf{R}\backslash 0; \tag{6.20}$$

and (iii) there exists a finite $N$ such that $|h_n(\omega)|<N$, $\forall\,n\in\mathbf{Z}_+$, $\omega\in\mathbf{R}$. Let $\{k_n\}$ be the sequence of functions on $\mathbf{R}$ defined by

$$\bar{k}_n(\omega) = f_\beta(\omega)\bar{h}_n(\omega). \tag{6.21}$$

Then it follows from Eq. (6.15) that $f_\beta$ is a multiplier[27] in $\mathcal{S}$ and that $|f_\beta(\omega)|\le\frac{1}{2}\beta$, $\forall\,\omega\in\mathbf{R}$. Hence $\{\bar{k}_n\}$ is a set of $\mathcal{S}$-class functions which satisfies conditions (i)–(iii). We shall denote by $k_n$ the function whose Fourier transform is $\bar{k}_n$.

It follows now from Eqs. (6.18), (6.21), and the fact that $\{\bar{h}_n\}$, $\{\bar{k}_n\}$ satisfy property (i) that

$$g = \int_0^t d\omega[\overline{K}_\beta(\hat{A},\hat{B};\omega)\bar{h}_n(\omega) - \overline{G}_\beta(\hat{A}\hat{\tilde{B}};\omega)\bar{k}_n(\omega)],$$

i.e.,

$$g = \int_{-\infty}^{\infty} dt\,[K_\beta(\hat{A},\hat{B};t)h_n(t) - G_\beta(\hat{A},\hat{\tilde{B}};t)k_n(t)], \quad \forall\,n\in\mathbf{Z}_+.$$

By Eqs. (3.6), (6.10), and (6.11), and the invariance of $\hat{\Omega}_\beta$ under $U_\beta(\mathbf{R})$, this last equation may be written in the form

$$g = -i\int_{-\infty}^{\infty} dt\,h_n(t)(\hat{\Omega}_\beta,(\hat{A}_\beta\hat{U}_\beta(-t)\hat{\tilde{B}}_\beta - \hat{\tilde{B}}_\beta\hat{U}_\beta(t)\hat{A}_\beta)\hat{\Omega}_\beta) + \int_{-\infty}^{\infty} dt\,k_n(t)(\hat{\Omega}_\beta,(\hat{A}_\beta\hat{U}_\beta(-t)\hat{\tilde{B}}_\beta + \hat{\tilde{B}}_\beta\hat{U}_\beta(t)\hat{A}_\beta)\hat{\Omega}_\beta), \quad \forall\,n\in\mathbf{Z}_+. \tag{6.22}$$

Let $\{\hat{E}_{\beta,\lambda}\}$ be the family of spectral projectors for $U_\beta(\mathbf{R})$, i.e., $U_\beta(t) = \int e^{i\lambda t}dE_{\beta,\lambda}$, the integral being taken as the strong limit of the Riemann sums. Then

$$\int_{-\infty}^{\infty} dt\,h_n(t)\hat{U}_\beta(\pm t) = \int_{-\infty}^{\infty} dt\,h_n(t)\left(\int_{-\infty}^{\infty} e^{\pm i\lambda t}d\hat{E}_{\beta,\lambda}\right) = (2\pi)^{1/2}\int_{-\infty}^{\infty}\bar{h}_n(\pm\lambda)d\hat{E}_{\beta,\lambda}$$

Hence, it follows from properties (i)–(iii) that

$$\lim_{n\to\infty}\int_{-\infty}^{\infty} dt\,h_n(t)\hat{U}_\beta(\pm t) = (2\pi)^{1/2}\hat{E}_\beta(0). \tag{6.23}$$

Likewise, using Eqs. (6.15) and (6.21),

$$\lim_{n\to\infty}\int_{-\infty}^{\infty} dt\,k_n(t)\hat{U}_\beta(t) = \tfrac{1}{2}\beta(2\pi)^{1/2}\hat{E}_\beta(0). \tag{6.24}$$

Thus, we can now use Eqs. (6.23) and (6.24) to equate $g$ to the limit, as $n\to\infty$, of the right-hand side of Eq. (6.22). Hence, using the fact that $\hat{\Omega}_\beta\in\hat{E}_\beta(0)\hat{\mathcal{H}}_\beta$,

$$g = -i(2\pi)^{1/2}(\hat{\Omega}_\beta,[\hat{E}_\beta(0)\hat{A}_\beta\hat{E}_\beta(0),\hat{E}_\beta(0)\hat{\tilde{B}}_\beta\hat{E}_\beta(0)]_-\hat{\Omega}_\beta) + (2\pi)^{1/2}\tfrac{1}{2}\beta(\hat{\Omega}_\beta,[\hat{E}_\beta(0)\hat{A}_\beta\hat{E}_\beta(0),\hat{E}_\beta(0)\hat{\tilde{B}}_\beta\hat{E}_\beta(0)]_+\hat{\Omega}_\beta). \tag{6.25}$$

Now it follows from Lemma 3.2 together with Eq. (3.6) and the definition of $\hat{E}_\beta(0)$ that, for all $t\in\mathbf{R}$,

$$\hat{E}_\beta(0)\hat{\tilde{B}}_\beta\hat{E}_\beta(0) = \hat{E}_\beta(0)\hat{\tilde{B}}_\beta(t)\hat{E}_\beta(0) = \frac{d}{dt}\hat{E}_\beta(0)\hat{B}_\beta(t)\hat{E}_\beta(0) = \frac{d}{dt}\hat{E}_\beta(0)\hat{B}_\beta\hat{E}_\beta(0) = 0.$$

Thus, the first inner product in Eq. (6.25) vanishes. Further, the second inner product also vanishes in the case where $\{E_\beta(0)\hat{\mathfrak{A}}_\beta''E_\beta(0)\}''$ is Abelian. Hence, in this case, $g=0$; and consequently Eq. (6.18) reduces to the required formula (6.16). QED

*Comment:* This theorem provides a relation between the "linear part" of the response of $\hat{\mathbf{S}}$ to an external force, on the one hand, and the correlation function $G_\beta$ on the other. Since this latter function depends on the spectrum of $\hat{H}_\beta$ [generator of $\hat{U}_\beta(\mathbf{R})$], we see that the FD theorem provides a relationship between the response of $\hat{\mathbf{S}}$ to external forces, on the one hand, and the spectrum of $\hat{H}_\beta$ on the other. This relationship could be of some significance for the purpose of obtaining information, by experimental means, on the spectrum of $\hat{H}_\beta$.

### C. Classical Limit for $\tilde{\mathbf{S}}$

We shall formulate conditions which suffice to ensure that the response functional $\mathfrak{F}$ reduces in an appropriate limit to the response of $\mathbf{S}$ to a "classical" force (suitably defined).

*Definition 6.4:* We term $\tilde{\phi}$ to be $a$-quasicoherent with respect to $(\tilde{B},\tilde{\tau})$ if:

(i) $\tilde{\phi},\tilde{B}$ are functions of a real-valued parameter $a$, in which case we shall indicate the $a$ dependence of $\tilde{\phi},\tilde{B},\mathfrak{F},F_r$ by a suffix $a$; and

(ii) there exists a real-valued function $F$ on $\mathbf{R}$ such that

$$\lim_{a\to 0}\tilde{\phi}_a(\tilde{B}_a(t)\cdots\tilde{B}_a(t_r)) = \prod_{j=1}^{r} F(t_j), \qquad \forall\, t_1,\ldots,t_r \in \mathbf{R},\ r<\infty.$$

*Note:* According to this definition, $a$-quasi coherence is a weaker property than coherence, in the sense used by Glauber[2]: for the latter property requires the factorization of $\tilde{\phi}(\tilde{B}(t_1)\cdots\tilde{B}(t_r))$ into the product $\prod_{j=1}^{r}\tilde{\phi}(\tilde{B}(t_j))$, without any limiting procedure. We shall construct a class of $a$-quasicoherent states in the Appendix.

*Theorem 6.2:* With the above definitions and assumptions, let $\tilde{\phi}$ be an $a$-quasicoherent state with respect to $(\tilde{B},\tilde{\tau})$. Then

$$\lim_{a\to 0}\mathfrak{F}_a(\lambda,t;A) = \hat{\phi}_\beta(\hat{A}) + \sum_{r=1}^{\infty}(i\lambda)^r\int_0^t dt_1\int_0^{t_1}dt_2\cdots\int_0^{t_{r-1}}dt_r \times F(t_1)\cdots F(t_r)\langle\hat{\Phi}_\beta;\hat{\eta}_{\beta,r-1}(t_r)\cdots\hat{\eta}_{\beta,1}(t_1)\hat{A}_\beta(t)\rangle, \qquad \forall\,\hat{A}\in\hat{\mathfrak{A}},\ \lambda,t\in\mathbf{R}. \quad (6.26)$$

*Proof:* Assume that $\tilde{\phi}$ is $a$-quasicoherent with respect to $(\tilde{B},\tilde{\tau})$. Then it follows from Defs. (6.2) and (6.4) that

$$\lim_{a\to 0}F_{1,a}(t) = F(t), \quad (6.27)$$

and

$$\lim_{a\to 0}F_{r,a}(s_2,\ldots,s_r;t_r) = \begin{cases} F(t_1)\cdots F(t_r) & \text{if } s_2=s_3=\cdots=s_r=-1\,. \\ 0 & \text{otherwise}\end{cases} \quad (6.28)$$

Consider now the form of Eq. (6.9), with suffixes $a$ added to $\mathfrak{F},F_r,\tilde{\phi},\tilde{B}$. The modulus of the coefficient of $\lambda^r$ in this equation is still majorized by $\|A\|(2|t|\times\|\tilde{B}\|\,\|\hat{B}\|)^r/r!$; and thus the right-hand side of the equation converges uniformly with respect to $a$. The required result then follows trivially from Eqs. (6.9), (6.27), and (6.28). QED

*Comment:* One can re-express Eq. (6.26) in the form

$$\lim_{a\to 0}\mathfrak{F}_a(\lambda,t;A) = \hat{\Phi}_\beta(\hat{U}_{\beta F}(t)\hat{A}_\beta\hat{U}^*_{\beta F}(t)),$$

where $\{\hat{U}_{\beta F}(t)\mid t\in\mathbf{R}\}$ is the set of unitary operators in $\hat{\mathfrak{K}}_\beta$ defined by

$$\frac{d}{dt}\hat{U}_{\beta F}(t) = i(\hat{H}_\beta + F(t)\hat{B}_\beta)\hat{U}_{\beta F}(t), \qquad \hat{U}_{\beta F}(0)=\hat{I}_\beta,$$

where $\hat{H}_\beta$ is the generator of $\hat{U}_\beta(\mathbf{R})$. Thus, in the limit $a\to 0$, the effect of $\tilde{\mathbf{S}}$ on $\hat{\mathbf{S}}$ is that of a time-dependent perturbation $F(t)\hat{B}$, where $F$ is a real-valued function on $\mathbf{R}$. Thus, $\mathbf{S}$ acts as the source of a "classical" force on $\hat{\mathbf{S}}$ in the $a$-quasicoherent limit ($a\to 0$).

## 7. CONCLUSION

We have constructed a $C^*$-algebraic formulation of the dynamics of a pair of coupled systems, of which one ($\tilde{\mathbf{S}}$) is finite and the other ($\hat{\mathbf{S}}$) infinite. This formulation has been based on the physical assumptions (i)–(iii), specified in Sec. 1.

The principal consequences of these assumptions are as follows.

(i) The dynamics of the Compound system ($\tilde{\mathbf{S}}+\hat{\mathbf{S}}$) is given by Theorem 4.1. In particular (Corollary to Theorem 4.1), the $\tilde{\mathbf{S}}$ always remains normal and that of $\hat{\mathbf{S}}$ always remains in the island $\hat{\vartheta}_\beta$. This last result thus exhibits some of the physical significance of the concept of an "island of states."

(ii) The evolution of $\tilde{\mathbf{S}}$ is given by the GME stated and proved in Theorem 5.1. This GME may be regarded as the generalization of the Liouville equation to open systems. This GME should find natural applications in the theories of irreversibility and ergodicity.

(iii) In cases where the $\tilde{\mathbf{S}}$–$\hat{\mathbf{S}}$ coupling is of the type given by Eq. (6.1), the response of $\hat{\mathbf{S}}$ to the driving force generated by $\tilde{\mathbf{S}}$ corresponds to the functional $\mathfrak{F}$ [Eq. (6.7)]. The linear part of $\mathfrak{F}$ obeys a generalization of the fluctuation theorem to infinite systems (Theorem 6.1): Apart from its theoretical significance, this theorem might have some empirical usefulness for reasons indicated in the Comment following Theorem 6.1. Finally, in cases where the initial state of $\tilde{\mathbf{S}}$ possesses the $a$-quasicoherent property specified in Def. 6.4, the effect of $\tilde{\mathbf{S}}$ on $\hat{\mathbf{S}}$ reduces, in the limit $a\to 0$, to that of a "classical" time-dependent external force. Thus, the $a$-quasicoherence limit corresponds to a classical limit.

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## APPENDIX

We shall now construct an example of an $a$-quasicoherent state. It may be seen that the state will correspond to that of a simple harmonic oscillator, appropriately displaced from its mean equilibrium configuration.

Let $\tilde{W}$ be a strongly continuous map from $\mathbf{C}$ into the unitary operators in $\tilde{\mathfrak{K}}$, such that

$$\tilde{W}(z)\tilde{W}(z') = \tilde{W}(z+z)\exp\tfrac{1}{2}i(\mathrm{Im}\bar{z}z'), \qquad \forall\, z,z'\in\mathbf{C}, \quad (A1)$$

and

$$\tilde{W}(0) = \tilde{I}. \quad (A2)$$

Then $\tilde{W}$ is a regular Weyl representation[28] of the canonical commutation relations in $\tilde{\mathfrak{K}}$. It follows from Eq. (A1) that

$$\tilde{W}(z_0)\tilde{W}(z_2)\cdots\tilde{W}(z_l)\tilde{W}(-z_0) = \tilde{W}(z_1+z_2+\cdots+z_l)\exp i\left\{\sum_{m=1}^{l}(\mathrm{Im}\bar{z}_0z_m) + \frac{1}{2}\sum_{\substack{m,n=1\\ m<n}}^{l}\mathrm{Im}(\bar{z}_m z_n)\right\}, \qquad \forall\, z_0,z_1,\ldots,z_l\in\mathbf{C}. \quad (A3)$$

Assume now that $\tilde{\mathfrak{A}}$ is the $W^*$-algebra generated by $\{\tilde{W}(z)|z \in \mathbf{C}\}$, and that the group $\tilde{\tau}(\mathbf{R})(\in \mathrm{Aut}\,\tilde{\mathfrak{A}})$ is given by

$$\tilde{\tau}(t)\tilde{W}(z) = \tilde{W}(ze^{it}), \quad \forall\, t \in \mathbf{R},\ z \in \mathbf{C}. \tag{A4}$$

By choosing $\tilde{W}$ to be the Fock representation of the Weyl algebra, we ensure[29] that $\tilde{\tau}(\mathbf{R})$ is a group of spatial automorphisms of $\tilde{\mathfrak{A}}$, unitarily implemented in $\tilde{\mathcal{H}}$ by a strongly continuous representation of $\mathbf{R}$.

For $a \in \mathbf{R}$, we specify $\tilde{B}_a(\in \tilde{\mathfrak{A}})$ by the formula

$$\tilde{B}_a = a^{-1}\int_R dk\, f(k/a)\tilde{W}(k). \tag{A5}$$

where $f$ is a continuous function, of class $L^{(1)}$, on $\mathbf{R}$, and where the integral is the strong limit of Riemann sums. We also define $\phi_a$ to be a normal state on $\mathfrak{A}$, of the form

$$\tilde{\phi}_a(\cdot) = \tilde{\psi}(\tilde{W}(ix_0/a)(\cdot)\tilde{W}(-ix_0/a)), \tag{A6}$$

where $x_0(\in \mathbf{R}\backslash 0)$ and $\tilde{\psi}(\in \tilde{\mathfrak{A}}_*^+)$ are independent of $a$. It follows from Eqs. (3.1) and (A3)–(A6) that, for $l < \infty$,

$$\begin{aligned}\tilde{\phi}_a(\tilde{B}_a(t_1)\cdots\tilde{B}_a(t_l)) &= a^{-l}\int_{R^l} dk_1\cdots dk_l f(k_1/a)\cdots f(k_l/a)\\ &\quad\times \tilde{\psi}(\tilde{W}(k_1e^{it_1} + \cdots + k_le^{it_l}))\\ &\quad\times \exp\left(\frac{ix_0}{a}\sum_{n=1}^{l} k_n \cos t_n\right)\\ &\quad\times \exp\left(\frac{i}{2}\sum_{\substack{m,n=1\\ m<n}}^{l} k_m k_n \sin(t_m - t_n)\right).\end{aligned}$$

Hence, using a change of variables $k_m \to ak_m$,

$$\begin{aligned}\tilde{\phi}_a(\tilde{B}_a(t_1)\cdots\tilde{B}_a(t_l)) &= \int_{R^l} dk_1\cdots dk_l f(k_l)\exp\left(ix_0\sum_{n=1}^{l} k_n \cos t_n\right)\\ &\quad\times \tilde{\psi}(\tilde{W}(ak_1e^{it_1} + \cdots + ak_le^{it_l}))\\ &\quad\times \exp\left(\tfrac{1}{2}ia^2\sum_{\substack{m,n=1\\ m<n}}^{l} k_m k_n \sin(t_m - t_n)\right).\end{aligned} \tag{A7}$$

Since $\tilde{W}(0) = \tilde{I}$ and $f \in L^{(1)}(\mathbf{R})$, it follows from the normality of $\tilde{\psi}$ and the strong continuity of $\tilde{W}$ that the application of Lebesgue's theorem to Eq. (A7) yields

$$\lim_{a\to 0} \tilde{\phi}_a(\tilde{B}_a(t_1)\cdots\tilde{B}_a(t_l)) = F(t_1)\cdots F(t_l), \quad \forall\, t, \ldots, t_l \in \mathbf{R}, \tag{A8}$$

where $F(t) = \int_R dk f(\mathrm{k})\exp(ik\cos t)$, $\forall\, t \in \mathbf{R}$.

Thus, by Eq. (A8) and Def. 6.4, $\tilde{\phi}$ is an $a$-quasicoherent state with respect to $(\tilde{B}, \tilde{\tau})$, as required.

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# Complex Time, Contour Independent Path Integrals, and Barrier Penetration

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By developing an analogy between the Feynman path integral and contour integral representations of the special functions, we obtain WKB formulas for barrier penetration from a path integral. We first show that there exists for the path integral a notion of contour independence in the time parameter. We then select an appropriate contour to describe the physical situation of barrier penetration and obtain asymptotic formulas from the function space integral. The method is interpreted as a path integral derivation of the complex ray description of barrier penetration. In the last three sections we investigate several canonical problems of the theory of complex rays with these path integral techniques.

## 1. INTRODUCTION

Many asymptotic formulas of quantum mechanics have been derived from the Feynman path integral (Refs. 1–6). However, formulas associated with barrier penetration have not been obtained in this manner. Here we obtain these "nonclassical" effects from a path integral representation. Our method may be viewed as an analogue in function space of contour representations of the special functions. That is, we perform an analytic continuation of the function space integral with respect to the time parameter and develop a notion of contour independence in this parameter. Then, by selecting an appropriate contour, we extract the asymptotic behavior of the function space integral.

Consider the Green's function $G$ for the one-dimensional time independent Schrödinger equation

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}G(x,x'|E) + (E - V(x))\,G(x,x'|E) = \hbar\delta(x-x'). \tag{1.1}$$

$G$ may be represented as a Fourier transform,

$$G(x,x'|E+i\epsilon) = -i\int_0^\infty dt\,\exp[(i/\hbar) \times (E+i\epsilon)t]K(x,t|x',0), \quad \epsilon > 0, \tag{1.2}$$

where $K$, the kernel of the time-dependent Schrödinger equation, is represented as a path integral,[7]

$$K(x,t|x',0) = \int \mathfrak{D}x(\cdot)\,\exp\{(i/\hbar)S\,[x(\cdot),t]\}, \quad x(\cdot) \in P(x,t|x',0). \tag{1.3}$$

Here $P(x,t|x',0)$ is the set of paths connecting the space–time points $(x',0)$ and $(x,t)$. $S[x(\cdot),t]$ is the action functional of classical mechanics.

When $x$ and $x'$ lie in the same classically allowed region of space, one may extract the asymptotic behavior of $G$ (as $\hbar$ vanishes) directly from representation (1.2) and (1.3). In this case the method of stationary phase in function space is applicable. However, when $x$ and $x'$ do not lie in the same allowed region, the method fails since no real, critical path at energy $E$ connects $x$ and $x'$.

To treat this case we introduce an equivalent function space integral representation of $G$. This equivalent representation is based upon an explicit analytic continuation of $K(x,t|x',0)$ into the lower half $t$ plane by means of a function space integral. As will be discussed in more detail later, existing path integrals, valid in the lower half $t$ plane, are not directly applicable. In Sec. 2, in order to obtain a useful representation, we introduce a notion of the path integral being independent of contour in the $t$ plane, and we show that the representations in question possess this property. In Sec. 3, we utilize this contour independence by selecting a particular contour which is appropriate to the problem at hand. From the function space integral along this contour, we extract the asymptotic behavior of $G$.

Usually barrier penetration is not considered a semiclassical phenomena. Certainly it cannot be described in terms of real classical paths at fixed energy, which is the primary reason that the effect has not been obtained in previous asymptotic evaluations of path integrals.[8] However, it is known[9,10] that complex valued solutions of Newton's equations do penetrate forbidden regions. Further, if these complex rays are used to construct semiclassical wavefunctions, agreement with WKB calculations is obtained. It is this complex ray description of barrier penetration which we obtain from the path integral, as may be seen from the final formula specialized to one barrier, Eq. (3.9). In fact the path integral provides the most direct derivation of the complex ray formulas, in that both the equation defining the dominant path and the approximate Green's function are obtained directly from an exact representation of $G$.

Complex ray methods, while useful in many specific problems,[11] have been plagued with mathematical difficulties. For one, in the general case, no rule exists which provides a rationale to select the parameter with respect to which the analytic continuation is to be made. For quantum mechanics the path integral provides the rule. Our calculations show that the time $t$ is the natural parameter.[12] Secondly, the global validity of complex ray methods is difficult to establish. It is very unlikely that path integral methods will soon answer the questions of global existence by providing error estimates accurate "in the large." Nevertheless, the path integral provides an alternative view of the complex rays, a view based upon extremely direct calculations. As such, it should provide insight into these difficult problems. For this reason we use our methods to study several "canonical problems" in the theory of complex rays; the linear potential (Sec. 4), the parabolic barrier (Sec. 5), and the repulsive coulomb potential for the radial Schrödinger equation (Sec. 6). The last example is included primarily to extend the theory to include the radial Schrödinger equation.

In the first two examples there is a feature of particular interest, namely, integrands possessing critical points which coalesce. In the linear case, when both $x$ and $x'$ lie in the classically forbidden region, a pair of such points produces the relative factor of $\frac{1}{2}\exp(\frac{1}{2}i\pi)$ between the "direct" and "reflected" terms, Eq. (4.14). In the quadratic case, as $E$ approaches the top of the barrier, an infinite number of

critical points coalesce at infinity (Fig. 7), preventing the approximation from being uniform.

The idea of an analytic continuation of the path integral with respect to time is not new. Our starting point, Eq. (2.1), was used by Babbitt[13] and by Feldman[14] in early proofs of the existence of the path integral. However, to our knowledge, we are the first to formulate this notion of the contour independence of the Feynman path integral and to utilize this property for calculational purposes. The present work may be viewed as the first application of the "existence formulas" of Babbitt and Feldman.

While the general analogy between this work and contour representations is striking, it does not cover the specific details of the actual continuation procedure. In fact, no natural analogue of this procedure exists for classical, $N$-dimensional integrals. Such an analogue would be the continuation of an integral such as $\int \cdots \int dx_1 \cdots dx_N f(x_1, \ldots, x_N)$ with respect to the labeling indices $(1, 2, \ldots, N)$. In function space this labeling is continuous, making the entire procedure possible.

## 2. PATH INDEPENDENCE OF THE REPRESENTATIONS

In this section we define the basic representations and develop the notion of contour independence for these representations. Consider any point $t_0$ in the lower half complex $t$ plane. To define $K(x, t_0 | x', 0)$, it seems natural to partition into $N$ subdivisions the ray connecting the origin with $t_0$ (Fig. 1), and to construct the path integral as a limit of $N$-fold integrals

$$K(x, t_0 | x', 0) = \lim_{N\to\infty} \left(\frac{mN}{2\pi i\hbar t_0}\right)^{N/2} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 \cdots dx_{N-1} \times \exp\left[\frac{i}{\hbar} \sum_{j=1}^{N} \left(\frac{mN}{2t_0}(x_j - x_{j-1})^2 - V(x_j)\frac{t_0}{N}\right)\right], \quad x_0 \equiv x', \; x_N \equiv x. \tag{2.1}$$

Certainly if $V(\cdot)$ is (real) continuous and bounded below, the $N$-fold integral exists—convergence being guaranteed by the Gaussian term. In fact for such potentials Babbitt has proven that (2.1) is a valid representation of $K$ in the lower half $t$ plane, and Feldman has extended this class to include all potentials which are Riemann approximable and bounded below.[15] He also established that the limit is independent of the partition of the ray. In this paper we consider the $N$-fold averaging together with the limit on $N$ as the definition of a function space integral and denote it by

$$K(x, t_0 | x', 0) = \int_{x(\cdot)\in P(x,t_0|x',0)} \mathfrak{D}x(\cdot) \times \exp\{(i/\hbar) S[x(\cdot), t_0]\} \tag{2.2}$$

In definition (2.1) the variables of integration $\{x_j\}$ are real. This forces the class of paths $P(x, t_0 | x', 0)$ to be composed of real-valued functions along the ray, that is

$$P(x, t_0 | x', 0) \equiv \{x(\cdot) : \text{ray} \to R \mid x(0) = x', x(t_0) = x\}. \tag{2.3}$$

However, this representation is not particularly suitable for asymptotic evaluation. The saddle point method (in function space) indicates that, as $\hbar$ vanishes, certain critical paths should dominate the behavior of the integral. These critical paths are defined by the variational problem,

$$\delta S[x(\cdot), t_0] = 0, \quad x(0) = x', \quad x(t_0) = x, \tag{2.4}$$

or equivalently by the two point boundary value problem,

$$m\frac{d^2x(\tau)}{d\tau^2} = -\frac{dV}{dx}, \quad x(0) = x', \quad x(t_0) = x. \tag{2.5}$$

In general the solution $\bar{x}(\cdot)$ of (2.5) will not be real valued along the ray connecting the origin with $t_0$. [This may be easily seen by solving (2.5) in a simple case such as the linear potential.] Thus, the critical path $\bar{x}(\cdot)$ will not be a member of the class $P$.

One's first thought is to modify representation (2.2) by enlarging the class $P$ to include complex valued paths. We are hesitant to do this, however, because of the extreme convergence difficulties which would result.[16] We prefer to replace the ray connecting the origin and $t_0$ with a general rectifiable contour $\Gamma : \tau = \tau(s), s \in [0,1]$, $\tau(0) = 0$, $\tau(1) = t_0$. This replacement is permissible because, as we will now show, there exists a notion of contour independence. In Sec. 3 we show that the replacement is useful for asymptotic evaluations.

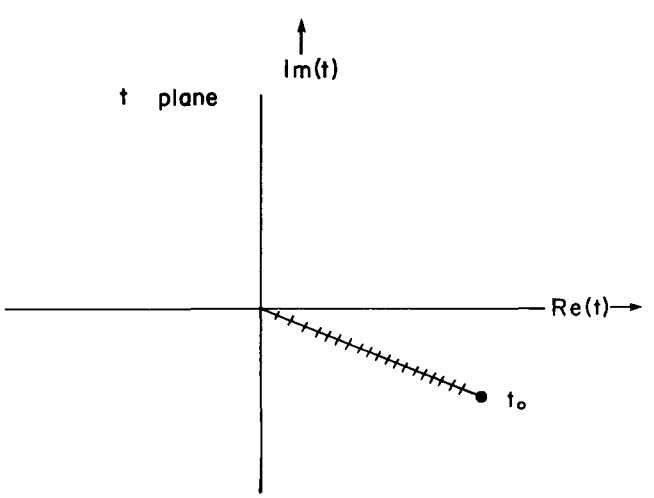


FIG. 1. Partition of ray.

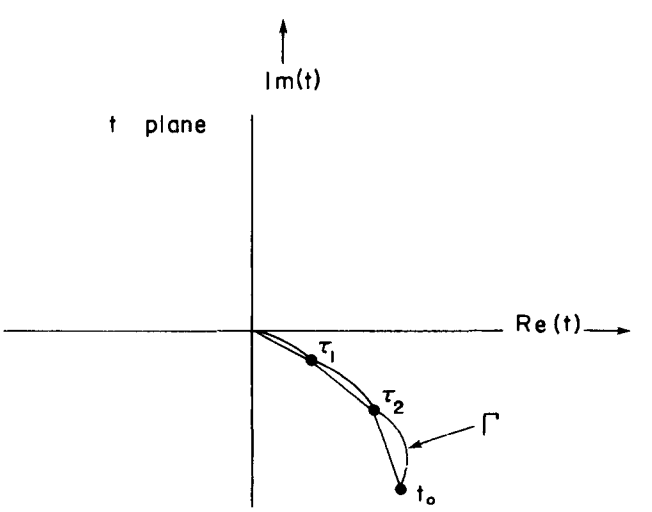


FIG. 2. A typical contour $\Gamma$.

If contour $\Gamma$ has decreasing imaginary part (Fig. 2),

$$\mathrm{Im}(\tau(s_1)) < \mathrm{Im}(\tau(s_2)), \quad s_1 > s_2, \tag{2.6}$$

an $N$-fold partition of $\Gamma$ will certainly yield an $N$ fold convergent integral. The following simple lemma makes it clear that the path integral exists along $\Gamma$, actually being independent of $\Gamma$.

For notational convenience we define the operators $K^t$ as

$$(K^t\psi)(x) \equiv \int_{-\infty}^{\infty} K(x,t\,|\,x',0)\,\psi(x')dx', \qquad \psi \in L^2(R),\ \mathrm{Im}\,t \le 0, \tag{2.7}$$

and $K_N^t$ as

$$(K_N^t\psi)(x) = \left(\frac{mN}{2\pi i\hbar t}\right)^{N/2} \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dx_0\cdots dx_{N-1} \times \exp\left[\frac{i}{\hbar}\sum_{j=1}^{N}\left(\frac{mN}{2t}(x_j - x_{j-1})^2 - V(x_j)\frac{t}{N}\right)\right]\psi(x_0),$$
$$\psi \in L^2(R), \quad \mathrm{Im}\,t \le 0, \quad x_N = x. \tag{2.8}$$

The operators $K^t$ form a holomorphic semigroup in $C^-$, the lower half $t$ plane union the real axis, and the operators $K_N^t$ are uniformly bounded (in $N$) by 1.[17,18]

*Lemma:* For any $\tau$ and $\tau_1$ such that $\tau, \tau_1$, and $(\tau - \tau_1)$ all lie in the lower half complex plane,

$$K^\tau\psi = \lim_{N\to\infty} K_N^{\tau_1}K_N^{\tau-\tau_1}\psi \text{ for all } \psi \in L^2(R).$$

*Proof:* Consider two complex numbers $\tau$ and $\tau_1$, satisfying $\mathrm{Im}\,\tau < 0$, $\mathrm{Im}\,\tau_1 < 0$, and $\mathrm{Im}(\tau - \tau_1) < 0$. Since $K^\tau$ is a holomorphic semigroup in $C^-$;

$$K^\tau = K^{\tau_1}K^{(\tau-\tau_1)}. \tag{2.9}$$

Applying representation (2.1), one obtains

$$K^\tau = (\lim_{N\to\infty} K_N^{\tau_1})\cdot(\lim_{N\to\infty} K_N^{(\tau-\tau_1)}), \tag{2.10}$$

where the limits are taken in the strong sense. The operators $K_N^\tau$ are uniformly bounded (in $N$) by 1. Using the fact that the product of two strongly convergent, uniformly bounded sequences of operators in a Hilbert space is itself strongly convergent, converging to the product of the limits, one concludes

$$K^\tau\psi = \lim_{N\to\infty}(K_N^{\tau_1}K_N^{(\tau-\tau_1)}\psi) \quad \forall\ \Psi \in L^2(R). \tag{2.11}$$

This lemma extends to finite products. Consider any rectifiable contour $\Gamma$ possessing property (2.6), and select any polygonal approximation of $\Gamma$, with vertices $(\tau_0 \equiv 0, \tau_1, \ldots, \tau_{M-1}, \tau_M \equiv t_0)$ lying upon $\Gamma$. The extension of the lemma applies, yielding

$$K^{t_0}\psi = K^{\tau_1}K^{(\tau_2-\tau_1)}\cdots K^{(\tau_M-\tau_{M-1})} = \lim_{N\to\infty}[K_N^{\tau_1}K_N^{(\tau_2-\tau_1)}\cdots K_N^{(\tau_M-\tau_{M-1})}]. \tag{2.12}$$

Since the same operator $K^{t_0}$ is obtained for finer and finer polygonal approximations, we may pass to the limit. Thus, for contours $\Gamma$ satisfying (2.6), we have the notion of a path integral representation of $K^{t_0}$ along $\Gamma$, along with the fact that such representations actually are contour independent. As long as the path integral exists for real $t_0$,[19,20] the above results immediately extend to include contours $\Gamma$ satisfying

$$\mathrm{Im}\,\tau(S_1) \le \mathrm{Im}\,\tau(S_2), \quad S_1 > S_2. \tag{2.6'}$$

## 3. BARRIER PENETRATION FORMULAS

In this section, armed with this notion of contour independence, we define a contour $\Gamma$ appropriate to the problem of barrier penetration and extract from the path integral along $\Gamma$ the asymptotic behavior. Throughout this section we assume that $V(\cdot)$ is smooth enough to guarantee needed existence, uniqueness, and analyticity properties (Appendix).

We consider Eq. (2.5) for the critical path $\bar{x}(\tau)$ and seek those contours in the $t$ plane along which the analytic function $\bar{x}(\tau)$ has constant (in fact no) imaginary part. To describe these contours, we first solve the intitial value problem at energy $\xi = \xi_R + i\xi_I$,

$$\tau(\bar{x}) = \sqrt{\frac{m}{2}}\int_{x'}^{\bar{x}} dz\,[\xi - V(z)]^{-1/2}, \qquad z, x', \bar{x} \in R. \tag{3.1}$$

As long as $\xi_I \neq 0$, the branch point of the square root lies off the real $z$ axis. We restrict ourselves to $\xi_I > 0$ and, without loss of generality, fix $x > x'$. Select that branch of the square root defined by

$$(\xi - V)^{1/2} = +\left(\frac{(\xi_R - V) + [(\xi_R - V)^2 + \xi_I^2]^{1/2}}{2}\right)^{1/2} + i\left(\frac{-(\xi_R - V) + [(\xi_R - V)^2 + \xi_I^2]^{1/2}}{2}\right), \tag{3.2}$$

where all radicals are positive. Under these restrictions, contours defined by (3.1) have decreasing imaginary parts (as $\bar{x}$ increases from $x'$ to $x$).

Define $D$, a subset of the $t$ plane, by

$$D \equiv \{t \in C^- \,|\, t = \sqrt{m/2}\int_{x'}^{x} dz\,[\xi - V(z)]^{-1/2}; \ x, x', z \in R; x > x'; \text{ for some } \xi = \xi_R + i\xi_I, \xi_I > 0\}. \tag{3.3}$$

Consider any $t_0 \in D$. Define $\xi = \xi(t_0)$ by

$$t_0 = \sqrt{m/2}\int_{x'}^{x} dz\,[\xi(t_0) - V(z)]^{-1/2}. \tag{3.1'}$$

Further, define a contour $\Gamma$ by

$$\Gamma: \tau(\bar{x}) \equiv \sqrt{m/2}\int_{x'}^{\bar{x}} dz\,[\xi(t_0) - V(z)]^{-1/2}. \tag{3.1''}$$

$\Gamma$ satisfies (2.6) and defines $\bar{x}(\tau)$, a real-valued solution of (2.5). Since $\Gamma$ satisfies (2.6), the results of Sec. 2 justify selecting it as a contour along which path to integrate.

But now, by construction, the critical path of this function space integral $\bar{x}(\tau)$ is real on $\Gamma$, hence, a member of the class of paths $P$. Expanding the action functional $S[x(\cdot), t_0]$ about $\bar{x}(\cdot)$ while retaining terms through second order, we approximate the path integral by

$$K(x, t_0\,|\,x', 0) \simeq \tilde{K}(x, t_0\,|\,x', 0) \quad \text{as } \hbar \to 0, \tag{3.4}$$

where

$$\tilde{K}(x, t_0\,|\,x', 0) \equiv \exp\left\{\frac{i}{\hbar}\int_{\Gamma^0}^{t_0}\left[\frac{m}{2}\left(\frac{d\bar{x}}{d\tau}\right)^2 - V(\bar{x}(\tau))\right]d\tau\right\} \times \int_{P(0,t_0\,|\,0,0)} \mathfrak{D}x(\cdot)$$

$$\times \exp\left\{\frac{i}{2\hbar}\int_0^{t_0}\left[m\left(\frac{dx}{d\tau}\right)^2 - \alpha(\tau)x^2\right]d\tau\right\},$$

$$\alpha(\tau) \equiv \left(\frac{d^2V}{dx^2}\right)_{x=\bar{x}(\tau)}. \tag{3.5}$$

This path integral, being Gaussian, may be calculated explicitly to yield

$$\tilde{K}(x,t_0|x',0) = \left(\frac{m}{2\pi i\hbar}\right)^{1/2}\left|\frac{\partial^2 S(x,t_0|x',0)}{\partial x\partial x'}\right|^{1/2}$$
$$\times \exp[(i/\hbar)\,S(x,t_0|x',0)],$$
$$S(x,t_0|x',0) = \int_{\Gamma^0}^{t_0} d\tau\left[\frac{1}{2}m\left(\frac{d\bar{x}}{d\tau}\right)^2 - V(\bar{x}(\tau))\right]. \tag{3.6}$$

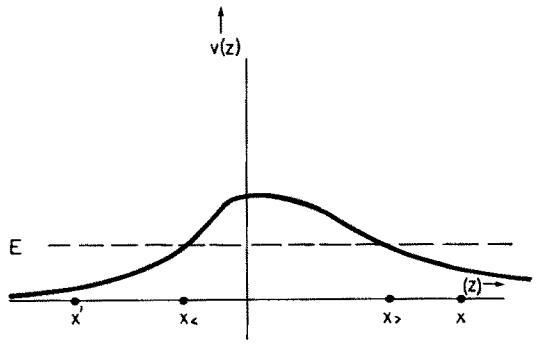


FIG. 3. A typical barrier.

Finally, we relate this calculation to the problem of barrier penetration. Returning to Eq. (1.2) and the case where no real classical path at energy $E$ connects $x$ and $x'$, we deform the path of integration of the Fourier transform to pass through the region $D$. In this region we replace $K$ with its asymptotic approximation (3.6), and find that the integrand which results possesses a critical point $t_0$ in $D$, namely

$$t_0 = \sqrt{\frac{m}{2}}\int_{x'}^{x} dz\,(\xi - V)^{-1/2}, \qquad \xi = E + i\epsilon,\ \epsilon > 0. \tag{3.7}$$

The dominant behavior of $G$ will be given by a neighborhood of $t_0$ and may be calculated by the saddle point method to yield

$$\tilde{G}(x,x'|E + i\epsilon) = e^{(-3\pi i)/4}\left[\left(\frac{m}{2}\right)\left(\frac{\partial^2 S}{\partial x\partial x'}\right)\left(\frac{\partial^2 S}{\partial t_0^2}\right)^{-1}\right]^{1/2}$$
$$\times \exp\{(i/\hbar)\,[(E + i\epsilon)t_0 + S]\}, \quad S \equiv S(x,t_0|x',0). \tag{3.8}$$

When (3.8) is specialized to a single barrier (Fig. 3), (3.7) is used to express $t_0$ in terms of $\xi$, and $\epsilon$ is set at zero, $\tilde{G}$ becomes

$$\tilde{G}(x,x'|E) = -m[k(x)k(x')]^{-1/2}\left[\exp\left(\frac{i}{\hbar}\int_x^{x<} k(x)dx - \frac{1}{\hbar}\right.\right.$$
$$\left.\left.\times \int_{x<}^{x>} K(x)dx + \frac{i}{\hbar}\int_{x>}^{x'} k(x)dx\right)\right],$$

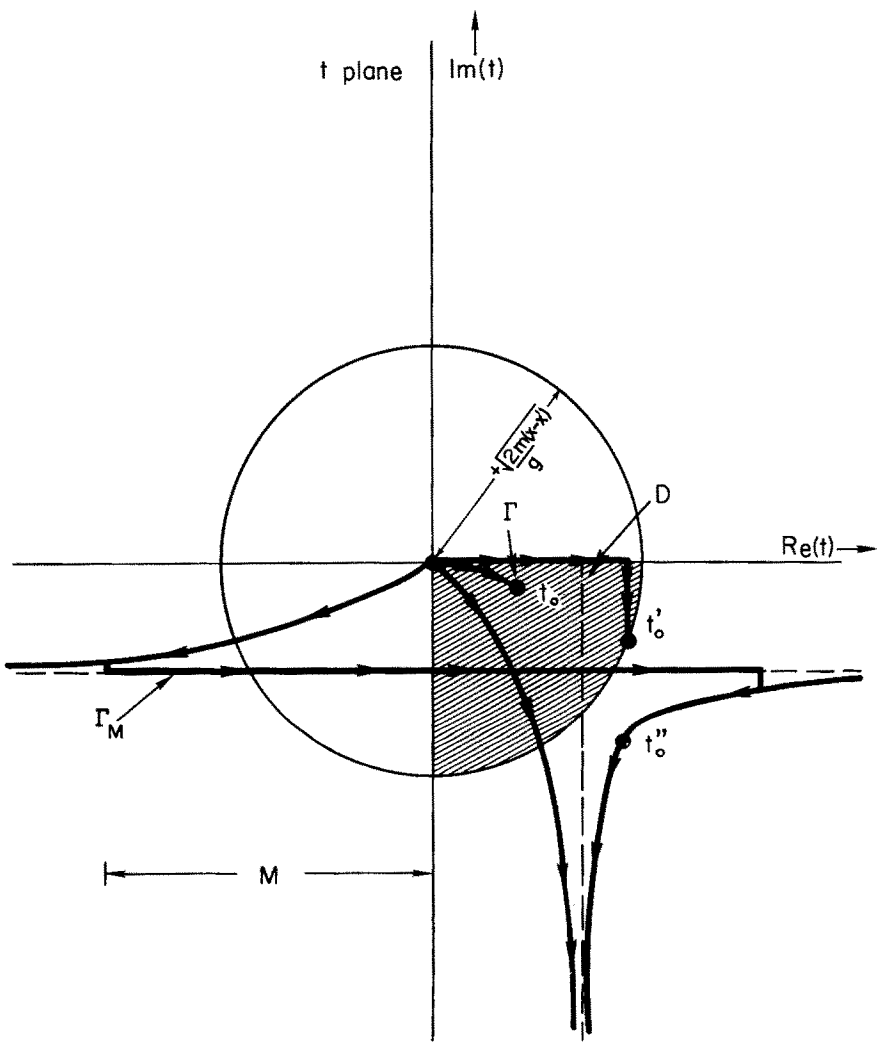


FIG. 4. Region $D$ with typical contours $\Gamma$ and $\Gamma_M$, linear potential.

where $k(x) \equiv +\{2m[E - V(x)]\}^{1/2}$,

$K(x) \equiv +\{2m[V(x) - E]\}^{1/2}$,

$x' < (x_<) < (x_>) < x'$. (3.9)

Here the turning points are defined as $x_<$ and $x_>$ (Fig. 4).

Notice that (3.9) contains the WKB barrier penetration factor, as it should. We have succeeded in obtaining a complex ray description of barrier penetration from the path integral. The entire calculation of Sec. 3 is formal. As with all path integral calculations, no estimate of the error has been made. Nevertheless, Eqs. (3.1′), (6)–(9) provide explicit equations for the complex ray and approximate amplitudes. While we have restricted ourselves to one dimension, it is reasonable to expect that the methods will generalize to higher dimensions. There, of course, the formulas will not be as explicit. We now apply these methods to study several canonical problems in the theory of complex rays, canonical because they are local approximations to many potentials. For these examples we have explicitly verified that the formulas are asymptotic to $G$.

## 4. LINEAR POTENTIAL

Let $V(x)$ equal $gx$, $g > 0$. Further denote the turning point by $x_0$, $x_0 \equiv (E/g)$, and fix $x$ and $x'$ satisfying $x' < x_0 < x$. In this case the region $D$ (Fig. 4) is the intersection of the fourth quadrant with the interior of the circle centered at the origin with radius $r$:

$$r^2 \equiv (2m/g)(x - x') \tag{4.1}$$

We remark that for $t$ restricted to the boundary of this circle, the energy $\xi$ for the solution of the classical Eqs. (2.5) is real, while for points $t$ inside $D$, $\mathrm{Im}\xi > 0$. For points $t$ in $D$, $\Gamma$ is given by

$$\Gamma: \tau(\bar{x}) = (2m/g^2)^{1/2}[(\xi - gx')^{1/2} - (\xi - g\bar{x})^{1/2}],$$

$$\xi \equiv \frac{m}{2t^2}\left(\frac{g^2t^4}{4m^2} + \frac{gt^2(x + x')}{m} + (x - x')^2\right). \tag{4.2}$$

Along $\Gamma$, formula (3.5) yields

$$\tilde{K}(x, t\,|\,x', 0) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \exp\left[\frac{i}{\hbar}\left(\frac{m}{2}\frac{(x - x')^2}{t} - \frac{g}{2} \times (x + x')t - \frac{g^2}{24m}t^3\right)\right], \quad t \in D. \tag{4.3}$$

Finally we apply (4.3) in the approximation of the Fourier tranform to obtain

$$\tilde{G}(x, x'\,|\,E) = -m[K(x)k(x')]^{-1/2} \exp\left(\frac{i}{\hbar}\int_{x'}^{E/g} k(x)dx - \frac{1}{\hbar}\int_{E/g}^{x} K(x)dx\right), \tag{4.4}$$

where

$K(x) \equiv +[2m(gx - E)]^{1/2}$,

$k(x') \equiv +[2m(E - gx')]^{1/2}$. (4.5)

A similar calculation with $x$ and $x'$ fixed satisfying $x_0 < x' < x$ yields

$$\tilde{G}(x, x'\,|\,E) = -m[K(x)K(x')]^{-1/2} \exp\left(-\frac{1}{\hbar}\int_{x'}^{x} K(x)dx\right). \tag{4.6}$$

In this simple case it is instructive to verify these formulas by actual application of the method of steepest descent. For the linear potential $\tilde{K}$, formula (3.5) is exact for all $t$ in $C^-$. [For any $t$ in $C^-$ one need only to calculate the $N$-fold integral (2.1) explicitly and take the limit to verify $K$ equals $\tilde{K}$.] Fixing $x' < E/g < x$, we consider the Fourier transform

$$G(x, x'\,|\,E + i\epsilon) = e^{-3\pi i/4}\left(\frac{m}{2\pi\hbar}\right)^{1/2}\int_0^\infty \frac{dt}{t^{1/2}} \times \exp\{(i/\hbar)[(E + i\epsilon)t + S]\}, \tag{4.7}$$

$$S \equiv \frac{m}{2}\frac{(x - x')^2}{t} - \frac{g}{2}(x + x')t - \frac{g^2t^3}{24m}.$$

Except at the origin, the integrand is an analytic function of $t$. It possesses four critical points

$$\pm(g^2/m)^{1/2}t = \{[(E - gx') + ((E - gx')^2 + \epsilon^2)^{1/2}]^{1/2} + i[-(E - gx') + ((E - gx')^2 + \epsilon^2)^{1/2}]^{1/2}\} \pm \{[(E - gx) + ((E - gx)^2 + \epsilon^2)^{1/2}]^{1/2} + i[-(E - gx) + ((E - gx)^2 + \epsilon^2)^{1/2}]^{1/2}\}, \tag{4.8}$$

where all roots are taken to be positive. Of these, denote the one in the fourth quadrant by $t_0$, and define a contour $\gamma$ from the origin through $t_0$ to infinity by the following conditions:

(1) $\mathrm{Re}[S(x, t\,|\,x', 0) + (E + i\epsilon)t] = \mathrm{Re}[S(x, t_0\,|\,x', 0) + (E + i\epsilon)t_0]$ on $\gamma$ and

(2) $\gamma$ approaches the asymptote

$\mathrm{Im}(t) = -(3)^{-1/2}\,\mathrm{Re}(t)$ as $t \to \infty$. (4.9)

The contour $\gamma$ is a line of steepest descent, to which

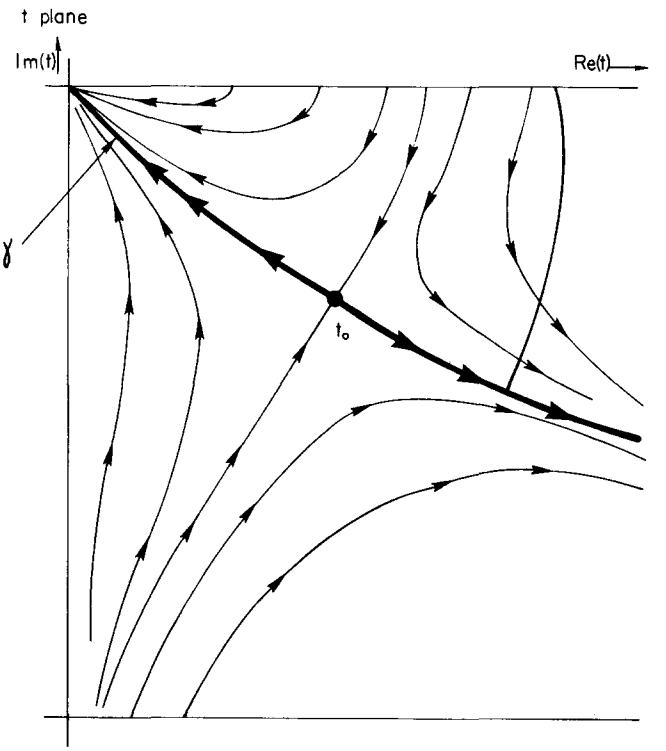


FIG. 5. Lines of constant $\mathrm{Re}(S + Et)$, linear potential, $x' < E/g < x$. Arrows denote direction of increasing $\mathrm{Im}(S + Et)$. $t_0$ is the critical point.

the path of integration may be deformed (Fig. 5). Along $\gamma$ we calculate the integral by the method of steepest descent.[21,22] This simple calculation establishes that $G$ is asymptotic to $\tilde{G}$, Eq. (4.4):

$$G(x,x'|E) \simeq \tilde{G}(x,x'|E) + O(\hbar^{\delta}\tilde{G}), \quad 0 < \delta < \tfrac{1}{2}, \text{ as } \hbar \to 0. \tag{4.10}$$

Expression (4.10) is not uniformly valid as $x$ and $x'$ approach the turning point $(E/g)$. In our framework, the origin of the nonuniformity is that the critical points "coalesce." As $x$ approaches $(E/g)$ from above, $x'$ fixed, the complex conjugate pairs of critical points approach the real axis, colliding when $x = (E/g)$[23]; as $x'$ approaches $(E/g)$ from below, $x$ fixed, those critical points with identical real parts collide at the imaginary axis; and as both $x$ and $x'$ approach $(E/g)$, all four critical points collide at the origin. In these cases it is unreasonable to expect any one member $t_0$ of a colliding set to dominate. When two critical points coalesce, both must be taken into account.[24,25] We turn now to a case where colliding critical points play a particularly important role.

Fix $x$ and $x'$ such that $(E/g) < x' < x$. Equations (4.7) and (4.8) still apply. As shown in Fig. 6, the contour $\gamma$ defined by conditions (4.9) now passes through both critical points in $C^-$, $t_0$, and $t_0'$. Once again the path of integration may be deformed to coincide with $\gamma$. Breaking $\gamma$ at $t_0'$, we separate the Fourier transform into two integrals

$$G(x,x'|E) = e^{(-3\pi i)/4}(m/2\pi\hbar)^{1/2}[I_1 + I_2], \tag{4.11}$$

where

$$I_1 \equiv \int_{\gamma}^{t_0'} \frac{dt}{t^{1/2}} \exp\left(\frac{i}{\hbar}(Et + S)\right) \tag{4.12}$$

and

$$I_2 \equiv \int_{\gamma}^{\infty} \frac{dt}{t^{1/2}} \exp\left(\frac{i}{\hbar}(Et + S)\right). \tag{4.13}$$

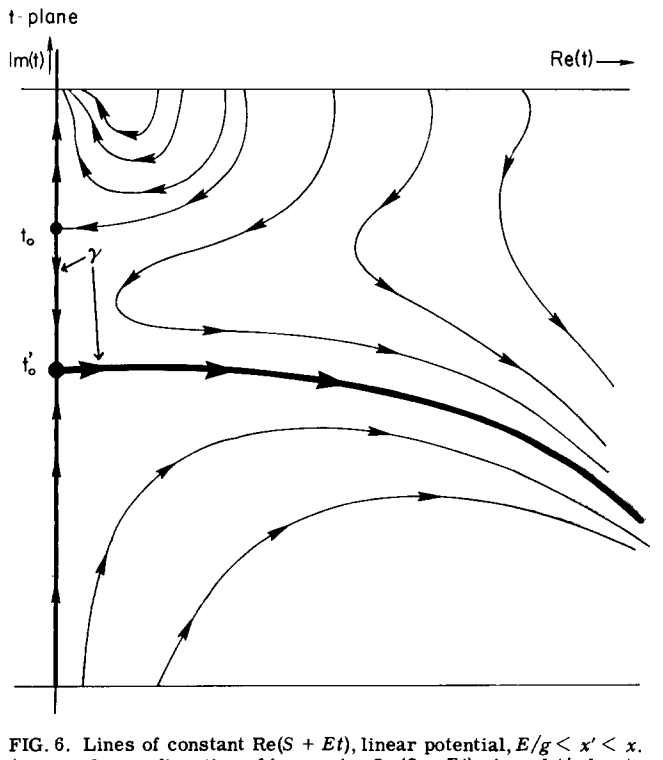


FIG. 6. Lines of constant Re$(S + Et)$, linear potential, $E/g < x' < x$. Arrows denote direction of increasing Im$(S + Et)$. $t_0$ and $t_0'$ denote the critical points.

Applying the method of steepest descent to both $I_1$ and $I_2$, noticing that $I_2$ is only "one-half Gaussian," we obtain

$$G(x,x'|E)^{1/2} = -m[K(x)K(x')^{-1/2}\left[\exp\left(-\frac{1}{\hbar}\int_{x'}^{x} K(x)dx\right) + \frac{e^{(i\pi)/2}}{2}\exp\left(\frac{1}{\hbar}\int_{x'}^{E/g} K(x)dx - \frac{1}{\hbar}\int_{E/g}^{x} K(x)dx\right)\right] + 0\left[\hbar^{\delta}\exp\left(-\frac{1}{\hbar}\int_{x'}^{x} K(x)dx\right)\right], \quad 0 < \delta < \tfrac{1}{2}. \tag{4.14}$$

For fixed $E/g < x' < x$, the second term in (4.14) is exponentially small when compared with the first, and Eq. (4.6) yields the correct asymptotic behavior of $G$. However, the second factor in (4.14) must be kept if the approximation is to be uniformly valid as $x'$ approaches the turning point $E/g$. As mentioned above, two critical points coalesce and both contribute to the asymptotic value of $G$.

The relative factor $\frac{1}{2}\exp(\frac{1}{2}i\pi)$ between the two terms in (4.14) is particularly interesting. Seckler and Keller interpret this factor as the result of a loss of "one half the wave" into the allowed region, together with a phase change due to reflection from the turning point. In their work the factor arises due to the boundary condition of a purely outgoing wave at $(-\infty)$. In our derivation, the $\frac{1}{2}$ may be traced to the fact that $I_2$ is only "one half a Gaussian," while the $e^{i\pi/2}$ is due to the rotation of $\gamma$ by $e^{i\pi/2}$ at $t_0'$.

Finally this example indicates that the path integral representation may be extended beyond $D$, and that it must be so extended if uniformly valid approximations are sought. Here $\tilde{K}$ is exact for all $t$ in $C^-$ indicating that the region $D$ is somehow artificial. Noticing that the critical point $t_0'$, lying outside of $D$, is reached by a change in branches of the $t$ versus $E$ relation, one is tempted to extend $D$ by a switch of branches. In fact, for the linear case, a candidate for the contour $\Gamma$ [satisfying conditions such as (2.6′)] does exist for points lying outside of $D$. However, as shown in Fig. 5, it possesses an asymptote which makes it necessary to tie together $(-\infty)$ and $(+\infty)$ in some fashion. One way to accomplish this is to follow $\Gamma_M$, also depicted in Fig. 5. Since $K^t$ is a semigroup in $C^-$, it may be path integrated along $\Gamma_M$, the critical path becoming real as $M \to +\infty$. In this way it should be possible to extend the region $D$.

## 5. PARABOLIC BARRIER

Let $V(x) = -\frac{1}{2}gx^2$, $g > 0$, denote the turning points by $x_{\pm} = \pm(\sqrt{2|E|})/g$, and fix $x' < x_- < x_+ < x$. In this case formula (3.9) yields

$$\tilde{G}(x,x'|E) = -m[k(x)k(x')^{-1/2}\exp\left\{\frac{i}{\hbar}\left[\int_{x'}^{x_-} k(x)dx + \int_{x_+}^{x} k(x)dx + i|E|\pi\left(\frac{m}{g}\right)^{1/2}\right]\right\}, \tag{5.1}$$

where

$$k(x) = +[2m(E + \tfrac{1}{2}gx^2)]^{1/2}. \tag{5.2}$$

Again it is instructive to verify this formula by the method of steepest descent. $\tilde{K}$ is exact for all $t$ in $C^-$. We consider the Fourier transform

$$G(x,x'\,|\,E+i\epsilon) = e^{(-3\pi i)/4}\left(\frac{(mg)^{1/2}}{2\pi\hbar}\right)^{1/2}\int_0^\infty \times\{\sinh[(g/m)^{1/2}t]\}^{-1/2}\exp\{(i/\hbar)\,[(E+i\epsilon)t+S]\}dt, \tag{5.3}$$

where

$$S \equiv S(x,t\,|\,x',0) = (\tfrac{1}{4}mg)^{1/2}\{(x^2+x'^2)\coth[(g/m)^{1/2}t] - 2xx'\,\mathrm{csch}[(g/m)^{1/2}t]\}. \tag{5.4}$$

The integrand is an analytic function of $t$ with the exception of the points $t = in\pi(m/g)^{1/2}$, $n\epsilon(0,\pm1,\pm2,\ldots)$. As $\epsilon$ vanishes, the critical points are defined by $t_n = t_{nR} + it_{nI}$,

$$t_{nI} = (2n+1)\pi(m/g)^{1/2},$$
$$\frac{2E}{g}\sinh^2((g/m)^{1/2}t_{nR}) = x^2 + x'^2 + 2xx'\cosh(\sqrt{g/m}\,t_{nR}). \tag{5.5}$$

For each value of $n$, (5.5) admits four solutions (Fig. 7).

We now choose an appropriate contour $\gamma$. This choice is not uniquely determined, the only requirement being that one must bound the error along it. In the fourth quadrant the two critical points for $n=-1$, $t_<$ and $t_>$ in Fig. 8, lie closest to the real axis and would be expected to dominate the integral. We define the first part of $\gamma$ as that line of constant $\mathrm{Re}[Et+S]$ connecting the origin with $t_<$, along which $\mathrm{Im}[Et+S]$ is monotonically decreasing from the origin to $t_<$ (Fig. 8). From $t_<$, $\gamma$ is defined as the line $(\mathrm{Im}t) = -\pi(m/g)^{1/2}$ through $t_>$ on to infinity. Notice that along this second portion of $\gamma$, $\mathrm{Im}[Et+S]$ is constant, and the method of stationary phase is applicable. Once again a standard calculation establishes that the path of integration may be deformed to coincide with $\gamma$.

Breaking $\gamma$ at $t_<$, we separate the Fourier transform into two integrals,

$$G(x,x'\,|\,E+i\epsilon) = e^{-3\pi i/4}\left(\frac{(mg)^{1/2}}{2\pi\hbar}\right)^{1/2}\{I_1+I_2\}, \tag{5.6}$$

$$I_1 \equiv \int_{\gamma 0}^{t_<}\left[\sinh\left(\sqrt{\frac{g}{m}}\,t\right)\right]^{-1/2}\exp\left(\frac{i}{\hbar}[(E+i\epsilon)t+S]\right), \tag{5.7}$$

and

$$I_2 \equiv \int_{\gamma t_<}^{\infty}\left[\sinh\left(\sqrt{\frac{g}{m}}\,t\right)\right]^{-1/2}\exp\left(\frac{i}{\hbar}((E+i\epsilon)t+S)\right). \tag{5.8}$$

Calculating the first by the method of steepest descent and the second by that of stationary phase, we obtain

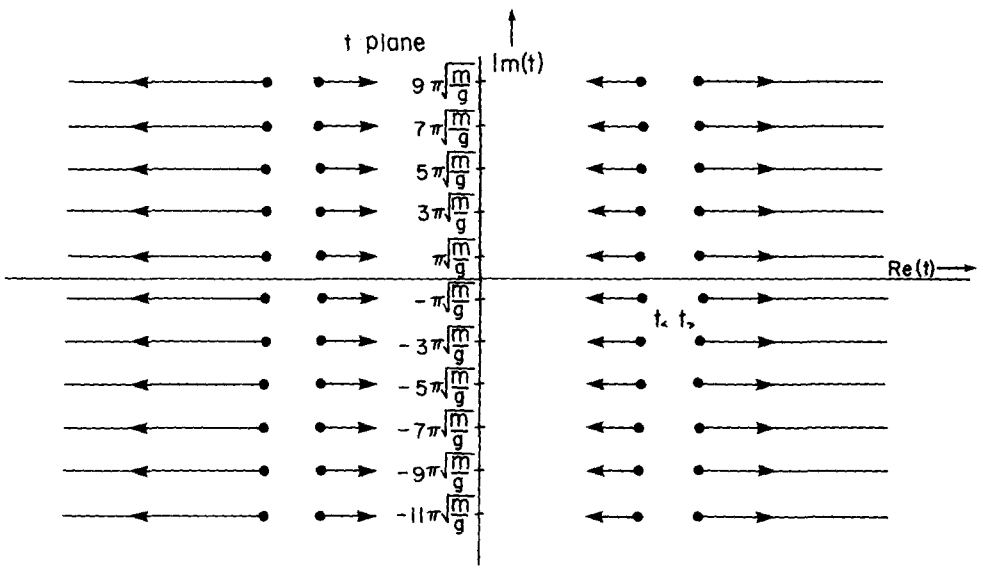


FIG. 7. Critical points for parabolic barrier, $x' < x_- < x_+ < x$. Arrows denote motion of critical points as $E$ approaches the top of the barrier from below. "Outer" critical points coalesce at $\infty$.

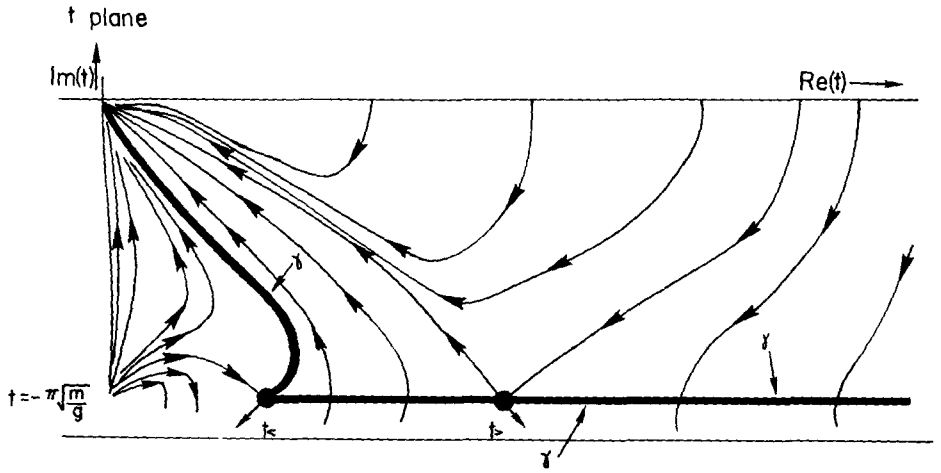


FIG. 8. Lines of constant $\mathrm{Re}(S+Et)$, parabolic potential, $x' < -(2|E|/g)^{1/2} < +(2|E|/g)^{1/2} < x$. Arrows denote direction of increasing $\mathrm{Im}(S+Et)$. $t_<$ and $t_>$ denote the critical points.

$$I_1 = -e^{(i\pi)/4}\exp\left(\frac{i}{\hbar}(Et_< + S)\right)\left\{(\pi\hbar)\left[2\left(\frac{\partial^2 S}{\partial t_<^2}\right)^{1/2} \times \sinh\left(\sqrt{\frac{g}{m}}\,t_<\right)\right]^{-1}\right\}^{1/2}[1 + O(\hbar^\delta)],$$
$$0 < \delta < \tfrac{1}{2}, \tag{5.9}$$

and

$$I_2 = e^{(i\pi)/4}\exp\left(\frac{i}{\hbar}(Et_< + S)\right)\left\{(\pi\hbar)\left[2\left(\frac{\partial^2 S}{\partial t_<^2}\right) \times \sinh\left(\sqrt{\frac{g}{m}}\,t_<\right)\right]^{-1}\right\}^{1/2}[1 + O(\hbar^\delta)]$$
$$+ e^{(-i\pi)/4}\exp\left(\frac{i}{\hbar}(Et_> + S)\right)\left\{(2\pi\hbar)\left[\left|\frac{\partial^2 S}{\partial t_>^2}\right| \times \sinh\left(\sqrt{\frac{g}{m}}\,t_>\right)\right]^{-1}\right\}^{1/2}[1 + O(\hbar^\delta)], \quad 0 < \delta < \tfrac{1}{2}. \tag{5.10}$$

Adding, we compute that $G$ is asymptotic to $\tilde{G}$, Eq. (5.1),

$$G(x,x'|E) = \tilde{G}(x,x'|E) + O(\hbar^\delta \tilde{G}), \quad 0 < \delta < \tfrac{1}{2}. \tag{5.11}$$

Here we have used (5.5) to express $t_>$ in terms of $E$.

This result may be interpreted as a particle traveling in real time until it strikes the turning point where its real time "freezes." It then penetrates the barrier by taking an excursion into complex time. Upon striking the second turning point, its complex time freezes, and it leaves the barrier with increasing real time. Notice that the calculation establishes that $\tilde{G}$ depends only upon $t_>$ and not upon $t_<$. (Physically one might have expected $t_<$ not to contribute since it may be interpreted as arising from a motion "backwards in real time" due to a change in branch of the $t$ versus $E$ relation.)[26]

Finally, we remark that $\tilde{G}$ is not uniformly valid as $E$ vanishes, since one half of the critical points move to infinity, Fig. 8. The change of varible $t' = 1/t$ establishes that the transformed integrand has a countable number of critical points coalescing at the origin. Certainly one member of this set, $t_>^{-1}$, does not dominate the behavior of the integral. However, other techniques[27] show the uniformly valid expansion will depend upon a countable number of these critical points. Since countable numbers of coalescing critical points arise in physical problems involving resonances and "above barrier reflections," it may be necessary to understand such critical point behavior in order to treat these problems with the path integral.

## 6. TWO ADDITIONAL EXAMPLES

In this section we mention two additional potentials for which the formula may be checked by other methods. First, let $V(x) = V_0[\cosh(\alpha x)]^{-2}$, $\alpha > 0$, $V_0 > 0$. Clearly formula (3.9) applies ($x'$ is to the left) of the barrier, $x$ to the right).

Since in this case no closed form of $K(x,t|x',0)$ is known, $\tilde{G}$ may not be verified as directly as were the preceding two examples. Nevertheless, the time-independent Schrödinger equation in this potential may be solved terms of hypergeometric functions.[28] By using these to construct $G$, and then evaluating it asymptotically as $\hbar$ vanishes, one can verify $\tilde{G}$. We mention this only because this potential, due to its behavior at infinity, may provide a better model for above barrier reflection than the parabolic barrier.

Rather than present the details of this verification, we prefer to consider an example involving the radial Schrödinger equation. Let $V(r)$ be a repulsive potential, and let the energy $E$ be high enough that the effective potential $[l(l+1)\hbar^2]/(2mr^2) + V(r)$ has only one turning point $r_0$. Fix $r' > r_0 > r$. We seek the asymptotic behavior of $G$ as $\hbar$ vanishes:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right)G(r,r'|E,l) = -\delta(r-r'). \tag{6.1}$$

Following Langer,[29] we transform the singularity at the origin to infinity by the change of variable $r = e^{-x}$,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + W(x) + L\right)g(x,x'|E,L) = -\delta(x-x'), \tag{6.2}$$

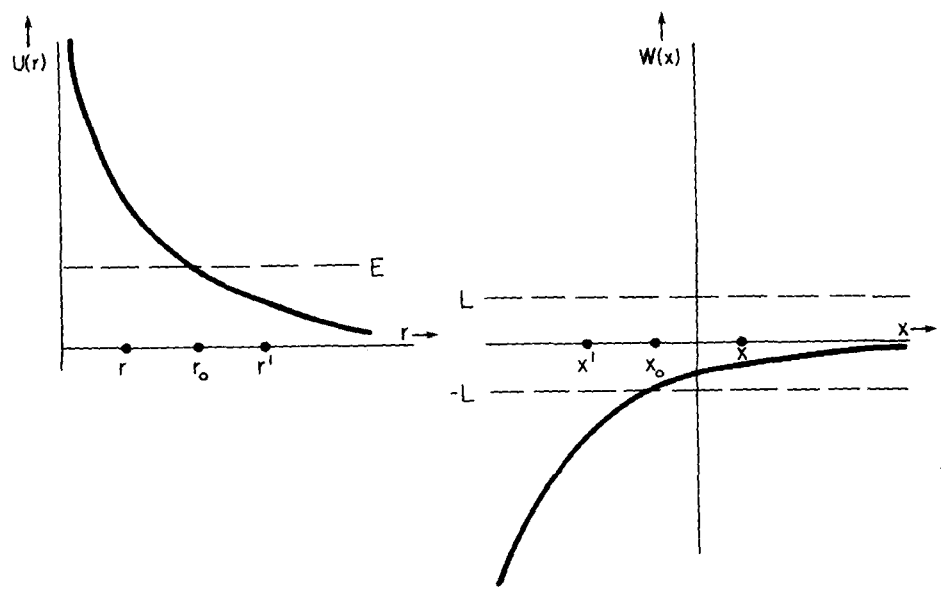


FIG. 9. (a) $U(r) = [l(l+1)\hbar^2/2mr^2] + V(r)$; (b) $W(x) = [V(e^{-x}) - E]e^{-2x}$.

where

$$r' = e^{-x'}, \quad r_0 = e^{-x_0}, \quad L = \frac{\hbar^2}{2m}\left(l+\frac{1}{2}\right)^2,$$
$$W(x) = [V(e^{-x}) - E]e^{-2x}, \quad \text{and} \quad g = (r'r)^{-1/2}G. \tag{6.3}$$

In order to place (6.3) in a form suitable for path integration,[30] we Fourier transform on the variable $L$. The transform $\hat{g}$ satisfies

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + W(x) - i\hbar\frac{\partial}{\partial\lambda}\right)\hat{g}(x,x'|E,\lambda) = 0 \tag{6.4}$$
$$\lim_{\lambda\to 0+}\hat{g}(x,x'|E,\lambda) = \delta(x-x'), \quad \hat{g}\equiv 0,\ \lambda<0,$$

and may be represented as a path integral,

$$\hat{g}(x,x'|E,\lambda) = \int_{x(\cdot)\in P(x,\lambda|x',0)} \mathfrak{D}x(\cdot)\ \exp\left(\frac{i}{\hbar}S(x(\cdot),\lambda)\right),$$
$$S(x(\cdot),\lambda) = \int_0^\lambda \left[\frac{1}{2}m\left(\frac{dx}{d\tau}\right)^2 - W[x(\tau)]\right]d\tau. \tag{6.5}$$

$g$ is then given by

$$g(x,x'|E,L) = \frac{i}{\hbar}\int_0^\infty d\lambda\ \exp\left(-\frac{i}{\hbar}\lambda L\right)\hat{g}(x,x'|E,\lambda). \tag{6.6}$$

We seek to evaluate this "λ-path" integral asymptotically as $\hbar$ vanishes, $L$ fixed. The situation is sketched in Fig. 9, from which it is clear that there is no real critical path. However, the technique of Sec. 3 applies with λ playing the role of time. In this case, formula (3.8) becomes

$$\tilde{g}(x,x'|E,L) = m[K_w(x)k_w(x')]^{-1/2} \times \exp\left(\frac{i}{\hbar}\int_{x'}^{x_0} k_w(x)dx - \frac{1}{\hbar}\int_{x_0}^{x} K_w(x)dx\right), \tag{6.7}$$

where

$$K_w(x) = +\{2m[L+W(x)]\}^{1/2},$$
$$k_w(x') = +\{2m[-L-W(x')]\}^{1/2}. \tag{6.8}$$

Returning to the physical variables $r, r'$, and $l$, we obtain

$$\tilde{G}(r,r'|E,l) = m[K(r)k(r')]^{-1/2} \exp\left(-\frac{i}{\hbar}\int_{r'}^{r_0} k(r)dr + \frac{1}{\hbar}\int_{r_0}^{r} K(r)dr\right), \tag{6.7'}$$

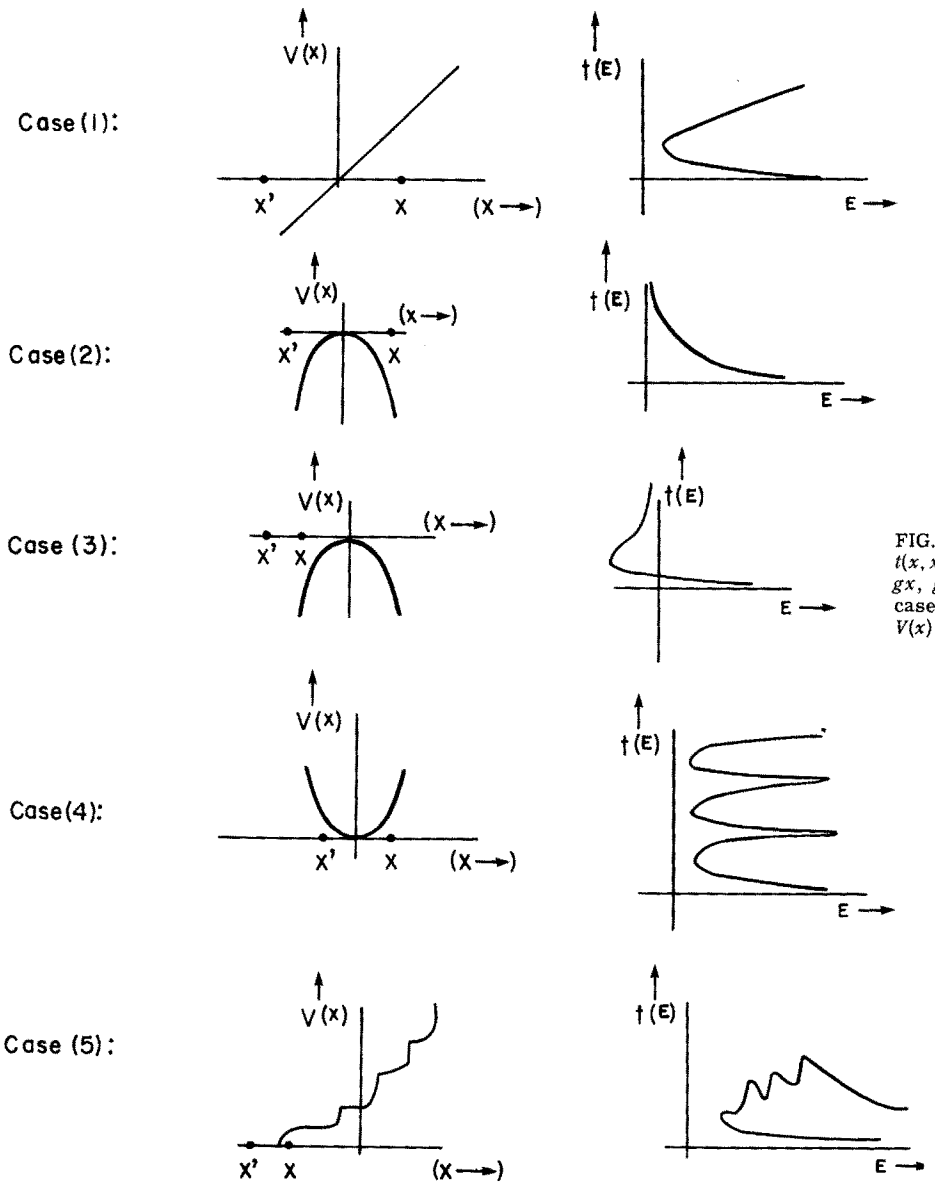


FIG. 10. Sketches of potentials and their $t(x,x'|E)$ vs $E$ relation. Case (1): $V(x) = gx$, $g>0$; case (2): $V(x) = -\frac{1}{2}gx^2$, $g>0$; case (3): $V(x) = -\frac{1}{2}gx^2$, $g>0$; case (4): $V(x) = \frac{1}{2}gx^2$, $g>0$.

where

$$K(r) = +\left[2m\left(-E + V(r) + \frac{(l+\frac{1}{2})^2}{2mr^2}\hbar^2\right)\right]^{1/2},$$
$$k(r') = \left[2m\left(E - V(r') - \frac{(l+\frac{1}{2})^2}{2mr'^2}\hbar^2\right)\right]^{1/2}. \quad (6.8')$$

For $V(r) = g/r$, $g > 0$, we have verified formula (6.7') by solving (6.1) in terms of Whittaker functions and then evaluating its asymptotic expansion.

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## APPENDIX

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*Note added in proof:* Since this work was submitted, Karl Freed[31] has published results on barrier penetration obtained by an analytic continuation of the sum over classical paths. His approach, which is similar to one we employed earlier,[32] does not continue the function space integral, but rather its asymptotic approximation.

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## I. INTRODUCTION

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$$K(r) = +\left[2m\left(-E + V(r) + \frac{(l+\frac{1}{2})^2}{2mr^2}\hbar^2\right)\right]^{1/2},$$
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As in the Schrödinger case if $\nu$ is the $O(2)$ quantum number of the radial wavefunction in the basis $O(2,1) \supset O(2)$, then $r^k D_{\nu/\nu+q}, k, q$ integers, is proportional to the $q$th component of a tensor operator. Here $D_a$ is a dilatation operator defined such that $D_a f(x) = f(ax)$. A generalized Pasternack and Sternheimer selection rule exists and matrix elements diagonal in the $O(2)$ quantum number can be derived group theoretically.

Crubellier and Feneuille[7] have used the Infeld and Hull generalized Kepler equation to generalize Armstrong's[8] $O(2,1)$ treatment of the nonrelativistic hydrogen atom to the $k$ Dirac atom. The method in this paper differs from that of Crubellier and Feneuille[7] who introduced a nonphysical two variable wavefunction. Here dilatation operators and one variable physical wavefunctions are used.

## II. GROUP STRUCTURE OF THE GENERALISED KEPLER EQUATION

Consider the equation

$$\left(\nabla^2 - \frac{(\lambda - l)(l + \lambda + 1)}{\rho^2} + \frac{2Z}{\rho} - \frac{Z^2}{\nu^2}\right) u(\rho\theta\varphi) = 0. \tag{1}$$

$\lambda$ here is a monotonic function of $l$, where $l$ and $\nu - \lambda$ are integers. $Z$ is the charge on the nucleus. This separates in the usual manner giving the solution

$$u = R_\nu^\lambda(\rho) Y_m^l(\theta\varphi),$$

where $Y_m^l(\theta\varphi)$ is a spherical harmonic and $R_\nu^\lambda(\rho)$ satisfies the radial equation

$$\left(\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} + \frac{2Z}{\rho} - \frac{Z^2}{\nu^2} - \frac{\lambda(\lambda+1)}{\rho^2}\right) R_\nu^\lambda = 0, \tag{2}$$

which is apart from minor variations of the generalized Kepler equation of Infeld and Hull.[4] A solution to (2) is

$$R_\nu^\lambda = N_{\lambda\nu} e^{-Z\rho/N} \left(\frac{2Z\rho}{\nu}\right)^\lambda L_{\nu-\lambda-1}^{2\lambda+1}\left(\frac{2Z\rho}{\nu}\right), \tag{3}$$

where $L_{\nu-\lambda-1}^{2\lambda+1}\left(\frac{2Z\rho}{\nu}\right)$ is a generalized Laguerre polynomial defined by

$$L_b^a(x) = \sum_{n=0}^{b} \frac{\Gamma(a+b+1)(-x)^n}{n!(b-n)!\Gamma(a+n+1)}.$$

We have

$$\int_0^\infty R_\nu^\lambda R_{\nu'}^\lambda \rho^2 d\rho = \delta(\nu\nu'), \tag{4}$$

which requires

$$N_{\lambda\nu} = \frac{2}{\nu^2}\left(\frac{Z^3(\nu - \lambda - 1)!}{\Gamma(\nu + \lambda + 1)}\right)^{1/2}.$$

We now take the quantities

$$K_\pm = \mp\left(\frac{\nu \pm 1}{\nu}\right) D_{\nu/\nu\pm1}\,(x_\nu \partial/\partial x_\nu \mp x_\nu \pm \nu + 1) \tag{5}$$

and $K_0 = \nu$ under the inner product,

$$\int_{\rho_0}^\infty \int_\Omega R_\nu^\lambda Y_m^l x_\nu^2 R_{\nu'}^{\lambda'} Y_{m'}^{l'} x_{\nu'} \frac{\nu^2\nu'}{Z^3} dx_{\nu'} d\Omega = \delta(\nu\nu')\delta(ll') = \delta(\nu\nu')\delta(ll')\delta(\lambda\lambda'), \tag{6}$$

since $\lambda$ is a monotonic function of $l$. Here

$$x_\nu = Z\rho/\nu \text{ and } d\Omega = \sin\theta d\theta d\varphi.$$

As in I, $D_{\nu/\nu\pm1}$ is a dilatation operator defined such that $D_a f(\rho) = f(a\rho)$, which implies that

$$D_{\nu/\nu'} f(x_\nu) = f(x_{\nu'}).$$

This gives

$$K_\pm R_\nu^\lambda = [(\nu \mp \lambda)(\nu \pm \lambda \pm 1)]^{1/2} R_{\nu\pm1}^\lambda,$$
$$K_0 R_\nu^\lambda = \nu R_\nu^\lambda,$$

and

$$\begin{aligned}\int_0^\infty \int_\Omega & R_\nu^\lambda Y_m^l x_\nu^2 [K_+K_-] R_\nu^\lambda Y_m^l \frac{\nu^3}{Z^3} dx_\nu d\Omega \\ &= -\int_0^\infty \int_\Omega R_\nu^\lambda Y_m^l x_\nu^2 [D_{\nu-1/\nu}(x_{\nu-1}\partial/\partial x_{\nu-1} - x_{\nu-1} + \nu) \\ &\quad \times D_{\nu/\nu-1}(x_\nu \partial/\partial x_\nu + x_\nu - \nu + 1) \\ &\quad - D_{\nu+1/\nu}(x_{\nu+1}\partial/\partial x_{\nu+1} + x_{\nu+1} - \nu) \\ &\quad \times D_{\nu/\nu+1}(x_\nu \partial/\partial x_\nu - x_\nu + \nu + 1)] R_\nu^\lambda Y_m^l (\nu^3/Z^3) dx_\nu d\Omega \\ &= \int_0 \int_\Omega R_\nu^\lambda Y_m^l x_\nu^2 (-2K_0) R_\nu^\lambda Y_m^l \frac{\nu^3}{Z^3} dx_\nu d\Omega.\end{aligned}$$

Similarly $[K_0 K_\pm] = \pm K_\pm$.

Hence as in I, since the $Y_m^l$ form a basis for a representation of $O(3)$, the wavefunctions $R_\nu^\lambda Y_m^l$ for fixed $m$ form the basis for a representation of the group $O(2,1) \times O(3)$. We note the important point that in this scheme, it is the $O(2,1) \times O(3)$ states $|\lambda\nu m\rangle$ for fixed $m$ and not the $O(2,1)$ states $|\lambda\nu\rangle$ which form the basis of the Hilbert space. In this physical realization the radial wavefunctions $R_\nu^\lambda$ alone are not orthogonal with respect to $\lambda$.

Following I, we find the eigenvalues of the Casimir invariant

$$G = K_0^2 - \tfrac{1}{2}(K_+K_- + K_-K_+)$$

to be $\lambda(\lambda + 1)$, and hence the wavefunctions $R_\nu^\lambda Y_m^l$ for fixed $m$ for a basis for the representation $D_{\lambda+1}^+$ of $O(2,1)$ and $\mathfrak{D}^l$ of $O(3)$.

Note that Eq. (2) is in fact equivalent to $GR_\nu^\lambda = \lambda(\lambda + 1)R_\nu^\lambda$ and hence is very similar to a type $B$ Infeld and Hull factorization,[4] with $K_\pm$ acting as the step upstep down operators.

Four special cases are considered by specifying $\lambda$ and $\rho$. The radial equations become

(1) Schrödinger hydrogen atom $\rho = r, \lambda = l$,

(2) Klein–Gordon "hydrogen atom" $\rho = r$,

$$\lambda = -\tfrac{1}{2} + [(l + \tfrac{1}{2})^2 - Z^2\alpha^2]^{1/2},$$

(3) $k$ Dirac hydrogen atom $\rho = ar$ where $a = \mu\epsilon\alpha/\eta$, $\mu$ mass of nucleus and

$$\epsilon = \left(1 + \frac{\alpha^2 Z^2}{(n + \lambda)^2}\right)^{-1/2}, \quad \lambda = (k^2 - \alpha^2 Z^2)^{1/2},$$

(4) Biedenharn's[6] $S$ Dirac hydrogen atom. In this case we have two iterated second order equations and $\rho = r$,

$$\lambda = +(k^2 - Z^2\alpha^2)^{1/2} - \tfrac{1}{2} + \tfrac{1}{2}\,\mathrm{sgn}(k).$$

The representation structures hence derived are in agreement with those given by Bacry and Richard,[9] Barut and Bornzin[10] and Lanik.[11]

## III. TENSOR OPERATORS AND THE RACAH ALGEBRA

Having established our formalism the extension of I to this more general case is straightforward. First we consider the commutation relations of the $O(2,1)$ generators with the quantity $(\rho^k/(\nu+q)^{k-1})D_{\nu/\nu+q}A^l_{l'}(\theta\varphi)$, $k$ and $q$ integers, where

$$A^l_{l'}(\theta\varphi)Y^l_m = Y^{l'}_m$$

and find that it transforms according to the $q$th component of a tensor operator whose representation is of finite dimension equal to $-2k-3$ if $k \leq -2$ and is labeled $D_{-k-2}$ and of finite dimension and reducible but not fully reducible if $k > -2$. This representation is labeled $D'_{k+1}$. Both of these representations are nonunitary since the eigenvalues of $K_\mp K_\pm$ are not positive definite.[12]

As in I the Wigner–Eckart theorem holds so

$$\langle \lambda\nu m \,|\, T^k_q \,|\, \lambda'\nu' m\rangle = \langle \lambda \| T^k \| \lambda'\rangle C^{\lambda' k\lambda}_{\nu' q\nu},$$

where $C^{\lambda' k\lambda}_{\nu' q\nu}$ is an $O(2,1)$ Clebsch–Gordan coefficient. In I the representations were characterized by integers only; however, the derivation of the Clebsch–Gordan coefficients in this case is unchanged except for the replacement of factorials by gamma functions at the appropriate places. Binomial identities used in their derivation are still applicable since the addition theorem for binomial coefficients, namely

$$\sum_p \binom{k_1}{p}\binom{k_2}{r-p} = \binom{k_1+k_2}{r},$$

where

$$\binom{a}{b} = \frac{\Gamma(a+1)}{\Gamma(b+1)(a-b+1)}$$

holds for all values of $k_1$ and $k_2$.

We recall from I that the technique for deriving Clebsch–Gordan coefficients due to van de Waerden[13] and Bargmann[14] requires the representation states be realized by normalized multispinors $N_{ab}\xi^a\eta^b$. We then form an invariant coupling of two representations and a contragradient representation giving Eq. (12) of I, namely

$$\delta_1^{k_1}\delta_2^{k_2}\delta_3^{k_3} = \sum_{m_1 m_2 m_3} C^{\Phi_1\Phi_2\Phi_3}_{m_1 m_2 m_3} N_1 \xi_1^{\Phi_1+m_1}\eta_1^{\Phi_1-m_1} \times N_2\xi_2^{\Phi_2+m_2}\eta_2^{\Phi_2-m_2}N_3\xi_3^{\Phi_3-m_3}\eta_3^{\Phi_3+m_3} \quad (6')$$

Here the $\delta_i$ are the three determinantal invariants

$$\delta_1 = \xi_2\eta_3 - \xi_3\eta_2, \quad \delta_2 = \xi_3\eta_1 - \xi_1\eta_3, \quad \delta_3 = \xi_1\eta_2 - \xi_2\eta_1.$$

This implies

$$k_2 + k_3 = 2\Phi_1, \quad k_3 + k_1 = 2\Phi_2, \quad k_2 + k_3 = 2\Phi_3 \quad (7)$$

or equivalently

$$k_1 = \Phi_2 + \Phi_3 - \Phi_1, \quad k_2 = \Phi_3 + \Phi_1 - \Phi_2, \quad k_3 = \Phi_1 + \Phi_2 - \Phi_3. \quad (8)$$

Expanding the left hand-side of (6′) gives

$$\sum_{pqr}\binom{k_1}{p}\binom{k_2}{q}\binom{k_3}{r}(-1)^{k_1-p+q+r}\xi_1^{k_3-r+q}\eta_1^{k_2-q+r}\xi_2^{p+r} \times \eta_2^{k_1+k_3-p-r}\xi_3^{k_2+k_1-p-r}\eta_3^{p+q} \quad (9)$$

In order that the correct representations are coupled, we require $k_1$ and $k_3$ to be positive integers. This means that $\xi_1$, $\xi_2$, and $\eta_3$ are bounded below and $\eta_2$ is bounded above as required. Then by (7), $\Phi_2$ is a positive integer. The selection rule for negative $k$ follows from (8),

$$\Phi_1 + \Phi_2 - \Phi_3 = k_1 \geq 0$$
$$\Phi_2 + \Phi_3 - \Phi_1 = k_3 \geq 0 \quad \text{and} \quad \Phi_2 \geq 0$$

implies $0 \leq \Phi_2 \leq |\Phi_1 - \Phi_3|$.

Substituting

$$\Phi_1 = -\lambda - 1, \quad \Phi_3 = -\lambda' - 1, \quad \Phi_2 = -k - 2 = s - 2$$

gives

$$2 \leq s \leq |\lambda - \lambda'| + 1.$$

Comparing coefficients between (6′) and (9) now gives the unnormalized Clebsch–Gordan coefficients. To normalize an orthogonality condition is required. This is derived by closer consideration of the direct product state $|\lambda\nu; kq\rangle$, where the state $|kq\rangle$ corresponds to the tensor $D_{\nu/\nu\pm1}A^l_{l'}$. The $l$ quantum numbers have been omitted as being unimportant. The set of states $|\lambda\nu\rangle$ form a basis for the unitary representation $D^+_{\lambda+1}$, so in this basis $K^+_\pm = K_\mp$ under the inner product $\langle\lambda'\nu'|\lambda\nu\rangle = \delta_{\lambda\lambda'}\delta_{\nu\nu'}$. However, the set $|kq\rangle$ does not form a unitary representation, so if we demand that $K^+_\pm = K_\mp$ in the direct product space, we must define the inner product in this basis to be

$$\langle k'q'|kq\rangle = (-1)^q\delta(qq').$$

This is so since

$$\langle k'q'|K_\pm kq\rangle = \mp[(k\mp q)(k\pm q\pm 1)]^{1/2}\langle k'q'|kq\rangle \quad (10)$$

from I, Sec. V.

So (10) equals

$$\mp(-1)^q[(k\mp q)(k\pm q\pm 1)]^{1/2} = \langle K_\pm k'q'|kq\rangle, \quad (11)$$

i.e., $K^+_\pm = K_\mp$.

Now if $|\lambda\nu\rangle = \sum_{\nu' q} C^{\lambda' k\lambda}_{\nu' q\nu}|\lambda'\nu'; kq\rangle$, taking the inner product with $\langle kq; \lambda''\nu''|$ gives as the required orthogonality condition

$$\sum_{\nu q} C^{\lambda k\lambda'}_{\nu q\nu'} C^{*\lambda k\lambda''}_{\nu q\nu''}(-1)^q = \delta(\lambda'\lambda'')\delta(\nu'\nu''). \quad (12)$$

Finally then

$$C^{\lambda\, k\lambda'}_{\nu\, q\nu'} = (-1)^{k+q}\left(\frac{\Gamma(\lambda'-\lambda-k-1)\Gamma(\lambda+\lambda'+k+3)\Gamma(\lambda-\lambda'-k-1)}{\Gamma(\lambda+\lambda'-k)}\right)^{1/2}$$
$$\times\left(\frac{\Gamma(\nu'-\lambda')\Gamma(\nu'+\lambda')\Gamma(2\nu'+2)(-k-2-q)!}{\Gamma(\nu+\lambda+1)\Gamma(\nu-\lambda)(-k-2+q)!}\right)^{1/2}$$
$$\times\sum_t(-1)^{t+k+q}\binom{\lambda'-\nu'+t}{-k-1-q}\binom{k+\nu'+\lambda-t}{\nu'+\lambda'}\binom{\lambda+\nu}{t},\quad k>-2; \tag{13a}$$

$$C^{\lambda\, k\lambda'}_{\nu\, q\nu'} = \frac{\Gamma(\lambda-\lambda'+k+3)\Gamma(\lambda'+\nu'+1)}{(k+1+q)!}\sum_t\frac{\Gamma(k+\nu'-\lambda-t+1)}{\Gamma(k+3+\lambda-\nu'+t)\Gamma(\lambda'+\nu'-t+1)\Gamma(\nu'-\lambda'-t)\Gamma(\nu-\lambda-t)t!},$$
$$k\leqslant -2,\quad k+q\geqslant 0. \tag{13b}$$

In the second case, $k+q<0$ has not been considered as the case $q=0$ is of most interest.

## IV. MATRIX ELEMENTS

To complete this paper the reduced matrix elements for the generalized Kepler problem are derived. This is done by considering the matrix element

$$\langle\lambda'\lambda+1|\,T^k_0\,|\lambda\lambda+1\rangle = C^{\lambda}_{\lambda+1\ 0\ \lambda+1}\langle\lambda'\|T^k\|\lambda\rangle,\quad \lambda\geqslant\lambda'.$$

Since $L_0^{2l+1}$ is a constant, the integral becomes a sum of integrals of the form

$$\int_0^\infty e^{-ax}x^b dx = \Gamma(b+1)/a^{b+1},$$

provided that $b>-1$, i.e., provided that $\lambda+\lambda'+k+2>-1$. Substituting for

$$C^{\lambda}_{\lambda+1\ 0\ \lambda+1}$$

from (13) gives

$$\langle\lambda'\|T^k\|\lambda\rangle = \frac{1}{2}\,\frac{1}{(2Z)^k}\,\frac{\Gamma(\lambda+\lambda'+k+3)\Gamma(\lambda-\lambda'-1)}{\Gamma(\lambda+\lambda')},\quad k\leqslant -2, \tag{14a}$$

or

$$\frac{1}{2}\,\frac{1}{(2Z)^k}\left(\frac{\Gamma(\lambda+\lambda'+k+3)}{\Gamma(\lambda'-\lambda-k-1)\Gamma(\lambda-\lambda'-k-1)\Gamma(\lambda+\lambda'-k)\Gamma(2l'+2)}\right)^{-1/2}. \tag{14b}$$

To illustrate this technique, we shall derive a matrix element for the $k$ Dirac hydrogen atom important in the theory of hyperfine structure.[5] Using the notation of Bethe and Salpeter,[5] we note first that

$$\chi_1 = (\epsilon a/2Z)^{1/2}(1/2\gamma)[(\gamma_2+\gamma_1)(\epsilon k-\gamma)^{1/2}\rho R^{\gamma}_{l}{}^{-1} + (\gamma_2-\gamma_1)(\epsilon k+\gamma)^{1/2}\rho R^{\gamma}_{l}]$$

and

$$\chi_2 = (\epsilon a/2Z)^{1/2}(1/2\gamma)[(\gamma_2-\gamma_1)(\epsilon k-\gamma)^{1/2}\rho R^{\gamma}_{l}{}^{-1} + (\gamma_2+\gamma_1)(\epsilon k+\gamma)^{1/2}\rho R^{\gamma}_{l}],$$

where

$$\gamma_1 = (k-\alpha Z)^{1/2},\quad \gamma_2 = (k+\alpha Z)^{1/2},\quad \lambda=\gamma=\gamma_1\gamma_2.$$

Consider now the matrix element $\int_0^\infty \chi_1\chi_2 dr/r^2$. This equals

$$\frac{\epsilon a^2}{8Z^2\nu^3\gamma^2}\left((\gamma_2^2-\gamma_1^2)(\epsilon k-\gamma)\int_0^\infty R^{\gamma}_{l}{}^{-1}\frac{\nu^3}{\rho^2}R^{\gamma}_{l}{}^{-1}\rho^2 d\rho + (\gamma_2^2-\gamma_1^2)(\epsilon k+\gamma)\int_0^\infty R^{\gamma}_{\nu}\frac{\nu^3}{\rho^2}R^{\gamma}_{\nu}\rho^2 d\rho\right),$$

since by the selection rule the terms containing different $\gamma$ vanish. Substituting from Eqs. (12) and (13) gives finally

$$\int_0^\infty\frac{\chi_1\chi_2 dr}{r^2} = \frac{\epsilon a^2\alpha Z}{\nu^3}\left(\frac{2\epsilon k-1}{\gamma(4\gamma^2-1)}\right)$$

in agreement with Crubellier and Feneuille.[7] In the same way a second matrix element important in hyperfine structure evaluates as

$$\int_0^\infty\frac{(\chi_1^2+\chi_2^2)dr}{r^3} = \frac{\epsilon a^3 k}{2\gamma^3\nu^3}\left(\frac{(\epsilon k-\gamma)}{(\gamma-\frac{1}{2})(\gamma-1)} + \frac{(\epsilon k+\gamma)}{(\gamma+\frac{1}{2})(\gamma+1)}\right) + \frac{2a^3\epsilon\alpha Z}{\gamma^2\nu^4(4\gamma^2-1)}$$
$$\times[(\epsilon^2k^2-\gamma^2)(\nu^2-\gamma^2)]^{1/2}.$$

## V. CONCLUSIONS

As in I a formal solution for off diagonal matrix elements of $\rho^k$ can be given. A closed expression for these matrix elements cannot however be given as it is $D_{\nu/\nu+q}\rho^k$ and not $\rho^k$ that is proportional to a tensor operator in this scheme. Two variable models are also incapable of finding these matrix elements.[7,8] Considerable refinement of the technique will be necessary before a closed formula could be found for this difficult problem. Further progress would now appear to lie in the direction of the many electron problem which awaits some approximate group structure to describe complex atoms.


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## Solutions of a Class of Nonlinear Coupled Partial Differential Equations

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A class of nonlinear coupled partial differential equations are solved. These are generalizations of the general relativistic equations arising for a static distribution of massive charged particles.

Nordtvedt[1] has recently found an exact solution of the general relativistic field equations of Einstein and Maxwell for a general static distribution of massive charged particles. This solution resulted from a pair of coupled nonlinear partial differential equations of the type

$$F^3\nabla^2 F = -\tfrac{1}{4}(\nabla\psi)^2 - 2\pi\rho F^8 \tag{1}$$

and

$$\nabla^2\psi = -4\pi\rho F^6, \tag{2}$$

where $F, \rho$ and $\psi$ are functions of $x_1, \ldots, x_\mu$, with $\mu = 3$ for Nordtvedt's problem, although in the following $\mu$ is arbitrary unless stated otherwise. In this note a general class of coupled nonlinear equations, of which Eqs. (1) and (2) are a special case, is studied and solved in the sense that $F$ is expressed as an explicit function of $\psi$ resulting in an equation which $\psi$ satisfies. These equations for $\psi$ are discussed and in a variety of special cases are well known.

First, a generalization of Eqs. (1) and (2) for $\rho = 0$, which turns out to be simpler, will be looked at. Consider

$$(F)^n\nabla^2 F = -(\nabla\psi)^2, \tag{3}$$

where $\psi$ satisfies Laplace's equation

$$\nabla^2\psi = 0. \tag{4}$$

By treating $F$ as a functional of $\psi$ and using Eq. (4), write

$$F^n\nabla^2 F = F^n\frac{d^2F}{d\psi^2}(\nabla\psi)^2 = -(\nabla\psi)^2, \tag{5}$$

and assuming $\nabla\psi$ is not zero,

$$F^n\frac{d^2F}{d\psi^2} = -1. \tag{6}$$

The cases $n = \pm 1$ will be handled separately, so for now these two values of $n$ are excluded. With the substitution

$$F = (d + a\psi)^l, \tag{7}$$

solutions to Eq. (6) are obtained for $l$ and $a$ satisfying

$$l = 2/(n+1) \quad \text{and} \quad a^2 = (n+1)^2/2(n-1) \tag{8}$$

or

$$F_\pm = \left(d \pm \frac{(n+1)}{\sqrt{2(n-1)}}\psi\right)^{2/n+1}, \tag{9}$$

where $d$ is an arbitrary constant, and $\psi$ is a solution of Laplace's equation. These are solutions for any $n$ except $n = \pm 1$. For $n = -1$ the solution is

$$F = d_1\sin\psi + d_2\cos\psi. \tag{10}$$

For $n = +1$, Eq. (6) has a first integral which is

$$\frac{dF}{d\psi} = \mp\sqrt{2}\sqrt{c - \ln F}\,. \tag{11}$$

Introducing a new variable $y$ by

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Eq. (10) can be solved at once to obtain

$$\psi = D \pm \sqrt{2}e^c\int_0^y e^{-t^2}\,dt, \tag{13}$$

or

$$\psi = D \pm (\tfrac{1}{2}\pi)^{1/2}e^c\,\mathrm{erf}(c - \ln F)^{1/2}, \tag{14}$$

where erf is the error function, which must be inverted if one wants $F$ as a function of $\psi$.

As a side remark, if one has the nonlinear $m$th order one-dimensional equation for $F = F(x)$,

$$F^n\frac{d^mF}{dx^m} = c = \text{const}, \tag{15}$$

then it has the solution

$$F = (d + ax)^{m/n+1} \tag{16}$$

with $d$ arbitrary and $a$ satisfying

$$a^m = c(n+1)^m\{(m)(m-n-1)\cdots \times [m - (m-1)(n+1)]\}^{-1}. \tag{17}$$

Returning to the original equations, Eqs. (1) and (2), let us generalize them to the forms

$$F^n\nabla^2 F = -a(\nabla\psi)^2 - bF^l \tag{18}$$

and

$$\nabla^2\psi = -cF^m, \tag{19}$$

where Eqs. (1) and (2) are recovered for $n = 3$, $a = \frac{1}{4}$, $b = 2\pi\rho$, $l = 8$, $c = 4\pi\rho$, and $m = 6$. Using arguments similar to those in the above paragraphs, one observes that Eqs. (18) and (19) can be readily solved as long as the constants $b$ and $c$ are not zero when

$$n = 2(l - m) - 1 \tag{20}$$

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Returning to the original equations, Eqs. (1) and (2), let us generalize them to the forms

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$$n = 2(l - m) - 1 \tag{20}$$

and

$$a = (b^2/c^2)(l - m - 1) \tag{21}$$

in which cases

$$F = [d + (l - m)(b/c)\psi]^{1/(l-m)}, \tag{22}$$

where $d$ is an arbitrary constant. If $l = m$, this is not applicable and the appropriate expression is

$$F = d \exp(b\psi/c) \tag{23}$$

with $a, b$ and $c$ satisfying

$$b^2 = -ac^2. \tag{24}$$

Before discussing the resulting equations for $\psi$, it is perhaps worthwhile to point out that when both $b$ and $c$ are zero one should recover the result obtained in studying Eqs. (3) and (4). To show this, first restrict $n$ so that $n \neq \pm 1$. From Eq. (20) one has

$$l - m = \tfrac{1}{2}(n + 1) \tag{25}$$

and from Eq. (21),

$$b/c = \pm\, [2a/(n - 1)]^{1/2}, \tag{26}$$

which is the appropriate expression to use when $b$ and $c$ go to zero. Via Eqs. (25) and (26), Eq. (22) becomes

$$F_{\pm} = \left( d \pm \frac{a^{1/2}(n + 1)}{[2(n - 1)]^{1/2}}\, \psi \right)^{2/(n+1)}. \tag{27}$$

The limit of $b$ and $c$ going to zero can now be taken in Eq. (27), and one recovers Eq. (9), after setting $a = 1$ as is appropriate. For $n = -1$, $l = m$, so Eq. (23) must be used. From Eq. (24), one has

$$b/c = \pm\, i\sqrt{a}, \tag{28}$$

which yields from Eq. (23)

$$F = d \exp(\pm\, i\sqrt{a}\,\psi). \tag{29}$$

From this, Eq. (10) is recovered at once. As long as $b$ and $c$ are not zero, Eqs. (20)–(22) yield acceptable solutions to Eqs. (18) and (19) for $n = +1$, which from Eqs. (20) and (21) imply $a = 0$, namely,

$$F = [d + b/c\psi] \tag{30}$$

is a solution of the equations

$$F\nabla^2 F = -bF^{m+1} \tag{31}$$

and

$$\nabla^2\psi = -cF^m. \tag{32}$$

However, for this $n$ value one can not recover Eq. (14).

The coupled set of equations, Eqs. (18) and (19), for the values of parameters given by Eqs. (20) and (21) or Eq. (24) are completely solved by Eqs. (22) or (23) as soon as $\psi$ is known as a function of $x_1, \ldots, x_\mu$. Next let us discuss the equations satisfied by $\psi$. From Eq. (19) plus Eq. (22) or (23) one finds, respectively,

$$\nabla^2\psi = -c[d + (l - m)b\psi/c]^{m/(l-m)} \tag{33}$$

and

$$\nabla^2\psi = -cd^m \exp[(mb\psi)/c]. \tag{34}$$

Nonlinear partial differential equations, of which the above are examples, are the subject of much recent and present research in mathematics.[2-5] Some comments specific to the above are found below. As a side remark, for one dimension both of the above equations can be solved at once by standard techniques since neither the independent variable nor the first derivative occurs.

First consider Eq. (34) with $cd^m \equiv \alpha$ and $mb/c \equiv \beta$ which is

$$\nabla^2\psi + \alpha \exp(\beta\psi) = 0. \tag{35}$$

This equation has been widely studied in one, two, and three dimensions and it has arisen in various physical problems. Discussions of some of these are found in Ref. 2, Sec. 4.16 and Ref. 6, Vol. 1, p. 838 and Vol. 2, p. 679.

Next consider Eq. (33), change the dependent variable by introducing

$$y = d + (l - m)(b\psi/c) \tag{36}$$

and define

$$k \equiv (l - m)b \quad \text{and} \quad (m/l - m) \equiv \gamma \tag{37}$$

which results in an equation for $y$,

$$\nabla^2 y + ky^\gamma = 0, \tag{38}$$

where it should be observed from Eq. (37) that $k \neq 0$, since $l \neq m$ in Eq. (33). As far as the author knows, this type of nonlinear equation has not been extensively studied in arbitrary dimensions for arbitrary $\gamma$ unless a particular symmetry is present. Some general discussions which are appropriate can be found in Refs. 2, 4, 5, and 6, Vol. 1, pp. 784-93. In three dimensions for some specific values of $\gamma$, Eq. (38) has been studied. For $\gamma = 0$, one has Poisson's equation. For $\gamma = 1$, it is Helmholtz's equation studied in most mathematical physics books (Ref. 6, Vol. 1, p. 829). For $\gamma = 2$, one has an equation which arises in diffusion controlled chemical reactions and is discussed in Sec. 6.4 of Ref. 2. Other situations where Eq. (38) has been studied is when it can be reduced to a nonlinear ordinary differential equation.[7] This occurs either in one dimension, in which case the solution is immediate since neither the first derivative nor independent variable appears explicitly, or in higher dimensions when the symmetry of the solution is known. For example, consider a solution which is spherically symmetric. Then, in three dimensions, Eq. (38) reduces to

$$\frac{d^2y}{dr^2} + \frac{2}{r}\frac{dy}{dr} + ky^\gamma = 0, \tag{39}$$

which is known as an equation of the Lane–Emden

type.[8,9] More generally, symmetry consideration may lead to a nonlinear equation of the form

$$ay'' = F(x, y, y') \tag{40}$$

and many cases for different $F$'s have been treated.[7-9]

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The author wishes to express his appreciation to the referee for many helpful suggestions and references and to Professor K. N. Nordtvedt, Jr. for a copy of his preprint and related comments.

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# On Multigroup Transport Theory with a Degenerate Transfer Kernel*

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(Received 3 September 1971)

The multigroup transport equation is studied in plane geometry assuming that the transfer kernel is representable in a degenerate form. The eigenvalue spectrum is analyzed and the associated eigensolutions are obtained in terms of generalized functions. Full-range orthogonality relation is demonstrated. The full-range completeness of the eigensolutions is established under rather general conditions. For the half-range completeness to hold, it is additionally required that the scattering kernel be self-adjoint and possesses reflection symmetry.

## I. INTRODUCTION

In a recent series of papers[1] the one-dimensional multigroup transport equation has been analyzed applying the method of singular eigensolution expansions. The transfer kernel is assumed to be representable in a degenerate form; consequently, the technique developed is amenable at least to situations where the scattering operator is compact. In this paper the formalism is extended to the energy-dependent total cross section. A preliminary report was presented at a recent conference.[2]

A modal expansion in the energy variable of the linear homogeneous Boltzmann equation yields the $N$-group approximation[3]

$$\mu \frac{\partial}{\partial x}\psi(x,\mu) + \mathbf{\Sigma}\psi(x,\mu) = \int_{-1}^{1} \mathbf{K}(\mu,\mu')\psi(x,\mu')\,d\mu'. \tag{1}$$

The notation is standard.[1] $\psi$ has $N$ components, namely the density in each energy group. $\mathbf{\Sigma}$ and $\mathbf{K}$ are $N \times N$ matrices representing the total removal and group-to-group scattering cross sections, respectively.

In the present study it is assumed that the removal matrix is diagonal—as obtained by an elementary derivation of the multigroup approximation—or diagonalizable. However, certain subsequent considerations, e.g., full range biorthogonality and the identity of the direct and adjoint eigenvalue spectra, are trivially extended to a general $\mathbf{\Sigma}$ matrix. The groups are ordered so that the diagonal elements $\sigma_i$ obey

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_N = 1. \tag{2}$$

To make the problem tractable in an explicit form, the kernel $\mathbf{K}(\mu,\mu')$ is assumed to be degenerate;

$$\mathbf{K}(\mu,\mu') = \sum_{i=1}^{M} \mathbf{L}_i(\mu)\mathbf{M}_i(\mu'). \tag{3}$$

We emphasize that a compact operator $\mathbf{K} \in L^2(-1,1)$ can be arbitrarily well approximated by a kernel of this form.[4]

The discrete eigenfunctions of Eq. (1) have been analyzed previously.[5] The continuum "eigensolutions" are obtained by appropriately extending the formalism of Ref. 1. Therefore the details are omitted in the subsequent sections. A more comprehensive discussion can be found elsewhere.[6]

As is customary, the completeness property of the eigensolutions is studied by first reducing the proof to a matrix Hilbert problem. Full-range completeness can be demonstrated under relatively weak conditions. In fact, it can be expected to hold even for nondegenerate transfer kernels.[7] For half-range completeness to hold it is additionally required that the transfer kernel be self-adjoint and possess reflection symmetry. These rather stringent conditions are necessitated by the index consideration pertaining to the Hilbert problem. We might mention that numerous earlier investigations have been incomplete or have made assumptions in this respect.[8]

## II. EIGENVALUES AND EIGENFUNCTIONS

The usual separation of variables in Eq. (1),

$$\psi(x,\mu) = e^{-x/\nu}\phi(\nu,\mu), \tag{4}$$

leads to the eigenvalue equation

$$\left(\mathbf{\Sigma} - \frac{\mu}{\nu}\mathbf{I}\right)\phi(\nu,\mu) = \int_{-1}^{1} \mathbf{K}(\mu,\mu')\phi(\nu,\mu')\,d\mu'. \tag{5}$$

Similar manipulation in the equation adjoint to Eq. (1) yields

$$\left(\mathbf{\Sigma} - \frac{\mu}{\nu}\mathbf{I}\right)\phi^{\dagger}(\nu,\mu) = \int_{-1}^{1} \mathbf{K}^{T}(\mu',\mu)\phi^{\dagger}(\nu,\mu')\,d\mu'. \tag{6}$$

In fact $\mathbf{\Sigma}^T$ would appear in Eq. (6); but the assumption of diagonalizability is employed. It should also be

type.[8,9] More generally, symmetry consideration may lead to a nonlinear equation of the form

$$ay'' = F(x, y, y') \tag{40}$$

and many cases for different $F$'s have been treated.[7-9]

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## I. INTRODUCTION

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In fact $\mathbf{\Sigma}^T$ would appear in Eq. (6); but the assumption of diagonalizability is employed. It should also be

mentioned that Eq. (6) is not the adjoint in the technical sense[4] but rather is convenient in the analysis. For example, the orthogonality relation

$$\int_{-1}^{1} \mu\,(\boldsymbol{\phi}^{\dagger}(\nu',\mu))^{T}\boldsymbol{\phi}(\nu,\mu)d\mu = 0, \qquad \nu \neq \nu' \tag{7}$$

can be obtained immediately.

The residual eigenvalue spectrum is empty,[5] despite the fact that the above operators are not normal. The discrete eigenvalues are zeros of the dispersion function $\Omega(z)$, where

$$\Omega(z) = \det\Lambda(z), \tag{8}$$

and $\boldsymbol{\Lambda}$ is a block matrix, with block elements

$$[\Lambda(z)]_{ij} = \delta_{ij}\mathbf{I} - \int_{-1}^{1} \mathbf{M}_i(\mu)\mathbf{D}(z,\mu)\mathbf{L}_j(\mu)\,d\mu \tag{9}$$

and

$$\mathbf{D}(z,\mu) = \left(\Sigma - \frac{\mu}{z}\mathbf{I}\right)^{-1}. \tag{10}$$

The discrete modes can be written as

$$\boldsymbol{\phi}(\nu_k,\mu) = \mathbf{D}(\nu_k,\mu)\sum_{i=1}^{M}\mathbf{L}_i(\mu)\mathbf{n}_i(\nu_k), \tag{11}$$

$$\mathbf{n}_i(z) = \int_{1}^{1} \mathbf{M}_i(\mu)\boldsymbol{\phi}(z,\mu)d\mu. \tag{12}$$

The continuous spectrum is degenerate in the usual way.[6] Thus, on the interval

$$\nu \in \left(-\frac{1}{\sigma_n}, -\frac{1}{\sigma_{n-1}}\right)\cup\left(\frac{1}{\sigma_{n-1}}, \frac{1}{\sigma_n}\right) \equiv (n), \tag{13}$$

$\boldsymbol{\phi}(\nu,\mu)$ is $(N-n+1)$-fold degenerate,

$$\boldsymbol{\phi}_j^{(n)}(\nu,\mu) = [\mathbf{D}(\nu,\mu) + \lambda_j^{(n)}(\nu)\delta^{(n)}(\nu,\mu)] \times \sum_{i=1}^{M}\mathbf{L}_i(\mu)\mathbf{n}_{ij}^{(n)}(\nu), \quad n \leq N, \quad j \leq N-n+1, \tag{14}$$

where $\lambda_j^{(n)}(\nu)$ is a root of the secular equation

$$\det\{[\Lambda^{+}(\nu) + \Lambda^{-}(\nu)] + (i/\pi\nu)\lambda^{(n)}(\nu)[\Lambda^{+}(\nu) - \Lambda^{-}(\nu)]\} = 0, \qquad \nu \in (n), \tag{15}$$

and $\delta(\nu,\mu)$ is implicitly defined by the relation

$$[\Lambda^{\pm}(\nu)]_{ij} = \delta_{ij}\mathbf{I} - \int_{-1}^{1}\mathbf{M}_i(\mu)[\mathbf{D}(\nu,\mu) \mp i\pi\nu\delta^{(n)}(\nu,\mu)] \times \mathbf{L}_j(\mu)\,d\mu. \tag{16}$$

In an explicit form $\boldsymbol{\delta}^{(n)}(\nu,\mu)$ is a diagonal matrix with elements

$$[\delta^{(n)}(\nu,\mu)]_{ii} = \delta(\sigma_i\nu - \mu), \qquad \nu \in (n). \tag{17}$$

The rank of the matrix appearing in Eq. (15) is $NM$. However, the characteristic polynomial is only of degree $N-n+1$ in $\lambda^{(n)}$.[6] The vectors $\mathbf{n}_{ij}^{(n)}(\nu)$, $i \leq M, j \leq N-n+1, n \leq N-n+1$ are defined in analogy with Eq. (12). As in the case of the discrete spectrum, the ratio of the components of $\mathbf{n}_{ij}(\nu)$ is intrinsically determined by a linear system of equations.

The functions $\lambda_j^{(n)}(\nu)$ are the same for the direct and adjoint problems.[6] In order to determine them explicitly a special combination of the eigensolutions is more conveniently employed. The details may be found elsewhere.[1]

## III. COMPLETENESS OF THE EIGENSOLUTIONS

We wish to begin the study of the completeness of the eigensolution set with a general framework of the formalism assuming an arbitrary range $L$.

Letting $\boldsymbol{\psi}(\mu)$ represent an arbitrary vector whose components satisfy the entended Holder condition, we find that the expansion in terms of the continuous modes alone is

$$\boldsymbol{\psi}(\mu) = \sum_{n=1}^{N}\sum_{j=1}^{N-n+1}\int_{(n)}\alpha_j^{(n)}(\nu)\boldsymbol{\phi}_j^{(n)}(\nu,\mu)d\nu, \quad \mu \in L, \tag{18}$$

where

$$(n)_L = (n) \cap L, \tag{19}$$

and $\alpha_j^{(n)}(\nu)$ is an expansion coefficient.

By substituting the explicit forms of the $\boldsymbol{\phi}_i^{(n)}(\nu,\mu)$ into this equation one obtains, after some algebra

$$\boldsymbol{\psi}(\mu) = \sum_{n=1}^{N}\sum_{i=1}^{M}\int_{(n)_L}[\mathbf{D}(\nu,\mu)\mathbf{L}_i(\mu)\mathbf{N}_i^{(n)}(\nu)\boldsymbol{\alpha}^{(n)}(\nu) + \boldsymbol{\delta}^{(n)}(\nu,\mu)\mathbf{L}_i(\mu)\mathbf{N}_i^{(n)}(\nu)\lambda^{(n)}(\nu)\boldsymbol{\alpha}^{(n)}(\nu)]d\nu, \quad \mu \in L \tag{20}$$

where

$$[\lambda^{(n)}(\nu)]_{ij} = \lambda_j^{(n)}(\nu)\delta_{ij}, \quad i,j \leq N-n+1 \tag{21}$$

and

$$[\mathbf{N}_l^{(n)}(\nu)]_{ij} = [\mathbf{n}_{li}^{(n)}(\nu)]_j, \quad i \leq N-n+1, \; j \leq N. \tag{22}$$

In order to proceed further, it is necessary to put Eq. (20) in "dominant" form.[9] Hence we circumvent the occurrence of a Fredholm term which would eliminate any conclusive statement of completeness.[10] This is achieved by the change of variable

$$\mu \to \mu/\sigma_i \tag{23}$$

in the $i$th equation of the system. Simultaneously introducing matrices $\mathbf{L}_{\sigma i}(\mu)$ defined as

$$[\mathbf{L}_{\sigma i}(\mu)]_{kl} = [\mathbf{L}_i(\sigma_k\nu)]_{kl}h_k(\nu), \tag{24}$$

where

$$h_k(\nu) = 1, \quad \nu \in [-1/\sigma_k, 1/\sigma_k] \qquad = 0 \quad \text{otherwise}, \tag{25}$$

Eq. (20) has the form

$$\Sigma\boldsymbol{\psi}_{\sigma}(\mu) = \sum_{i=1}^{M}\mathbf{L}_{\sigma i}(\mu)\left(\int_L \frac{\nu}{\nu-\mu}\sum_{n=1}^{N}\mathbf{N}_i^{(n)}(\nu)\boldsymbol{\alpha}^{(n)}(\nu)g_n(\nu)d\nu + \sum_{n=1}^{N}\mathbf{N}_i^{(n)}(\mu)\boldsymbol{\lambda}^{(n)}(\mu)\boldsymbol{\alpha}^{(n)}(\mu)g_n(\mu)\right). \tag{26}$$

Here $\boldsymbol{\psi}_{\sigma}$ has been obtained from a single column operation performed pursuant to Eq. (24), i.e.,

$$[\boldsymbol{\psi}_{\sigma}(\mu)]_i = [\boldsymbol{\psi}(\sigma_i\mu)]_i h_i(\mu) \tag{27}$$

and

$$g_n(\mu) = 1, \quad \mu \in (n)_L, \qquad = 0 \quad \text{otherwise}. \tag{28}$$

Generalizing the procedure presented previously, Eq. (26) is multiplied by $\mathbf{M}_i^{\sigma}(\mu)$, $i = 1, 2, \cdots M$, where

$$[\mathbf{M}_i^{\sigma}(\mu)]_{kl} = [\mathbf{M}_i(\sigma_l\nu)]_{kl}h_l(\nu). \tag{29}$$

Defining $\boldsymbol{\xi}_i(\mu)$ by

$$\xi_i(\mu) = \mathbf{M}_i^{\varrho}(\mu)\Sigma\psi_o(\mu), \tag{30}$$

we obtain

$$\mu\xi_i(\mu) = \frac{1}{2\pi i}\sum_{j=1}^{M}[\Lambda^+(\mu) - \Lambda^-(\mu)]_{ij}\Big(\int_L \frac{\nu}{\nu-\mu}\sum_{n=1}^{N} \mathbf{N}_j^{(n)}(\nu)\alpha^{(n)}(\nu)g_n(\nu)\,d\nu + \sum_{n=1}^{N}\mathbf{N}_j^{(n)}(\mu)\lambda^{(n)}(\mu) \times \alpha^{(n)}(\mu)g_n(\mu)\Big). \tag{31}$$

Furthermore, using the identity[6]

$$i\pi\nu\sum_{j=1}^{M}[\Lambda^+(\nu) + \Lambda^-(\nu)]_{ij}\mathbf{N}_j^{(n)}(\nu) = \sum_{i=1}^{M}[\Lambda^+(\nu) - \Lambda^-(\nu)]_{ij}\mathbf{N}_j^{(n)}(\nu)\alpha^{(n)}(\nu) \tag{32}$$

in Eq. (31) leads to

$$\mu\xi_i(\mu) = \sum_{j=1}^{M}\Big(\frac{1}{2\pi i}[\Lambda^+(\mu) - \Lambda^-(\mu)]_{ij}\int_L \frac{\nu}{\nu-\mu}\rho_j(\nu)\,d\nu + \tfrac{1}{2}\mu[\Lambda^+(\mu) + \Lambda^-(\mu)]_{ij}\rho_j(\mu)\Big), \tag{33}$$

where

$$\rho_j(\mu)g_n(\mu) = \mathbf{N}_j^{(n)}(\mu)\alpha^{(n)}(\mu). \tag{34}$$

Considering Eq. (33) for all values of $i \le M$, we have a system of $NM$ equations

$$\mu\xi(\mu) = \frac{1}{2\pi i}[\Lambda^+(\mu) - \Lambda^-(\mu)]\int_L \frac{\nu}{\nu-\mu}\rho(\nu)\,d\nu + \tfrac{1}{2}\mu[\Lambda^+(\mu) + \Lambda^-(\mu)]\rho(\mu), \tag{35}$$

where the vectors $\xi(\mu)$ and $\rho(\mu)$ consist of all the components $[\xi_i(\mu)]_j$ and $[\rho_i(\mu)]_j$, $i \le M \le j \le N$, respectively.

Finally, introducing the boundary values $\Phi^{\pm}(\mu)$ of a sectionally holomorphic vector $\Phi(z)$, where

$$\Phi(z) = \frac{1}{2\pi i}\int_L \frac{1}{\nu - z}\rho(\nu)\,d\nu, \tag{36}$$

one obtains

$$\mu\xi(\mu) = \Lambda^+(\mu)\Phi^+(\mu) - \Lambda^-(\mu)\Phi^-(\mu), \qquad \mu \in L. \tag{37}$$

The canonical form of this equation is

$$\Phi^+(\mu) = \mathbf{g}(\mu)\Phi^-(\mu) + \mathbf{f}(\mu), \qquad \mu \in L, \tag{38}$$

where the transformation matrix $\mathbf{g}(\mu)$ is

$$\mathbf{g}(\mu) = [\Lambda^+(\mu)]^{-1}\Lambda^-(\mu) \tag{39}$$

and

$$\mathbf{f}(\mu) = \mu[\Lambda^+(\mu)]^{-1}\xi(\mu). \tag{40}$$

It is obvious that some special consideration is needed if $\Lambda^{\pm}(\mu)$ is a singular matrix on $\mu \in L$. This is tantamount to the occurrence of a discrete eigenvalue embedded in the continuous spectrum.[11] We assert that the normal modes are complete, $\nu \in L$, where Eq. (38) has a unique solution, $\mu \in L$, such that $\Phi(z) \to \mathbf{0}$ as $|z| \to \infty$.

The essential problem is to establish the existence of a nonsingular fundamental matrix $\mathbf{X}(z)$ whose boundary conditions obey the equation

$$\mathbf{g}(\mu) = \mathbf{X}^+(\mu)[\mathbf{X}^-(\mu)]^{-1}, \qquad \mu \in L. \tag{41}$$

If such a matrix exists, then

$$\Phi(z) = \frac{1}{2\pi i}\mathbf{X}(z)\Big(\int_L [\mathbf{X}^+(\mu)]^{-1}\mathbf{f}(\mu)\frac{d\mu}{\mu - z} + \mathbf{p}(z)\Big), \tag{42}$$

where $\mathbf{p}(z)$ is a vector of polynomials.

Sufficient conditions for the existence of a matrix $\mathbf{X}(z)$ are studied extensively in the mathematical literature. If the Hilbert problem [Eq. (38)] has continuous coefficients (i.e., if the elements of $\mathbf{g}(\mu)$ are continuous functions on $L$ and at the endpoints), $\mathbf{g}(\mu)$ reduces to the identity matrix. Mandzavidze and Khvedelidze[12] have deduced the existence of a fundamental matrix for this case considering a certain convergent sequence of matrices.

The original theory of Vekua[9] is applicable if $\mathbf{g}(\mu)$ is piecewise Lipschitz continuous. The Hilbert problem is reduced to another one having continuous coefficients whereby an additional number $\rho$ enter the index equation. The Lipschitz condition is required because the theory is based on the solubility of a certain system of Fredholm equations.

In order for Eq. (42) to be the solution of Eq. (38) it is required that the inhomogeneous term $\mathbf{f}(\mu)$ satisfied the extended $H_{\epsilon}$-condition. The definition of $\mathbf{f}(\mu)$ and Eq. (30) then specify the conditions on an admissible function $\psi(\mu)$. Further restrictions on $\mathbf{f}(\mu)$ arise from the analyticity requirements of $\Phi(z)$. $\Phi(z)$ will vanish at infinity only if $m$ conditions of the form

$$\int_L [\omega_i(\mu)]^T\mathbf{f}(\mu)\,d\mu = 0, \tag{43}$$

(where the vectors $\omega_i(\mu)$, $i = 1, 2, \ldots, m$, are related to the $\mathbf{X}$ matrix) are imposed on $\mathbf{f}(\mu)$.

Denoting the number of arbitrary polynomial coefficients in Eq. (42) by $l$, all the parameters relevant to the solubility constitute the index equation[9]:

$$m - l = -(1/2\pi)\Delta_L \arg \det \mathbf{g}(\mu) + \rho, \tag{44}$$

where $\Delta_L$ denotes the change of the operand on $L$. In particular, if $L$ is the full-range then

$$n = (1/2\pi)\Delta_{-1,1}\arg \det \mathbf{g}(\mu), \tag{45}$$

where $n$ is the total number of discrete eigenfunctions.

Requiring $\rho = 0$, one has a proper number of discrete expansion coefficients provided that $l$ also vanishes. This is certainly sufficient, and at this point it appears that $l + \rho = 0$ may guarantee a unique solution. The number $l$ is manifestly nonnegative. It is the sum of all positive partial indices of the $\mathbf{X}$ matrix. It is known[9] that $\mathbf{X}$ can be put in normal form at infinity, i.e.,

$$\lim_{z\to\infty}\mathbf{X}(z)\begin{bmatrix} z^{k_1} & & 0 \\ & \ddots & \\ 0 & & z^{k_{NM}} \end{bmatrix} = I, \tag{46}$$

where $k_i$ is a partial index.

The nonpositivity of the partial indices (i.e., $l = 0$), is readily established in the full-range case.[1] In the

half-range a general proof has been also proposed[1] assuming the reflection symmetry of the dispersion matrix:

$$\mathbf{\Lambda}(z) = \mathbf{\Lambda}(-z). \tag{47}$$

The proof is not entirely conclusive because of some details arising from the fact that the direct and adjoint problems have to be considered simultaneously. For a self-adjoint kernel, where

$$\mathbf{K}(\mu, \mu') = \mathbf{K}^T(\mu', \mu), \tag{48}$$

and therefore

$$\mathbf{\Lambda}(z) = \mathbf{\Lambda}^T(z), \tag{49}$$

a rigorous proof has been given.[13] Although this restriction may seem severe, in many nonself-adjoint problems the scattering kernel can be symmetrized; for example, in the thermal neutron case Maxwellian weights can be introduced.[14]

In full-range problems a constructive proof could have been given. This follows from the fact that Eq. (39) already represents an appropriate Wiener–Hopf factorization. The solution of the expansion coefficients can, however, be obtained more conveniently from the orthogonality relation Eq. (7).

## IV. CONCLUSION

The multigroup transport equation was considered assuming that the transfer kernel can be represented in a degenerate form. The analysis was carried out using the method of singular eigensolutions. We wish briefly to capitulate the results of the preceding sections by including the relevant conclusions established earlier[1]:

(1) Full range biorthogonality of the Case eigenfunctions is shown (rather trivially). In fact, it holds for even a nondegenerate kernel.

(2) The eigenfunctions are complete on the full range if any of the following conditions holds:

(a) If $\mu \mathbf{M}_i(\mu)\boldsymbol{\psi}(\mu)$ obeys the extended Hölder condition [$\boldsymbol{\psi}(\mu)$ is the vector being expanded, and we say that the function is "extended Hölder" if it is a weak limit of a sequence of Hölder functions][15];

(b) if the elements of the matrix $\mathbf{g}(\mu) = [\mathbf{\Lambda}^+(\mu)]^{-1}\mathbf{\Lambda}^-(\mu)$ are continuous, and if $\lim g[\pm(1-\epsilon)] = I$. Here $\mathbf{\Lambda}(z)$ is the dispersion matrix.] Also, a certain vector $\mathbf{f}(\mu)$, which is constructed from $[\mathbf{\Lambda}^+(\mu)]^{-1}$, $\boldsymbol{\psi}(\mu)$, and the matrices $\mathbf{M}_i(\mu)$ must be "extended Hölder."

(c) if $\mathbf{g}(\mu)$ is Lipschitz continuous almost everywhere, and an index $\rho$ (which must be calculated, from the discontinuities in $g$, for each particular case) vanish. (For negative $\rho$, the set is overcomplete).

The case (a) above is the classic case, in that all known problems fall into this category. However, case (b) is of great interest, because it is most readily generalizable to the half-range case. In fact, all known specific examples of half-range completeness do fall into category (b). Case (c) is rather uninteresting because of the stringency of the Lipschitz condition.

Half-range completeness holds if either (b) or (c) above holds and, if in addition, the elements $\mathbf{K}(\mu, \mu')$ are bounded in a neighborhood of $\mu, \mu' = 0$. There are two other requirements as well, which arise from the condition that no polynomial occur in the solution of the Hilbert problem. They are

(a′) $\mathbf{\Lambda}(z) = \mathbf{\Lambda}(-z)$. This is always true, if $\mathbf{K}(\mu, \mu') = \mathbf{K}(-\mu, -\mu')$, certainly a physically meaningful assumption.

(b′) More stringently, the transfer kernel $\mathbf{K}$ is self-adjoint, i.e.,

$$\mathbf{K}(\mu, \mu') = \mathbf{K}^T(\mu', \mu). \tag{48′}$$

While we did not find any analytic solution to the bounded medium problems, we wish to use our results to analyze those boundary value problems (1) by expressing the solutions in terms of the emergent distribution and the infinite medium Green's function, which is readily derived in a closed form,[6] (2) to justify the numerical solutions, either the direct iteration or the invariant embedding approaches, and (3) to derive the half-range orthogonality weight function in terms of the $H$ function along the lines proposed recently for a special case of our kernel.

Since the completeness proofs are crucial for a work of this kind some attempt should be directed to extend the validity of our theorems. It appears that the classical conditions[9,12] could be relaxed. Equally importantly, the half-range index considerations are likely to hold even for nonself-adjoint kernels; but a proof has not yet been established.

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# Radial Moments of Folding Integrals for Nonspherical Distributions

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Simple relations are exhibited between the radial moments of two nonspherical distributions when one is obtained by folding a scalar function into the other. Some applications are mentioned, and the generalization to nonscalar functions is indicated.

## I. INTRODUCTION

It is well known that when one spherical distribution $h(r_1)$ is obtained by folding a scalar function $g(s)$ into another spherical distribution $f(r_2)$,

$$h(r_1) = \int f(r_2)g(s)\,d\mathbf{r}_2, \tag{1}$$

where $\mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2$, then there are simple relations between the volume integrals $J_0$ and mean square radii $\langle r^2\rangle$ of the distributions. If

$$J_0(j) = 4\pi \int j(r)r^2 dr, \tag{2}$$

then

$$J_0(h) = J_0(f)J_0(g), \tag{3}$$

and if

$$\langle r^2\rangle_j = 4\pi \int j(r)r^4 dr/J_0(j), \tag{4}$$

then

$$\langle r^2\rangle_h = \langle r^2\rangle_f + \langle r^2\rangle_g. \tag{5}$$

These results are used extensively, for example, in applications of the so-called reformulated optical model of elastic scattering from nuclei.[1]

We present here some generalizations of these relations, for distributions $f$ (and hence $h$) which are nonspherical, which do not seem to be well known. These find application, for example, in studies of inelastic scattering from nuclei, e.g., by electrons. They also provide checks on the numerical accuracy of calculations of folded functions like (1).

We define the generalization of (1) as

$$h(\mathbf{r}_1) = \int f(\mathbf{r}_2)g(s)\,d\mathbf{r}_2, \tag{6}$$

where $g(s)$ is still a scalar function of the magnitude of $\mathbf{s}$. The nonspherical distribution $f$ can be expressed by the multipole expansion[2]

$$f(\mathbf{r}_2) = \sum_{lm} f_{lm}(r_2)Y_l^m(\Omega_2), \tag{7}$$

where

$$f_{lm}(r_2) = \int f(\mathbf{r}_2)Y_l^m(\Omega_2)^*\,d\Omega_2. \tag{8}$$

There is a similar expansion for $h$,

$$h(\mathbf{r}_1) = \sum_{LM} h_{LM}(r_1)Y_L^M(\Omega_1). \tag{9}$$

Given the Slater expansion[2] of $g$

$$g(|\mathbf{r}_1 - \mathbf{r}_2|) = 4\pi \sum_{kq} g_k(r_1, r_2)Y_k^q(\Omega_1)Y_k^q(\Omega_2), \tag{10}$$

these multipole coefficients are related by

$$h_{LM}(r_1) = 4\pi \int f_{LM}(r_2)g_L(r_1, r_2)r_2^2 dr_2. \tag{11}$$

We also define generalizations of quantities (2) and (4):

$$J_n(j) = 4\pi \int j(r)r^{n+2}dr \tag{12}$$

and

$$\langle r^n\rangle_j = J_n(j)/J_0(j). \tag{13}$$

We note from the definitions above that

$$J_L(j_{LM}) = 4\pi q_{LM}^*(j), \tag{14}$$

where $q_{LM}(j)$ is the usual[2,3] multipole moment of a distribution $j(\mathbf{r})$,

$$q_{LM}(j) = \int j(\mathbf{r})r^L Y_L^M(\theta, \phi)\,d\mathbf{r}.$$

We also define for the multipole coefficient $j_{LM}(r)$ the quantity

$$R_{tr}^2(j_{LM}) = J_{L+2}(j_{LM})/J_L(j_{LM}). \tag{15}$$

In studies of electron scattering, $R_{tr}$ is often referred to as the "transition radius."

It is relations between these various quantities that we discuss here. The main results are given in Eqs. (17)–(19) below.

## II. RESULTS

The results are obtained by a straightforward application of standard techniques[2] to the integrals

$$\int h(\mathbf{r}_1)r_1^{L+k}Y_L^M(\Omega_1)d\mathbf{r}_1.$$

In particular we use the solid harmonic expansion which holds for $\mathbf{r}_1 = \mathbf{s} + \mathbf{r}_2$,

$$r_1^L Y_L^M(\Omega_1) = \sum_{\lambda\mu}\left[\frac{4\pi}{2\lambda+1}\binom{2L+1}{2\lambda}\right]^{1/2} s^\lambda Y_\lambda^\mu(\Omega_s)r_2^{L-\lambda} \times Y_{L-\lambda}^{M-\mu}(\Omega_2)\langle L-\lambda, \lambda, M-\mu, \mu\,|\,LM\rangle, \tag{16}$$

where

$$\binom{a}{b} = \frac{a!}{b!(a-b)!},$$

and $\langle ab\alpha\beta\,|\,c\gamma\rangle$ is the usual[2] Clebsch–Gordan or Wigner coefficient.

We soon obtain for $k = 0, 2$ the relations

$$J_L(h_{LM}) = J_L(f_{LM})J_0(g) \tag{17}$$

and

$$J_{L+2}(h_{LM}) = J_{L+2}(f_{LM})J_0(g) + \tfrac{1}{3}(2L+3)J_L(f_{LM})J_2(g). \tag{18}$$

Combining these two we have for the transition radii

$$R_{tr}^2(h_{LM}) = R_{tr}^2(f_{LM}) + \tfrac{1}{3}(2L+3)\langle r^2\rangle_g. \tag{19}$$

Equations (17) and (19) reduce to Eqs. (3) and (5), respectively, for $L = 0$.

Relations between the quantities of higher order may be obtained, but become increasingly complicated and

less useful as $k$ increases. For example, for $k = 4$ we use the expression

$$|\mathbf{s} + \mathbf{r}_2|^4 = \sum_\mu [(32\pi/15)s^2 r_2^2 Y_2^\mu(\Omega_s) Y_2^\mu(\Omega_2)^* + (16\pi/3)s r_2 (s^2 + r_2^2)\, Y_1^\mu(\Omega_s) Y_1^\mu(\Omega_2)^*] + (s^4 + r_2^4 + \tfrac{10}{3} s^2 r^2) \quad (20)$$

to obtain

$$J_{L+4}(h_{LM}) = J_{L+4}(f_{LM}) J_0(g) + \tfrac{2}{3}(2L+5) J_{L+2}(f_{LM}) J_2(g) + \tfrac{1}{15}(2L+5)(2L+3) J_L(f_{LM}) J_4(g). \quad (21)$$

## III. EXTENSION TO NONCENTRAL "FORCES"

The function $g(s)$ itself may be generalized to noncentral forms by writing

$$G_{KQ}(\mathbf{s}) = (4\pi)^{1/2} g_{KQ}(s) Y_K^Q(\Omega_s), \quad (22)$$

which is normalized so that the scalar $g(s)$ of the previous sections is now $g_{00}(s)$. We may now proceed as before. The distribution $h$ now depends upon the indices $K$, $Q$ where

$$h^{KQ}(\mathbf{r}_1) = \int f(\mathbf{r}_2) G_{KQ}(\mathbf{s}) d\mathbf{r}_2, \quad (23)$$

as do its corresponding multipole coefficients

$$h^{KQ}(\mathbf{r}_1) = \sum_{LM} h_{LM}^{KQ}(r_1) Y_L^M(\Omega_1). \quad (24)$$

We soon find the generalization of the relation (17) for $k = 0$,

$$J_L(h_{LM}^{KQ}) = \alpha_{LM}^{KQ} J_{L-K}(f_{L-K,M-Q}) J_K(g_{KQ}), \quad (25)$$

where

$$\alpha_{LM}^{KQ} = \left(\frac{(2L+1)!}{(2K+1)!(2L-2K+1)!}\right)^{1/2} \times \langle L-K, K, M-Q, Q \mid LM\rangle = \left[\frac{2L+1}{(2K+1)(2L-2K+1)}\binom{L-M}{K-Q}\binom{L+M}{K+Q}\right]^{1/2}. \quad (26)$$

The previous result (17) is regained with $K = Q = 0$ since $\alpha_{LM}^{00} = 1$. We also have $\alpha_{LM}^{LM} = 1$ and $\alpha_{LM}^{KQ} = 0$ if $K > L$.

The higher order results become progressively more complicated. For $k = 2$, for example, the generalization of Eq. (18), we find $J_{L+2}(h_{LM}^{KQ})$ to be a linear combination of the products

$$J_K(g_{KQ}) J_{L-K+2}(f_{L-K,M-Q}),$$
$$J_K(g_{KQ}) J_{L-K+2}(f_{L-K+2,M-Q}),$$
$$J_{K+2}(g_{KQ}) J_{L-K}(f_{L-K,M-Q}),$$

and

$$J_{K+2}(g_{KQ}) J_{L-K}(f_{L-K-2,M-Q}).$$

## IV. CONCLUSIONS

The results of most interest are those presented in Eqs. (17) and (19) and are generalizations of the well-known results (3) and (5) for spherical distributions. An example of their application in studies of electron scattering from nuclei occurs when one folds a finite-sized distribution $g$ of the charge on a proton into a "point-proton" distribution $f$ in order to obtain the nuclear charge distribution $h$. Equation (17) shows that the transition charge density for a $2^L$-pole transition and the corresponding point-proton transition density have the same expectation value for $r^L$. Hence the reduced transition probability $B(EL)$ may be evaluated using either distribution. The transition radius $R_{tr}$, however, is increased by the folding by an amount given by Eq. (19).

## ACKNOWLEDGMENT

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# Variational Estimates and Generalized Perturbation Theory for the Ratios of Linear and Bilinear Functionals*

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(Received 20 October 1971; Revised Manuscript Received 15 March 1972)

Variational functionals are presented which provide an estimate of ratios of linear and bilinear functionals of the solutions of the direct and adjoint equations (inhomogeneous and homogeneous) governing linear systems. These variational functionals are used as the basis for a generalized perturbation theory for estimating the effects of changes in system parameters upon these ratios of linear and bilinear functionals. The relation of the present theory to the variational theory of Pomraning and to the generalized perturbation theory of Usachev and Gandini is discussed. Potential applications of the theory to nuclear reactor physics are outlined.

## 1. INTRODUCTION

If a variational functional can be written for a given property of a linear system, then that property can be computed to second-order accuracy (with respect to errors in the solution function) by evaluating the variational functional. For example, a variational functional for the eigenvalue of the linear system described by the equation[1]

$$(A - \lambda B)\phi_\lambda = 0 \quad (1)$$

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less useful as $k$ increases. For example, for $k = 4$ we use the expression

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## 1. INTRODUCTION

If a variational functional can be written for a given property of a linear system, then that property can be computed to second-order accuracy (with respect to errors in the solution function) by evaluating the variational functional. For example, a variational functional for the eigenvalue of the linear system described by the equation[1]

$$(A - \lambda B)\phi_\lambda = 0 \quad (1)$$

is[2]

$$\lambda[\phi_\lambda^*, \phi_\lambda] = \langle \phi_\lambda^*, A\phi_\lambda \rangle / \langle \phi_\lambda^* B \phi_\lambda \rangle, \tag{2}$$

where $\phi_\lambda^*$ must satisfy the adjoint equation

$$(A^* - \lambda B^*)\phi_\lambda^* = 0. \tag{3}$$

$A, B, A^*$, and $B^*$ are linear operators satisfying $\langle u, Av \rangle = \langle A^* u, v \rangle$, $\langle u, Bv \rangle = \langle B^* u, v \rangle$. If functions $\tilde{\phi}$ and $\tilde{\phi}^*$ which differ from the solutions to Eqs. (1) and (3) by $\delta\phi$ and $\delta\phi^*$, respectively, are used to evaluate Eq. (2), it may be shown that

$$\delta\lambda \equiv \lambda[\tilde{\phi}_\lambda^*, \tilde{\phi}_\lambda] - \lambda[\phi_\lambda^*, \phi_\lambda] = 0 + \text{order}\langle \delta\phi^*, \delta\phi \rangle.$$

Similarly, a variational estimate of the linear functional $\langle S^*, \phi \rangle$ of the solution to the inhomogeneous equation

$$(A - B)\phi = S \tag{4}$$

is given by the Roussopolos functional[3]

$$R[\phi^*, \phi] = \langle S^*, \phi \rangle + \langle \phi^*, [S - (A - B)\phi] \rangle \tag{5}$$

or the Schwinger functional[4]

$$J[\phi^*, \phi] = \langle\langle S^*, \phi \rangle \langle \phi^*, S \rangle\rangle / \langle \phi^*, (A - B)\phi \rangle, \tag{6}$$

where $\phi^*$ satisfies

$$(A^* - B^*)\phi^* = S^*. \tag{7}$$

Selengut[5] demonstrated that these latter two functionals are equivalent.

Pomraning[6] suggested the variational functional

$$P_1[\psi^*, \phi] = G[\phi] + \langle \psi^*, [S - (A - B)\phi] \rangle \tag{8}$$

for estimating the arbitrary linear functional $G[\phi]$ of the solution of Eq. (4). He demonstrated that $\psi^*$ must satisfy

$$(A^* - B^*)\psi^* = G'[\phi], \tag{9}$$

where the prime indicates the functional derivative.

Pomraning[7] also suggested the variational functional

$$P_2[\theta^*, \phi_\lambda] = G[\phi_\lambda] + \langle \theta^*, (A - \lambda B)\phi_\lambda \rangle \tag{10}$$

for estimating an arbitrary linear functional $G[\phi_\lambda]$ of the eigensolution of Eq. (1). He showed that $\theta^*$ must satisfy

$$(A^* - \lambda B^*)\theta^* = -G'[\phi_\lambda]. \tag{11}$$

A necessary condition for Eq. (11) to have a solution is that the rhs is orthogonal to the eigensolutions of Eq. (1) or

$$\langle \phi_\lambda, G'[\phi_\lambda] \rangle = 0,$$

which is just the basic property of homogeneous functionals.

In many practical situations, the property of interest is the ratio of two linear or bilinear functionals of the solution to the direct [Eqs. (1) or (4)] and/or adjoint [Eqs. (3) or (7)] equations describing the system. While Pomraning's functionals may be specialized to accommodate the case of ratios of linear functionals of the solution to the direct equations, no variational functionals have been presented which are suitable for estimating ratios of linear functionals of the solution to the adjoint equation or ratios of bilinear functionals of the solutions of the direct and adjoint equations.

The primary purpose of this paper is to present variational functionals which may be used to estimate ratios of linear and bilinear functionals of the direct and adjoint solutions of the equations which govern linear systems. A secondary purpose is to develop a perturbation theory from the variational functionals, which, for eigenvalue problems, is similar to the generalized perturbation theory developed from physical arguments for reactor physics problems by Usachev[8] and extended by Gandini.[9] Thus, an ancillary result is the provision of a firmer theoretical basis for the generalized perturbation theory, in addition to extending that theory to systems governed by inhomogeneous equations.

## II. LINEAR FLUX RATIOS—INHOMOGENEOUS SYSTEMS

Consider the problem of estimating the ratio of linear functionals of the solution $\phi$ of Eq. (4)

$$R_{ij} \equiv \langle \Sigma_i \phi \rangle / \langle \Sigma_j \phi \rangle, \tag{12}$$

where $\Sigma_i$ and $\Sigma_j$ are scalar operators. A direct estimate of $R_{ij}$ from Eq. (12) with a function $\tilde{\phi}$ which differed from the solution of Eq. (4) by a function $\delta\phi$ would introduce an error $\delta R_{ij} \propto \langle \delta\phi \rangle$; i.e., a first-order error.

However, the variational functional

$$F_1[\psi^*, \phi] = \langle\langle \Sigma_i \phi \rangle / \langle \Sigma_j \phi \rangle\rangle \{1 - \langle \psi^*, [(A - B)\phi - S] \rangle\} \tag{13}$$

provides an estimate of $R_{ij}$ with error $\delta R_{ij} \propto \langle \delta\psi^*, \delta\phi \rangle$; i.e., of second order. Here $\delta\phi$ is the difference between the trial function $\tilde{\phi}$ used to evaluate Eq. (13) and the solution of Eq. (4), and $\delta\psi^*$ is the difference between the trial function $\tilde{\psi}^*$ used to evaluate Eq. (13) and the solution of

$$(A^* - B^*)\psi^* = (\Sigma_i / \langle \Sigma_i \phi \rangle) - (\Sigma_j / \langle \Sigma_j \phi \rangle). \tag{14}$$

The proof of this follows from the easily verifiable fact that $F_1$ is stationary (i.e., $\delta F_1 = 0$ to first order) about functions $\psi^*$ and $\phi$ which satisfy Eqs. (14) and (4), respectively, and the stationary value is $R_{ij}$. Pomraning's results[6] reduce to this form when $G[\phi] = R_{ij}$.

A perturbation theory for changes in $R_{ij}$ corresponding to changes in the system parameters can be derived from the difference

$$\delta R_{ij} = F_1'[\psi^*, \phi] - F_1[\psi^*, \phi]. \tag{15}$$

The prime indicates that the perturbed values $\Sigma_i', \Sigma_j', A', B', S'$ are used in Eq. (13) to evaluate $F'$, while the unperturbed values are used to evaluate $F$. Trial functions which approximate (or are equal to) the unperturbed solutions to Eqs. (4) and (14) are used to evaluate both $F'$ and $F$. The result, accurate to second order, is

$$\frac{\delta R_{ij}}{R_{ij}} = \frac{\langle \delta\Sigma_i \phi\rangle}{\langle \Sigma_i \phi\rangle} - \frac{\langle \delta\Sigma_j \phi\rangle}{\langle \Sigma_j \phi\rangle} - \langle \psi^*, [(\delta A - \delta B)\phi - \delta S]\rangle, \tag{16}$$

where $\delta A \equiv A' - A$, etc. If the solution $\phi$ did not change with the introduction of the perturbation, the first two terms in Eq. (16) would rigorously describe the change $\delta R_{ij}/R_{ij}$. A conventional estimate (one in which the unperturbed flux is used) based on Eq. (12) yields just the first two terms. Thus, the final term in Eq. (16) accounts for the effect of the perturbation upon the solution $\phi$ and represents a refinement upon conventional methods.

## III. LINEAR FLUX RATIOS—HOMOGENEOUS SYSTEMS

Consider again the problem of estimating $R_{ij}$, this time with $\phi_\lambda$, the fundamental eigensolution of Eq. (1). Again, a direct estimate from Eq. (12) would yield a first-order error $\delta R_{ij}$. The variational functional

$$F_2[\psi^*, \phi_\lambda] = (\langle \Sigma_i \phi_\lambda\rangle / \langle \Sigma_j \phi_\lambda\rangle)[1 - \langle \psi^*, (A - \lambda B)\phi_\lambda\rangle] \tag{17}$$

provides an estimate of $R_{ij}$ accurate to second order with respect to the differences $\delta\phi$ and $\delta\psi^*$ between the trial functions used in evaluating Eq. (17) and the solutions of Eq. (1) and

$$(A^* - \lambda B^*)\psi^* = (\Sigma_i / \langle \Sigma_i \phi_\lambda\rangle) - (\Sigma_j / \langle \Sigma_j \phi_\lambda\rangle), \tag{18}$$

respectively. Proof follows from consideration of the stationarity conditions for $F_2$. Pomraning's results[7] reduce to this form when $G[\phi] = R_{ij}$.

Equation (18) has a solution because the rhs is orthogonal to $\phi_\lambda$, the fundamental eigensolution of Eq. (1). The method of successive approximations yields a solution to Eq. (18) of the form (see Appendix for discussion of convergence)

$$\psi^* = \sum_{n=0}^{\infty} \psi_n^*, \tag{19}$$

where

$$A^*\psi_0^* = (\Sigma_i / \langle \Sigma_i \phi_\lambda\rangle) - (\Sigma_j / \langle \Sigma_j \phi_\lambda\rangle), \tag{20a}$$

$$A^*\psi_n^* = \lambda B^* \psi_{n-1}^*, \quad n > 0. \tag{20b}$$

A mutual orthogonality relation can be constructed from Eqs. (20) and Eq. (1):

$$0 = \frac{\langle \Sigma_i \phi_\lambda\rangle}{\langle \Sigma_i \phi_\lambda\rangle} - \frac{\langle \Sigma_j \phi_\lambda\rangle}{\langle \Sigma_j \phi_\lambda\rangle} = \langle A^*\psi_0^*, \phi_\lambda\rangle = \langle \psi_0^*, A\phi_\lambda\rangle$$
$$= \langle \psi_0^*, \lambda B \phi_\lambda\rangle = \langle \lambda B^*\psi_0^*, \phi_\lambda\rangle = \langle A^*\psi_1^*, \phi_\lambda\rangle$$
$$= \langle \psi_1^*, A\phi_\lambda\rangle = \langle \psi_1^*, \lambda B\phi_\lambda\rangle = \cdots = \langle \psi_n^*, \lambda B\phi_\lambda\rangle = \cdots.$$

Thus, the $\psi_n^*$, and hence $\psi^*$, are biorthogonal to $\phi_\lambda$ with respect to the operator $B$. This suggests that Eqs. (20) be replaced by

$$A^*\xi_0^* = (\Sigma_i / \langle \Sigma_i \phi_\lambda\rangle) - (\Sigma_j / \langle \Sigma_j \phi_\lambda\rangle), \tag{21a}$$

$$A^*\xi_n^* = \lambda B^* \psi_{n-1}^*, \quad n > 0, \tag{21b}$$

$$\psi_n^* = \xi_n^* - [(\langle \xi_n^*, B\phi_\lambda\rangle / \langle \phi_\lambda^*, B\phi_\lambda\rangle)\phi_\lambda^*], \tag{21c}$$

where the second term in Eq. (21c) was added to remove any fundamental mode contamination which may arise from numerical roundoff.

A perturbation theory for changes in $R_{ij}$ corresponding to changes in the system parameters can be derived from the difference

$$\delta R_{ij} = F_2'[\psi^*, \phi_\lambda] - F_2[\psi^*, \phi_\lambda], \tag{22}$$

where both $F_2'$ and $F_2$ are evaluated with approximations to the solutions of Eqs. (1) and (18) for the unperturbed system parameters, while perturbed and unperturbed system parameters are used in Eq. (17) to evaluate $F_2'$ and $F_2$, respectively. The result, accurate to second order, is

$$\frac{\delta R_{ij}}{R_{ij}} = \frac{\langle \delta\Sigma_i \phi_\lambda\rangle}{\langle \Sigma_i \phi_\lambda\rangle} - \frac{\langle \delta\Sigma_j \phi_\lambda\rangle}{\langle \Sigma_j \phi_\lambda\rangle} - \langle \psi^*, [\delta A - \delta(\lambda B)]\phi_\lambda\rangle, \tag{23}$$

where, again, $\delta A \equiv A' - A$, etc. As before, the third term in Eq. (23) accounts for the effect of the perturbation upon the eigensolution $\phi_\lambda$ and represents a refinement upon conventional theory, which would approximate $\delta R_{ij}/R_{ij}$ with the first two terms of Eq. (23).

Usachev[8] obtained a perturbation expression equivalent to Eq. (23), and prescriptions equivalent to Eqs. (19) and (21), from physical arguments for the case of neutron transport within a critical nuclear reactor. His results are subject to the additional constraint $\delta(\lambda B) = \lambda \delta B$. It is indicative of the power of variational principles that the straightforward derivation given above led to the same results as the convoluted physical arguments of Usachev.

## IV. LINEAR ADJOINT RATIOS—INHOMOGENEOUS SYSTEMS

Now consider the problem of estimating the ratio of linear functionals of the solution of Eq. (7)

$$R_{ij}^* \equiv \langle \phi^* s_i\rangle / \langle \phi^* s_j\rangle, \tag{24}$$

where $s_i$ and $s_j$ are scalar operators. A direct estimate from Eq. (24) results in errors $\delta R_{ij}^*$ which are first order in the difference $\delta\phi^*$ between the trial function used to evaluate Eq. (24), $\tilde{\phi}^*$, and the solution of Eq. (7), $\phi^*$.

The variational functional

$$F_3[\phi^*, \psi] = (\langle \phi^* s_i\rangle / \langle \phi^* s_j\rangle) \times \{1 - \langle [(A^* - B^*)\phi^* - S^*], \psi\rangle\} \tag{25}$$

provides a second-order estimate of $R_{ij}^*$ relative to the functions $\delta\phi^*$ mentioned above and $\delta\psi$, which is the difference between a trial function $\tilde{\psi}$ used to evaluate Eq. (25) and the solution to

$$(A - B)\psi = (s_i / \langle \phi^* s_i\rangle) - (s_j / \langle \phi^* s_j\rangle). \tag{26}$$

Proof of this follows from consideration of the stationarity properties of $F_3$.

A perturbation theory for changes in $R_{ij}$ corresponding to changes in the system parameters can be derived from the difference

$$\delta R_{ij}^* = F_3'[\phi^*, \psi] - F_3[\phi^*, \psi], \tag{27}$$

where both $F'_3$ and $F_3$ are evaluated with approximations to the solutions of the unperturbed Eqs. (7) and (26), $F'_3$ is evaluated with the perturbed system parameters, and $F_3$ is evaluated with the unperturbed system parameters. The result, accurate to second order, is

$$\frac{\delta R^*_{ij}}{R^*_{ij}} = \frac{\langle \phi^* \delta s_i \rangle}{\langle \phi^* s_i \rangle} - \frac{\langle \phi^* \delta s_j \rangle}{\langle \phi^* s_j \rangle} - \langle [(\delta A^* - \delta B^*)\phi^* - \delta S^*], \psi \rangle. \tag{28}$$

Because the first two terms in Eq. (28), which correspond to the conventional method of estimation, are exact in the case where the perturbation does not change the adjoint, the third term in Eq. (28) represents a refinement to account for the effect of the perturbation on the adjoint.

## V. LINEAR ADJOINT RATIOS—HOMOGENEOUS SYSTEMS

In this case, a variational estimate of $R^*_{ij}$ is sought for the case in which the ratio involves linear functionals of the fundamental eigensolution $\phi^*_\lambda$ of Eq. (3). The variational functional

$$F_4[\phi^*_\lambda, \psi] = (\langle \phi^*_\lambda s_i \rangle / \langle \phi^*_\lambda s_j \rangle)[1 - \langle \phi^*_\lambda, (A - \lambda B)\psi \rangle] \tag{29}$$

provides a second-order estimate of $R^*_{ij}$ relative to the difference $\delta\phi^*_\lambda$ between the trial function used to evaluate Eq. (29) and the solution to Eq. (3), and the difference $\delta\psi$ between the trial function used to evaluate Eq. (29) and the solution to

$$(A - \lambda B)\psi = (s_i / \langle \phi^*_\lambda s_i \rangle) - (s_j / \langle \phi^*_\lambda s_j \rangle). \tag{30}$$

Proof follows from the stationarity properties of $F_4$.

Equation (30) has a solution because the rhs is orthogonal to $\phi^*_\lambda$, the fundamental eigensolution of Eq. (3). The method of successive approximation applied to Eq. (30) yields a solution of the form (see Appendix for discussion of convergence)

$$\psi = \sum_{n=0}^{\infty} \psi_n, \tag{31}$$

where

$$\psi_n = \xi_n - [(\langle \phi^*_\lambda, B\xi_n \rangle / \langle \phi^*_\lambda, B\phi_\lambda \rangle)\phi_\lambda] \tag{32}$$

and the $\xi_n$ are generated recursively:

$$A\xi_0 = (s_i / \langle \phi^*_\lambda s_i \rangle) - (s_j / \langle \phi^*_\lambda s_j \rangle), \tag{33a}$$

$$A\xi_n = \lambda B \psi_{n-1}, \quad n > 0. \tag{33b}$$

The second term in Eq. (32) is included to remove fundamental mode contamination which may arise from numerical roundoff. (A mutual biorthogonality relation exists which requires that $\langle \phi^*_\lambda, B\psi_n \rangle = 0$, $n \geq 0$.)

A perturbation theory may be derived, similar to the previous section, from the difference

$$\delta R^*_{ij} = F'_4[\phi^*_\lambda, \psi] - F_4[\phi^*_\lambda, \psi], \tag{34}$$

where the unperturbed trial solutions are used to evaluate $F'_4$ and $F_4$. Perturbed system parameters are used to evaluate $F'_4$, while $F_4$ is evaluated with the unperturbed parameters. The result, accurate to second order, is

$$\frac{\delta R^*_{ij}}{R^*_{ij}} = \frac{\langle \phi^*_\lambda \delta s_i \rangle}{\langle \phi^*_\lambda s_i \rangle} - \frac{\langle \phi^*_\lambda \delta s_j \rangle}{\langle \phi^*_\lambda s_j \rangle} - \langle \phi^*, [\delta A - \delta(\lambda B)]\psi \rangle. \tag{35}$$

The reasoning of the previous section indicates that the third term in Eq. (35) is a refinement upon conventional theory which accounts for the effect of the perturbation on the adjoint. Gandini[9] obtained an expression equivalent to Eq. (35), subject to the constraint $\delta(\lambda B) = \lambda \delta B$, and algorithms equivalent to Eqs. (31)–(33), in his extension of Usachev's generalized perturbation theory.

## VI. BILINEAR RATIOS—INHOMOGENEOUS SYSTEMS

In many practical situations an estimate of the ratio of bilinear functionals of the solutions $\phi$ of Eq. (4) and $\phi^*$ of Eq. (7)

$$\rho_{ij} \equiv \langle \phi^*, H_i \phi \rangle / \langle \phi^*, H_j \phi \rangle. \tag{36}$$

is required. Here $H_i$ and $H_j$ are arbitrary linear operators. A direct estimate from Eq. (36) leads to errors which are of first order in $\delta\phi^*$ and $\delta\phi$, the differences between the trial functions $\tilde{\phi}^*$ and $\tilde{\phi}$ used to evaluate Eq. (36) and the solutions to Eqs. (7) and (4), respectively.

The variational functional

$$F_5[\phi^*, \Gamma^*, \phi, \Gamma] = (\langle \phi^*, H_i \phi \rangle / \langle \phi^*, H_j \phi \rangle) \times \{1 - \langle \Gamma^*, [(A - B)\phi - S] \rangle - \langle [(A^* - B^*)\phi^* - S^*], \Gamma \rangle\} \tag{37}$$

provides an estimate of $\rho_{ij}$ which is accurate to second order in $\delta\phi^*$, $\delta\phi$ and the functions $\delta\Gamma^*$ and $\delta\Gamma$, which are the differences between the trial functions $\tilde{\Gamma}^*$ and $\tilde{\Gamma}$ used to evaluate Eq. (37) and the solutions of

$$(A^* - B^*)\Gamma^* = (H_i^* \phi^* / \langle \phi^*, H_i \phi \rangle) - (H_j^* \phi^* / \langle \phi^*, H_j \phi \rangle) \tag{38}$$

and

$$(A - B)\Gamma = (H_i \phi / \langle \phi^*, H_i \phi \rangle) - (H_j \phi / \langle \phi^*, H_j \phi \rangle), \tag{39}$$

respectively. Proof follows from the stationarity properties of $F_5$.

A perturbation theory for changes in $\rho_{ij}$ corresponding to perturbation in the system parameters can be derived from the difference

$$\delta\rho_{ij} = F'_5[\phi^*, \Gamma^*, \phi, \Gamma] - F_5[\phi^*, \Gamma^*, \phi, \Gamma], \tag{40}$$

where both $F'_5$ and $F_5$ are evaluated with approximations to Eqs. (4), (7), (38), and (39) for the unperturbed system; and $F'_5$ is evaluated with the perturbed parameters, while $F_5$ is evaluated with the unperturbed parameters. The result, accurate to second order, is

$$\frac{\delta\rho_{ij}}{\rho_{ij}} = \frac{\langle \phi^*, \delta H_i \phi \rangle}{\langle \phi^*, H_i \phi \rangle} - \frac{\langle \phi^*, \delta H_j \phi \rangle}{\langle \phi^*, H_j \phi \rangle} - \langle \Gamma^*, [(\delta A - \delta B)\phi - \delta S] \rangle - \langle [(\delta A^* - \delta B^*)\phi^* - \delta S^*], \Gamma \rangle. \tag{41}$$

The first two terms in Eq. (41) correspond to the conventional theory and would be exact if the perturbation did not alter $\phi^*$ or $\phi$. The third and fourth terms are refinements which account for the effect of the perturbation upon $\phi$ and $\phi^*$, respectively.

## VII. BILINEAR RATIOS—HOMOGENEOUS SYSTEMS

Consider again the problem of estimating $\rho_{ij}$ of Eq. (36), this time with $\phi_\lambda^*$ and $\phi_\lambda$, the fundamental eigensolutions of Eqs. (3) and (1), respectively. As before, a direct estimate from Eq. (36) would have an error which was first order in $\delta\phi_\lambda^*$ and $\delta\phi_\lambda$, the differences between the trial functions $\tilde{\phi}_\lambda^*$ and $\tilde{\phi}_\lambda$ used to evaluate Eq. (36) and the solutions of Eqs. (3) and (1), respectively.

The variational functional

$$F_6[\phi_\lambda^*, \Gamma^*, \phi_\lambda, \Gamma] = (\langle \phi_\lambda^*, H_i\phi_\lambda\rangle / \langle \phi_\lambda^*, H_j\phi_\lambda\rangle) \times [1 - \langle \phi_\lambda^*, (A - \lambda B)\Gamma\rangle - \langle \Gamma^*, (A - \lambda B)\phi_\lambda\rangle] \quad (42)$$

provides an estimate of $\rho_{ij}$ which is accurate to second order in $\delta\phi_\lambda^*$, $\delta\phi_\lambda$, and the differences $\delta\Gamma^*$ and $\delta\Gamma$ between the trial functions used to evaluate Eq. (42) and the solutions of

$$(A^* - \lambda B^*)\Gamma^* = (H_i^*\phi_\lambda^* / \langle \phi_\lambda^*, H_i\phi_\lambda\rangle) - (H_j^*\phi_\lambda^* / \langle \phi_\lambda^*, H_j\phi_\lambda\rangle) \quad (43)$$

and

$$(A - \lambda B)\Gamma = (H_i\phi_\lambda / \langle \phi_\lambda^*, H_i\phi_\lambda\rangle) - (H_j\phi_\lambda / \langle \phi_\lambda^*, H_j\phi_\lambda\rangle), \quad (44)$$

respectively. Proof follows from the stationarity properties of $F_6$.

Equation (43) has a solution because the rhs is orthogonal to $\phi_\lambda$, the fundamental eigensolution of Eq. (1). Application of successive approximations to Eq. (43) yields (see Appendix for discussion of convergence)

$$\Gamma^* = \sum_{n=0}^{\infty} \Gamma_n^*, \quad (45)$$

where

$$\Gamma_n^* = \xi_n^* - (\langle \xi_n^*, B\phi_\lambda\rangle / \langle \phi_\lambda^*, B\phi_\lambda\rangle)\phi_\lambda^*, \quad (46)$$

and the $\xi_n^*$ are generated recursively:

$$A^*\xi_0^* = (H_i^*\phi_\lambda^* / \langle \phi_\lambda^*, H_i\phi_\lambda\rangle) - (H_j^*\phi_\lambda^* / \langle \phi_\lambda^*, H_j\phi_\lambda\rangle), \quad (47a)$$

$$A^*\xi_n^* = \lambda^* B^*\Gamma_{n-1}^*, \quad n > 0. \quad (47b)$$

Similarly, a solution to Eq. (44) may be constructed from

$$\Gamma = \sum_{n=0}^{\infty} \Gamma_n, \quad (48)$$

where

$$\Gamma_n = \xi_n - (\langle \phi_\lambda^*, B\xi_n\rangle / \langle \phi_\lambda^*, B\phi_\lambda\rangle)\phi_\lambda, \quad (49)$$

and the $\xi_n$ are generated recursively:

$$A\xi_0 = (H_i\phi_\lambda / \langle \phi_\lambda^*, H_i\phi_\lambda\rangle) - (H_j\phi_\lambda / \langle \phi_\lambda^*, H_j\phi_\lambda\rangle), \quad (50a)$$

$$A\xi_n = \lambda B\Gamma_{n-1}, \quad n > 0. \quad (50b)$$

The second terms in Eqs. (46) and (49) are included to remove any fundamental mode contamination which may arise from numerical roundoff. (Mutual biorthogonality relations exist which require that $\langle \Gamma_n^*, B\phi_\lambda\rangle = 0$, $\langle \phi_\lambda^*, B\Gamma_n\rangle = 0$, $n \geq 0$.)

A perturbation theory for changes in $\rho_{ij}$ corresponding to perturbations in the system parameters can be derived from the difference

$$\delta\rho_{ij} = F_6'[\phi_\lambda^*, \Gamma^*, \phi_\lambda, \Gamma] - F_6[\phi_\lambda^*, \Gamma^*, \phi_\lambda, \Gamma]. \quad (51)$$

As before, $F_6'$ and $F_6$ are both evaluated with trial functions which approximate the solution of the unperturbed Eqs. (1), (3), (43), and (44). Perturbed parameters are used to evaluate $F_6'$, while unperturbed parameters are used to evaluate $F_6$. The result, accurate to second order, is

$$\frac{\delta\rho_{ij}}{\rho_{ij}} = \frac{\langle \phi_\lambda^*, \delta H_i\phi_\lambda\rangle}{\langle \phi_\lambda^*, H_i\phi_\lambda\rangle} - \frac{\langle \phi_\lambda^*, \delta H_j\phi_\lambda\rangle}{\langle \phi_\lambda^*, H_j\phi_\lambda\rangle} - \langle \phi_\lambda^*, [\delta A - \delta(\lambda B)]\Gamma\rangle - \langle \Gamma^*, [\delta A - \delta(\lambda B)]\phi_\lambda\rangle. \quad (52)$$

Again, the first two terms in Eq. (52) correspond to the conventional result. The third and fourth terms are refinements which account for the effect of the perturbation upon $\phi_\lambda^*$ and $\phi_\lambda$, respectively.

Gandini[9] obtained a perturbation expression similar to Eq. (52), subject to the constraint $\delta(\lambda B) = \lambda\delta B$, and algorithms equivalent to Eqs. (45)–(50) in his extension of Usachev's generalized perturbation theory. The functional $F_6$ specializes to a variational principle given by Delves[10] for estimating quadratic functionals, rather than ratios, when the operators are assumed to be self-adjoint and the formalism is revised to omit the term in the denominator.

## VIII. POSSIBLE APPLICATIONS TO NUCLEAR REACTOR PHYSICS

Potential applications to problems in reactor physics are considered to illustrate the use of the theory presented in the previous sections. Hopefully, these examples will suggest applications in other fields by analogy.

Frequently, the solution to a problem slightly different from the problem of interest is either available or readily obtainable, and one would like to use this solution to compute a ratio of functionals for the problem of interest, or one would like to assess the change in the ratio of functionals corresponding to the changes leading from the problem for which a solution is available to the problem of interest. In the former case, the variational functionals $F_1$ through $F_6$ provide a more accurate estimate of the ratio of functionals than would be obtained by a direct evaluation of the ratio using the available solution. In the latter case, the perturbation expressions provide a means, accurate to second order, of assessing the change in the ratio of functionals without the necessity of calculating the solution for the problem of interest. Changes in material composition, material arrangement, mathematical model, nuclear data, source, and fuel temperature arise in reactor analysis.

Material composition changes occur when one material is substituted for another (e.g., insertion of a control rod, experimental device, detector, etc.) and when changes in isotopic composition due to fission, activation, and radioactive decay take place. Changes in material arrangement may arise from thermal expansion or changes in the loading pattern. In a somewhat different vein, the material in a reactor may be homogenized in the calculational model to facilitate obtaining a solution. This homogenized solution could be used, together with the actual hete-

rogeneous material configuration, in a variational functional to obtain an estimate of a ratio in the actual system, or in a perturbation expression to assess the difference between the ratio in the fictitious homogenized model and in the actual heterogeneous model. (Variational and perturbation expressions for the eigenvalue have been applied to this end.[11,12])

In the same vein, a simplified mathematical model may be used to obtain an approximate solution. This solution may be used in a variational functional constructed for a more rigorous mathematical model to obtain an estimate of a ratio. Alternately, the perturbation expression, with $\delta A$ and $\delta B$ corresponding to the differences between the more rigorous and approximate operators, could be used with the approximate solution to assess the effect of the difference between the more rigorous and approximate models on the ratio. Replacing high-order neutron transport approximations with low-order approximations, such as diffusion theory, and neglecting anisotropy in the neutron angular scattering distributions are typical simplifications.

Perturbation expressions of the form presented in this paper have been used to assess the effect of nuclear data uncertainties upon ratios of functionals, both for the purpose of assessing the implied uncertainty in the performance of nuclear reactors[13,14] and for adjusting averaged cross sections to obtain agreement with integral experiments.[15,16] Use of the variational functionals would allow an estimate of the corresponding ratios when new data became available without the necessity of obtaining a solution corresponding to the new data.

The variational functionals $F_1$ and $F_2$ are appropriate for estimating reaction rates or activation ratios in subcritical ($F_1$) or critical ($F_2$) reactors. In this case $\Sigma_i$ and $\Sigma_j$ are the cross sections appropriate to the reactions, distributed or localized in space and energy according to the dictates of the problem. The functionals can also provide an estimate of relative local flux or power peaking if $\Sigma_i = \delta(r - r_i)$ or $\Sigma_f \delta(r - r_i)$ and $\Sigma_j = 1$ or $\Sigma_f$, respectively. $\delta(r - r_i)$ is the Dirac delta, $r$ is the spatial variable, and $\Sigma_f$ is the macroscopic fission cross section distributed in space and energy. Another use of these functionals is to estimate the relative neutron flux above some energy $E_{\min}$. In this case, $\Sigma_i = U(E - E_{\min})$ and $\Sigma_j = 1$, where $U$ is the step function.

An estimate of the relative importance of neutron sources $s_i$ and $s_j$ to the reaction rate $\langle S^*, \phi \rangle$ in a subcritical reactor is provided by the variational functional $F_3$. Both $F_3$ (subcritical) and $F_4$ (critical) provide an estimate of the relative local adjoint when $s_i = \delta(r - r_i)$ and $s_j = 1$.

The variational functionals $F_5$ (subcritical) and $F_6$ (critical) provide an estimate of reactivity worths, effective delayed neutron fraction, and effective prompt-neutron lifetime, depending upon the choice of $H_i$ and $H_j$. When $H_i$ is the change in the neutron balance operator $-\Delta(A - \lambda B)$ (critical) or $-\Delta(A - B)$ (subcritical) due to a sample inserted into a reactor, and $H_j$ is the integral operator

$$\chi(E) \int_0^\infty dE' \, \nu\Sigma_f(E', r),$$

then the variational functionals provide an estimate of the reactivity worth of the sample. Here $E$ is the neutron energy, $\nu$ is the number of neutrons per fission, and $\chi$ is the energy distribution of fission neutrons. When $H_i$ is the integral operator

$$\chi_d(E) \int_0^\infty dE' \, \nu\beta\Sigma_f(E', r),$$

and $H_j$ remains the same, an estimate of the effective delayed neutron fraction is provided by the variational functionals. Here, $\beta$ is the fraction of delayed fission neutrons, and $\chi_d$ is the distribution in energy of these delayed neutrons. If $H_i$ is the inverse neutron speed, and $H_j$ remains the same, $F_5$ and $F_6$ provide an estimate of the prompt-neutron lifetime. A ratio of reactivity worths results when both $H_i$ and $H_j$ are changes in the neutron balance operator.

Thus, there are many potential applications of the theory to nuclear reactor physics, only a few of which have been examined to date. Certainly, fruitful applications must exist in other fields as well.

## APPENDIX

The method of successive approximations was used to construct a solution to the flux importance equation

$$(A - \lambda B)\chi = S \tag{A1}$$

of the form

$$\chi = \sum_{n=0}^{\infty} \chi_n, \tag{A2}$$

where

$$A\chi_0 = S, \tag{A3}$$

$$A\chi_n = \lambda B\chi_{n-1}, \quad n > 0. \tag{A4}$$

Solving Eqs. (A3) and (A4), which requires the assumption that $A^{-1}$ exists,

$$\chi_n = A^{-1}\lambda B\chi_{n-1} = (A^{-1}\lambda B)^n A^{-1}S, \; n \geq 0, \tag{A5}$$

and substituting in Eq. (A2) yields

$$\chi = \sum_{n=0}^{\infty} (A^{-1}\lambda B)^n A^{-1}S. \tag{A6}$$

It was shown previously that

$$\langle \phi_\lambda^*, S \rangle = 0,$$

where $\phi_\lambda^*$ is the fundamental ($i = 0$) eigenfunction of

$$(A^* - \lambda_i B^*)\phi_i^* = 0. \tag{A7}$$

Thus, $S$ can be represented by an expansion in the higher harmonic ($i > 0$) eigenfunctions $\phi_i$ of

$$(A - \lambda_i B)\phi_i = 0, \tag{A8}$$

assuming that these eigenfunctions form a complete set. Writing

$$S = \sum_{i=1}^{\infty} a_i \lambda_i B\phi_i,$$

it follows that

$$(A^{-1}\lambda B)^n A^{-1}S = \sum_{i=1}^{\infty} a_i (\lambda_0/\lambda_i)^n \phi_i.$$

If it can be established that $\lambda_0 < |\lambda_i|$, $i \geq 1$, then the sum in Eq. (A6) converges and may be written

$$\chi = \sum_{n=0}^{\infty} (A^{-1}\lambda B)^n A^{-1}S = (I - A^{-1}\lambda B)^{-1}A^{-1}S = (A - \lambda B)^{-1}S, \quad \text{(A9)}$$

which is the solution of Eq. (A1). For example, when $A$ and $B$ correspond to the removal and fission operators in the multigroup, finite-difference representation of neutron diffusion theory, there are positivity proofs[17] which assure the convergence of the series in Eq. (A9).

A somewhat more general proof may be developed from a theorem of linear algebra,[18] which states that if the range of $(A - \lambda B)$ is closed, which is assumed, then Eq. (A1) has a solution for a given $S$ if, and only if, $S$ is biorthogonal to every solution of the adjoint homogeneous equation

$$(A - \lambda B^*)\phi^* = 0. \quad \text{(A10)}$$

The vectors $S$ defined by the right-hand sides of Eqs. (30) and (43) have this property, which establishes the existence of a solution to Eq. (A1), at least for those situations in which Eq. (A10) has a solution.

Assuming that $A^{-1}$ exists, Eq. (A1) may be written

$$(I - A^{-1}\lambda B)\chi = A^{-1}S. \quad \text{(A11)}$$

By defining

$$z_N \equiv \sum_{n=0}^{N} (A^{-1}\lambda B)^n \equiv \sum_{n=0}^{N} P^n, \quad \text{(A12)}$$

it will be shown that the condition sufficient for convergence of the series in Eq. (A6) to the solution of Eq. (A1) is: That for all vectors $y$, there exists a constant $\gamma$, independent of $y$, such that $0 < \gamma < 1$ and such that

$$|A^{-1}\lambda By| \equiv |Py| < \gamma |y|, \quad \text{(A13)}$$

where $|\ |$ denotes the norm.

First, it will be shown that Eq. (A13) is sufficient to insure convergence of the sequence $z_N x$. For any vector $x (M \leq N)$,

$$|z_N x - z_M x| = \left| \sum_{n=M+1}^{N} P^n x \right| \leq \sum_{n=M+1}^{N} |P^n x| \leq \sum_{n=M+1}^{N} \gamma^n |x| = \gamma^{M+1} \sum_{n=M+1}^{N} \gamma^{n-M-1} |x| < [\gamma^{M+1}/(1-\gamma)]\,|x|.$$

Thus, it follows that an integer $M_0$ exists such that for all $M > M_0, \gamma^{M+1} < \epsilon(1-\gamma)$ for any $\epsilon > 0$. Hence, the sequence $z_n x$ converges in the Cauchy sense.

Assuming a complete vector space, the sequence $z_n x$ will converge to some limit vector $q$. Define the operator $K$

$$q \equiv Kx \equiv \lim_{N\to\infty} z_N x. \quad \text{(A14)}$$

Consider the product

$$z_N(I-P)x = \left( \sum_{n=0}^{N} P^n - \sum_{n=1}^{N+1} P^n \right) x = (I - P^{N+1})x.$$

Since Eq. (A13) obtains, with $\gamma < 1$,

$$\lim_{N\to\infty} z_N(I-P)x = x. \quad \text{(A15)}$$

It also may be shown that (A13) is sufficient to insure that

$$K(I-P)x = \lim_{N\to\infty} z_N(I-P)x = x$$

and

$$(I-P)Kx = \lim_{N\to\infty} (I-P)z_N x = x.$$

Hence, $\lim_{N\to\infty} z_N$ is the inverse of $(I-P)$.

Consequently, relation (A13) is sufficient to insure the convergence of Eq. (A6) to the solution of Eq. (A1).

In general, the solution of Eq. (A1) is not unique because Eq. (A8) has a nontrivial solution which may be added to any solution of Eq. (A1), and the sum remains a solution of Eq. (A1). However, the successive approximation solution technique applied to Eq. (A1) leads to biorthogonality relations $\langle \phi^*, B\chi \rangle = 0$ which exclude solutions to Eq. (A8), and thus a unique solution to Eq. (A1) is obtained.

Similar proofs may be readily constructed for the adjoint importance equation.

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1 We shall speak of an "equation" throughout. However, the formalism is appropriate for matrix operations as well and, hence, is applicable to systems of equations.

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# Amplitude Dispersion and Stability of Nonlinear Weakly Dissipative Waves

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A method to solve nonlinear dissipative wave equations using ideas of Luke, Krylov, and Bogolyubov is presented. The method is compared to Whitham's theory. Dispersion relations for nonlinear dissipative waves, including amplitude dispersion, are discussed. Furthermore, stability problems of such waves are investigated.

## INTRODUCTION

Mathematical progress during the last years makes it possible to investigate the dispersion of nonlinear wave equations.

Lashinsky[1] has discussed in detail the motivation to investigate mathematical models for nonlinear modes in plasmas, and he also presented such a model[2] starting from a weakly nonlinear oscillator equation

$$\ddot{x} + \omega_0^2 x = -\epsilon F(x, \dot{x}). \tag{1}$$

To discuss the solutions of this equation, Lashinsky used the method of averaging in conjunction with the technique of variation of parameters (Krylov–Bogolyubov method[3]). For $\epsilon = 0$, Eq. (1) has the solution

$$x = A\cos(\omega_0 t + \psi), \tag{2}$$

where now $A \to A(t), \psi \to \psi(t)$ for $\epsilon \neq 0$. Under the assumptions $\epsilon \ll 1, \dot{A}/A \ll \omega_0, \dot{\psi}/\psi \ll \omega_0$, which express a *weak nonlinearity*, by the so-called method of averaging (over one period) the leading terms in a Fourier expansion can be found, and finally

$$\langle \dot{A} \rangle = -\frac{\epsilon}{2\pi\omega_0} \int_0^{2\pi} F(A\cos\theta - \omega_0 A \sin\theta)\sin\theta\, d\theta, \tag{3}$$

where $\theta = \omega_0 t + \psi$.

The right-hand sides are functions of the amplitude $A$ only since the time was averaged out over one period. From (3), the amplitude $A(t)$ as a function of time $t$ can be computed.[2] Lashinsky also considered weakly nonlinear waves in bounded plasmas. He investigated the equation

$$(1/c^2)\phi_{tt} - \nabla^2\phi = -\epsilon F(\phi, \phi_t) \tag{4}$$

by using expansions of the type

$$\phi = \sum_\lambda a_\lambda(t)\phi_\lambda(x). \tag{5}$$

The orthogonality conditions of the $\phi_\lambda$ and the period averaging process result in similar equations like (3).

The averaging over the period was also used by Tam.[4] He considers the propagation of nonlinear dispersive waves in a cold nondissipative plasma. He uses a perturbation technique and introduces fast and slow variables giving the periodic and the nonlinear (averaged) part of the solution. Also, Luke[5] uses this method in his investigation of the nonlinear wave equation

$$(1/c^2)\phi_{tt} - \nabla^2\phi = F(\phi). \tag{6}$$

He demonstrates that his technique is equivalent to Whitham's averaged Lagrangian method.[6-8]

In this paper we extend Whitham's theory of the averaged Lagrangian to dissipative waves. Tam[9] points out that the effect of collisional dissipation on nonlinear dispersion is important. Collisional damping may reduce the effect of nonlinear instability.

## DISPERSION RELATION AND AVERAGED LAGRANGIAN

We consider waves $\phi(\mathbf{x}, t)$ which satisfy a *strongly* nonlinear weakly dissipative partial differential equation of such a form that the linear wave equation can be split off. Rotating our coordinate system so that the wave vector $\mathbf{k}$ points into the direction of the $x$ axis we write for our wave equation

$$(1/c^2)\phi_{tt} - \phi_{xx} + b\phi + \epsilon g\phi_t = -V'(\phi) + \epsilon N(\phi_t) + \epsilon\phi_t G(\phi), \tag{7}$$

where $V', N$, and $G$ are nonlinear functions, $V' = dV/d\phi$, and $c, b$, and $g$ are constants which may depend on $\omega$. $\epsilon$ is a small parameter measuring the weakness of the dissipative terms. We now define a phase surface

$$\theta(x, t) = \text{const}, \tag{8}$$

which has the property that all points $(x, t)$ on it have the same value of the wavefunction $\phi$. From (8) we have

$$d\theta = \theta_x dx + \theta_t dt = 0, \tag{9}$$

so that points moving with the speed

$$\frac{dx}{dt} = \frac{-\theta_t}{\theta_x} \tag{10}$$

see a constant phase $\theta$. Defining wavenumber and frequency by

$$\theta_x = k, \quad -\theta_t = \omega \quad \text{or} \quad \frac{\partial\theta}{\partial t} + \omega = 0, \tag{11}$$

we see that (10) is the phase speed. In the three-dimensional case we have $\nabla\theta = \mathbf{k}$, and therefore

$$\text{curl}\,\mathbf{k} = 0, \tag{12}$$

which indicates that wavecrests are neither vanishing nor splitting into two or more crests.[10] From (11) and (12) the *conservation equation of wavecrests*, Eq. (13), follows:

$$\frac{\partial\mathbf{k}}{\partial t} + \nabla\omega = 0. \tag{13}$$

In a similar way it can be shown[10,11] that a point moving with the group velocity

$$\left(\frac{dx}{dt}\right)_g = \frac{d\omega}{dk} \tag{14}$$

sees $\omega$ unchanged. After this disgression, we return to Eq. (7). Its Lagrangian reads

$$L(\phi, \phi_x, \phi_t) = (1/c^2)\tfrac{1}{2}\phi_t^2 - \tfrac{1}{2}\phi_x^2 - \tfrac{1}{2}b\phi^2 - V(\phi). \tag{15}$$

Since the system is dissipative, the Euler Lagrange equations read[12-14]

$$\frac{\partial}{\partial x}\frac{\partial L}{\partial \phi_x} + \frac{\partial}{\partial t}\frac{\partial L}{\partial \phi_t} - \frac{\partial L}{\partial \phi} = -\epsilon g\phi_t + \epsilon N(\phi_t) + \epsilon\phi_t G(\phi), \tag{16}$$

where $N(\phi_t)$ may be of the form

$$N(\phi_t) = -\phi_t^{2n-1}, \tag{17}$$

where $n = 1\frac{1}{2}, 2, 2\frac{1}{2}, \cdots$. Substituting the Lagrangian (15) into (16) we immediately obtain our wave equation (7). We will now make a classification of our wave equation:

I. $N = 0, G = 0, V' = 0$: The equation is *linear; k* and $\omega$ are independent of $x$ and $t$.

1. $b = 0, g = 0$: no dispersion, no dissipation;

$$\phi = Ae^{ikx-i\omega t}, \quad \omega = \pm ck. \tag{18}$$

2. $b \neq 0, g = 0$: frequency dispersion, no dissipation;

$$\phi = Ae^{ikx-i\omega t}, \quad \omega = \pm c(k^2 + b^2)^{1/2}. \tag{19}$$

Any function $\omega(k)$, with exception of the definition (18) for $c$, is called a *dispersion relation of a linear wave equation*. Such dispersion relations may also be found by Laplace–Fourier transformation of the linear wave equation.[15]

3. $b = 0, g \neq 0$: Dissipative case, $\bar{g} = \epsilon g$;

$$\phi = Ae^{ikx-i\omega t}, \quad \omega = -\tfrac{1}{2}i\bar{g}c^2 \pm c(k^2 - \tfrac{1}{4}\bar{g}^2c^2)^{1/2}. \tag{20}$$

4. $b \neq 0, g \neq 0$: Dissipative case, $\phi$ like in (20);

$$D(\omega, k) \equiv (\omega^2/c^2) - k^2 - b + \bar{g}i\omega = 0. \tag{21}$$

II. If neither $N$, $G$, nor $V$ vanish, the wave equation is *nonlinear*. If the nonlinearity is *weak*, which we define by

$$\langle \theta_{xx} \rangle = \frac{1}{2\pi}\int_0^{2\pi} \theta_{xx}\,d\theta \approx 0, \qquad \langle \theta_{tt} \rangle = \frac{1}{2\pi}\int_0^{2\pi} \theta_{tt}\,d\theta \approx 0, \tag{22}$$

so that $\theta_x = k$ and $\theta_t = -\omega$ become constant "in the average", i.e., when appearing under an integral $\int_0^{2\pi} \cdots d\theta$, then a dispersion relation of a nonlinear wave equation can be derived. It turns out that $\omega$ is not only a function of $k$ (*frequency dispersion*), but also of the amplitude $A$ (*amplitude dispersion*). Using Luke's method of stretched variables, an amplitude dispersion relation can be derived also for *strongly nonlinear* waves.

In the dissipationless case ($g = G = N = 0$), Whitham suggested[6,7,16] the existence of a variational principle

$$\frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \theta_t} + \frac{\partial}{\partial x}\frac{\partial \mathcal{L}}{\partial \theta_x} = 0 \tag{23}$$

for the averaged Lagrangian

$$\mathcal{L} = \frac{1}{2\pi}\int_0^{2\pi} L(\theta, \theta_x, \theta_t, A)\,d\theta = \mathcal{L}(\theta_x, \theta_t, A), \tag{24}$$

and he assumed that the variation of $\mathcal{L}$ with respect to the amplitude $A$ or to the energy $E = \frac{1}{2}A^2$, i.e.,

$$\mathcal{L}_E = 0 \quad \text{or} \quad \mathcal{L}_A = 0 \tag{25}$$

gives the dispersion relation of the nonlinear equation. Equations (13), (23), and (25) determine the three functions $k(x, t)$, $\omega(x, t)$, and $A(x, t)$. For exactly *linear nondissipative* vibrations and waves the condition (25) becomes[17]

$$\mathcal{L} = 0. \tag{26}$$

This is trivial since $L = T - U$ and the virial theorem states for periodic motion that $\langle T \rangle = \langle U \rangle$ so that the dispersion relation for linear motions, i.e., Eq. (26) follows from the virial theorem.

In the *dissipative* case a principle analogous to the Whitham principle (23) may be found by averaging (16). A proof of the result will be given in the next chapter. We first rewrite (16) using

$$\phi = \phi(\theta). \tag{27}$$

By substituting into (16) we get

$$\frac{\partial}{\partial x}\left(\frac{d\theta}{d\phi}\frac{\partial L}{\partial \theta_x}\right) + \frac{\partial}{\partial t}\left(\frac{d\theta}{d\phi}\frac{\partial L}{\partial \theta_t}\right) - \frac{\partial L}{\partial \theta}\frac{d\theta}{d\phi} = \epsilon\omega g\frac{d\phi}{d\theta} + \epsilon N - \epsilon\frac{d\phi}{d\theta}\omega G. \tag{28}$$

By averaging now Eq. (28) with $(1/2\pi)\int \cdots d\phi$ and using (24) we obtain

$$\frac{\partial}{\partial x}\frac{\partial \mathcal{L}}{\partial \theta_x} + \frac{\partial}{\partial t}\frac{\partial \mathcal{L}}{\partial \theta_t} = \frac{\epsilon g\omega}{2\pi}\int_0^{2\pi}\frac{d\phi}{d\theta}\,d\phi + \frac{\epsilon}{2\pi}\int_0^{2\pi} N d\phi - \frac{\omega\epsilon}{2\pi}\int_0^{2\pi} G\frac{d\phi}{d\theta}\,d\phi \equiv Q. \tag{29}$$

This is the variational principle which replaces (23) in the dissipative case. (13) remains unchanged, and an equation replacing (25) will be derived in the next chapter in the course of proving (29).

## THE TAM–LUKE METHOD APPLIED TO DISSIPATIVE WAVES

As mentioned earlier, all equations necessary to determine $k(x, t)$, $\omega(x, t)$, and $A(x, t)$ of (18) can be derived[4,5] using a special technique and without using a Lagrangian. We now extend this technique to the dissipative case. We prefer this technique because Whitham's method gives wrong results in special cases. (If one considers, e.g., (7), (15) for $V = N = G = g = 0$, then (25) or (26) do not give the right dispersion relation which is given by (19). Whitham thinks[7] that this restriction of the form of the Lagrangian presumably corresponds to the assumption of separability of the Hamilton–Jacobi equation in the classical theory of adiabatic invariants.) Following Luke,[5] we introduce *stretched variables* by

$$X = \epsilon x, \quad T = \epsilon t. \tag{30}$$

In order to include relatively fast local oscillations (through the dependence on the variable $\theta$) and to take care of the slow variations of $A$, $k$, and $\omega$ (through the dependence on the stretched variables $X$ and $T$), we make the expansions

$$\phi(x, t) = U(\theta, X, T) + \epsilon U_1(\theta, X, T) + O(\epsilon^2), \tag{31}$$

$$V'(\phi) = V'(U) + \epsilon U_1 V''(U) + O(\epsilon^2), \tag{32}$$

$$N(\phi_t) = N(-U_\theta\omega) + \epsilon(U_T - U_{1\theta}\omega)N'(-U_\theta\omega) + O(\epsilon^2), \tag{33}$$

$$G(\phi) = G(U) + \epsilon U_1 G'(U) + O(\epsilon^2). \tag{34}$$

Substituting (31)–(34) into (7) we obtain by equating the various powers of $\epsilon$ (and neglecting $\epsilon^{2\cdots}$)

$$U_{\theta\theta}[(\omega^2/c^2) - k^2)] + bU = -V'(U), \tag{35}$$

which replaces (25) and

$$U_{1\theta\theta}[(\omega^2/c^2) - k^2] + bU_1 + U_1 V''(U) = F, \tag{36}$$

where

$$F = (2/c^2)U_{\theta T}\omega + 2U_{\theta X}k + (1/c^2)U_\theta\omega_T + U_\theta k_X + gU_T + N(-\omega U_\theta) + G(U)U_T. \tag{37}$$

The dispersion relation is contained in (35). In order to show that (36) is equivalent to (29) we first show that $U_1 = U_\theta$ is a solution of the homogeneous equation (36). This is done by derivating (35) with respect to $\theta$ and showing that the result is identical to (36) for $F = 0$. In order to solve (36), we then write

$$U_1 = W(\theta)U_\theta; \tag{38}$$

substituting into (36) one receives

$$[(\omega^2/c^2) - k^2](W_{\theta\theta}U_\theta + 2W_\theta U_{\theta\theta}) = F. \tag{39}$$

Using the identity

$$\frac{\partial}{\partial\theta}(U_\theta^2 W_\theta) = W_{\theta\theta}U_\theta^2 + 2W_\theta U_{\theta\theta}U_\theta \tag{40}$$

and multiplying (39) by $U_\theta$, we obtain after elimination of $W$ by (38) and integration

$$[(\omega^2/c^2) - k^2](U_{1\theta}U_\theta - U_1 U_{\theta\theta}) = + \int_0^\theta FU_\theta d\theta. \tag{41}$$

In order to avoid[18] secular terms proportional to integer powers of $\theta$, $U_1$ and $U_{1\theta}$ must be bounded. But $U_1$ or $U_{1\theta}$ are not periodic and are unbounded unless the integral in (41) is bounded for large $\theta$. Now, if $U$ (and $U_\theta$, $U_T = -\omega U_\theta$) are periodic, then the integrals are bounded and secular terms can be avoided. The integration has to be carried out only up to the period $\tau$. Multiplication of (35) by $U_\theta$ and integration yields

$$U_\theta = [2E(X,T) - bU^2 - 2V(U)]^{1/2}[(\omega^2/c^2) - k^2]^{-1/2}. \tag{42}$$

Here the energy $E(X, T)$ is an integration constant. From (42) we see that $U(\theta)$ is a periodic function: For $V = 0$ we have a harmonic function, for $V = \sin U$ or polynomial up to the fourth degree, $U(\theta)$ is a Jacobi elliptic function, and for higher polynomials we have the inverse functions of hyperelliptic or Abelian integrals representing also periodic functions. If $U$ is periodic, then $U_\theta$, $U_X$, $U_T$, and $F$ are periodic. Then

$$\int_0^\tau FU_\theta d\theta = 0, \tag{43}$$

and from (37) we obtain

$$\frac{\partial}{\partial T}\left(\frac{\omega}{c^2}\int_0^\tau U_\theta dU\right) + \frac{\partial}{\partial X}\left(k\int_0^\tau U_\theta dU\right) = -g\omega\int_0^\tau U_\theta dU - \int_0^\tau NdU + \omega\int_0^\tau GU_\theta dU \tag{44}$$

since, during one period $\tau$, $dU = U_\theta d\theta$. Skipping the factor $1/2\pi$, replacing $2\pi$ by $\tau$, we see from (30), (24), and (15) that (44) is equivalent to (29). QED

The three equations (13), (35) instead of (25), and (44) determine $\omega(X, T)$, $k(X, T)$, $A(X, T) = \sqrt{2E(X, T)}$. The dispersion relation is obtained by integration of (42). With an appropriate choice of the integration constant we have

$$\left(\frac{\omega^2}{c^2} - k^2\right)^{1/2}\int_0^\tau (2E - bU^2 - 2V)^{-1/2}dU - 2\pi \equiv D(\omega, k, E) = 0. \tag{45}$$

This relation contains $E$ (and therefore the amplitude $A$) and describes *amplitude dispersion:* $\omega = \omega(k, E)$. It may be also written in the form (25). (35) and (42) are conservative equations; but (44) is not. If, however, $N = g = G = 0$, then also (44) reduces to the conservative case (23) and

$$A = \sqrt{2E} = \text{const}. \tag{46}$$

This result may also be derived by the Krylov–Bogolyubov method. For $V' = 0$, (35) has the generating solution

$$U = A\sin(\alpha\theta + \psi), \qquad U_\theta = A\alpha\cos(\alpha\theta + \psi), \tag{47}$$

where $A$, $\alpha$, $\psi$ are constants and

$$b/\alpha^2 = (\omega^2/c^2) - k^2. \tag{48}$$

Now, for $V' \neq 0$ according to Krylov–Bogolyubov we let $A \to A(\theta)$, $\psi \to \psi(\theta)$, and we then have from (47)

$$A\alpha\cos(\alpha\theta + \psi) = \dot{A}\sin(\alpha\theta + \psi) + A(\alpha + \dot{\psi})\cos(\alpha\theta + \psi) \tag{49}$$

and therefore ($\dot{A} = dA/d\theta$)

$$\dot{A}\sin(\alpha\theta + \psi) + A\dot{\psi}\cos(\alpha\theta + \psi) = 0. \tag{50}$$

Substituting $U_{\theta\theta} = \dot{A}\alpha\cos(\alpha\theta + \psi) - A\alpha(\alpha + \dot{\psi})\sin(\alpha\theta + \psi)$ into (35) gives

$$\dot{A} = -(\alpha/b)V'\cos(\alpha\theta + \psi), \tag{51}$$

$$\dot{\psi} = (\alpha/Ab)V'\sin(\alpha\theta + \psi). \tag{52}$$

Expanding $V'(U)\sin(\alpha\theta + \psi)$ [resp. $V'(U)\cos(\alpha\theta + \psi)$] into Fourier series and integrating $(1/2\pi)\int_0^{2\pi}\cdots d\psi$ gives

$$-\langle\dot{A}\rangle = \frac{\alpha}{b}\frac{1}{2\pi}\int_0^{2\pi} V'(U)\cos\psi\, d\psi \tag{53}$$

—which might be compared to (3)—and

$$\langle\dot{\psi}\rangle = \frac{\alpha}{Ab}\frac{1}{2\pi}\int_0^{2\pi} V'(U)\sin\psi d\psi. \tag{54}$$

Via (47), (53) can be written $\int V'(A\sin\psi)d\sin\psi = 0$, and we then have the following.

*Theorem 1:* For any nonlinear conservative wave equation of the type (7) the amplitude $A$ (and therefore the energy $E$) is constant. Defining an effective frequency

$$\Omega = \alpha + \dot{\psi}, \tag{55}$$

we may write (47) in the form

$$U = A(\theta)\sin(\int \Omega d\theta + \psi_0), \tag{56}$$

where $\psi_0 = \text{const}$. Equation (54) and

$$\theta(x,t) = k(x,t)x - \omega(x,t)t \tag{57}$$

then give a dispersion relation for $\Omega$.

*Nonlinear dissipative case* ($V' = 0$): From (7) we now have

$$U_{\theta\theta}[(\omega^2/c^2) - k^2] + bU - \epsilon g\omega U = \epsilon N(-U_\theta\omega) - \epsilon G(U)U_\theta\omega \tag{58}$$

so that $V'$ in (53) and (54) has to be replaced by

$$\epsilon^{-1}V' \to g\omega A(\theta)\alpha\cos(\alpha\theta+\psi) + \omega G[A\sin(\alpha\theta+\psi)] \cdot A(\theta)\alpha\cos(\alpha\theta+\psi) - N[-\omega A\alpha\cos(\alpha\theta+\psi)].$$

Then from (54) we have $<\dot{\psi}> = 0$ and the following.

*Theorem 2:* For any nonlinear dissipative wave equation of the type (7) the frequency $\omega$ is not modified by the dissipation terms in first order of $\epsilon$.

The case $b = 0$ presents problems here, since in this case the Krylov–Bogolyubov method cannot be applied to (35).

## STABILITY

In many cases Eq. (35) cannot be solved exactly or the wave equation is not of the type (7). In these cases Lighthill[19] proposed for conservative systems an expansion of $\mathcal{L}$. We would like to follow up a similar way for the dissipative case. In general, $\mathcal{L} = \mathcal{L}(\omega, k, A)$. We are, however, able to eliminate, e.g., $A$ from one of the three equations determining $\omega, k, A$ or from the amplitude dispersion relation. With $\mathcal{L} = \mathcal{L}(\omega, k)$ we rewrite (29) by exchanging the order of differentiation

$$\theta_{tt}\mathcal{L}_{\omega\omega} - 2\theta_{xt}\mathcal{L}_{\omega k} + \theta_{xx}\mathcal{L}_{kk} = 2\pi Q. \tag{59}$$

A similar equation, namely

$$-\frac{1}{c^2}\theta_{tt}\int_0^\tau U_\theta dU - \frac{1}{c^2}\theta_t\frac{\partial}{\partial T}\int_0^\tau U_\theta dU + \theta_{xx}\int_0^\tau U_\theta dU + \theta_x\frac{\partial}{\partial X}\int_0^\tau U_\theta dU = g\theta_t\int_0^\tau U_\theta dU + \int_0^\tau N dU - \theta_t\int_0^\tau GU_\theta dU \tag{60}$$

may be derived from (44).

This is a partial differential equation for $\theta(x,t)$. We now expand $\mathcal{L}$. Since $\mathcal{L}_{\text{lin}} = 0$ according to (36), $\mathcal{L}$ measures exactly the derivation from the dispersion relation of the linear equation. In order to make this more explicit we expand

$$\mathcal{L}(\omega,k) \equiv \mathcal{L}(\tau,k) = a\tau^2 = a[\omega - f(k)]^2, \tag{61}$$

where $\omega_0 = f(k)$ is the dispersion relation of the linear equation, e.g., (21). We then have the correspondence

$$\frac{\partial}{\partial k} \to \frac{\partial}{\partial k} - f'\frac{\partial}{\partial \tau}, \quad \frac{\partial}{\partial \omega} \to \frac{\partial}{\partial \tau},$$

where $\tau$ and $k$ are now two independent variables. Since then $\mathcal{L}_k = 0$, $\mathcal{L}_\tau = 2a\tau$, $\mathcal{L}_{\tau\tau} = 2a$, (59) takes the form

$$\theta_{tt} + 2f'\theta_{xt} + (f'^2 - f''\tau)\theta_{xx} = \pi Q/a. \tag{62}$$

Since $f = f(k)$, $\theta_x = k(x,t)$, this is a quasilinear partial differential equation for $\theta(x,t)$. Applying usual characteristics method, see e.g., Ref. 20, one may write (62) in the form

$$A\theta_{xx} + B\theta_{xt} + C_{tt} = \pi Q/a. \tag{63}$$

Then the characteristics are:

*Real* (hyperbolic equation), if $B^2 - 4AC \equiv 4f''\tau > 0$;

*Complex* (elliptic equation), if $B^2 - 4AC \equiv 4f''\tau < 0$.

We see that the dissipative term $Q$ does not enter into this condition. So for (61) we have the following theorem.

*Theorem 3:* (a) The effect of nonlinear terms on the stability behavior is described by $f''(k)\cdot[\omega - f(k)]$. The stability behavior of the linear equation, described by $\omega_0 = f(k)$ is not altered by nonlinear terms, *if* $f''(k)\cdot[\omega - f(k)] > 0$. If, however, $f''(k)\cdot[\omega - f(k)] < 0$, then the nonlinear terms may destabilize, an otherwise stable solution of a linear equation.

(b) The inclusion of a dissipative term $Q$ does not by itself modify the character of the stability behavior; but the time behavior of unstable and stable modes is modified.

Examples and applications of this theorem will be given in forthcoming papers.

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# Structure of Simplexes of Equilibrium States in Quantum Statistical Mechanics

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The structure of Choquet simplexes of equilibrium states of infinite system in quantum statistical mechanics is investigated. It is shown that a facial simplex is a Bauer simplex whenever its extreme points form a physically equivalent class; however, the simplex of KMS states for a given inverse temperature is *not* a Bauer simplex if it is not a singleton.

## 1. INTRODUCTION

In the algebraic approach of statistical mechanics, the equilibrium state of infinite system is described by the state (the normalized positive linear form) on a suitable $C^*$-algebra. Some important features of the equilibrium states are their invariance under some group (translations in $\mathbb{Z}^\nu$, or $\mathbb{R}^\nu$, Euclidean transformations, etc.), and their analytic property known as the Kubo–Martin–Schwinger boundary condition. The mathematical structure of the equilibrium states with these properties, namely, the invariant states and KMS states, have been intensely studied. In many cases, the set of these states turns out to be a compact convex set and a Choquet simplex, e.g., the set of all states invariant under a group $G$ on a $G$-Abelian $C^*$-algebra,[1] and the set of all KMS states for a given inverse temperature.[2,3] Therefore, it would be interesting to study the mathematical structure of equilibrium states from the aspect of simplexes and compact convex sets, which have been highly developed and widely applied to different fields in mathematics.[4]

The nice simplexes are those with closed extreme boundary, namely, those of which the extreme points form a closed set, i.e., Bauer simplexes.[4] Hence, the first step in our study of the equilibrium states in this direction is to investigate whether they could form nice simplexes.

For the set of invariant states under a group, a characterization for a Bauer simplex has been found by Størmer.[5] Thus, we shall study mostly the characterizations of simplexes of KMS states in the present paper.

We begin with facial simplex (see definition in Sec. 3), which in many cases turns out to be a Bauer simplex. It is shown that a facial simplex of the state space of a $C^*$-algebra is a Bauer simplex if its extreme points form a physically equivalent class. However, in general, the simplex of KMS states is not a Bauer simplex. First, we give a characterization for Bauer simplex of KMS states on a separable $C^*$-algebra, then, we show that for a separable GCR $C^*$-algebra, the set of KMS states is *not* a Bauer simplex if it is not a singleton. And, a characterization for a separable simple $C^*$-algebra is found, which will be interested in the quantum lattice system or the $C^*$-algebra associated with canonical anticommutation relation.

In Sec. 2, we give some definitions and notations for the compact convex sets and simplexes. We recall some well-known results and show briefly that the KMS states for a given inverse temperature form a Choquet simplex from Refs. 2 and 3.

We study the facial simplexes in Sec. 3. Our main result in this section is Theorem 3.1, and we point out that the simplex of KMS state is a facial simplex of the simplex of invariant states under the time translation.

Section 4 deals with the simplexes of KMS states. The characterization of a Bauer simplex is given in Theorem 4.1. Theorem 4.2 shows the nonexistence of Bauer simplex on a separable GCR algebra. A characterization of Bauer simplex for a separable, simple $C^*$-algebra is in Theorem 4.3.

We apply topological method in the proof of our theorems, and Theorems 4.1 and 4.3 are two topological characterizations for Bauer simplexes.

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In this section we give some preliminary definitions and notations and recall some well-known results.

Let $X$ be a vector space and $Q$ a convex subset of $X$. A *face* of $Q$ is a convex subset $F$ of $Q$ such that for all $x, y, z \in Q$ with $z = \lambda x + (1-\lambda)y$, where $0 < \lambda < 1$, $z \in F$ implies $x, y \in F$. The extreme points of $Q$, denoted by $E(Q)$, are just the one-point faces of $Q$. We note that if $F$ is a face of $Q$, then $E(F) \subseteq E(Q)$.

If $C$ is a *cone* in $X$, i.e., $C$ is a subset of $X$ such that $C + C \subseteq C$, $\alpha C \subseteq C$ for $\alpha > 0$, and $C \cap (-C) = \{0\}$. We order the elements of $X$ by $x \preceq y$ if $y - x \in C$. $C$ is a *lattice cone* if for each $x$ and $y$ in $C$ there is a greatest lower bound $x \wedge y$ in $C$. It follows that each pair $x, y \in C$ have a least upper bound $x \vee y$ in $C$, and in fact both bounds exist for all elements in $C - C$ (Ref. 6, pp. 59–60). A *base* of $C$ is an intersection of $C$ with a hyperplane $H$, where $H$ is a hyperplane in $X$ not containing 0 that meets all generators of $C$, i.e., for all $x \in C - \{0\}$, there is an $\alpha > 0$ with $\alpha x \in H$. A convex set $K$ in $X$ is called a *simplex* if it is the base of a lattice cone. It is readily verified that a convex subset $F$ of $K$ will be a face of $K$ if and only if $x \in F$, $y \in K$, and $0 \preceq y \preceq \alpha x$ for some positive scalar $\alpha$ imply that

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# Structure of Simplexes of Equilibrium States in Quantum Statistical Mechanics

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The structure of Choquet simplexes of equilibrium states of infinite system in quantum statistical mechanics is investigated. It is shown that a facial simplex is a Bauer simplex whenever its extreme points form a physically equivalent class; however, the simplex of KMS states for a given inverse temperature is *not* a Bauer simplex if it is not a singleton.

## 1. INTRODUCTION

In the algebraic approach of statistical mechanics, the equilibrium state of infinite system is described by the state (the normalized positive linear form) on a suitable $C^*$-algebra. Some important features of the equilibrium states are their invariance under some group (translations in $\mathbb{Z}^\nu$, or $\mathbb{R}^\nu$, Euclidean transformations, etc.), and their analytic property known as the Kubo–Martin–Schwinger boundary condition. The mathematical structure of the equilibrium states with these properties, namely, the invariant states and KMS states, have been intensely studied. In many cases, the set of these states turns out to be a compact convex set and a Choquet simplex, e.g., the set of all states invariant under a group $G$ on a $G$-Abelian $C^*$-algebra,[1] and the set of all KMS states for a given inverse temperature.[2,3] Therefore, it would be interesting to study the mathematical structure of equilibrium states from the aspect of simplexes and compact convex sets, which have been highly developed and widely applied to different fields in mathematics.[4]

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We begin with facial simplex (see definition in Sec. 3), which in many cases turns out to be a Bauer simplex. It is shown that a facial simplex of the state space of a $C^*$-algebra is a Bauer simplex if its extreme points form a physically equivalent class. However, in general, the simplex of KMS states is not a Bauer simplex. First, we give a characterization for Bauer simplex of KMS states on a separable $C^*$-algebra, then, we show that for a separable GCR $C^*$-algebra, the set of KMS states is *not* a Bauer simplex if it is not a singleton. And, a characterization for a separable simple $C^*$-algebra is found, which will be interested in the quantum lattice system or the $C^*$-algebra associated with canonical anticommutation relation.

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$y \in F$. We refer the reader to Refs. 4 and 6 for the general theory of simplexes and compact convex sets.

Let $X$ be a locally convex Hausdorff space and $K$ a compact convex subset of $X$. If $K$ is a simplex, then $K$ is a *Choquet simplex*. Furthermore, a *Bauer simplex* $K$ is a Choquet simplex with the closed boundary, hence its extreme points $E(K)$, which is not empty, form a closed set in $K$. Hereafter a simplex will mean a Choquet simplex in a locally convex Hausdorff space.

In Ref. 7, Effros has introduced a topology on $E(K)$ for a simplex $K$, called the *structure topology*, whose closed sets are exactly those sets $E(F)$ for a closed face of $K$. $E(K)$ endowed with this topology is called the *structure space*. This structure topology is $T_1$ and compact, but, in general, not Hausdorff. It is Hausdorff if and only if $K$ is a Bauer simplex. Moreover, this topology is weaker than the relative topology on $E(K)$ induced by the given topology of $K$. And, these two topologies on $E(K)$ coincide if and only if $K$ is a Bauer simplex.[4] A detailed study of the structure of Choquet and Bauer simplexes can be found in Ref. 4.

Let $\mathfrak{A}$ be a $C^*$-algebra with identity 1. An ideal $I$ of $\mathfrak{A}$ is called primitive if $I$ is the kernel of an irreducible representation of $\mathfrak{A}$. We denote by Prim $(\mathfrak{A})$ the set of all primitive ideals of $\mathfrak{A}$. Prim $(\mathfrak{A})$ can be topologized by the *hull-kernel* operation as follows:

If $S$ is a subset of Prim $(\mathfrak{A})$, then the *kernel* of $S$ is the closed ideal

$$k(S) = \cap \{J; J \in S \cup \{\mathfrak{A}\}\}.$$

If $J$ is any subset of $\mathfrak{A}$, let

$$h(J) = \{I \in \text{Prim } (\mathfrak{A}); I \supseteq J\},$$

this is called the *hull* of $J$. Then

$$S \to S^- = hk(S)$$

is the closure operation of the *Jacobson topology* on Prim $(\mathfrak{A})$. And, the closed subsets of Prim $(\mathfrak{A})$ are just those of the form $h(J)$, where $J$ is any subset of $\mathfrak{A}$. The Jacobson topology is a $T_0$-space (Ref. 8, Sec. 3.1).

We denote by $S(\mathfrak{A})$ the state space of $\mathfrak{A}$ equipped with the $w^*$-topology. Let $\sigma_t$ for $t \in \mathbb{R}$ be a one-parameter automorphism group of $\mathfrak{A}$ such that the map $t \to \sigma_t(x)$ for $x \in \mathfrak{A}$ is continuous in the norm-topology of $\mathfrak{A}$. A state $\phi \in S(\mathfrak{A})$ is said to be a "KMS state" with respect to $\sigma_t$ for a given inverse temperature $\beta = 1/kT$, if it satisfies the KMS boundary condition, i.e., if

$$\int dt f(t - i\beta)\phi(x\sigma_t(y)) = \int dt f(t)\phi(\sigma_t(y)x)$$

holds for all $x, y \in \mathfrak{A}$ and for any function $f$ with Fourier transform in $\mathfrak{D}$. We refer to Ref. 9 and the references given there for further information about KMS states. Most of our analysis in the next sections will not use explicitly the analytic properties of KMS states, but their algebraic aspects.

If $K_\beta$ is the set of all KMS states of $\mathfrak{A}$ with respect to $\sigma_t$ for a given $\beta$, then $K_\beta$ is a compact convex subset of $S(\mathfrak{A})$.[9] In fact $K_\beta$ can be shown as a simplex as follows[2,3]:

Let $C_\beta$ be the positive cone associated with $K_\beta$, i.e., $C_\beta$ is the set of all positive linear functionals of $\mathfrak{A}$ satisfying KMS boundary condition. More precisely, $K_\beta = C_\beta \cap S(\mathfrak{A}) = C_\beta \cap H$, where $H = \{\phi \in \mathfrak{A}^*; \phi(1) = 1\}$ is the hyperplane in $\mathfrak{A}^*$, the Banach dual of $\mathfrak{A}$. Hence, we need only to show that $C_\beta$ is a lattice cone.

For a $\phi \in C_\beta$, let $\pi_\phi$ be the cyclic representation induced by $\phi$, and $\xi_\phi$ the cyclic vector. Then the KMS boundary condition can be extended to the weak-closure $\pi_\phi(\mathfrak{A})''$ of $\pi_\phi(\mathfrak{A})$, in fact, $\phi(x) = \omega_{\xi_\phi} \circ \pi_\phi(x)$ for $x \in \pi_\phi(\mathfrak{A})''$ satisfies KMS condition with respect to $\tilde{\sigma}_t$, the extension of $\sigma_t$ to $\pi_\phi(\mathfrak{A})''$, i.e., $\tilde{\sigma}_t$ is the modular automorphism of $\pi_\phi(\mathfrak{A})''$.[2] If $\psi \in C_\beta$ and satisfies the KMS condition with respect to $\tilde{\sigma}_t$, then $\psi(x) = \omega_{k\xi_\phi} \circ \pi_\phi(x)$ for $x \in \pi_\phi(\mathfrak{A})''$, with $k \in \mathfrak{Z}_\phi$ and $k \geq 0$, where $\mathfrak{Z}_\phi$ is the center of $\pi_\phi(\mathfrak{A})''$ (Ref. 2; Theorem 15.4.)

Let $\psi_1, \psi_2 \in C_\beta$, then $\psi_i = \omega_{k_i\xi_\phi} \circ \pi_\phi$ for $k_i \in \mathfrak{Z}_\phi$ with $k_i \geq 0$ $(i = 1, 2)$. Since $\mathfrak{Z}_\phi$ is an Abelian von Neumann algebra, its self-adjoint part is a lattice, hence $k_1 \wedge k_2 = k \in \mathfrak{Z}_\phi$. Let $\psi = \omega_{k\xi_\phi} \circ \pi_\phi$, then $\psi$ is the g.l.b. of $\psi_i (i = 1, 2)$. Clearly, $\psi$ satisfies KMS condition, hence $\psi \in C_\beta$. It follows that $C_\beta$ is a lattice cone associated with $K_\beta$.

Consequently, each $\phi \in K_\beta$ is the barycenter of a unique maximal measure $\mu_\phi$ from Choquet–Meyer's uniqueness theorem.[4,6] Furthermore, it has been shown by Emch et al[10] that $\mu_\phi$ is the central measure of $\phi$ in the sense of Sakai.[11] However, we shall not study any measure-theoretical aspect of K.M.S. states in the present paper.

## 3. FACIAL SIMPLEXES

Let $K$ be a compact convex subset of the state space $S(\mathfrak{A})$, which is endowed with the $w^*$-topology, and $E(K)$ the extreme points of $K$. $K$ is called a *facial simplex* of $S(\mathfrak{A})$ if $K$ is a simplex as well as $K$ is a face of $S(\mathfrak{A})$. Similarly, a facial simplex $K$ of a compact convex set $H$ of $S(\mathfrak{A})$ is a simplex as well as $K$ is a face of $H$. However, by a facial simplex, without referring to any compact convex subset of $S(\mathfrak{A})$, we shall mean a facial simplex of $S(\mathfrak{A})$.

In this section we shall show that in many cases a facial simplex turns out to be a Bauer simplex.

For a simplex $K$ in $S(\mathfrak{A})$, we have the following:

*Proposition 3.1:* Each closed face of a simplex $K$ is a facial simplex of $K$.

*Proof:* If $F$ is a closed face of $K$, then $F$ is a compact convex subset of $K$. Let $C_1$ and $C_2$ be the cones associated with $F$ and $K$, respectively. Since $F$ is a face of $K$, hence $C_1$ is an *hereditary* subcone of $C_2$, i.e., for each $\phi_1 \in C_1$, $\phi_2 \in C_2$, and $\phi_1 - \phi_2 \in C_2$ imply $\phi_2 \in C_1$ (Ref. 4, p. 82). Furthermore, $C_2$ is a lattice cone, hence $C_1$ is also a lattice cone from Ref. 6, p. 64: And, $F$ is the base of $C_1$, therefore $F$ is a simplex. By the given assumption, as $F$ is a face of $K$, thus $F$ is a facial simplex of $K$.

An immediate consequence is:

*Corollary 3.1:* Each closed face of a facial simplex is a facial simplex.

Furthermore, from the above proposition and Rogalski's lemma [i.e., each compact convex subset of a simplex $K$ is a face of $K$, if its extreme points belong to $E(K)$ (Ref. 12; lemme 28)], it is easy to show

*Corollary 3.2:* Let $F$ be a compact convex subset of a simplex $K$. If $E(F) \subseteq E(K)$, then $F$ is a facial simplex of $K$.

If $F$ is a facial simplex of a Bauer simplex $K$, then $F$ is also a Bauer simplex. In fact, $E(F) \subseteq E(K)$, then the structure space $E(F)$ is Hausdorff, since $E(K)$ is Hausdorff. Thus we have

*Proposition 3.2:* Each facial simplex of a Bauer simplex is a Bauer simplex.

If $\mathfrak{A}$ is Abelian then each facial simplex turns out to be a Bauer simplex. More precisely, we have

*Proposition 3.3:* If $\mathfrak{A}$ is a $C^*$-algebra with identity, consider the following three conditions:

(i) $\mathfrak{A}$ is Abelian;
(ii) $S(\mathfrak{A})$ is a Bauer simplex;
(iii) Each facial simplex is a Bauer simplex.

Then, (i) $\Leftrightarrow$ (ii) $\Rightarrow$ (iii).

(i) $\Leftrightarrow$ (ii) is well known. However, Bauer simplex follows also from the fact that $S(\mathfrak{A})$ satisfies Størmer's axiom.[13] (ii) $\Rightarrow$ (iii) see Proposition 3.2.

(iii) $\Leftarrow$ (ii) is not true, see Corollary 3.3 below.

Before going to discuss facial simplexes of a non-Abelian $C^*$-algebra, we recall an equivalent relation for states. Let $\rho, \phi \in S(\mathfrak{A})$, if $\pi_\rho$ and $\pi_\phi$ are the cyclic representations induced by $\rho$ and $\phi$, respectively. $\rho$ and $\phi$ are called *physically equivalent* if $\pi_\rho$ and $\pi_\phi$ have the same kernels, i.e., kern $\pi_\rho$ = kern $\pi_\phi$.[14] A subset $M$ of $S(\mathfrak{A})$ forms a *physically equivalent class* if all cyclic representations $\pi_\phi$ induced by all $\phi \in M$ are physically equivalent. Since Prim $(\mathfrak{A})$ equipped with the Jacobson topology is $T_0$-space; hence, for $I \in$ Prim $(\mathfrak{A})$, $\{I\}$ is not necessary closed. However, $\{I\}$ is closed in the Jacobson topology if and only if $I$ is a maximal primitive ideal (Ref. 8; 3.1.4).

Let $K$ be a compact convex subset of $S(\mathfrak{A})$, then $E(K)$ is nonempty. If $K$ is a face of $S(\mathfrak{A})$, then $E(K) \subseteq ES(\mathfrak{A})$. Moreover, if $E(K)$ forms a physically equivalent class, then all irreducible representations $\pi_\phi$ induced by all pure states $\phi$ from $E(K)$ are corresponding to a primitive ideal $I_0$ from Prim $(\mathfrak{A})$, such that kern $\pi_\phi = I_0$ for all $\phi \in E(K)$. The main property of $I_0$ is:

*Proposition 3.4:* Let $K$ be a closed split face[13] of $S(\mathfrak{A})$, $E(K)$ the extreme points in $K$. If $E(K)$ forms a physically equivalent class, then the corresponding primitive ideal $I_0$ of $\mathfrak{A}$ is a maximal primitive ideal.

*Proof:* Suppose that there is a primitive ideal $I \in$ Prim $(\mathfrak{A})$ such that $I \supseteq I_0$. Let $\pi$ be the irreducible representation of $\mathfrak{A}$ corresponding to $I$ such that kern $\pi = I$, then kern $\pi \supseteq$ kern $\pi_0$, where $\pi_0$ is the irreducible representation induced by each $\phi \in E(K)$ such that kern $\pi_0 = I_0$ as described above. We note that kern $\pi_0 = \cap_\phi$ kern $\pi_\phi$ for all $\phi \in E(K)$, hence

$$\text{kern } \pi \supseteq \bigcap_\phi \text{kern } \pi_\phi$$

for all $\phi \in E(K)$. Thus, $\pi$ is weakly contained in the set of $\pi_\phi$ for all $\phi \in E(K)$ (Ref. 8; 3.4.5).

Let $\rho$ be a pure state associated with $\pi$, then $\rho$ is a $w^*$-limit point of states associated with $\pi_\phi$ for $\phi \in E(K)$ (Ref. 8, Theorem 3.4.10). Hence, $\rho$ is a $w^*$-limit point of states $\phi_x$ of the form $x \to \phi_x(\cdot) = \phi(x^* \cdot x)$ for $x \in \mathfrak{A}$. (Ref. 8, 2.4.8). However, $K$ is an invariant face of $S(\mathfrak{A})$ (Ref. 13, Proposition 7.1); thus $\phi_x \in K$, and therefore $\rho \in K$. Then, $\rho \in E(K)$; otherwise $\rho$ is not in $ES(\mathfrak{A})$. And, by the assumption, kern $\pi_\rho$ = kern $\pi_0$, but $\pi_\rho$ and $\pi$ are (unitarily) equivalent; therefore, kern $\pi$ = kern $\pi_\rho$ = kern $\pi_0$, and $I = I_0$.

We are able to prove our main result in this section.

*Theorem 3.1:* Let $\mathfrak{A}$ be a $C^*$-algebra with identity and $K$ facial simplex on $S(\mathfrak{A})$. Suppose $K$ is split (in the sense of Ref. 13). If $E(K)$ forms a physically equivalent class, then $K$ is a Bauer simplex.

*Proof:* If $K$ is a singleton, this theorem is trivial, therefore we assume that $K$ is not a singleton. Let $ES(\mathfrak{A})$ and Prim $(\mathfrak{A})$ be equipped with $w^*$-topology and Jacobson topology, respectively. We define a map $\theta$ from $ES(\mathfrak{A})$ into Prim $(\mathfrak{A})$ by $\theta(\rho)$ = kern $\pi_\rho = I_\rho$ for $\rho \in ES(\mathfrak{A})$, $I_\rho \in$ Prim $(\mathfrak{A})$, then $\theta$ is continuous (Ref. 13, p. 439). (In fact $\theta$ is also open and onto; however, we do not need these properties here.)

By assumptions, $E(K) \subseteq ES(\mathfrak{A})$ and $E(K)$ forms a physically equivalent class; hence

$$\theta : E(K) \to \{I_0\},$$

where $I_0$ = kern $\pi_\phi$, and $\pi_\phi$ is irreducible representation induced by each $\phi \in E(K)$.

We claim that $\theta^{-1}(\{I_0\}) = E(K)$. Suppose that $\theta^{-1}(\{I_0\}) \times \backslash E(K) \neq \emptyset$, let $\rho \in \theta^{-1}(\{I_0\}) \backslash E(K)$ and $\theta(\rho) = I_0$, then kern $\pi_\rho$ = kern $\pi_\phi \cdot \pi_\rho$ can be considered as weakly contained in $\pi_\phi$, then by a similar argument given in the proof of Proposition 3.4, $\rho \in K$ and hence $\rho \in E(K)$.

Since $K$ is not a singleton, $I_0$ is a maximal primitive ideal from Proposition 3.4, hence $\{I_0\}$ is closed in the Jacobson topology. Therefore, due to the continuity of $\theta$, $E(K_\beta) = \theta^{-1}(\{I_\beta\})$ is closed in the $w^*$-topology, which completes the proof of theorem.

An immediate consequence is the following.

*Corollary 3.3:* For a simple $C^*$-algebra $\mathfrak{A}$, every facial simplex is a Bauer simplex.

A remark is given here as another consequence of Theorem 3.1: If $\mathfrak{A}$ is separable and $K$ is a facial simplex, then the structure space $E(K)$ is a complete metric space, whenever $E(K)$ forms a physically equivalent class. In fact, the structure topology and the $w^*$-topology are coincided, since $E(K)$ is $w^*$-closed; and the $w^*$-topology is metrizable for a separable $C^*$-algebra.

We note that the Choquet simplex $K_\beta$ of KMS states defined in Sec. 2 is not a facial simplex of $S(\mathfrak{A})$; but $K_\beta$ is a facial simplex of some compact convex subset of $S(\mathfrak{A})$. This can be seen as follows: Let $\mathfrak{A}$ be a $C^*$-algebra equipped with a one-parameter automorphism group $\sigma_t$ with suitable continuity, for $t \in \mathbb{R}$, and $I(\mathfrak{A})$ denote the compact convex subset of $S(\mathfrak{A})$ such that $\phi \in I(\mathfrak{A})$ iff $\phi = \phi \circ \sigma_t$ for all $t \in \mathbb{R}$. If $\mathfrak{A}$ is asymptotically Abelian with respect to the additive group $\mathbb{R}$ (e.g. time translation), then $K_\beta$ is a subset of $I(\mathfrak{A})$.[9] Let $\phi \in E(K_\beta)$, then $\pi_\phi$ is a factor representation on $\mathcal{H}_\phi$,[15] and the center of $\pi_\phi(\mathfrak{A})''$, $\mathfrak{Z}_\phi = \{\lambda I\}$. Let $\mathfrak{Z}_\phi \cap \mathfrak{U}(\phi)' = \{\lambda I\}$, where $\mathfrak{U}(\phi)$ is the group of the

unitary operators $U_\phi(t)$, such that $t \to U_\phi(t)$ for $t \in \mathbf{R}$ is a unitary representation of $\mathbb{R}$ on $\mathcal{H}_\phi$. Thus, it follows from Ref. 5, Corollary 5.5 that $\phi \in E(I(\mathfrak{A}))$ for any $\phi \in E(K_\beta)$. As $K_\beta$ is a compact convex subset of $I(\mathfrak{A})$, which is known as a simplex, (see, e.g., Refs. 1 and 5), then from Corollary 3.2 it follows that $K_\beta$ is a facial simplex of $I(\mathfrak{A})$.

## 4. SIMPLEXES OF KMS STATES

As we have noted in Sec. 2 that the set of KMS states $K_\beta$ with respect to a fixed one-parameter automorphism $\sigma_t$ of $\mathfrak{A}$ for a given inverse temperature $\beta$ is a simplex. Hence, the question of the structure of $K_\beta$ arises: Is $K_\beta$ also a Bauer simplex, or does $K_\beta$ have similar structure like facial simplexes? We study this problem in this section.

We assume hereafter that $\mathfrak{A}$ is *separable*. From Ref. 15, $\phi \in E(K_\beta)$ if and only if $\phi$ is primary, thus the kernel of $\pi_\phi$, the cyclic representation induced by $\phi \in E(K_\beta)$, is a primitive ideal of $\mathfrak{A}$ (Ref. 16, Corollaire 3). We may define a map $\gamma: E(K_\beta) \to \text{Prim}(\mathfrak{A})$ by

$$\gamma(\phi) = \text{kern } \pi_\phi,$$

where $E(K_\beta)$ and Prim $(\mathfrak{A})$ are endowed with the structure topology and the Jacobson topology, respectively.

Firstly, we want to show the continuity of $\gamma$ by applying a method given by Effro and Hahn.[17]

Let $F$ be a closed subset of Prim $(\mathfrak{A})$, then $F = h(J)$, where $J$ is a subset of $\mathfrak{A}$ such that $J = k(F)$. Define a subset $M_F$ of $K_\beta$ by

$$M_F = \{\phi \in K_\beta; \text{kern } \pi_\phi \supseteq J\},$$

then $\gamma^{-1}(F) = E(K_\beta) \cap M_F$.

For $\phi \in K_\beta$, $I_\phi = \{x \in \mathfrak{A}; \phi(x^*x) = 0\}$, the left kernel of $\phi$, is a two-side ideal of $\mathfrak{A}$ and $I_\phi = \text{kern } \pi_\phi$.[2] Take the quotient space $\mathfrak{A}/I_\phi$ with a scalar product $(x_\phi, y_\phi) = \phi(y^*x)$, where $x_\phi$ and $y_\phi$ are equivalent class containing $x$ and $y$, respectively. Thus, the completion of $\mathfrak{A}/I_\phi$ is the representation space $\mathcal{H}_\phi$ of the cyclic representation $\pi_\phi$ with the cyclic vector $\xi_\phi = 1_\phi$, here 1 is the identity of $\mathfrak{A}$: And, for $a \in \mathfrak{A}$, $\pi_\phi(a)$ is a bounded linear operator on $\mathcal{H}_\phi$ such that $\pi_\phi(a)x_\phi = (ax)_\phi$. This is the usual GNS construction of $\pi_\phi$. Moreover, since $I_\phi$ is a two-sided ideal of $\mathfrak{A}$, we may also define a bounded linear operator ${}_\phi\pi(a)$ (for $a \in \mathfrak{A}$) on $\mathcal{H}_\phi$ such that ${}_\phi\pi(a)x_\phi = (xa)_\phi$.

For $x \in \mathfrak{A}$, then $x \in \text{kern } \pi_\phi$ if and only if $x \in I_\phi$, and $\phi(x^*x) = \|\pi_\phi(x)\xi_\phi\|^2 = 0$ implies that

$$\pi_\phi(x)y_\phi = (xy)_\phi = {}_\phi\pi(y)x_\phi = {}_\phi\pi(y)(x1)_\phi$$
$$= {}_\phi\pi(y)\pi_\phi(x)\xi_\phi = 0$$

for all $y \in \mathfrak{A}$. Hence, for any $\psi$ associated with $\pi_\phi$, if $x \in J$ then $\psi(x^*x) = 0$, and $I_\psi \supseteq J$. And, furthermore, if $\psi \in K_\beta$, then kern $\pi_\psi \supseteq J$, so that $\psi \in M_F$. Therefore

$$M_F = \bigcap_{x \in J} \{\phi \in K_\beta; \phi(x^*x) = 0\},$$

which is $w^*$-closed in $K_\beta$. Moreover, if $\rho \leq \alpha\phi$ for $\rho \in K_\beta$, and $\phi \in M_F$ with $\alpha > 0$, then $\rho \in M_F$. Thus, $M_F$ is a face of $K_\beta$, so that $E(M_F) \subseteq E(K_\beta)$, hence,

$$\gamma^{-1}(F) = E(M_F),$$

which is closed in the structure topology on $E(K_\beta)$. Therefore, $\gamma$ is continuous in the structure topology. And we have proved the following:

*Lemma 4.1:* Let $\mathfrak{A}$ be a separable $C^*$-algebra with identity. If $\gamma$ is a map from $E(K_\beta)$ into Prim $(\mathfrak{A})$ defined by $\gamma(\phi) = \text{kern } \pi_\phi$ as described above, then $\gamma$ is structurally continuous.

Furthermore, we say that $E(K_\beta)$ is *decomposable in the sense of ensembles*, or briefly *decomposable*, as follows (cf. Ref. 18): kern $\pi_{\phi_1} = \text{kern } \pi_{\phi_2}$ implies that $\pi_{\phi_1}$ and $\pi_{\phi_2}$ are quasi-equivalent for any $\phi_1, \phi_2 \in E(K_\beta)$.

For different temperature of KMS states, the above condition is not true.[2] However, it holds for a GCR $C^*$-algebra $\mathfrak{A}$ as follows:

Let $\phi_i \in E(K_\beta)$ $(i = 1, 2)$, and kern $\pi_{\phi_1} = \text{kern } \pi_{\phi_2}$. Since $\mathfrak{A}$ is GCR and $\pi_{\phi_i}(i = 1, 2)$ are factor representations, thus $\pi_{\phi_i}(i = 1, 2)$ are quasi-equivalent to irreducible representations $\pi_i(i = 1, 2)$ (Ref. 8; 5.5.3). It follows that kern $\pi_1 = \text{kern } \pi_2$, which implies that $\pi_1$ and $\pi_2$ are equivalent (Ref. 8; 4.3.7). Consequently, $\pi_{\phi_1}$ and $\pi_{\phi_2}$ are quasi-equivalent.

*Lemma 4.2:* In addition to the assumption of Lemma 4.1, if $E(K_\beta)$ is decomposable, then $\gamma$ is injective, up to the equivalence.

*Proof:* Let $\phi_1, \phi_2 \in E(K_\beta)$ with $\phi_1 \neq \phi_2$. Suppose that kern $\pi_{\phi_1} = \text{kern } \pi_{\phi_2}$, then, by the hypothesis, $\pi_{\phi_1}$ and $\pi_{\phi_2}$ are quasi-equivalent. Moreover, $\phi_1$ and $\phi_2$ are separating[9]; hence $\pi_{\phi_1}(\mathfrak{A})''$ and $\pi_{\phi_2}(\mathfrak{A})''$ have separating and cyclic vector $\xi_{\phi_1}$ and $\xi_{\phi_2}$, respectively. As $\pi_{\phi_1}$ and $\pi_{\phi_2}$ are quasi-equivalent, they are also (unitarily) equivalent (Ref. 19, Theorem 3, p. 233). Therefore $\phi_1 = \phi_2$, up to the equivalence, which completes the proof of Lemma 4.2

Let $B$ be the range of $\gamma$, i.e.,

$$\gamma(E(K_\beta)) = B,$$

then $B$ is a subset of Prim $(\mathfrak{A})$. And, $\gamma$ is a surjective mapping from the structure space $E(K_\beta)$ onto $B$.

*Lemma 4.3:* As the assumption given in Lemma 4.1, if $\gamma$ is surjective mapping from $E(K_\beta)$ onto $B$, then $\gamma$ is a (structurally) closed mapping.

*Proof:* Let $F$ be a closed subset of $E(K_\beta)$, then $F = E(K_\beta) \cap T$, where $T$ is a $w^*$-closed face of $K_\beta$. It is easy to see that $\gamma(F) \subseteq h(J)$ for some $J \subseteq \mathfrak{A}$. In fact, we have $h(J) = \{\text{kern } \pi_\phi \in B; \text{kern } \pi_\phi \supseteq J\}$ with $J = \bigcap_{\phi \in F} \text{kern } \pi_\phi$.

Conversely, we have to show: $\gamma(F) \supseteq h(J)$. Let $I_\rho = \text{kern } \pi_\rho \in h(J)$, then there is a state $\rho \in E(K_\beta)$ such that $\gamma(\rho) = I_\rho$, since $\gamma(E(K_\beta)) = B$. Hence we need only to show that $\rho \in T$.

Since $I_\rho = \text{kern } \pi_\rho \supseteq \bigcap_{\phi_i \in F} \text{kern } \pi_{\phi_i}$, thus $\rho$ is a $w^*$-limit of finite linear combinations of states associated with $\pi_{\phi_i}$ for all $\phi_i \in F$ (Ref. 8, Theoreme 3.4.4), i.e.,

$$\rho = w^* - \lim_n \sum_i^n \lambda_i \omega_{\xi_i} \circ \pi_{\rho_i}$$

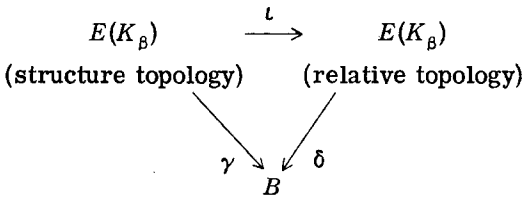
with $\sum_i^n \lambda_i = 1$ and $\xi_i \in \mathcal{H}_{\phi_i}$, which is the representation space of $\pi_{\phi_i}$.

Furthermore, since $\phi \in F$ is a KMS state, $\phi$ is separating.[9] Hence $\mathcal{H}_\phi = [\pi_\phi(\mathfrak{A})\xi_\phi] = [\pi_\phi(\mathfrak{A})'\xi_\phi]$.[20] Let $\eta = x'\xi_\phi$ for $x' \in \pi_\phi(\mathfrak{A})'$, then $\omega_\eta \circ \pi_\phi = \omega_{x'\xi_\phi} \circ \pi_\phi \leq \|x'\|^2\phi$. For $\xi \in \mathcal{H}_\phi$, $\omega_\xi \circ \pi_\phi$ is a norm limit of states $\omega_\eta \circ \pi_\phi$, thus $\omega_\xi \circ \pi_\phi \leq \alpha\phi$ with $\alpha = \|x'\|^2$. Consequently, $\sum_i^n \lambda_i \omega_\xi \circ \pi_{\phi_i} \leq \alpha \sum_i^n \lambda_i \phi_i$ with $\alpha = \max\{\alpha_i; i = 1, 2, \ldots, n\}$, and also its $w^*$-limit $\rho$, viz. $\rho \leq \alpha \sum_i^n \lambda_i \phi_i$. However, $T$ is a convex subset of $K_\beta$, hence $\sum_i^n \lambda_i \phi_i \in T$. Therefore, as $T$ is a face of $K_\beta$, $\rho \in T$, the proof of Lemma 4.3 is complete.

Let $E(K_\beta)$ be endowed with the relative topology which is induced by the $w^*$-topology of $K_\beta$ and the map from $E(K_\beta)$ into Prim $(\mathfrak{A})$ be denoted by $\delta$. In fact $\delta$ and $\gamma$ are the same map having a domain with different topologies. Since the relative topology is stronger than the structure topology,[7] thus $\delta$ is also continuous from Lemma 4.1. We denote by $B$ the range of $\delta$ again, then we are able to give a characterization for the structure of $K_\beta$ as follows:

*Theorem 4.1:* Let $\mathfrak{A}$ be a separable $C^*$-algebra with identity and $\delta$ the map from $E(K_\beta)$ onto $B$; here $E(K_\beta)$ is endowed with the relative topology and $B \subseteq$ Prim $(\mathfrak{A})$. If $E(K_\beta)$ is decomposable, then $K_\beta$ is a Bauer simplex if and only if $\delta$ is a closed mapping.

*Proof:* Consider the following commutative diagram




where $\iota$ is the identity map. Then, we have

$$\iota = \delta^{-1} \circ \gamma.$$

By the given hypothesis, $\delta$ is closed and also continuous from the previous argument. Hence $\delta$ is a homeomorphism, and $\delta^{-1}$ is continuous. Furthermore, the continuity of $\gamma$ follows from Lemma 4.1, therefore $\iota$ is a continuous identity map, which implies that the structure topology is stronger than the relative topology. It follows that two topologies on $E(K_\beta)$ coincide. Hence $E(K_\beta)$ is compact in the relative topology, and so $E(K_\beta)$ is $w^*$-compact. Therefore $K_\beta$ is a Bauer simplex.

Conversely, if $K_\beta$ is a Bauer simplex, then the structure topology and the weak topology are coincided.[4] And, from Lemma 4.3, $\gamma$ is structurally closed; therefore $\delta$ is also closed.

As we have noted that $E(K_\beta)$ is decomposable for a GCR $C^*$-algebra, therefore we may apply the above theorem to show the nonexistence of Bauer simplex in a GCR algebra.

*Theorem 4.2:* Let $\mathfrak{A}$ be a separable, GCR $C^*$-algebra with identity. If $K_\beta$ is not a singleton, then $K_\beta$ is *not* a Bauer simplex.

*Proof:* We need only to show a counter example that $\delta$ given in Theorem 4.1 is *not closed.*

Let $\mathfrak{A}$ be a separable, GCR $C^*$-algebra with identity, equipped with a one-parameter automorphism $\sigma_t$. Suppose $\mathfrak{A}$ has a *faithful* primary KMS state with respect to $\sigma_t$. Since $\delta$ is closed in the $w^*$-topology (which coincides with the relative topology now), hence $\delta(E(K_\beta)) = B$ is closed in Prim $(\mathfrak{A})$, so that $B = h(J) = \{I \in \text{Prim } (\mathfrak{A}); I \supseteq J\}$ for some subset $J$ of $\mathfrak{A}$. If $E(K_\beta)$ has a faithful primary KMS state, then $B =$ Prim $(\mathfrak{A})$; consequently, every primitive ideal of $\mathfrak{A}$ is the kernel of the cyclic representation induced by a K.M.S. state. We construct a counter example suggested by Takesaki[21] as follows:

Let $\mathcal{H}$ be a separable Hilbert space with an orthonormal basis $\{\xi_n; n = 1, 2, \cdots\}$, and $u$ be a isometric map of $\mathcal{H}$ defined by

$$u\xi_n = \xi_{n+1}, \quad n = 1, 2, \cdots.$$

If $e_n$ is the projection of $\mathcal{H}$ onto $\mathbb{C}\xi_n$, $n = 1, 2, \cdots$. For a sequence $\{\lambda_n\} \in l^1$ with $\lambda_n > 0$, put

$$h = \sum_{n=1}^\infty \lambda_n e_n.$$

Then $h$ is a modular operator on $\mathcal{H}$. If $\sum_{n=1}^\infty \lambda_n = 1$, $h$ induces a faithful normal state of $\mathfrak{B}(\mathcal{H})$, the algebra of all bounded operators on $\mathcal{H}$: And, the modular automorphism group of the state is induced by the one-parameter unitary group

$$h^{it} = \sum_{n=1}^\infty \lambda_n^{it} e_n.$$

Let $\mathfrak{A}$ be the $C^*$-algebra generated by $u$ and $u^*$ defined above. Then it is known that $\mathfrak{A}$ contains the $C^*$-algebra $\mathfrak{C}(\mathcal{H})$ of all compact operators on $\mathcal{H}$, and $\mathfrak{A}/\mathfrak{C}(\mathcal{H})$ is isomorphic to the algebra $C(\Gamma)$ of all continuous functions of the unit circle $\Gamma = \{\lambda \in \mathbb{C}; |\lambda| = 1\}$. For a suitable choice of $\{\lambda_n\}$, we want to show that

$$h^{it}\mathfrak{A}h^{-it} = \mathfrak{A}.$$

In fact, for $u \in \mathfrak{A}$,

$$\begin{aligned} h^{it}uh^{-it} &= h^{it}u \sum_{n=1}^\infty \lambda_n^{-it} e_n = h^{it} \sum_{n=1}^\infty \lambda_n^{-it} u e_n \\ &= h^{it} \sum_{n=1}^\infty \lambda_n^{-it} e_{n+1} u = \sum_{n=1}^\infty \lambda_{n+1}^{it} \lambda_n^{-it} e_{n+1} u \\ &= \left[\sum_{n=1}^\infty \left(\frac{\lambda_{n+1}}{\lambda_n}\right)^{it} e_{n+1}\right] u. \end{aligned}$$

Let $\lambda_n = 1/2^n$, then $\sum_{n=1}^\infty \lambda_n = 1$ and $\lambda_{n+1}/\lambda_n = \frac{1}{2}$; hence

$$\begin{aligned} h^{it}uh^{-it} &= \sum_{n=1}^\infty \left(\frac{1}{2}\right)^{it} e_{n+1} u \\ &= \left(\frac{1}{2}\right)^{it} \left(\sum_{n=1}^\infty e_{n+1}\right) u = \left(\frac{1}{2}\right)^{it} u \in \mathfrak{A}. \end{aligned}$$

Therefore, $h^{it}uh^{-it} \in \mathfrak{A}$, and the one-parameter automorphism group $\sigma_t(x) = h^{it}xh^{-it}$ of $\mathfrak{B}(\mathcal{H})$ is also a one-parameter automorphism group of $\mathfrak{A}$. However, $u - \sigma_t(u) = [1 - (\frac{1}{2})^{it}]u$ is *not* a compact operator on $\mathcal{H}$. Consider a state $\phi$ defined by

$$\phi(x) = \text{Tr}(xh),$$

then $\phi$ is a faithful KMS state of $\mathfrak{A}$ with respect to $\sigma_t$. Since $\mathfrak{A}$ is $\sigma$-weakly dense in $\mathfrak{B}(\mathfrak{H})$, we know that $\pi_\phi(\mathfrak{A})''$ is isomorphic to $\mathfrak{B}(\mathfrak{H})$. Hence $\phi$ is primary, i.e., $\phi \in E(K_\beta)$ for $\beta = 1$. Obviously, kern $\pi_\phi = \{0\}$. Therefore, $\mathfrak{A}$ has a faithful primary KMS state $\phi$ with respect to $\sigma_t$, and $\delta(E(K_\beta)) = \text{Prim}\,(\mathfrak{A})$. On the other hand, the automorphism $\sigma_t$ of $\mathfrak{A}$ induces naturally a one-parameter automorphism group $\tilde{\sigma}_t$ of $\mathfrak{A}/\mathfrak{C}(\mathfrak{H})$. Since $\sigma_t(u) - u \notin \mathfrak{C}(\mathfrak{H})$, hence $\tilde{\sigma}_t$ is not a trivial automorphism on the Abelian $C^*$-algebra $\mathfrak{A}/\mathfrak{C}(\mathfrak{H})$. However, any nontrivial one-parameter automorphism group of an Abelian $C^*$-algebra cannot induce a KMS state at all. Therefore, every primitive ideal of $\mathfrak{A}$, which contains $\mathfrak{C}(\mathfrak{H})$, is not the left kernel of any KMS state with respect to $\sigma_t$.

In quantum statistical mechanics, the $C^*$-algebra of quantum lattice system and the $C^*$-algebra associated with the canonical anticommutation relations are separable and simple. Hence we are interested in the structure of $K_\beta$ in these cases. As $\mathfrak{A}$ is simple, Prim $(\mathfrak{A}) = \{0\}$, hence the method given in the proof of Theorem 4.1 does not work for this case, since $\gamma^{-1}$ and $\delta^{-1}$ cannot exist. However we give another characterization of the structure of $K_\beta$ for this case.

Let $X$, $Y$ be topological spaces and $\gamma$ a mapping of $X$ into $Y$. $\gamma$ is said to be *proper* if $\gamma$ is continuous and the mapping $\gamma \times \iota_z : X \times Z \to Y \times Z$ is closed for every topological space $Z$, where $\iota_z$ is the identity mapping of $Z$ onto itself (Ref. 22, p. 97).

We return to mapping $\delta : E(K_\beta) \to \text{Prim}\,(\mathfrak{A}) = \{0\}$, here $E(K_\beta)$ is endowed with the relative topology induced by the $w^*$-topology of $K_\beta$.

Then $\delta$ is proper if and only if $E(K_\beta)$ is a compact space (Ref. 22, p. 103). Hence $E(K_\beta)$ is $w^*$-compact, and $E(K_\beta)$ is $w^*$-closed in $K_\beta$, i.e., $K_\beta$ is a Bauer simplex. We have therefore the following characterization:

*Theorem 4.3:* Let $\mathfrak{A}$ be a separable, simple $C^*$-algebra with a one-parameter automorphism group $\sigma_t$. Then, $K_\beta$ is a Bauer simplex if and only if the mapping $\delta : E(K_\beta) \to \text{Prim}\,(\mathfrak{A})$ is proper, where $E(K_\beta)$ is equipped with the relative topology.

We note from the previous arguments that this characterization holds not only for a simple $C^*$-algebra, but also for a separable $C^*$-algebra $\mathfrak{A}$ such that Prim $(\mathfrak{A})$ is a singleton. An immediate example: $\mathfrak{A}$ has only one irreducible representation, then it turns out $\mathfrak{A} = \mathfrak{C}(\mathfrak{H})$, the $C^*$-algebra of all compact operators on a Hilbert space $\mathfrak{H}$ (see e.g. Ref. 11, p. 236). This is a special case of a separable, simple, GCR $C^*$-algebra. However, for any separable, simple, GCR $C^*$-algebra $\mathfrak{A}$, it is easy to verify, from the proof of Lemma 4.2, that $E(K_\beta)$ is a singleton, hence the mapping $\delta : E(K_\beta) \to \text{Prim}\,(\mathfrak{A})$ in the Theorem 4.3 is proper. Therefore, we have an immediate

*Corollary 4.1:* If $\mathfrak{A}$ is a separable, simple, GCR $C^*$-algebra with a one-parameter automorphism group $\sigma_t$, then $K_\beta$ is a Bauer simplex.

Actually, by Krein–Milman theorem, $K_\beta$ is a singleton in this case.

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# Hypergeometric Structure of the Generalized Veneziano Amplitudes

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A multiple integral representation for a function of $n(n-1)/2$ variables, which reduces to the $(n+3)$-point generalized Veneziano amplitude for unit values of the variables, is integrated out once to obtain a recurrence formula for the amplitude. The result of complete integration obtained through repeated use of the recurrence formula is shown to belong to a class of generalized hypergeometric functions of many variables which are similar to but are more complex than the Lauricella functions. It is shown also that the $(n+3)$-point amplitude for $n \geq 3$ can be represented as a linear combination of an infinite number of ${}_{n+1}F_n[1]$ series with varying parameters.

## 1. INTRODUCTION

It is well known that the four- and five-point amplitudes are representable as the values for $x = 1$ of the hypergeometric functions ${}_2F_1[x]$ and ${}_3F_2[x]$, respectively. However, one will easily be convinced that this simple property of representing the $n$-point function in terms of a suitable ${}_pF_q[1]$ does not extend beyond $n = 5$. On the other hand, it was pointed out recently that the $n$-point functions may be regarded as the boundary values of a class of generalized hypergeometric functions that are Radon transforms of products of linear forms.[1] While it is undoubtedly an elegant way of describing the structure of these functions, it would still be desirable to bring out explicitly the hypergeometric nature of the functions on a more concrete and familiar bases.

In this paper it will be shown that the generalized Veneziano amplitudes can be represented as the boundary values of generalized hypergeometric functions of many variables of Lauricella type.[2] In addition, it will be shown that the $(n+3)$-point functions for $n \geq 3$ can also be represented as a linear combination of ${}_{n+1}F_n[1]$ series with varying parameters.

## 2. SOLUTIONS

Let us first define a function $V_n$ of variables $w_{ij}$ given as below:

$$V_n(\alpha_{01},\ldots,\alpha_{0n};\alpha_{11},\ldots,\alpha_{1n};\alpha_{21},\ldots,\alpha_{2,n-1};\ldots;\alpha_{n-1,1},\alpha_{n-1,2};\alpha_{n1}\,|\,w_{01},\ldots,w_{0n};w_{12},\ldots,w_{1n};\ldots;w_{n-1,n})$$
$$= \int_0^1\cdots\int_0^1 \prod_{i=1}^{n}\left\{du_i\,u_i^{\alpha_{0i}-1}(1-w_{i-1,i}\,u_i)^{\alpha_{1i}-1}\prod_{k=2}^{i}\left[1-u_i\left(w_{i-k,i}\prod_{j=0}^{k-2}u_{i-j-1}\right)\right]^{\alpha_{k,i-k+1}}\right\}. \tag{1}$$

By regarding $\alpha_{ij}$ to be functions of $n+3$ external particle momenta $p_1, p_2, \ldots, p_{n+3}$, $V_n$ may be looked upon as depending parametrically on these momenta, in addition to its being a function of the variables $w_{ij}$. Notice then that $V_n$ can readily be made to correspond to the known representation for the $(n+3)$-point function, for example, $B_{n+1}(p_0, p_1, \ldots, p_{n+2})$ given by Bardakci and Ruegg.[3] Moreover, for $w_{0i} = 1$, $i = 1, 2, \ldots, n$, $V_n$ will be seen to be easily identifiable, through a change of variables $x_i = \prod_{k=1}^{i} u_k$, for $i = 1, 2, \ldots, n$, with the function $F^{(n)}(a_i, b_i, c_{ij}; w_{ij})$ defined in Ref. 1.

With evaluation of Eq. (1) in mind consider the following relation[4]:

$$\int_0^1 du_i\,u_i^{\alpha_{0i}-1}(1-u_i)^{\alpha_{1i}-1}\times\prod_{k=2}^{i}(1-u_i x_{i,k-1})^{\alpha_{k,i-k+1}} = B(\alpha_{0i},\alpha_{1i})\times\sum\frac{(\alpha_{0i},\beta_{i,i-1})(-\alpha_{2,i-1},r_{2,i-1})\cdots(-\alpha_{i1},r_{i1})}{(\alpha_{0i}+\alpha_{1i},\beta_{i,i-1})(1,r_{2,i-1})\cdots(1,r_{i1})}\times(x_{i1})^{r_{2,i-1}}\cdots(x_{i,i-1})^{r_{i1}}. \tag{2}$$

In Eq. (2) $B$ stands for the beta function, the notation $(\alpha, r)$ under the summation symbol stands for the Pochhammer symbol $(\alpha)_r = \Gamma(\alpha+r)/\Gamma(\alpha)$ for ease of printing, and we set

$$\beta_{pq} = \sum_{k=p-g+1}^{p} r_{k,p-k+1}, \qquad p = 2,3,\ldots,n, \quad g = 1,2,\ldots,p-1. \tag{3}$$

Further, the sum in Eq. (2) equals $F_D(\alpha_{0i}; -\alpha_{2,i-1}, -\alpha_{3,i-2},\ldots,-\alpha_{i1}; \alpha_{0i}+\alpha_{1i}; x_{i1},\ldots,x_{i,i-1})$, where $F_D$ denotes one of the Lauricella functions which are a generalization to many variables of Appell's double series $F_i$, $i = 1, 2, 3,$ and 4, for two variables,[2] which in turn represent a generalization of Gauss' hypergeometric function of a single variable.

If we assume from now on that $w_{i-1,i} = 1$, for $i = 1, 2, \ldots, n$, we observe that we can carry out the integration in Eq. (1) in a successive manner by the use of Eq. (2) with $x_{i,k-1} = w_{i-k,i}\prod_{j=0}^{k-2}u_{i-j-1}$ for $i = 2, 3, \ldots, n$ and $k = 2, 3, \ldots, i$. Thus, the first integration over $u_n$ gives rise to

$$V_n(\alpha_{01},\ldots,\alpha_{0n};\alpha_{11},\ldots,\alpha_{1n};\ldots;\alpha_{n1}\,|\,1,w_{02},\ldots,w_{0n};\ldots;1,w_{n-2,n};1) = B(\alpha_{0n},\alpha_{1n})\times\sum\frac{(\alpha_{0n},\beta_{n,n-1})(-\alpha_{2,n-1},r_{2,n-1})\cdots(-\alpha_{n1},r_{n1})}{(\alpha_{0n}+\alpha_{1n},\beta_{n,n-1})(1,r_{2,n-1})\cdots(1,r_{n1})}\times(w_{n-2,n})^{r_{2,n-1}}(w_{n-3,n})^{r_{3,n-2}}\cdots(w_{0n})^{r_{n1}}\times V_{n-1}(\alpha_{01}+\beta_{n1},\ldots,\alpha_{0,n-1}+\beta_{n,n-1};\alpha_{11};\ldots;\alpha_{1,n-1};\ldots;\alpha_{n-1,1}\,|\,1,w_{02},\ldots,w_{0,n-1};\ldots;1,w_{n-3,n-1};1). \tag{4}$$

It is to be realized that Eq. (4) represents a recurrence formula for $V_n$.

A repeated use for $m$ times of the recurrence formula leads to[5]

$$V_n = \prod_{s=1}^{m}\left\{B(\alpha_{0,n-s+1},\alpha_{1,n-s+1})\times\prod_{t=0}^{n-s-1}\left[\sum_{r_{t+2,n-s-t}}\frac{(\alpha_{0,n-s+1},\delta_{n-s+1}^{(n)})}{(\alpha_{0,n-s+1}+\alpha_{1,n-s+1},\delta_{n-s+1}^{(n)})}\right.\right.$$

$$\times \frac{(-\alpha_{t+2,n-s-t},\gamma_{t+2,n-s-t})}{(1,\gamma_{t+2,n-s-t})}(w_{n-s-t-1,n-s+1})^{\gamma_{t+2,n-s-t}}\Big]\Big\}$$

$$\times V_{n-m}(\alpha_{01}+\delta_1^{(n)},\ldots,\alpha_{0,n-m}+\delta_{n-m}^{(n)};\ldots;\alpha_{n-m,1}|$$

$$\times 1,w_{02},\ldots,w_{0,n-m};\ldots;1,w_{n-m-2,n-m};1), \quad (5)$$

where we set

$$\gamma_q^{n,k}=\sum_{p=n-k+1}^{n}\beta_{pq} \quad (6)$$

and

$$\delta_j^{(n)}=\begin{cases}0, & \text{for } n=j=1,\\ \beta_{j,j-1}+\gamma_j^{n,n-j}, & \text{for } n=2,3,\cdots \text{ and } j=1,2,\ldots,n-1 \text{ with } \beta_{10}=\gamma_n^{n,0}=0.\end{cases} \quad (7)$$

Note that a use has been made of the relation

$$B(\alpha_{0j}+\gamma_j^{n,n-j},\alpha_{1j})\frac{(\alpha_{0j}+\gamma_j^{n,n-j},\beta_{j,j-1})}{(\alpha_{0j}+\alpha_{1j}+\gamma_j^{n,n-j},\beta_{j,j-1})}$$

$$=B(\alpha_{0j}+\delta_j^{(n)},\alpha_{1j})$$

$$=B(\alpha_{0j},\alpha_{1j})\frac{(\alpha_{0j},\delta_j^{(n)})}{(\alpha_{0j}+\alpha_{1j},\delta_j^{(n)})}, \quad (8)$$

which follows from the identity $(a,n+k)=(a+k,n)(a,k)$, in obtaining Eq. (5).

When $m=n-1$, we are left with $V_1$ which can be evaluated as

$$V_1(\alpha_{01}+\gamma_1^{n,n-1}\alpha_{11}|1)=B(\alpha_{01}+\delta_1^{(n)},\alpha_{11})$$

$$=B(\alpha_{01},\alpha_{11})(\alpha_{01},\delta_1^{(n)})/(\alpha_{01}+\alpha_{11},\delta_1^{(n)}), \quad (9)$$

where we noted $\gamma_1^{n,n-1}=\delta_1^{(n)}$ from Eq. (7). Upon substitution of Eq. (9) into Eq. (5) it is seen that the result of complete integration for $V_n$ is given by Eq. (5) with replacements $m\to n$, $V_0\to 1$, and $\prod_{t=0}^{n-s-1}[\cdots]\to(\alpha_{01},\delta_1^{(n)})/(\alpha_{01}+\alpha_{11},\delta_1^{(n)})$ for $s=n$.

If the result thus obtained is written out in the expanded form, namely,

$$V_n=B(\alpha_{0n},\alpha_{1n})B(\alpha_{0,n-1},\alpha_{1,n-1})\cdots B(\alpha_{01},\alpha_{11})$$

$$\times\sum_{r_{n1}}\sum_{r_{n-1,1},r_{n-1,2}}\cdots\sum_{r_{21},r_{22},\cdots r_{2,n-1}}\frac{(\alpha_{0n},\delta_n^{(n)})(\alpha_{0,n-1},\delta_{n-1}^{(n)})\cdots(\alpha_{01},\delta_1^{(n)})}{(\alpha_{0n}+\alpha_{1n},\delta_n^{(n)})(\alpha_{0,n-1}+\alpha_{1,n-1},\delta_{n-1}^{(n)})\cdots(\alpha_{01}+\alpha_{11},\delta_1^{(n)})}$$

$$\times\frac{(-\alpha_{n1},r_{n1})\cdot(-\alpha_{n-1,1},r_{n-1,1})(-\alpha_{n-1,2},r_{n-1,2})\cdots(-\alpha_{21},r_{21})(-\alpha_{22},r_{22})\cdots(-\alpha_{2,n-1},r_{2,n-1})}{(1,r_{n1})\cdot(1,r_{n-1,1})(1,r_{n-1,2})\cdots(1,r_{21})(1,r_{22})\cdots(1,r_{2,n-1})}$$

$$\times w_{0n}{}^{r_{n1}}w_{0,n-1}{}^{r_{n-1,1}}w_{1n}{}^{r_{n-1,2}}\cdots w_{02}{}^{r_{21}}w_{13}{}^{r_{22}}\cdots w_{n-1,n}{}^{r_{2,n-1}}, \quad (10)$$

$V_n$ is readily recognized to correspond to a generalization of the Gauss' hypergeometric function to a function of variables $w_{02},\ldots,w_{0n};w_{13},\ldots,w_{1n};\ldots;w_{n-2,n}$ whose number totals $n(n-1)/2$. We observe that the above result for $V_n$ which is renamed here as

$$G_n(\alpha_{01},\ldots,\alpha_{0n}|\alpha_{21},\ldots,\alpha_{2,n-1};\alpha_{31},\ldots,\alpha_{3,n-2};\ldots;$$
$$\alpha_{n1}|\alpha_{01}+\alpha_{11},\ldots,\alpha_{0n}+\alpha_{1n}\|w_{02},\ldots,w_{0n};$$
$$w_{13},\ldots,w_{1n};\ldots;w_{n-2,n}),$$

possesses a structure whose expansion coefficients are similar to but are more complex than those of Lauricella functions $F_A,F_B,F_C$ and $F_D$. That is, the coefficients are of type which is closer to

$$(\alpha,m+n+p)(\beta,m+n)(\beta',p)$$
$$\times[(\gamma,m)(\gamma',n)(\gamma'',p)(1,m)(1,n)(1,p)]^{-1}$$

mentioned on p. 115 of Ref. 2 than those for Lauricella functions. One could possibly regard $G_n$ as a generalization of $F_D(\alpha;\beta_1,\ldots,\beta_n;\gamma;x_1,\ldots,x_n)$ to a function with $n$ of $\alpha$'s (i.e., $\alpha_{0i}, i=1,2,\ldots n$), $n(n-1)/2$ of $\beta$'s (i.e., $\alpha_{21},\ldots,\alpha_{2n-1};\alpha_{31},\ldots,\alpha_{3,n-2};\ldots;\alpha_{n1}$), $n$ of $\gamma$'s (i.e., $\alpha_{0i}+\alpha_{1i}, i=1,2,\ldots,n$) and $n(n-1)/2$ of variables (i.e., $w_{02},\ldots,w_{0n};w_{13},\ldots,w_{1n};\ldots;w_{n-2,n}$).

It is of some interest to note that $V_n$ can also be represented as a linear combination of ${}_{n+1}F_n[w_{0n}]$ with varying parameters. To see this, let us use the relation expressed by the latter half of Eq. (8) to rewrite the final expression for $V_n$ which is obtainable from Eq. (5) in the manner prescribed earlier.

By so doing, we have

$$V_n=\prod_{s=1}^{n}\Big\{\prod_{t=0}^{n-s-1}\Big[\sum_{r_{t+2,n-s-t}}\frac{(-\alpha_{t+2,n-s-t},\gamma_{t+2,n-s-t})}{(1,\gamma_{t+2,n-s-t})}$$
$$\times(w_{n-s-t,n-s+1})^{\gamma_{t+2,n-s-t}}\Big]$$
$$\times B(\alpha_{0,n-s+1}+\delta_{n-s+1}^{(n)},\alpha_{1,n-s+1})\Big\}, \quad (11)$$

where we take $\prod_{t=0}^{n-s-1}[\cdots]=1$ for $s=n$. If we single out $r_{n1}$ and write

$$\delta_j^{(n)}=r_{n1}+\epsilon_j^{(n)}, \quad (12)$$

we obtain

$$B(\alpha_{0j}+\delta_j^{(n)},\alpha_{1j})=\{(\alpha_{0j}+\epsilon_j^{(n)},r_{n1})$$
$$\times[(\alpha_{0j}+\alpha_{1j}+\epsilon_j^{(n)},r_{n1})]^{-1}\}B(\alpha_{0j}+\epsilon_j^{(n)},\alpha_{1j}). \quad (13)$$

Then the sum of all terms that contain $r_{n1}$, namely, the product for $j=1,2,\ldots,n$ of the first factor on the right-hand side of Eq. (13) and the factor $(-\alpha_{n1},r_{n1})(w_{01})^{r_{n1}}/(1,r_{n1})$ that represents the $t=n-2$ contribution of the $s=1$ part of Eq. (11), add up to form an ${}_{n+1}F_n[w_{0n}]$. Thus we obtain

$$V_n=\prod_{s=1}^{n}\Big\{\prod_{k=0}^{n-s-1}{}'\Big[\sum_{r_{t+2,n-s-t}}\frac{(-\alpha_{t+2,n-s-t},\gamma_{t+2,n-s-t})}{(1,\gamma_{t+2,n-s-t})}$$
$$\times(w_{n-s-t-1,n-s+1})^{\gamma_{t+2,n-s-t}}$$

$$\times B(\alpha_{0,n-s+1}+\epsilon_{n-s+1}^{(n)},\alpha_{1,n-s+1})$$

$$\times {}_{n+1}F_n\left[\begin{matrix}\alpha_{01}+\epsilon_1^{(n)},\ldots,\alpha_{0n}+\epsilon_n^{(n)},-\alpha_{n1};w_{0n}\\ \alpha_{01}+\alpha_{11}+\epsilon_1^{(n)},\ldots,\alpha_{0n}+\alpha_{1n}+\epsilon_n^{(n)}\end{matrix}\right], \tag{14}$$

where it is understood that the beta function alone be retained for $n=1$ and the prime on the product symbol for $t$ indicates that the contribution from $t=n-s-1$ for $s=1$ (i.e., $t=n-2$) is to be deleted.

Returning to the determination of $\epsilon_j^{(n)}$ for $n=2,3,\cdots$ [the case of $n=1$ is of no interest since we have $\delta_j^{(n)}=0$ for $n=j=1$ from Eq. (7)], we find from Eq. (7) that

$$\epsilon_j^{(n)}=\begin{cases}\beta_{j,j-1}+\gamma_j^{n-1,n-1-j}+\sum_{k=n-j+1}^{n-1}\gamma_{k,n-k+1}, & \\ \qquad\text{for } j=1,2,\ldots,n-1\\ \sum_{k=2}^{n-1}\gamma_{k,n-k+1}, & \text{for } j=n.\end{cases} \tag{15}$$

We may point out that the result for $V_n$ given by Eq. (14) can also be obtained directly through stepwise integration in the direction opposite to that we adopted, that is, by using the result for $V_n$ in evaluating $V_{n+1}$ for $n=2,3,4,\cdots$. Thus, in evaluating $V_2$ we may first obtain $B(\alpha_{02},\alpha_{12})\ {}_2F_1[\alpha_{02},-\alpha_{21};\alpha_{02}+\alpha_{12};w_{02}u_1]$ by integrating it over $u_2$ and then $B(\alpha_{02},\alpha_{12})B(\alpha_{01},\alpha_{11}){}_3F_2[\alpha_{01},\alpha_{02},-\alpha_{21};\alpha_{01}+\alpha_{11},\alpha_{02}+\alpha_{12};w_{02}]$ by integrating over $u_1$ with the help of the well-known formula on the integration of ${}_pF_q$.[6] Proceeding to $V_3$ we may integrate first over $u_2$ and $u_3$ by expanding the factors $(1-w_{02}u_1u_2)^{\alpha_{21}}$ and $(1-w_{13}u_2u_3)^{\alpha_{22}}$. That part of the integration becomes a superposition of integrals which are of the same form as for $V_2$, i.e., ${}_3F_2[w_{03}u_1]$. The remaining integration over $u_1$ gives rise to a ${}_4F_3[w_{03}]$ again by the formula mentioned above. In this manner it is clear that an expression for $V_n$ as given by Eq. (14) can be found by this procedure.

## 3. REMARKS

In what follows we will give some remarks that have to do with the generalized Veneziano amplitudes of various orders.

(1) As was mentioned in the beginning the $(n+3)$-point function is given as the value for $w_{ij}=1$ of the hypergeometric expressions for $V_n$, namely, Eq. (10) or Eq. (14).

(2) The function $F^{(n)}(a_i,b_i,c_{ij};w_{ij})$ which derives from Eq. (1) by taking $w_{0i}=1$ for $i=1,2,\ldots,n$ does not directly lend itself to the method of integration used in the above. This is because the method presupposes integrals of the type that appears in Eq. (2) which corresponds to taking $w_{i-1,i}=1$, rather than $w_{0i}=1$, in Eq. (1). Nonetheless, we can indirectly apply the method to $F^{(n)}$ by expanding $(1-w_{i-1,i}u_i)^{\alpha_{1i}-1}$ and considering, with $w_{0i}=1$, $\sum[(-\alpha_{1i}+1,r_{1i})(w_{i-1,i})^{r_{1i}}/(1,r_{1i})]u_i^{\alpha_{0i}+r_{1i}-1}(1-u_i)^{\gamma-1}$ in place of $u_i^{\alpha_{0i}-1}(1-u_i)^{\alpha_{1i}-1}$ in Eq. (2).

(3) In spite of the fact that the four- and five-point functions are representable as a single term ${}_2F_1[1]$ and ${}_3F_2[1]$ series, respectively, it is clear from Eq. (14) that such a property is no longer available for $(n+3)$-point functions with $n\geq 3$. That is, except for $n=1$ and 2 for which $\delta_j^{(n)}=0$ and $\epsilon_j^{(n)}=0$, respectively, hold, an $(n+3)$-point function is represented generally by a linear combination of an infinite number of ${}_{n+1}F_n[1]$ series with varying parameters.

(4) Here we point out the relationship that exists between the Appell's or Lauricella's functions and the $F^{(n)}$ function of Ref. 1 [and hence the $(n+3)$-point function when $w_{ij}=1$].

First, we note that there exists an integral representation for the Appell's $F_3(\alpha,\alpha';\beta,\beta';\gamma;x,y)$ function given in terms of a ${}_2F_1$ function.[7] With the choice of $x=1$ and $y=w_{12}$ the $F_3$ becomes expressible in terms of a ${}_3F_2[w_{12}]$ [or an $F^{(2)}(w_{12})$], which implies that the five-point function may be given as an appropriate $F_3(..;..;..;1,1)$.

Next, if we take $x=-1$ and $y=w_{12}$ in the double integral representation for[8] $F_2(\alpha;\beta,\beta';\gamma,\gamma';x,y)$ and expand the factor $(1+\xi)^{-\alpha}$ in the integrand by writing $\xi=u-w_{12}v$, we obtain an expression that gives the $F_2(..;..;..;-1,w_{12})$ as a linear combination of $F^{(2)}(..;w_{12})$. It follows from this that $F_2(..;..;..;-1,1)$ is expressible as a superposition of five-point functions. Conversely, if we expand the factor $\xi^{c_{12}}=[1-(1-\xi)]^{c_{12}}$ that appears in the integral representation for $F^{(2)}(a_i,b_i,c_{12};w_{12})$ (for integration variables $u$ and $v$) in powers of $1-\xi=1-(u-w_{12}v)$ and further choose $w_{12}=1$, we see that a five-point function can be given as a superposition of $F_2(..;..;..;1,-1)$.

Finally, in the $n$-fold integral representation for the Lauricella function[9] $F_A(\alpha;\beta_1,\ldots,\beta_n:\gamma_1,\ldots,\gamma_n;x_1,\ldots,x_n)$ we may write the expression $1-\sum u_ix_i$ as

$$1-\sum_{i=1}^{n}u_ix_i=1-\sum_{i<j}(u_i-w_{ij}u_j)\equiv 1-\sum_{i=1}^{m}y_i.$$

Here we set

$$x_i=(n-i)-\sum_{k=1}^{i-1}w_{ki}\qquad\text{for } i=1,2,\ldots,n$$

(with $\sum_{k=1}^{i-1}w_{ki}=0$ for $i=1$) and labeled $y_i$ such that

$$y_1=u_1-w_{12}u_2,\cdots,\quad y_{n-1}=u_1-w_{1n}u_n,$$

$$y_n=u_2-w_{23}u_3,\cdots,\quad y_m=u_{n-1}-w_{n-1,n}u_n,$$

where $m=n(n-1)/2$. If we recall the multinomial expansion

$$\left(1-\sum_{i=1}^{m}y_i\right)^{-\alpha}=\sum\frac{(\alpha,r_1+r_2+\cdots+r_m)}{(1,r_1)\cdots(1,r_m)}y_1^{r_1}\cdots y_m^{r_m}$$

[which may also be written as $F_A(\alpha;\kappa_1,\kappa_2,..,\kappa_m;\kappa_1,\kappa_2,..,\kappa_m;y_1,y_2,\ldots,y_m)$], the $F_A$ under consideration is expressed as a linear combination of $F^{(n)}(..,..,r_1,..,r_m;w_{ij})$. By taking $w_{ij}=1$ it follows that $F_A(..;..;..;n-1,n-3,\ldots,-(n-3),-(n-1))$ can be given as a superposition of $F^{(n)}(..,\ldots,r_1,..,r_m;w_{ij}=1)$ or $(n+3)$-point functions.

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[1] A. C. T. Wu, J. Math. Phys. 12, 2035 (1971). For earlier works see the references contained therein.

[2] P. Appell and J. Kampé de Fériet, *Fonctions hypergéométriques et hypersphériques—polynomes d'Hermite* (Gauthier-Villars, Paris, 1926).

[3] K. Bardakci and H. Ruegg, Phys. Rev. 181, 1884 (1969).

[4] In Eq. (2) and similar expressions that follow the summation indexes $r_{st}$ and their limits 0 and $\infty$ are often left out. The validity of Eq. (2) may be seen by applying the binomial theorem to the terms with $k = 2, 3, \ldots, i$ on the left-hand side. See also Eq. (4), p. 114, and Eq. (8), p. 116, of Ref. 2.

[5] The product notation $\Pi[\sum \cdots]$ for the summation symbol is used for the sole benefit of the operational convenience.

[6] See, for example, Y. L. Luke, *The Special Functions and Their Approximations* (Academic, New York, 1969), Vol. 1, Eq. (10), p. 58.

[7] Equation (11), p. 35, Ref. 2.

[8] Equation (2), p. 28, Ref. 2.

[9] Equation (5), p. 115, Ref. 2.

# Is the Maxwell Field Local?*

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Is the classical Maxwell field truly local? This question is raised by several observations, among them the Aharonov–Bohm effect; but the question cannot be answered without a systematic definition and characterization of local subalgebras of observables. This paper reformulates classical field theory in analogy to axiomatic quantum field theory and introduces a precise statement for local independence. (Synonyms for local independence are Einstein causality and principle of maximum signal velocity.) The formal answer of the analysis is: The free Maxwell field does *not* have local independence. This conclusion is critically discussed.

## 1. INTRODUCTION

It is distressing to see a field act where it isn't, as in the Aharonov–Bohm effect.[1,2] Such an experience necessarily brings up the question: Is the Maxwell field local? And this question inevitably evokes the counterquestion: What does locality mean?[3,4] Because of the unsatisfactory state of quantum electrodynamics, and of the absence of a precise definition of locality in classical field theory and in particle quantum mechanics, the debate on these questions has necessarily been characterized by a certain vagueness both of the physical interpretation and of the structure of the mathematical theory. But the key to the riddle may be in the more elementary theory of the free Maxwell field—quantized or even classical—and these theories are simple enough to be discussed rigorously.

Is even the free Maxwell field local? This question is not frivolous. The constraint $\mathrm{div}\mathbf{B} = 0$ implies that the magnetic flux through one hemisphere determines the flux through the other, simultaneously in some reference frame. This may be taken as a violation of locality, because the state in some space–time region causes a constraint on the state in another spacelike region. Clearly, a more precise definition of the concepts is called for, and we have attempted to give a clear answer—at least for the classical free Maxwell field. This turns out to be a nontrivial task. Fortunately, a mathematically and interpretatively satisfactory formulation of local independence for classical physics is now available.[5] (Synonyms for local independence are Einstein causality and maximum signal velocity.) While the concomitant concepts of the algebra of observables and its local subalgebras have been defined and discussed for quantum field theory,[6–8] we had to do this long-overdue job for classical field theory. Fortunately, the well-known difficulty of integrating and differentiating in function space has not been an obstacle for our purpose. While the mathematical problem turns out to be simpler than anticipated, we have not been able to give a conclusive answer to the physical question.

The main point of physical interpretation that distinguishes the present paper from the large literature on the subject concerns the precise definition of locality or, more felicitously, local independence. While quantum field theory has always had—or has claimed to have—a precise theoretical expression for locality through the commutativity of local operators at spacelike points, the concept of locality in particle quantum theory and in classical field theory has remained imprecise ("informal" in Bohm's language[2]) until recently.

Of course, special consequences of local independence are known in classical field theory. In particular, for linear partial differential equations the Green's function must vanish outside the light cone. This condition, however, is not sufficient; although the vector potential $A_\mu$ has this property, it is reputed to be nonlocal.

## 2. POSTULATES COMMON TO CLASSICAL AND QUANTUM THEORIES

In order to study the consequences of the postulate of local independence for classical and quantum theories, it is desirable first to state the postulate in an operational manner without theoretical prejudices and then to combine it with the theoretical postulates of the two theories. For this purpose, classical theory is formulated so that it shares the general conceptual and mathematical framework that is customary for quantum theory.

Classical physics is then obtained as a special case rather than as a limit of a sequence of quantum theories. This approach is suggested by two previous developments. The first, by one of the present authors, is a reformulation of quantum mechanics[9] in which the algebra of observables appears as an algebra of functions—commutative for the classical theory and noncommutative for the quantum theory. The other is Prosser's unified theory of nonrelativistic particles.[10]

We assume a topological algebra $\mathfrak{A}$ of observables, some of whose members (forming, one hopes, a generating set) are images of well-specified nonmathematical entities, namely, observation procedures that are defined operationally. $\mathfrak{A}$ is either a real algebra or a complex *-algebra. Mean values of many observations (expectation values) are obtained by letting an object prepared by a state-preparing procedure interact with an observation apparatus. The map from $\mathfrak{A}$ to the set of expectation values obtained by a state-preparing procedure (a state) is assumed to be a linear, continuous, positive,[11] and normalized form on $\mathfrak{A}$. It is assumed that states

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separate the algebra $\mathfrak{A}$ so that the condition $\omega(A) = 0$ for all states $\omega$ implies $A = 0$.

Some observation procedures are localized within a space–time region $R$. This does not necessarily mean that the physical apparatus is confined to $R$, but that the procedure is so contrived that its result is independent of events outside $R$. Images of these local sets of procedures are, by assumption, local algebras $\mathfrak{A}(R)$. Common sense dictates the additivity postulate

$$\overline{\mathfrak{A}(R_1) \cup \mathfrak{A}(R_2)} = \mathfrak{A}(R_1 \cup R_2), \tag{2.1}$$

where $\overline{\mathcal{S}}$ denotes the closure (in the topology defined in Sec. 3) of the polynomial algebra generated by any set $\mathcal{S}$ of elements: We say that $\overline{\mathcal{S}}$ is the algebra topologically generated by $\mathcal{S}$. In words, Eq. (2.1) says that the algebra topologically generated by the union of two subalgebras associated to two regions is the algebra associated to the union of the two regions. It is also assumed that the union of all local algebras $\mathfrak{A}(R)$ generates topologically the total algebra, i.e.,

$$\overline{\bigcup_R \mathfrak{A}(R)} = \mathfrak{A}. \tag{2.2}$$

To avoid vagueness in the physical interpretation, Eqs. (2.1) and (2.2) must be understood not as stating the existence of a certain algebraic structure of $\mathfrak{A}$, but as statements concerning the map from nonmathematical procedures into the algebra $\mathfrak{A}$.

*Causality*[6] (sometimes called primitive causality) means that the present determines the future. Consider a local algebra $\mathfrak{A}(R_{s\tau})$, where $R_{s\tau}$ is a segment of thickness $\tau$ between two parallel spacelike hyperplanes $s$. Causality requires that this algebra should be equal to $\mathfrak{A}$, so that the expectation value "later" is known if all expectation values "now" are known. The statement is rather weak if it asserts merely the existence of such segments with a finite $\tau$. It seems reasonable to strengthen it by requiring that

$$\mathfrak{A}(R_s) = \mathfrak{A}, \tag{2.3}$$

where $R_s$ is any spacelike hyperplane.

In quantum field theory, causal independence of spacelike events (i.e., the existence of a finite signal velocity or of Einstein causality) is often considered to be expressed by the commutativity of relatively spacelike local subalgebras. For the present construction, this association is useless, because the algebras $\mathfrak{A}$ of observables are Abelian in classical physics. A more general and directly operational formulation is local independence.[12] Let any $\omega_1, \omega_2$ be two states and $\mathfrak{A}_r$, $\mathfrak{A}_s$ two local algebras associated to regions $R_r, R_s$ that are relatively spacelike. Then, there exists a state $\omega_3$ such that

$$\omega_1 | \mathfrak{A}_r = \omega_3 | \mathfrak{A}_r \quad \text{and} \quad \omega_2 | \mathfrak{A}_s = \omega_3 | \mathfrak{A}_s. \tag{2.4}$$

That is, any two partial states on spacelike subalgebras have a common extension.

In this definition, "state" (short for "normal state") means a certain subset of the linear, continuous, positive, and normalized forms on the algebra $\mathfrak{A}$ of observables. It is necessary to make this restriction to normal states also in quantum theory because some states have little physical meaning.[5] The precise definition of normal states for classical fields will be given in Sec. 5.

## 3. ABELIAN ALGEBRAS OF OBSERVABLES FOR CLASSICAL FIELDS

The irreducible representations of Abelian topological algebras are isomorphic to the complex numbers.[13] Therefore, classical physics differs from quantum theory in that the irreducible representations, which are of prime importance in quantum theory, are trivial.

The algebra of observables for classical fields will be constructed by analogy with the observables of an $n$-particle system.[10] The observation procedures corresponding to the initial positions and momenta $\{q_1, p_1, \ldots, q_n, p_n\}$ are operationally well defined. They correspond to unbounded functions on phase space. The piecewise continuous functions of these basic functions may be chosen as the algebra of observables. Their physical interpretation by procedures is obvious.

The main feature of this construction is the existence of a set of observables that are images of operationally defined procedures at one instant $t$ such that: (A) the set generates the algebra of observables, and (B) the members of the set are algebraically independent. We want field theory to share this feature to the largest possible extent.

The phenomena that are the subjects of classical field theories, such as acoustics and heat conduction, have—or are idealized as having—certain common features which determine the algebra of observables and its physical interpretation, particularly its local subalgebras. The instant observation of the pressure or the temperature at a point is, of course, an idealization; but there is no reason to believe that it is not adequate within the conceptual framework of classical physics. Fields $\varphi_i(x)$ at a point $x$ and at an instant $t = 0$ are exemplified by temperature, pressure, or electric field components at points $x$ of Euclidean 3-space. Let $\Omega$ be a topological space of real vector-valued functions $\{\psi_i(x)\}$ on Euclidean 3-space $R^3$. A class $G$ of functionals

$$F_{i,x}(\psi) = \psi_i(x) \tag{3.1}$$

will be considered as the images of the corresponding procedures $\varphi_i(x)$. Continuous functions of a finite number $n$ of such functionals $F_{i,x_1}, \ldots, F_{i,x_n}$ have an obvious operational interpretation, and they will be considered as elements of the algebra $\mathfrak{A}$ of observables. More general functionals of the $\varphi_i(x)$, such as

$$\int G_1[\varphi_1(x_1)] G_2[\varphi_2(x_2)] \cdots G_n[\varphi_n(x_n)] \times f(x_1, x_2, \ldots, x_n) dx_1\, dx_2 \cdots dx_n,$$

where $f$ is an integrable function in $R^{3n}$ and the $G_i(y)$ are bounded and continuous, have images

$$F(\psi) = \int G_1[\psi_1(x_i)] G_2[\psi_2(x_2)] \cdots G_n[\psi_n(x_n)] \times f(x_1, x_2, \ldots, x_n) dx_1 dx_2 \cdots dx_n \tag{3.2}$$

which are also elements of $\mathfrak{A}$. More generally, we assume that the set of continuous functionals $F$ that are images of procedures at the instant $t = 0$ is sufficiently large so that its closure is the algebra $C(\Omega)$

of all continuous functionals on $\Omega$. In this somewhat restricted sense we conform to the commonly held view that classical physics has a self-evident physical interpretation.

For mathematical precision, we will make a number of assumptions which are justified more by convenience than by physical necessity.

(1) $\Omega$ is a topological vector space. The points $\psi \in \Omega$ are real vector-valued functions on $R^3$, piecewise differentiable and bounded, equipped with the norm

$$\|\psi\| = \sup_{x \in R^3} \left(\sum_i |\psi_i(x)|^2\right)^{1/2}.$$

The space $\Omega$ does not necessarily include all functions of this class, and no closure is required.

(2) The algebra of observables is the algebra $C(\Omega)$ of all real continuous functionals $F$ on $\Omega$ and is equipped with the $c$-topology.[14] In this topology, a subbasis is constituted by the sets of functions

$$(A, B) \equiv \{F \in C(\Omega) \,|\, F(A) \subset B, (A \subset \Omega) \text{ is compact}, (B \subset R^1) \text{ is open}\}. \quad (3.3)$$

That is, if a function $F \in C(\Omega)$ restricted to a compact subset $A \in \Omega$ has values in the open subset $B$ of the real line, then all functions $F'$ "near" it are required to satisfy the same condition. This definition seems strange at first; but since $\Omega$ is a metric space, sequential convergence is precisely the classical uniform convergence of functions on any compact subset.[15]

The class of functions $\psi \in \Omega$ must be inferred from the empirical properties of the observation and state-preparing procedures that are the domain of the particular field theory.

These properties restrict the algebra; but since the algebra was generally defined in terms of functions on the carrier space $\Omega$, the empirical properties restrict $\Omega$. Again, since $\Omega$ was generally defined as a linear space of piecewise differentiable bounded vector-valued functions, these properties restrict the number of vector components and impose constraints on the functions.

Since, by assumption, $C(\Omega)$ includes all continuous functions, the elements of $G$ defined by Eq. (3.1) are algebraically independent. Hence, $G$ includes the images of those point observation procedures that are not subject to any constraints. In the case of heat conduction, the choice $G = \{F_x\}$ with

$$F_x(\psi) \equiv \theta(x) = \psi(x)$$

is indicated, because the time derivatives of the temperature field $\theta(x, t)$ at $t = 0$ are, by the equations of motion, determined by the set $\{F_x\}$. On the other hand, no restriction on the initial temperature $\theta(x)$ is known, so that $\Omega$ must include all piecewise differentiable scalar functions. For a pressure field $p(x)$, this choice would be inadequate. Observation procedures measuring the time derivatives $\dot{p}(x, 0)$ are algebraically independent of the $\{p(x, 0)\}$, because there exists no function $F$ of elements $p(x_i, 0)$ and of $\dot{p}(x_j, 0)$ such that $\omega(F) = 0$ for all states $\omega$. Indeed, by virtue of the assumed separation of $\mathfrak{A}$ by states, this means that no such function $F[p(x_1), \ldots, p(x_n), \dot{p}(x_m), \ldots, \dot{p}(x_N)] = 0$ exists, and hence the elements $\{\dot{p}(x, 0)\}$ are algebraically independent of $\{p(x, 0)\}$.

Hence, the proper choice for $\Omega$ will be the space of all piecewise differentiable two-component vector functions $\psi$, where $\psi_1$ corresponds to the pressure and $\psi_2$ to its time derivative. That is,

$$\begin{aligned} p(x, 0) &\mapsto F_{1,x}(\psi) = \psi_1(x), \\ \dot{p}(x, 0) &\mapsto F_{2,x}(\psi) = \psi_2(x). \end{aligned} \quad (3.4)$$

For the electromagnetic field, there are six vector components of $\psi_i(x)$, namely $E_i(x)$ and $B_i(x)$. Here, however, algebraic independence of the set $G$ forbids the choice of *all* piecewise differentiable bounded functions. In virtue of the assumed separation of $\mathfrak{A}$ by states, such a choice would imply the existence of a state in which

$$\int_S \sum_{i=4}^{6} F_{i,x}(\psi) n_i \, ds,$$

i.e., the image of the observation procedure $\int_S B_n ds$ (where $S$ is a closed surface), has a nonvanishing expectation value. The functions $\psi$ must be subjected to the constraints

$$\sum_{i=1}^{3} \frac{\partial}{\partial x_i} \psi_i = 0, \qquad \sum_{i=4}^{6} \frac{\partial}{\partial x_{i-3}} \psi_i = 0,$$

so that the predictions of the theory will exclude the existence of a state such that the expectation value of the magnetic or electric flux through a closed surface is nonvanishing. The linearity of the constraint makes it compatible with the linearity of the space $\Omega$.

It is not clear whether the set $G$ generates topologically the algebra $C(\Omega)$, as in particle theory. No theorems sufficiently powerful for a proof are known to us.

## 4. LOCAL SUBALGEBRAS ON SPACELIKE HYPERPLANES

Consider a region $R$ of space–time consisting of $n$ simultaneous points $R = \{x_1, \ldots, x_n\}$. The corresponding local subalgebra $\mathfrak{A}(R)$ contains the algebra generated by the images of the point observation procedures $\varphi_i(x_1), \ldots, \varphi_i(x_n)$, i.e., by the functionals $F_{i,x_j}(\psi) = \psi_i(x_j)$. Thus, $\mathfrak{A}(R)$ contains all continuous functions $G$ of the functionals $F_{i,x_j}$ with $x_j \in R$. To generalize this construction to a space-volume $R = V_0$ at the instant $t = 0$, it is necessary to postulate rather than to deduce.

We wish to express mathematically the fact that the observation procedures corresponding to $\mathfrak{A}(V_0)$ "see" only the events in $V_0$ or that they are "blind" toward things outside $V_0$. Consider the set of functionals

$$\mathfrak{A}_c(V_0) = \{F \,|\, F(\psi) = F(\chi_{V_0}\psi)\}, \quad (4.1)$$

where $\chi_{V_0}$ is the characteristic function of $V_0$. An element $F_g \in \mathfrak{A}_c(V_0)$ is constant on all functions $\psi$ that agree with a given function $g$ in $V_0$. Clearly, the set $\mathfrak{A}_c(V_0)$ is a subalgebra of $\mathfrak{A}$ if all functionals $F$ in (4.1) are in $\mathfrak{A}$. This subalgebra does just what the intuitive definition requires: It assigns values to functions only on the basis of their behavior in $V_0$. Hence we postulate

$$\mathfrak{A}_c(V_0) \subset \mathfrak{A}(V_0). \quad (4.2)$$

In general, $\mathfrak{A}_c(V_0)$ does not contain the time derivatives of the observables $F_{i,xj}$ at the instant $t = 0$ and cannot be considered as the local instant subalgebra $\mathfrak{A}(V_0)$. However, in all realistic field theories—such as the theories of heat conduction, acoustics, and *a fortiori* in relativistic theories—these time derivatives are in fact functions of the observables $F_{i,x_j}$ and of their space derivatives at $t = 0$. This "action at short distances" in field theories is not a necessary feature of nonrelativistic theories; for instance, integrodifferential equations are possible alternatives. In the following, we shall restrict ourselves to theories in which Eq. (4.2) can be replaced by the action-at-a-short-distance formula

$$\mathfrak{A}_c(V_0) = \mathfrak{A}(V_0). \tag{4.3}$$

We have to show consistency between the assumed form of instant local algebras given by Eqs. (4.1) and (4.3) on the one hand and the additivity and completeness properties expressed by Eqs. (2.1) and (2.2) on the other. The proof of Eq. (2.2) is trivial, since $\chi_V$ tends to the unit as $V$ becomes large. The proof of Eq. (2.1) is somewhat technical and has been relegated to Appendix A.

To define local algebras in general space–time regions $R$, we must consider the dynamics of the theory. The dynamics of the physical system is associated to a group $T(t)$ of automorphisms of the algebra $C(\Omega)$ which is in turn induced by homeomorphisms $\tau(t)$: $\psi(x) \mapsto \psi(x, t)$ of $\Omega$ through $[T(t)F](\psi) = F[\tau(t)\psi]$. Traditionally, this transformation results from the solution of a partial differential equation with $\psi(x)$ as initial condition, but this is not the most general case. The local instant algebra $\mathfrak{A}(V, t)$ for the space-volume $V$ at the instant $t$ contains the functionals with the property

$$[T(t)F](\psi) = F[\chi_V \tau(t)\psi].$$

A space–time region $R$ can be obtained by the union

$$R = \cup_{t_i} V(t_i)$$

of instant space volumes, and the algebra $\mathfrak{A}(R)$ is defined by the topological closure

$$\mathfrak{A}(R) = \overline{\cup_{t_i} \mathfrak{A}[V(t_i)]}.$$

Since no use is made of these more general local algebras, they will not be further discussed.

## 5. INSTANT LOCAL INDEPENDENCE WITHOUT CONSTRAINTS

We will prove instant local independence in the absence of constraints, i.e., causal independence of local subalgebras associated with nonintersecting volumes of a spacelike hypersurface for situations in which the carrier space $\Omega$ contains *all* piecewise differentiable bounded functions $\psi_i(x)$, with $i = 1, \ldots, n$.

Intuitively, normal states are those that can be produced by adding fields to the vacuum. We define an accrual operator $T_\varphi$ on the observables by

$$(T_\varphi F)(\psi) = F(\varphi + \psi). \tag{5.1}$$

Loosely speaking, this operator increases the existing field by the field $\varphi$. Let $S_0$ be the vacuum state defined by

$$S_0(F) = F(0), \tag{5.2}$$

where 0 is an element of $\Omega$. Then, a class of states defined by

$$S(F) = \sum \lambda_i S_0(T_{\varphi_i} F), \quad \lambda_i \geq 0, \ \sum \lambda_i = 1 \tag{5.3}$$

may be called normal because it is the class of states produced by accrual from the vacuum. In the same way, normal states which are only a "little" different from the vacuum are implemented in Fock space by density operators.

Consider the two normal states of a special class

$$S_\psi(F) = F(\psi), \quad S_\varphi(F) = F(\varphi). \tag{5.4}$$

On the local subalgebras $\mathfrak{A}(V_1)$ and $\mathfrak{A}(V_2)$, respectively, the states are

$$S_\psi(F_1) = F_1(\psi) = F_1(\chi_{V_1}\psi) \quad \text{and} \quad S_\varphi(F_2) = F_2(\chi_{V_2}\varphi), \tag{5.5}$$

where $F_i \in \mathfrak{A}(V_i)$. If there are no constraints, there exists a third function $\eta \in \Omega$ such that for two disjoint volumes $V_1, V_2$, one has

$$\eta(x) = \psi(x), \quad x \in V_1, \tag{5.6a}$$

and

$$\eta(x) = \varphi(x), \quad x \in V_2. \tag{5.6b}$$

Then, if $F_i \in \mathfrak{A}(V_i)$ with $i = 1, 2$,

$$\begin{aligned} S_\psi(F_1) = F_1(\psi) = F_1(\chi_{V_1}\psi) = F_1(\chi_{V_1}\eta) \\ = F_1(\eta) = S_\eta(F_1) \end{aligned} \tag{5.7}$$

and

$$\begin{aligned} S_\varphi(F_2) = F_2(\varphi) = F_2(\chi_{V_2}\varphi) = F_2(\chi_{V_2}\eta) \\ = F_2(\eta) = S_\eta(F_2). \end{aligned} \tag{5.8}$$

Hence, the state $S_\eta$ is a common extension of the two states $S_\varphi$ and $S_\psi$.

Consider now two states $S_i$ over $\mathfrak{A}(V_i)$, $i = 1, 2$, defined by convex linear combinations of states of the class (5.4), namely

$$\begin{aligned} S_1 &= \sum_k \lambda_k S_{\psi_k}, \quad 0 \leq \lambda_k \leq 1, \ \sum_k \lambda_k = 1, \\ S_2 &= \sum_m \delta_m S_{\varphi_m}, \quad 0 \leq \delta_m \leq 1, \ \sum_m \delta_m = 1. \end{aligned} \tag{5.9}$$

Again, if there are no constraints, there exists a set of functions $\{\eta_{km}\}$ such that

$$\eta_{km}(x) = \begin{cases} \psi_k(x) & x \in V_1, \\ \varphi_m(x) & x \in V_2, \end{cases} \tag{5.10}$$

and therefore the state

$$S_3 = \sum_{m,k} \delta_m \lambda_k S_{\eta_{km}} \tag{5.11}$$

is the common extension of $S_1$ and $S_2$. Indeed, let $F_1 \in \mathfrak{A}(V_1)$. Then we have

$$\begin{aligned} S_3(F_1) &= \sum_{m,k} \delta_m \lambda_k S_{\eta_{k,m}}(F_1) \\ &= \sum_{m,k} \delta_m \lambda_k F_1(\eta_{km}) \\ &= \sum_m \delta_m \sum_k \lambda_k F_1(\psi_k) = S_1(F_1), \end{aligned} \tag{5.12}$$

and similarly for $F_2 \in \mathfrak{A}(V_2)$. Thus we have shown the existence of a common extension for all normal states and, therefore, instant local independence for action-at-a-short-distance field theories without constraints.

It can be shown that all states of the type (5.4) are pure, but that not all pure states belong to this class.

## 6. CONSTRAINTS OF THE MAXWELL FIELD

Consider two contiguous space volumes $V_1$ and $V_2$, e.g., two open hemispheres separated by an equatorial plane. For the Maxwell field, the vector-valued functions $\psi_i$ are the electric and magnetic field intensities. A possible state $S_\psi$ of the type (5.3) is labeled by a constant magnetic field **B** parallel to the $z$ direction in a region including the hemisphere $V_1$, and another state $S_\varphi$ is labeled by a constant magnetic field—**B** extending at least through $V_2$. Since only divergenceless vector fields are points in $\Omega$, there is no common extension of the two states and, therefore, no local independence.

This result is surprising if one believes that the statement of local independence adopted here is the precise expression of Einstein's principle of limited signal velocity. (Note that for a scalar wave equation without constraints, local independence is confirmed.) We consider some possibilities for a solution of the paradox.

*1. Redefinition of the local algebras:* Consider the well-known representation of the free Maxwell field by a Fourier integral of plane waves. The coefficients $a_i(\mathbf{k})$ are linear combinations of four real functions of $\mathbf{k}$, not otherwise restricted. The Fourier transforms $a_i(x)$ of these could be considered as the basic observation procedures of which the functionals (3.1) are images. The space $\Omega$ would then consist of *all* piecewise differentiable four-component functions. Clearly, the algebra $C(\Omega)$ of functionals on this new carrier space is only another representation of the same algebra. However, if now the local subalgebra $\mathfrak{A}(V_0)$ is defined so that it contains images $F_{i,x_l}(\psi) = \psi_i(x_l)$ of the procedures $a_i(x_l)$ with $x_l \in V_0$, a different result is obtained, viz. local independence. The choice between these possibilities is not mathematical. The operational definition of the fields **E** and **B** agrees with the definition of local observation procedures, while the quantities $a_i(x)$ are complicated integrals of the fields and cannot be measured by instruments confined to a small volume.

Similar objections rule out a redefinition of local subalgebras in terms of the vector potential $A_\mu$.

*2. Incompleteness of the Maxwell theory:* We remember that a similar lack of local independence was found for a theory of a finite number of relativistic classical particles.[5] It is easy to show that such a theory cannot have the property of local independence; but it is easy to see how this defect is removed. Since the statement of local independence involves the *existence* of certain states, it suffices to remember that a theory with a finite number of particles is artificially truncated because in reality there exist states with more particles. In other words, the paradox is resolved here by pointing out that the general principle cannot reasonably be expected to apply to manifestly incomplete theories.

A similar argument could be made for the constraint $\operatorname{div}\mathbf{E} = 0$ of the Maxwell field. In a theory with charges, this constraint is canceled; but the constraint $\operatorname{div}\mathbf{B} = 0$ could be lifted only if there were magnetic monopoles. The possibility of magnetic monopoles has been discussed extensively, and there seems to be no theoretical reason to reject their existence. The present argument is probably the first to favor the postulation of magnetic charges for the sake of "saving sanity."

*3. Rejection of the proposed statement of local independence:* The difficulty is that there is no alternative proposal for a precise expression of finite signal velocity in classical physics. In quantum theory, various forms of commutativity, "strict locality," are equivalent to finite signal velocity[5]; for classical field theories no other formula has been proposed. One could, however, consider a *weak* local independence by postulating that only local algebras associated to regions with finite but arbitrarily small spacelike separation are causally independent. Then no states with discontinuous magnetic field intensities are required to exist. However, we show in Appendix B that the physical interpretation of this weakened requirement is also incompatible with the properties of the Maxwell field.

*4. Change of topology:* Some of our assumptions are more technical than physical, and one might wonder whether a subtle change in the assumed topology might not eliminate the paradox. Without claiming a decisive argument against this conjecture, we feel that thinking about alternative reasonable topologies seems unfruitful.

*5. Accept the inevitable:* Finally, it is conceivable that the nonlocal nature of the Maxwell field points toward a genuine physical feature. Consider the following possibility. The true local "elementary" field is a spin-$\frac{1}{2}$ field, and photons are "composite particles" in the sense that the spin-$\frac{1}{2}$ fields associated to a region $R$ generate the local algebra $\mathfrak{A}(R)$; but the electromagnetic fields (which we assume to be generated by the spin-$\frac{1}{2}$ fields) do not have this local property. This possibility is in general agreement with the ideas of Heisenberg,[16] and it may be supported by recent results on relativistic wave equations in external fields. From these, it seems that only a spin-$\frac{1}{2}$ field can be described in a natural manner without inconsistencies.[17,18]

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## APPENDIX A

The algebra defined by Eq. (4.1) can be described as follows. A set $s$ of constancy[19] for $\mathfrak{A}(V_0)$ is a set of points $\psi$ such that all functionals $F \in \mathfrak{A}(V_0)$ are constant on it, i.e., it is a set such that

$$[(\psi_1, \psi_2) \in s)] \Rightarrow [F(\psi_1) = F(\psi_2)] \quad \text{for} \quad F \in \mathfrak{A}(V_0). \tag{A1}$$

By (4.1) and (4.3), a set $s_f$ of constancy for $\mathfrak{A}(V_0)$ is the class of functions $\psi$ that agree with a given func-

tion $f$ in $V_0$. Then $\mathfrak{A}(V_0)$ is the algebra of all continuous functionals with sets of constancy defined by functions $f$ in the region $V_0$. An algebra $\mathfrak{A}(V_1 \cup V_2)$ associated to the region $V_1 \cup V_2$ correspondingly has sets of constancy defined by functions $g$ in $V_1 \cup V_2$. Two functions $\psi_1, \psi_2 \in \Omega$ that agree in $V_1 \cup V_2$ must agree *a fortiori* in $V_1$. Hence, a set of constancy of $\mathfrak{A}(V_1)$ is a union of sets of constancy of $\mathfrak{A}(V_1 \cup V_2)$. Hence

$$\mathfrak{A}(V_i) \subset \mathfrak{A}(V_1 \cup V_2), \quad i = 1, 2, \tag{A2a}$$

and

$$\mathfrak{A}(V_1) \cup \mathfrak{A}(V_2) \subset \mathfrak{A}(V_1 \cup V_2). \tag{A2b}$$

We show next that the polynomial algebra generated by $\mathfrak{A}(V_1) \cup \mathfrak{A}(V_2)$ is dense in $\mathfrak{A}(V_1 \cup V_2)$. Consider the many-one map $J$: $\varphi \mapsto \tilde{\varphi}$ from $\Omega$ to the space $\tilde{\Omega}$ of the constancy sets for $\mathfrak{A}(V_1 \cup V_2)$, the function $\tilde{\varphi}$ being the set of constancy to which $\varphi$ belongs.

The topology of $\tilde{\Omega}$ is defined by the norm

$$\| \tilde{\varphi} \| = \sup_{x \in V_1 \cup V_2,\ \varphi \in \tilde{\varphi}} |\varphi(x)|, \tag{A3}$$

where $\varphi$ is any function in the set $\tilde{\varphi}$.

It is easy to show that $J$ maps open sets in $\Omega$ onto open sets in $\tilde{\Omega}$. For, let $S_\epsilon$ be a sphere of radius $\epsilon$ in $\Omega$. Then $J(S_\epsilon)$ contains all sets in $\tilde{\Omega}$ with norm less than $\epsilon$. That is,

$$J(S_\epsilon) = \tilde{S}_\epsilon,$$

where $\tilde{S}_\epsilon$ is the open sphere of radius $\epsilon$ in $\tilde{\Omega}$. Furthermore, compact sets in $\Omega$ are mapped on compact sets in $\tilde{\Omega}$; and if $A_a$ runs on all compact subsets of $\Omega$, the sets $\{J(A_a)\}$ exhaust all compact subsets of $\tilde{\Omega}$.

We now define a map $K$ from $\mathfrak{A}(V_1 \cup V_2)$ onto $C(\tilde{\Omega})$, the set of *all* continuous functions $F$ on $\tilde{\Omega}$, by

$$KF = \tilde{F}, \quad \tilde{F}(\tilde{\varphi}) = F(\varphi), \tag{A4}$$

and require that the topology of $C(\tilde{\Omega})$ will be constructed by the subbasis $K[(A, B)]$, in which the sets $(A, B)$ are the subbasis for the topology of $C(\Omega)$ defined in Eq. (3.3). This inherited topology is nothing but the $c$-topology, since

$$K[(A, B)] = \{K(F) | [K(F)](A) \subset B\} = \{\tilde{F} | \tilde{F}(\tilde{A}) \subset B\}, \tag{A5}$$

where $A \subset \Omega$ is compact, $B \subset R$ is open, and from the previous discussion $\tilde{A} \subset \tilde{\Omega}$ is compact. From the definition of $K$ it follows that it is a continuous isomorphism. The gain in the last maneuver is the demonstration that although $\mathfrak{A}(V_1 \cup V_2)$ is *not* the set of *all* real continuous functions on some space, $K[\mathfrak{A}(V_1 \cup V_2)]$ is.

Since $\mathfrak{A}(V_1)$ and $\mathfrak{A}(V_2)$ are subalgebras of $\mathfrak{A}(V_1 \cup V_2)$, the map $F \mapsto \tilde{F}$ of $\mathfrak{A}(V_1 \cup V_2)$ induces injective mappings $\mathfrak{A}(V_i) \mapsto \tilde{\mathfrak{A}}(V_i)$ of $\mathfrak{A}(V_i)$ into $C(\tilde{\Omega})$. To show that the algebra generated by the union $\tilde{\mathfrak{A}}(V_1) \cup \tilde{\mathfrak{A}}(V_2)$ is dense in $C(\tilde{\Omega})$ (in the $c$-topology), we use the Stone–Weierstrass theorem.

*Stone–Weierstrass Theorem*[20]: Let $C(\tilde{\Omega}, c)$ be the sets of all continuous real functions on an arbitrary space $\tilde{\Omega}$, equipped with the $c$-topology, and $D \subset C(\tilde{\Omega}, c)$ a family that contains a nonzero constant function and is separating. Then the algebra $A(D)$ generated by $D$ is dense in $C(\tilde{\Omega}, c)$.

To show that the union $\tilde{\mathfrak{A}}(V_1) \cup \tilde{\mathfrak{A}}(V_2)$ separates the points $\tilde{\Omega}$, consider two distinct points $\tilde{\varphi}_1$ and $\tilde{\varphi}_2$ in $\tilde{\Omega}$, and let $\varphi_1$ and $\varphi_2$ be elements of $\Omega$ that map into $\tilde{\varphi}_1$ and $\tilde{\varphi}_2$, respectively. Then there must be a point $x_0 \in V_1 \cup V_2$ such that $\varphi_1(x_0) \neq \varphi_2(x_0)$. Consider now the functional

$$F_{x_0}(\psi) = \psi(x_0).$$

It is an element of $\mathfrak{A}$ because it is continuous, and if $x_0 \in V_i$ it is an element of $\mathfrak{A}(V_i)$ because

$$F_{x_0}(\chi_{V_i}\psi) = F_{x_0}(\psi).$$

Hence, $F(\varphi_1) \neq F(\varphi_2)$; and from the definition of the map $F \mapsto \tilde{F}$, it follow that $\tilde{F}_{x_0}(\tilde{\varphi}_1) \neq \tilde{F}_{x_0}(\tilde{\varphi}_2)$.

Hence, by the Stone–Weierstrass theorem, the topologically closed algebra $\tilde{\mathfrak{A}}_{12} = \overline{\tilde{\mathfrak{A}}(V_1) \cup \tilde{\mathfrak{A}}(V_2)}$ generated by the union $\tilde{\mathfrak{A}}(V_1) \cup \tilde{\mathfrak{A}}(V_2)$ is equal to $\tilde{\mathfrak{A}}(V_1 \cup V_2)$. Because of the continuity of the isomorphism of the map $\mathfrak{A} \to \tilde{\mathfrak{A}}$, the same statement applies to the algebras $\mathfrak{A}(V_1)$ and $\mathfrak{A}(V_2)$. This proves Eq. (2.1) and, hence, the consistency of the definition of instant local algebras in accordance with Eq. (4.1).

## APPENDIX B

Contact between a theoretical principle and an experiment is made by attempted refutations (falsifications) of the principle. If the principle states the impossibility of accomplishing a result, then evidence in its favor consists in the failure of sustained efforts to accomplish the result, or, in finding it more and more difficult to approach the desired end. As pointed out in Ref. 12, p. 1330, evidence in favor of the principle of energy conservation consists in the failure of many clever attempts to construct a machine that delivers large quantities of work for a long time without input. Similarly, evidence in favor of a claimed causal independence consists in the failure of attempts to prevent the existence of a partial state *here* and *now* by creating a partial state *there* and *now*—e.g., by shooting a bullet with infinite velocity. Conversely, evidence *against* causal independence consists in failure of attempts to create a partial state *here* and *now*, whatever the partial state *there* and *now* may be. For instance, a homogeneous strong magnetic north-field *here* is difficult to maintain in presence of a strong magnetic south field in the immediate surrounding. Failure to invent a magnetic Faraday cage is evidence against causal independence of two algebras associated to simultaneous and very close space regions. Practically, gradients $\partial B_z/\partial z$ of a magnetic field component $B_z$ above roughly $10^{10}$ gauss/cm. cannot be created by state-preparing procedures. Hence, empirical evidence against the feasibility of arbitrarily large gradients (the requirement of weak locality) is as strong as evidence against the feasibility of a discontinuity of the normal component of the magnetic field (the requirement of local independence). In this argument, use was made of empirical facts rather than of Maxwell's theory. However, we maintain that, in testing a theory for compliance with a causal independence principle, it is

necessary to consider not only the states whose existence the theory asserts, but also the means for preparing the state which should be part of a physical theory. Even if no experiment had ever been made to test Maxwell's theory, the above conclusion could be derived from detailed calculations on the energies necessary to create extreme gradients of the magnetic field. The conclusion would be the same: The difficulties in preparing states with very high gradients become insurmountable as the value of the gradient increases. Hence, even weak local independence is incompatible with the Maxwell theory.

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The origin–origin value of the Green's function for a simple cubic lattice with axial anisotropy is evaluated exactly.

There has been much interest recently in the evaluation of integrals of the Watson type

$$I(z) = \iiint_P d^3k \, \frac{f(k_1,k_2,k_3)}{z - g(k_1,k_2,k_3)}, \tag{1}$$

where $f$ and $g$ are trigonometric polynomials, and the integral extends over some finite polyhedron $P$. These are ubiquitous in lattice problems and are so named in honor of Watson[1] who evaluated $I$ in the cases $f = 1$:

(i) B.C.C. $g_1(\mathbf{k}) = \cos k_1 \cos k_2 \cos k_3$, $z = 1$;

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where $P$ is the parallelopiped $-\pi \leq k_i \leq \pi$. In this paper we shall evaluate $I$ for the case $f = 1$, $P$ as above, and

$$g(\mathbf{k}) = g_1(\mathbf{k}) + g_2(\mathbf{k}) + g_3(\mathbf{k}).$$

This case is of practical interest in studying the properties of a Heisenberg ferromagnet with axial anisotropy and has been examined numerically by Nakamura.[2]

Let us begin by assuming that $z > 7$, so the integrand is nonsingular. Then the integral over $k_3$, say, is elementary and the $k_2$ integration can be reduced to the complete elliptic integral of the first kind. Thus we have, after making the substitution $u = \cos k$,

$$I = \frac{32\pi}{z+1} \int_0^1 du(1-u^2)^{-1/2} \, \mathbf{K}[u(8/(z+1))^{1/2}]. \tag{2}$$

The complete elliptic integral $\mathbf{K}$ has the representations

$$\mathbf{K}(k) = \frac{\pi}{2} \sum_{n=0}^{\infty} \left(\frac{(2n-1)!!}{2^n n!}\right)^2 k^{2n} = \tfrac{1}{22}\pi F_1(\tfrac{1}{2}, \tfrac{1}{2}; 1; k^2), \quad |k| < 1 \tag{3}$$

with the understanding that $(-1)!! = 1$. By integrating term by term one finds

$$\int_0^1 x^{2\rho-1}(1-x^2)^{\sigma-1} \, \mathbf{K}(xz)dx = \frac{\pi}{4} \frac{\Gamma(\rho)\Gamma(\sigma)}{\Gamma(\rho+\sigma)} \, {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, \rho; 1, \sigma+\rho; z^2), \tag{4}$$

which is valid for $\mathrm{Re}\rho > 0$, $\mathrm{Re}\sigma > 0$, $|\arg(1-z^2)| < \pi$. Now by using (4) with $\rho = \sigma = \frac{1}{2}$, (2) becomes

$$I = [8\pi^3/(z+1)] \, {}_3F_2(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}; 1, 1; [8/(z+1)]). \tag{5}$$

Clausen's theorem which states

$${}_3F_2(2\alpha, 2\beta, \alpha+\beta; 2(\alpha+\beta), \alpha+\beta+\tfrac{1}{2}; z) = \{{}_2F_1(\alpha, \beta; \alpha+\beta+\tfrac{1}{2}; z)\}^2$$

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$$I = [8\pi^3/(z+1)][{}_2F_1(\tfrac{1}{2}, \tfrac{1}{2}; 1; a^2)]^2, \tag{6}$$

where $a^2 = \frac{1}{2}[(z+1)^{1/2} - (z-7)^{1/2}]/(z+1)^{1/2}$. Finally, noting that the hypergeometric function in (6) is again the complete elliptic integral we find the simple result

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$$I(7)=\Gamma^4(\tfrac{1}{4})\cong 172.792\,266\cdots$$

which complements Watson's results.

The function $\varphi(x)$ tabulated by Nakamura[2] is related to our results by

$$\varphi(x)=\frac{2}{\pi^3 x}\,I\left(\frac{8}{x}-1\right)=16\pi x\,(\mathbf{K}\{[\tfrac{1}{2}(1-\sqrt{1-x})]^{1/2}\})^2,$$

which reproduces his tabulated results for $0\le x\le 1$.

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# Multigroup Neutron Transport*

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We investigate the nature of the approximations involved in the multigroup treatment of the time-dependent neutron transport equation by using the method of approximating sequences of Banach spaces. We prove that solutions of the multigroup system converge, in a suitable sense, to the corresponding solutions of the exact transport equation. Moreover, we indicate the order of magnitude of the rate of convergence.

## 1. INTRODUCTION

The multigroup neutron transport equation is a powerful tool for investigating spectrum regeneration problems.[1] It is usually assumed that solutions of the multigroup transport equations approximate the corresponding solutions of the exact transport equation, in which the velocity (or energy) variable is not discretized. However, it is not clear how multigroup solutions approximate exact solutions and, correspondingly, evaluations of the errors involved in such a procedure are never given.

In this paper, we show that the nature of the multigroup treatment in the time-dependent case may be investigated by using the theory of semigroups of linear operators (Ref. 2, Chap. 9; Ref. 3) in connection with the method of the approximating sequences of Banach spaces (Ref. 2 p. 512; Refs. 4, and 5).

Moreover, we prove that solutions of the multigroup system converge, in a suitable sense, to the corresponding solutions of the exact transport equation. Finally, we indicate the order of magnitude of the rate of convergence.

## 2. MATHEMATICAL PRELIMINARIES

Following Trotter,[4] we say that a sequence of Banach spaces $\{X_n\}$ together with a sequence of linear operators $\{P_n\}$, $P_n\in\mathfrak{B}(X,X_n)$ (Ref. 2, p. 149), is a sequence of Banach spaces approximating a given Banach space $X$ if

$$\|P_n\|\le 1,\qquad n=1,2,3,\ldots, \tag{1}$$

$$\lim_{n\to\infty}\|P_n f\|_n=\|f\|\qquad \text{for every } f\in X, \tag{2}$$

where $\|\cdot\|_n$ is a norm in $X_n$ and $\|\cdot\|$ is a norm in $X$. As it will be clear in the sequel, $P_n f$ is a representation of $f\in X$ in the approximating space $X_n$. Hence, condition (2) roughly means that the norm of $f$ is close to the norm of its representation provided $n$ is big enough.

We also note that, if $\|P_n f\|_n\to\|f\|$ for every $f$ of a dense subset of $X$, then condition (2) is satisfied.

Let us now consider a sequence $\{f_n\}$ with $f_n\in X_n$, $n=1,2,\cdots$, by definition, we say that $\{f_n\}$ converges to $f\in X$ if $\lim\|f_n-P_n f\|_n=0$ as $n\to\infty$. Correspondingly, we call $f$ the limit of $\{f_n\}$ and write $f=\lim f_n$ as $n\to\infty$.

Finally, assume that $\{B_n\}$ is a sequence of operators with $B_n\in\mathfrak{B}(X_n)$ and that $B\in\mathfrak{B}(X)$. We say that $\{B_n\}$ converges to $B$ if $\lim_{n\to\infty}B_nP_nf=Bf$ for every $f\in X$, i.e., if $\|B_nP_nf-P_nBf\|\to 0$ for every $f\in X$.

By starting from the preceding definitions, the following theorem can be proved on the approximation of a given semigroup in $X$ by means of a sequence of semigroups in $X_n$ (Ref. 4, Theorem 5.1, p. 900).

*Theorem 1:* Let $T$ be a linear operator of class $\mathcal{G}(M,\beta_0)$ in $X$, and let $T_n$ be of class $\mathcal{G}(M,\beta_0)$ in $X_n$, $n=1,2,\cdots$; if

$$\lim_{n\to\infty}R(\lambda,T_n)P_nf=R(\lambda,T)f \tag{3}$$

for some $\lambda$ with $\mathrm{Re}\lambda>\beta_0$ and for every $f\in X$, where $R(\lambda,T_n)=(\lambda I-T_n)^{-1}$ and $R(\lambda,T)=(\lambda I-T)^{-1}$, then

$$\lim_{n\to\infty}\exp(t\,T_n)P_nf=\exp(t\,T)f \tag{4}$$

uniformly in any finite interval of $t\ge 0$ (notations are those of Ref. 2, Chap. 9). Hence, the convergence of the sequence of semigroups generated by the $T_n$ follows from the convergence of the resolvent operators $R(\lambda,T_n)$. Of course, this convergence must be understood in the sense of the definition given a few lines above.

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As we shall see in the following sections, due to Theorem 1, a given initial-value problem may be ap-

proximated by means of a suitable sequence of initial-value problems.

We conclude this section with the following perturbation theorem:

*Theorem 2:* Under the assumptions of Theorem 1, if

$$\lim_{n\to\infty} B_n P_n f = Bf \quad \text{for every } f \in X, \tag{5}$$

where $B_n \in \mathcal{B}(X_n)$ and $B \in \mathcal{B}(X)$, then

$$\lim_{n\to\infty} \exp[t(T_n + B_n)]P_n f = \exp[t(T + B)]f, \tag{6}$$

provided that the $B_n$ are uniformly bounded, i.e., $\|B_n\| \leq N$ where $N$ is a constant independent of $n$.

In fact, let $F = R(\lambda, T)B$, $F_n = R(\lambda, T_n)B_n$; since $T_n \in \mathcal{G}(M, \beta_0)$ (Ref. 2, p. 485), we have that $\|F_n\| \leq M\|B_n\|(\mathrm{Re}\lambda - \beta_0)^{-1}$. Hence, $\|F_n\| \leq 1$ provided that $\mathrm{Re}\lambda > \beta_0 + MN$ and, consequently,

$$\|R(1, F_n)\| \leq (1 - \|F_n\|)^{-1} \leq (\mathrm{Re}\lambda - \beta_0)/(\mathrm{Re}\lambda - \beta_0 - MN).$$

On the other hand, we have

$$\begin{aligned}\|P_n R(1, F)f - R(1, F_n)P_n f\|_n &\leq \|R(1, F_n)\\ &\times (P_n F - F_n P_n)R(1, F)f\|_n\\ &\leq [(\mathrm{Re}\lambda - \beta_0)/(\mathrm{Re}\lambda\\ &- \beta_0 - MN)]\,\|(P_n F - F_n P_n)g\|_n \to 0,\end{aligned}$$

where $g = R(1, F)f$ and where we used (5).

Finally, by taking into account that $R(\lambda, T + B) = R(1, F)R(\lambda, T)$, $R(\lambda, T_n + B_n) = R(1, F_n)R(\lambda, T_n)$, we obtain

$$\begin{aligned}\|R(\lambda, T_n + B_n)P_n f - P_n R(\lambda, T + B)f\|_n &\leq \|R(1, F_n)\\ &\times [R(\lambda, T_n)P_n f - P_n R(\lambda, T)f]\|_n\\ &+ \|[R(1, F_n)P_n\\ &- P_n R(1, F)]R(\lambda, T)f\|_n\\ &\leq [(\mathrm{Re}\lambda - \beta_0)/(\mathrm{Re}\lambda - \beta_0\\ &- MN)]\,\|R(\lambda, T_n)P_n f - P_n R(\lambda, T)f\|_n\\ &+ \|R(1, F_n)\\ &\times P_n\varphi - P_n R(1, F)\varphi\|_n,\end{aligned}$$

where $\varphi = R(\lambda, T)f$ and $\mathrm{Re}\lambda > \beta_0 + MN$. We conclude that

$$\lim_{n\to\infty} R(\lambda, T_n + B_n)P_n f = R(\lambda, T + B)f$$

for any $\lambda$ such that $\mathrm{Re}\lambda > \beta_0 + MN$; hence, due to theorem 1, (6) is proved.

## 3. THE MULTIGROUP TRANSPORT EQUATIONS

For the sake of simplicity, we shall consider the transport equation and the corresponding multigroup approximation in a homogeneous slab of thickness $2a$ surrounded by vacuum. Only a slightly more involved formalism is needed to study more complicated multiplying media.

As in Refs. 6 and 7, the Banach space $X$ is the set of all functions $f = f(x, \mu, v)$ which are integrable over the rectangle $|x| \leq a$, $|\mu| \leq 1$, $0 < v_m \leq v \leq v_M < +\infty$, with norm $\|f\| = \int_{v_m}^{v_M} dv \int_{-1}^{1} d\mu \int_{-a}^{a} |f|\,dx$.

The abstract version in $X$ of the initial-value problem for neutron transport in the homogeneous slab reads as follows:

$$\frac{du}{dt} = Tu - Bu + JHu, \quad t > 0, \quad u \in D(T) \subset X, \tag{7}$$

$$\lim_{t\to 0^+} \|u(t) - u_0\| = 0, \quad u_0 \in D(T), \tag{8}$$

where $u = u(x, \mu, v, t)$ is the neutron density, $du/dt$ is a strong derivative (Ref. 2, pp. 7 and 132), $u_0$ is a given element of $D(T)$, the domain of the operator $T$. Moreover, $T, B, J$, and $H$ are linear operators in $X$ defined by the following relations:

$$\begin{aligned}&Tf = -\mu v \frac{\partial f}{\partial x}, \quad Hf = \int_{v_m}^{v_M} H(v, v')f(x, \mu, v')dv',\\ &Jf = \tfrac{1}{2}\int_{-1}^{+1} f(x, \mu', v)d\mu', \quad Bf = v\Sigma(v)f,\end{aligned} \tag{9}$$

where $\Sigma(v)$ is the total cross section and $H(v, v')$ is a kernel which takes into account scattering and fission. Finally, $D(T)$ is the set of those elements $f \in X$ such that (a) $Tf \in X$, (b) $f(-a, \mu, v) = 0$ if $\mu \in (0, 1]$, and (c) $f(a, \mu, v) = 0$ if $\mu \in [-1, 0)$. It is easily proved that $D(T)$ is dense in $X$.

As it is well known (Ref. 8, p. 113; Ref. 9, p. 1554), the resolvent $R(\lambda, T)$ has the form

$$\left.\begin{aligned}R(\lambda, T)g &= (1/v\mu)\int_{-a}^{x} \exp[-(\lambda/v\mu)(x - y)]g(y, \mu, v)dy, \quad \mu > 0\\ &= -(1/v\mu)\int_{x}^{a} \exp[-(\lambda/v\mu)(x - y)]g(y, \mu, v)dy, \quad \mu < 0\end{aligned}\right\} \tag{10}$$

provided $\mathrm{Re}\lambda > 0$ and $g \in X$. Moreover, $R(\lambda, T)$ is such that

$$\|R(\lambda, T)\| \leq 1/\mathrm{Re}\lambda, \quad \mathrm{Re}\lambda > 0 \tag{11}$$

(Ref. 9, p. 1554). It follows that $T \in \mathcal{G}(1, 0)$, (Ref. 2, p. 485).

Let us now consider the multigroup version of system (7) + (8). First of all, the velocity range $V \equiv [v_m, v_M]$ is divided into $n$ subintervals $V_j \equiv [v_{j-1}, v_j]$, $j = 1, 2, \ldots, n$, with $v_0 = v_m$ and $v_n = v_M$. Correspondingly, the Banach space $X_n$ is composed of all vectors

$$\varphi = \varphi(x, \mu) = \begin{pmatrix}\varphi_1(x, \mu)\\ \cdots\\ \varphi_n(x, \mu)\end{pmatrix},$$

such that $\|\varphi\|_n = \sum_{j=1}^{n} \int_{-1}^{+1} d\mu \int_{-a}^{a} |\varphi_j(x, \mu)|\,dx < \infty$.

The abstract version in $X_n$ of the initial-value problem for multigroup neutron transport reads as follows

$$\frac{dw^{(n)}}{dt} = T_n w^{(n)} + J_n H_n w^{(n)}, \quad t > 0, \qquad w^{(n)} \in D(T_n) \subset X_n, \tag{12}$$

$$\lim_{t\to 0^+} \| w^{(n)}(t) - w_0^{(n)} \|_n = 0, \quad w_0^{(n)} \in D(T_n), \tag{13}$$

where $w^{(n)} = \begin{pmatrix} w_1 \\ \cdots \\ w_n \end{pmatrix}$ is the multigroup neutron density vector, $w_0^{(n)}$ is a given element of the domain of $T_n$, which is dense in $X_n$. Moreover, $T_n$, $B_n$, $J_n$, and $H_n$ are matrix-operators, defined by the following relations:

$$\left.\begin{aligned} T_n &= -\{v_{j-1}\delta_{ij}\}\frac{\partial}{\partial x}, \quad J_n = \{\delta_{i,j}\}J \\ H_n &= \{K_{i,j}\}, \quad B_n = \{b_j \delta_{i,j}\}, \quad i,j = 1,2,\ldots,n \end{aligned}\right\}, \tag{14}$$

where $\delta_{i,j}$ is the Kronecker symbol and where the constants $b_j$ and $K_{i,j}$ are such that

$$\left.\begin{aligned} &\{\inf[v\Sigma(v)], v \in V_j\} \leq b_j \leq \{\sup[v\Sigma(v)], v \in V_j\} \\ &\{\inf[\textstyle\int_i H(v,v')dv], v' \in V_j\} \leq K_{i,j} \\ &\leq \{\sup \textstyle\int_i H(v,v')dv, v' \in V_j\} \\ &\leq (v_i - v_{i-1}) \sup H(v,v'), \end{aligned}\right\} \tag{15}$$

where $\int_i \cdot dv = \int_{v_{i-1}}^{v_i} \cdot dv$ and $\Sigma(v)$ and $\int_i H(v,v')dv$ are assumed to be bounded pointwise continuous functions.

The resolvent operator $R(\lambda, T_n)$ is such that the $j$th component of the vector $R(\lambda, T_n)\varphi$ has the form

$$[R(\lambda, T_n)\varphi]_j = \frac{1}{\mu v_{j-1}} \int_{-a}^{x} \exp\left(\frac{-\lambda}{\mu v_{j-1}}(x-y)\right)\varphi_j(y,\mu)dy, \quad \mu > 0,$$

$$= -\frac{1}{\mu v_{j-1}} \int_{x}^{a} \exp\left(-\frac{\lambda}{\mu v_{j-1}}(x-y)\right) \times \varphi_j(y,\mu)dy, \quad \mu < 0 \tag{16}$$

provided that $\mathrm{Re}\lambda > 0$. Moreover, we have

$$\| R(\lambda, T_n) \| \leq 1/\mathrm{Re}\lambda, \quad \mathrm{Re}\lambda > 0. \tag{17}$$

It follows that $T_n \in \mathcal{G}(1,0)$ in $X_n$.

## 4. CONVERGENCE OF $\{R(\lambda, T_n)\}$ TO $R(\lambda, T)$

Let us now define the linear map $P_n$ from $X$ to $X_n$ as follows:

$$P_n f = \varphi = \begin{pmatrix} \varphi_1 \\ \cdots \\ \varphi_n \end{pmatrix}, \quad \varphi_j = \varphi_j(x,\mu) = \int_j f(x,\mu,v')dv', \quad j = 1,2,\ldots,n. \tag{18}$$

Clearly, we have $\| P_n f\|_n \leq \| f \|$. Hence, $\| P_n \| \leq 1$ and $P_n \in \mathcal{B}(X, X_n)$. As far as condition (2) is concerned, if $f(x,\mu,v)$ does not change its sign when $x$ and $\mu$ are arbitrarily fixed and $v$ runs over the interval $[v_m, v_M]$, we have that $\| P_n f\|_n = \| f \|$, $n = 1,2,\cdots$.

On the other hand, let $\Omega$ be the set of all polynomials defined over the set $\{(x,\mu,v): |x| \leq a, |\mu| \leq 1, v_m \leq v \leq v_M\}$, and assume that $p = p(x,\mu,v)$ is a polynomial of degree $m$. It follows that $p$ changes its sign $m$ times at most as $v$ runs over $[v_m, v_M]$, given any $x$ and $\mu$. Hence

$$0 \leq \sum_{j=1}^{n} \{\textstyle\int_j |p| dv' - |\int_j p\, dv'|\} = \sum{}' \{\textstyle\int_j |p| dv' - |\int_j p\, dv'|\} \leq 2m\bar{p}h^{(n)}, \quad n \geq m,$$

where $\bar{p} = \{\max |p(x,\mu,v)|, |x| \leq a, |\mu| \leq 1, v_m \leq v \leq v_M\}$, $h^{(n)} = \{\max h_j, j = 1,2,\ldots,n\}$, $h_j = v_j - v_{j-1}$ and where $\sum'$ is a sum extended over the $m$ subintervals over which $p$ changes its sign (given $x$ and $\mu$). We conclude that condition (2) is satisfied by any $g \in \Omega$, provided that $\lim_{n\to\infty} h^{(n)} = 0$.

We conclude that $\{X_n\}$ together with the $P_n$ is a sequence of Banach spaces approximating $X$, since $\Omega$ is dense in $X$.

In order to make use of the results of Theorems 1 and 2 of Sec. 2, we are now going to prove that relation (3) is valid if $T$ and $T_n$ are given by (9) and (14).

Given any $g \in X$ and assuming that $\lambda$ is any fixed positive real number, we have from (10) and from (16)

$$[P_n R(\lambda, T)g]_j = (\mu v)^{-1} \int_j dv \int_{-a}^{x} \exp(-\alpha/v) g(y,\mu,v)dy, \quad \mu > 0,$$

$$[R(\lambda, T_n)P_n g]_j = (\mu v_{j-1})^{-1} \int_{-a}^{x} dy \exp(-\alpha/v_{j-1}) \int_j g(y,\mu,v)dy, \quad \mu > 0,$$

where $\alpha = \lambda(x-y)/\mu > 0$. It follows

$$|[P_n R(\lambda, T)g - R(\lambda, T_n)P_n g]_j| = \Delta_j \leq (\mu v)^{-1} \int_j dv \int_{-a}^{x} dy \left\{\exp\left(-\frac{\alpha}{v}\right) \left|1 - \frac{v}{v_{j-1}} \times \exp\left[-\alpha\left(\frac{1}{v_{j-1}} - \frac{1}{v}\right)\right]\right| \cdot |g(y,\mu,v)|\right\}, \quad \mu > 0.$$

On the other hand, we have

$$|1 - (v/v_{j-1}) \exp\{-\alpha[(1/v_{j-1}) - (1/v)]\}| \leq h_j/v_{j-1} + (v/v_{j-1})(1 - \exp\{-\alpha[(1/v_{j-1}) - (1/v)]\})$$

since $\alpha$ is positive and $v \in V_j$. Hence, we obtain

$$\Delta_j \leq (h_j/\mu v_{j-1}) \int_j dv \int_{-a}^{x} \exp(-\alpha/v)|g(y,\mu,v)|dy/v + (1/\mu v_{j-1}) \int_j dv \int_{-a}^{x} [\exp(-\alpha/v) - \exp(-\alpha/v_{j-1})]|g(y,\mu,v)|dy.$$

Integration with respect to $x$ leads now to the following inequality:

$$\int_{-a}^{a} \Delta_j dx \leq (2h^{(n)}/\lambda v_m) \int_j dv \int_{-a}^{a} |g| dy, \quad \mu > 0. \tag{19}$$

Since a similar inequality can be obtained if $\mu > 0$, from (19) it follows that

$$\| P_n R(\lambda, T)g - R(\lambda, T_n)P_n g\|_n \leq (2h^{(n)}/\lambda v_m) \| g \|. \tag{20}$$

We conclude that (3) is satisfied provided that $\lim_{n\to\infty} h^{(n)} = 0$.

## 5. CONVERGENCE OF $\{B_n\}$ AND OF $\{J_nH_n\}$

First of all, we note that $\{J_nH_n\}$ and $\{B_n\}$ are uniformly bounded. In fact, we have

$$\|J_nH_n\varphi\|_n = \sum_{i=1}^{n}\int_{-1}^{1}d\mu\int_{-a}^{+a}dx\left|\tfrac{1}{2}\int_{-1}^{+1}d\mu'\sum_{j=1}^{n}K_{i,j}\varphi_j(x,\mu')\right| \leq H_M\|\varphi\|_n$$

and, in an analogous way

$$\|B_n\varphi\|_n \leq b_M\|\varphi\|_n,$$

where $H_M = (v_M - v_m)\{\sup[H(v,v')];\ v\in V, v'\in V\}$ and $b_M = \{\sup[v\Sigma(v)],\ v\in V\}$. Hence

$$\|B_n\| \leq b_M, \qquad \|J_nH_n\| \leq H_M, \qquad n = 1,2,\cdots. \tag{21}$$

On the other hand, given any $g\in X$, we have from (9) and (14)

$$|[P_nBg - B_nP_ng]_j| \leq \int_j|v\Sigma(v) - b_j|\,|g|dv \leq k^{(n)}\int_j|g|dv,$$

where $k^{(n)} = \max_{1\leq j\leq n}(\{\sup[v\Sigma(v)],\ v\in V_j\} - \{\inf[v\Sigma(v)],\ v\in V_j\})$.

It follows that

$$\|P_nBg - B_nP_ng\|_n \leq k^{(n)}\|g\|. \tag{22}$$

As far as the sequence $\{J_nH_n\}$ is concerned, we have

$$|[P_nJHg - J_nH_nP_ng]_j| \leq \tfrac{1}{2}\int_{-1}^{+1}d\mu'\sum_{i=1}^{n}\int_i dv'\,|g(x,\mu',v')| \times\left|\int_j H(v,v')dv - K_{j,i}\right| = \tfrac{1}{2}\int_{-1}^{+1}d\mu'\sum_{i=1}^{n}\int_i dv' \times|g(x,\mu',v')|\cdot\left|\int_j[H(v,v') - H_{j,i}]dv\right|,$$

where $H_{j,i} = K_{j,i}/(v_j - v_{j-1})$. Hence, we obtain

$$\|P_nJHg - J_nH_nP_ng\|_n \leq l^{(n)}\|g\|, \tag{23}$$

where

$$l^{(n)} = \max_{1\leq i\leq n}\left[\left\{\sup\left(\sum_{j=1}^{n}\left|\int_j[H(v,v') - H_{j,i}]dv\right|\right),\ v'\in V_i\right\}\right].$$

From (22) and (23) it follows that $\{B_n\}$ and $\{J_nH_n\}$ converge to $B$ and to $JH$, respectively, provided that $\lim_{n\to\infty}k^{(n)} = 0$ and $\lim_{n\to\infty}l^{(n)} = 0$.

## 6. CONCLUDING REMARKS

If we put

$$A = T - B + JH, \qquad A_n = T_n - B_n - J_nH_n, \tag{24}$$

from (20), (22), (23) and by using Theorems 1 and 2 of Sec. 2, we conclude that the sequence of semigroups $\{\exp(tA_n)\}$ converges to the semigroup $\exp(tA)$ generated by $A$, provided that

$$\text{(a) } \lim h^{(n)} = 0, \quad \text{(b) } \lim k^{(n)} = 0, \quad \text{(c) } \lim l^{(n)} = 0, \quad \text{as } n\to\infty. \tag{25}$$

Let conditions (25) be then satisfied and assume that the initial multigroup distribution $w_0^{(n)}$ on the right-hand side of (13) is such that

$$w_0^{(n)} = P_nu_0, \tag{26}$$

where $u_0$ is the exact initial distribution [see (8)]. On the other hand, the solutions of the initial-value problems (7) + (8) and (12) + (13) have the following form (Ref. 2, p. 481):

$$u = \exp(tA)u_0, \qquad w^{(n)} = \exp(tA_n)w_0^{(n)} = \exp(tA_n)P_nu_0.$$

Hence

$$\lim_{n\to\infty}\|P_nu - w^{(n)}\|_n = \lim_{n\to\infty}\|P_n\exp(tA)u_0 - \exp(tA_n)P_nu_0\|_n = 0, \tag{27}$$

and, consequently, the sequence $\{w^{(n)}\}$ converges to the exact solution $u$, according to the definition of convergence given in Sec. 2. In other words, the $j$th component $[P_nu]_j = \int_j udv$ of the representation in $X_n$ of the exact solution is close to the $j$th component of the $n$-group solution $w^{(n)}$, provided $n$ is large enough.

Let us now discuss briefly the nature of conditions (25). The meaning of (25a) is clear: the amplitude of the largest subinterval must approach zero as $n\to\infty$. As far as (25b) is concerned, we observe that, if $v\Sigma(v)$ is a continuous function of $v\in V$, then $v\Sigma(v)$ is also uniformly continuous. Hence $k^{(n)}\to 0$, provided that $h^{(n)}\to 0$. Moreover, if $v\Sigma(v)$ satisfies a Lipschitz condition

$$|v\Sigma(v) - v'\Sigma(v')| \leq L_1|v - v'|, \qquad v, v'\in V, \tag{28}$$

where $L_1$ is a positive constant, we have that $k^{(n)} \leq L_1h^{(n)}$.

Finally, let us consider condition (25c). If we assume that $H(v,v')$ is continuous (and hence uniformly continuous) over the square $V\times V$, it follows without difficulty that $l^{(n)}\to 0$ if $h^{(n)}\to 0$. Moreover, if $H(v,v')$ satisfies the following Lipschitz condition with respect to the variable $v'$:

$$|H(v,v') - H(v,\bar{v}')| \leq L_2|v' - \bar{v}'|, \tag{29}$$

where $L_2$ is a positive constant, we obtain that $l^{(n)} \leq L_2(v_M - v_m)h^{(n)}$.

## 7. EVALUATION OF THE ERROR

We are now going to evaluate an upper bound of the norm $\|P_nu - w^{(n)}\|_n$ [see (27)]. With this aim in mind, we first observe that, by using some results of perturbation theory for linear operators (Ref. 2, Theorem 2.1, p. 495), it is not difficult to prove that $A\in\mathcal{G}(1,\beta_0)$ in $X$ and $A_n\in\mathcal{G}(1,\beta_0)$ in $X_n$, where $\beta_0 = H_M + b_M$. Moreover, the following inequality is valid (see appendix):

$$\|P_nR(\lambda,A) - R(\lambda,A_n)P_n\| \leq \chi^{(n)}, \tag{30}$$

where

$$\chi^{(n)} = (\lambda - \beta_0)^{-2}[(2\lambda h^{(n)}/v_m) + k^{(n)} + l^{(n)}] \tag{31}$$

and $\lambda$ is an arbitrarily fixed real number, such that $\lambda > \beta_0$. On the other hand, a straightforward modification of formula (2.27) of Kato (Ref. 2, p. 501) gives

$$R(\lambda,A_n)[P_n\exp(tA) - \exp(tA_n)P_n]R(\lambda,A)f = \int_0^t\exp[(t-s)A_n][P_nR(\lambda,A) - R(\lambda,A_n)P_n] \times\exp(sA)f\,ds, \tag{32}$$

where $f$ is any element of $X$ and $\lambda > \beta_0$. It follows from (30) and from (32),

$$\|R(\lambda, A_n)[P_n \exp(tA) - \exp(tA_n)P_n]R(\lambda, A)\|_n \leq t \exp(\beta_0 t)\chi^{(n)}\|f\|, \quad \text{for every } f \in X. \tag{33}$$

Given now any $g \in D(A) = D(T)$, if we put $f = (\lambda I - A)g$, then we obtain from (33):

$$\|R(\lambda, A_n)[P_n \exp(tA) - \exp(tA_n)P_n]g\|_n \leq t \exp(\beta_0 t)\chi^{(n)}\|(\lambda I - A)g\|, \quad g \in D(A), \tag{34}$$

where $D(A) = D(T)$ is dense in $X$.

Furthermore, the following two inequalities can be deduced from (30):

$$\|\exp(tA_n)P_n R(\lambda, A)f - R(\lambda, A_n)\exp(tA_n)P_n f\|_n \leq \exp(\beta_0 t)\chi^{(n)}\|f\|, \tag{35}$$

$$\|P_n \exp(tA)R(\lambda, A)f - R(\lambda, A_n)P_n \exp(tA)f\|_n \leq \exp(\beta_0 t)\chi^{(n)}\|f\|, \tag{36}$$

where $f$ is any element of $X$.

By using (34)–(36), we get

$$\|[\exp(tA_n)P_n - P_n \exp(tA)]R(\lambda, A)g\|_n \leq \chi^{(n)} \exp(\beta_0 t)[2\|g\| + t\|(\lambda I - A)g\|], \quad g \in D(A). \tag{37}$$

Finally, assume that $u_0 \in D(A^2)$ (which is dense in $X$, Ref. 2, p. 480) and put $g = (\lambda I - A)u_0$. It then follows from (37)

$$\|[\exp(tA_n)P_n - P_n \exp(tA)]u_0\|_n \leq \chi^{(n)} \exp(\beta_0 t)[2\|(\lambda I - A)u_0\| + t\|(\lambda I - A)^2 u_0\|], \quad u_0 \in D(A^2). \tag{38}$$

Inequality (38) gives us an upper bound of the error $\|w^{(n)} - P_n u\|_n$ as a function of $t$, $\chi^{(n)}$ and of the initial distribution $u_0$. Moreover, the coefficient $\chi^{(n)}$ given by (31) is proportional to $h^{(n)}$, provided that condition (28) and (29) are satisfied. Finally, we observe that the parameter $\lambda$, appearing on the right-hand side of (38), is an arbitrarily fixed frequency larger than $\beta_0$. It is then reasonable to assume that $\lambda$ is a frequency of some physical interest, i.e., to put for instance $\lambda = 2\beta_0$.

## APPENDIX

From (24) it is not difficult to obtain the following relations:

$$R(\lambda, A) = R(1, C)R(\lambda, T),$$
$$R(\lambda, A_n) = R(1, C_n)R(\lambda, T_n), \quad \mathrm{Re}\lambda > \beta_0,$$

where

$$C = R(\lambda, T)[JH - B] \in \mathfrak{B}(X),$$
$$C_n = R(\lambda, T_n)[J_n H_n - B_n] \in \mathfrak{B}(X_n)$$

and where

$$\|R(1, C)\| \leq \mathrm{Re}\lambda/(\mathrm{Re}\lambda - \beta_0),$$
$$\|R(1, C_n)\| \leq \mathrm{Re}\lambda/(\mathrm{Re}\lambda - \beta_0).$$

Moreover, we have

$$\|P_n Cg - C_n P_n g\|_n \leq \|[P_n R(\lambda, T) - R(\lambda, T_n)P_n](JH - B)g\|_n + \|R(\lambda, T_n)[P_n(JH - B) - (J_n H_n - B_n)P_n]g\|_n.$$

Hence, by using (20), (22), and (23) we obtain

$$\|P_n C - C_n P_n\| \leq \gamma^{(n)}/\lambda, \quad \lambda > \beta_0,$$

where $\gamma^{(n)} = (2\beta_0/v_m)h^{(n)} + k^{(n)} + l^{(n)}$.

By a similar procedure we get

$$\|P_n R(1, C) - R(1, C_n)P_n\| = \|R(1, C)[P_n C - C_n P_n]R(1, C)\| \leq \lambda(\lambda - \beta_0)^{-2}\gamma^{(n)}, \quad \lambda > \beta_0.$$

Hence, we finally have

$$\|P_n R(\lambda, A) - R(\lambda, A_n)P_n\| \leq \|[P_n R(1, C) - R(1, C_n)P_n]R(\lambda, T)\| + \|R(1, C_n)[P_n R(\lambda, T) - R(\lambda, T_n)P_n]\| \leq (\lambda - \beta_0)^{-2}\gamma^{(n)} + 2[v_m(\lambda - \beta_0)]^{-1}h^{(n)}$$

provided that $\lambda > \beta_0$.

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# Local and Covariant Quantization of Linearized Einstein's Equations

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An analysis is given of all the possible quantizations of the linearized Einstein equations in terms of a weakly local and/or covariant potential $h_{\mu\nu}(x)$. The discussion is done without making the apparently arbitrary choices which characterize the standard formulations, and special attention is paid in proving those general features which follow from basic principles and are therefore common to all local and/or covariant formulations. It is shown that the requirement of locality and/or covariance alone implies that the Einstein equations cannot hold as mean values on a dense set of states, and therefore unphysical states must be introduced in an essential way. Moreover, the requirement that the Einstein equations hold as mean values on the physical states forces the existence of states of negative norm in order to define $h_{\mu\nu}$ as a local and/or covariant operator. Thus the characteristic features of Gupta's formulation are shown to be shared by any local and/or covariant theory. The arbitrary choices which occur in the representation of the field operator $h_{\mu\nu}$, in the definition of the metric operator and in the choice of the subsidiary condition which identifies the physical states, are shown to lead to only a one-parameter family of theories. They can be classified according to the subsidiary condition

$$(\partial^\mu h_{\mu\nu} + q\partial_\nu h_\mu{}^\mu)^+\Psi = 0,$$

each $q \neq -\frac{1}{4}$ identifying a possible theory. This arbitrariness, which makes the literature on the subject rather confusing, is resolved by proving that all the theories are (isometrically) equivalent. Such formulations are discussed in the framework of axiomatic quantum field theory, with particular emphasis on their group theoretical contents. Finally, an extensive treatment of Gupta's formulation is given along the lines discussed by Wightman and Gärding for quantum electrodynamics.

## 1 INTRODUCTION

The aim of the present paper is to characterize the possible quantizations of the linearized Einstein equations in terms of a weakly local and covariant potential $h_{\mu\nu}(x)$. An essential point of our analysis will be to avoid any choice or restriction on the theory, which might look arbitrary and therefore questionable. Our aim will be to discuss only those properties which follow from general principles and are therefore shared by any formulation of the theory. Of course, no commitment is made to particular gauge conditions so that the discussion is gauge independent.

Special attention is paid in proving that very general and physically motivated assumptions already give rather strong restrictions on the theory and essentially lead to the Gupta formulation. This shows that the characteristic features of the Gupta formulation are much more general than one might think.

In Secs. 2–6 we will discuss the restrictions imposed by locality and/or covariance. It has been shown in a previous paper[1] that if the potential is defined as a weakly local and/or covariant operator, the linearized Einstein equations cannot hold not even in the weak form

$$\begin{aligned} &R_{\mu\nu}(f)\Psi_0 = 0, \\ &\epsilon^{\lambda\mu\nu\rho}\,\partial_\mu R_{\alpha\beta\nu\rho}(f)\Psi_0 = 0 \end{aligned} \tag{1}$$

($\Psi_0$ being the vacuum state). In the present paper we will first analyze how weakly the Einstein equations must be required to hold in order that the difficulties due to locality and covariance do no longer appear. Furthermore we will investigate the conditions imposed on the metric by the requirements of locality and covariance. Our analysis is performed in the framework of axiomatic quantum field theory[2]. The conclusion we will arrive at is the following: Locality and covariance imply that the Einstein equations can hold only as mean values on a set of states which cannot be dense in the Hilbert space. Furthermore, the metric operator $\eta$ cannot be positive definite or semidefinite.

As a consequence, *the presence of unphysical states and the introduction of an indefinite metric appear unavoidable in a local and/or covariant theory*. This suggests that a local and covariant quantization of the Einstein equations can be performed only along the lines indicated by Gupta.[3]

In Sec. 6 and 7 the arbitrariness involved in (i) the representation of the operator $h_{\mu\nu}$, (ii) the choice of the metric operator $\eta$, and (iii) the choice of the subsidiary condition, is discussed in detail. At first sight one might think that there are as many possible quantizations of the linearized Einstein equations as the possible choices (i)–(iii). We will show that actually the arbitrariness involved in (i)–(iii) can lead to only one parameter family of theories, as a consequence of general principles. The possible theories may be classified in terms of the parameter $q$ which occurs in the subsidiary condition.

Finally, the relation between the possible theories parametrized by $q$ is discussed. Since different values of $q$ lead to different propagators, the arbitrariness in the choice of $q$ has sometimes been a source of discussion in the literature.[4] As we will show in Sec. 9, even if the different theories have formally different properties, they are related to one another by a generalized isometry. This will be proved in a rigorous way by analyzing the Wightman functions and without making use of gauge transformations, whose mathematical meaning is not very clear.

In conclusion, without loss of generality as a consequence of the previous results, a detailed discussion is given of the formulation corresponding to the Gupta subsidiary condition ($q = -\frac{1}{2}$). The implications of the negative results of Ref. 1, in connection with the Gupta formulation are also discussed.

## 2. BASIC DEFINITIONS

We start by defining the problem we are going to discuss. Since we are interested in the Einstein

equations, the basic fields are the fields $R_{\mu\nu\rho\sigma}(x)$, which satisfy the following identities[5]:

$$R_{\lambda\mu\nu\rho} = -R_{\mu\lambda\nu\rho} = R_{\mu\lambda\rho\nu} = R_{\nu\rho\lambda\mu},$$
$$R_{\lambda\nu\rho\sigma} + R_{\lambda\rho\sigma\nu} + R_{\lambda\sigma\nu\rho} = 0. \tag{2}$$

We further assume that

(a) the fields $R_{\mu\nu\rho\sigma}(x)$ are defined as operator-valued (tempered) distributions in a Hilbert space $H$.[6]

(b) There exists a "unitary"[7] representation of the Poincaré group $\{a, \Lambda\} \to U(a, \Lambda)$ in the Hilbert space $H$, and the fields $R_{\mu\nu\rho\sigma}(x)$ transform as tensor fields under $U(a, \Lambda)$:

$$U(a, \Lambda)\, R_{\mu\nu\rho\sigma}(x)\, U(a, \Lambda)^{-1} = \Lambda_{\mu}^{-1\,\alpha}\Lambda_{\nu}^{-1\,\beta}\Lambda_{\rho}^{-1\,\gamma}\Lambda_{\sigma}^{-1\,\delta} R_{\alpha\beta\gamma\delta}(\Lambda x + a)$$

(c) There exists a state $\Psi_0$ (vacuum state) which is invariant under $U(a, \Lambda)$:

$$U(a, \Lambda)\Psi_0 = \Psi_0.$$

(d) The spectrum of the generators of $U(a, 1)$ is contained in $V_+$:

$$V_+ \equiv \{\text{set of four vectors p such that } p^2 \geq 0,\ p^0 \geq 0\}.$$

The above conditions are rather mild assumptions and are satisfied in the standard quantizations of the Einstein equations, like the Gupta formulation or the radiation gauge method.[8]

In order to simplify the discussion, we will work in the weak field approximation. In this case $R_{\mu\nu\rho\sigma}(x)$ may be written in terms of lower order tensors $h_{\mu\nu}(x) = h_{\nu\mu}(x)$ (the gravitational potentials) in the following way[5]:

$$R_{\mu\nu\rho\sigma}(x) = \tfrac{1}{2}(\partial_\nu\partial_\rho\delta_\mu^\alpha\delta_\sigma^\beta + \partial_\mu\partial_\sigma\delta_\nu^\alpha\delta_\rho^\beta - \partial_\nu\partial_\sigma\delta_\mu^\alpha\delta_\rho^\beta - \partial_\mu\partial_\rho\delta_\nu^\alpha\delta_\sigma^\beta)h_{\alpha\beta}(x). \equiv D_{\mu\nu\rho\sigma}{}^{\alpha\beta}h_{\alpha\beta}(x) \tag{3}$$

Then, the quantization of the fields $R_{\mu\nu\rho\sigma}(x)$ reduces to the quantization of the fields $h_{\mu\nu}(x)$.

Corresponding to assumptions (a) and (b) we now make the following assumptions:

(a′) The fields $h_{\mu\nu}(x)$ are defined as operator valued distributions in $H$, and $\Psi_0$ is in the domain of $h(f) \equiv h_{\mu\nu}(f^{\mu\nu})$ for any test function $f^{\mu\nu}$.

(b′) The fields $h_{\mu\nu}(x)$ have the following transformation properties under the space-time translation group

$$U(a, 1)h_{\mu\nu}(x)U(a, 1)^{-1} = h_{\mu\nu}(x + a).$$

For a more detailed discussion of these assumptions, see Ref. 1.

In the following by covariant and/or weakly local theory we mean a theory in which we have

$$U(a, \Lambda)h_{\mu\nu}(x)U(a, \Lambda)^{-1} = \Lambda_{\mu}^{-1\,\rho}\Lambda_{\nu}^{-1\,\sigma}\, h_{\rho\sigma}(\Lambda x + a)$$

and/or

$$(\Psi_0, [h_{\mu\nu}(x), h_{\rho\sigma}(y)]\Psi_0) = 0 \quad \text{if } (x - y)^2 < 0.$$

We recall that the classical equations, whose quantization we are looking for, are the following ones:

$$R_{\mu\nu} = 0, \qquad \epsilon^{\alpha\beta\gamma\delta}\partial_\beta R_{\rho\sigma\gamma\delta} = 0.$$

They are the Einstein equations in the weak field approximation in vacuum.[5]

## 3. WEAK LOCAL COMMUTATIVITY AND UNPHYSICAL STATES

It has been previously shown[1] that in a weakly local theory satisfying the assumptions (a)–(d), (a′) and (b′), one cannot have

$$R_{\mu\nu}\Psi_0 = 0, \qquad \epsilon^{\alpha\beta\gamma\delta}\partial_\beta R_{\rho\sigma\gamma\delta}\Psi_0 = 0.$$

Then, if the theory must have any contact with the quantization of the Einstein equations, one is forced to have them satisfied at least in the mean. The weakest assumption one can make is to require that the Einstein equations are satisfied at least when one takes the mean values on the "physical" states. By "physical" states we mean the set $D_0$ of vectors which can be obtained from the vacuum state by applying polynomials in the smeared fields $R(f) \equiv R_{\mu\nu\rho\sigma}(f^{\mu\nu\rho\sigma})$. Thus we assume that

$$(\Psi, R_{\mu\nu}(f^{\mu\nu})\Phi) = 0, \tag{4}$$

where $\Phi, \Psi \in D_0$.

It is important to stress that Eqs. (4) are rather weak equations: As shown by the following theorem, they can be satisfied only in a proper subspace of $H$.

*Theorem 1:* In a weekly local theory with the properties (a)–(d), (a′) and (b′), the set of "physical" states $D_0$ on which Eq. (4) holds in the mean cannot be dense in $H$.

*Proof:* Let us assume that $D_0$ is dense in $H$. Then, by putting $\Phi = \Psi_0$ in Eq. (4) and by defining

$$\Phi = R_{\mu\nu}(f^{\mu\nu})\Psi_0,$$

one would get

$$(\Psi, \tilde{\Phi}) = 0,$$

where $\Psi$ runs over a dense subset of $H$. From this it follows

$$(\Psi_0, h_{\rho\sigma}\tilde{\Phi}) = 0,$$

i.e.,

$$(\Psi_0, h_{\rho\sigma}R_{\mu\nu}\Psi_0) = 0.$$

As proved in Ref. 1 this equation leads to a trivial theory.

As a consequence of Theorem 1, one cannot hope to realize a local quantum field theory of the Einstein equations in a Hilbert space $H$ in which the physical states form a dense subset of $H$. The unphysical states must be introduced in an essential way. If one denotes by $\bar{D}_0$ the closure of $D_0$, one has that $H - \bar{D}_0$ cannot be empty.

Moreover, one cannot expect that the unphysical states will play an irrelevant role. The presence of unphysical states is essential in order that $h_{\mu\nu}(x)$

be defined as a weakly local operator. As a matter of fact, one cannot hope to define $h_{\mu\nu}(x)$ as a weakly local operator leaving $\bar{D}_0$ invariant

$$h_{\mu\nu}(f^{\mu\nu})\bar{D}_0 \subset \bar{D}_0.$$

If this could be possible, one would get a Hilbert space $\bar{D}_0$ in which the Einstein equations would hold in the mean on a dense subset of states. As discussed in the previous theorem, this would lead to a trivial theory.

It is worthwhile to remark that the same results are obtained if, instead of weak local commutativity, one adds the requirements of covariance to assumptions (a)–(d), (a'), and (b'). Indeed, in a covariant nontrivial theory one cannot have[9]

$$(\Psi_0, h_{\rho\sigma}R_{\mu\nu}\Psi_0) = 0.$$

Thus the conclusions of the above theorem apply equally well.

Then, the introduction of unphysical states is a necessary step if one wants to define $h_{\mu\nu}(x)$ as a weakly local *and/or* covariant operator.

## 4. WEAK LOCAL COMMUTATIVITY AND INDEFINITE METRIC

It has been shown that the Einstein equations can be written in terms of a weakly local gravitational potential $h_{\mu\nu}(x)$, provided they are required to hold only as mean values on the "physical" states, which cannot be dense in $H$. One can strengthen the above result by showing that the equation

$$(\Phi, R_{\mu\nu}\Psi) = 0, \quad \forall\Phi, \Psi \in D_0 \tag{5}$$

can be satisfied only in a Hilbert space equipped with indefinite metric. Thus W.L.C. not only requires the introduction of unphysical states, but also the use of an idefinite metric, as stated in the following theorem.

*Theorem 2:* A weakly local gravitational potential satisfying the Einstein equations in the weak form (5) can be defined as an operator valued distribution with properties (a)–(d), (a'), and (b') of Sec. 2 only in a Hilbert space with indefinite metric. More precisely Eq. (5) may be assumed to hold only if the product $(\ ,\ )$ is defined as a sesquilinear form

$$(\Phi, \Psi) = \langle \eta\Phi, \Psi \rangle,$$

where $\langle\ ,\ \rangle$ is the scalar product in $H$, and $\eta$ is an indefinite Hermitian operator.

*Proof:* Putting $\Psi = \Psi_0 \in D_0$ and $\Phi = R_{\mu\nu}\Psi_0 \in D_0$ in Eq. (5), we have

$$\|R_{\mu\nu}\Psi_0\|^2 = 0. \tag{6}$$

If the metric is positive definite, Eq. (6) yields

$$R_{\mu\nu}\Psi_0 = 0$$

and consequently

$$(\Psi_0, h_{\rho\sigma}R_{\mu\nu}\Psi_0) = 0,$$

which allows us to conclude that the theory is trivial, as discussed in the previous section.

On the other hand, if $\eta \geq 0$, one may single out the subspace $H_0 \subset H$ consisting of vectors with vanishing norm

$$\Psi \in H_0 \quad \text{iff } (\Psi, \Psi) = 0.$$

By Lemma 4 of Ref. 1, the following property holds:

$$\Psi \in H_0 \quad \text{iff } (\Phi, \Psi) = 0 \quad \forall\Phi \in H.$$

Thus, Eq. (6) implies

$$R_{\mu\nu}\Psi_0 \in H_0$$

and, by putting $\Phi = h_{\rho\sigma}\Psi_0$, $\Psi = R_{\mu\nu}\Psi_0$ in Eq. (5) one has again

$$(\Psi_0, h_{\rho\sigma}R_{\mu\nu}\Psi_0) = 0.$$

This implies that the theory is trivial.

In conclusion, a quantum field theory of the Einstein equations can be formulated in terms of a weakly local potential $h_{\mu\nu}(x)$ only if one is prepared to have unphysical states and indefinite metric as essential features of the Hilbert space in which the theory is defined.

## 5. LORENTZ COVARIANCE AND INDEFINITE METRIC

The results of the previous section can be easily extended to the case of a covariant theory in which the Einstein equations are required to hold in the mean. We have the following.

*Theorem 3:* A covariant gravitational potential satisfying the Einstein equations in the weak form (5) can be defined as an operator valued distribution with properties (a'), (b'), (c), and (d) of Sec. 2 only in a Hilbert space with indefinite metric.

*Proof:* By the same technique used in the proof of Theorem 2, if $\eta \geq 0$ one finds

$$(\Psi_0, h_{\rho\sigma}R_{\mu\nu}\Psi_0) = 0,$$

which, together with the assumption of covariance, implies that the theory is trivial.

This result is not strictly connected with the request of having a theory of the Einstein equations. Indeed, if we add the hypothesis of weak local commutativity, we find that *any covariant theory of spin two massless particles* must be formulated in a Hilbert space equipped with indefinite metric.

*Theorem 4:* A field $h_{\mu\nu}(x)$ describing massless spin-2 particles can be defined as a weakly local and covariant operator valued distribution only in a Hilbert space with indefinite metric.

*Proof:* Let us assume that the metric operator may be semipositive ($\eta \geq 0$).

The two point function

$$W_{\mu\nu\rho\sigma} = (\Psi_0, h_{\mu\nu}(x)h_{\rho\sigma}(y)\Psi_0) \tag{7}$$

transforms according to a representation of the Lorentz group

$$W_{\mu\nu\rho\sigma}(\Lambda^{-1}x) = \Lambda_{\mu}^{-1\,\alpha}\Lambda_{\nu}^{-1\,\beta}\Lambda_{\rho}^{-1\,\gamma}\Lambda_{\sigma}^{-1\,\delta}W_{\alpha\beta\gamma\delta}(x).$$

Weak local commutativity implies that $W_{\mu\nu\rho\sigma}(x)$ can be regarded as the boundary value of a function $W_{\mu\nu\rho\sigma}(z)$ which is analytic in the extended tube $\mathcal{T}'$, and that Eq. (7) can be analytically continued to complex $\Lambda$.[10] Thus, $W_{\mu\nu\rho\sigma}(z)$ yields a representation of the complex Lorentz group $L_+(C)$ and one may use the Araki–Hepp theorem[11] to prove that $W_{\mu\nu\rho\sigma}(x)$ can be written in the following way[9]:

$$\begin{aligned}W_{\mu\nu\rho\sigma}(x) &= (g_{\mu\rho}g_{\nu\sigma} + g_{\gamma\sigma}g_{\mu\sigma})F_1(x) + g_{\mu\nu}g_{\rho\sigma}F_2(x)\\ &+ g_{\mu\nu}\partial_\rho\partial_\sigma F_3(x) + g_{\rho\sigma}\partial_\mu\partial_\nu F_4(x) + \partial_\rho\partial_\sigma\partial_\nu F_5(x)\\ &+ (g_{\mu\nu}\partial_\nu\partial_\sigma + g_{\nu\sigma}\partial_\mu\partial_\rho + g_{\nu\rho}\partial_\mu\partial_\sigma + g_{\mu\sigma}\partial_\nu\partial_\rho)F_6(x),\end{aligned}$$

where $F_i(x)$, $i = 1, \ldots, 6$, are Lorentz invariant distributions. Now, the invariant distributions are multiplied by independent tensors.[12] Thus, the analyticity of $W_{\mu\nu\rho\sigma}(z)$ in $\mathcal{T}'$ yields the analyticity in $\mathcal{T}'$ of each invariant function $F_i(x)$. This implies that each distribution $F_i(x)$ must satisfy weak local commutativity

$$F_i(x) = F_i(-x), \qquad \text{if } x^2 < 0.$$

Furthermore, since the field $h_{\mu\nu}(x)$ describes massless particles, it must obey the equation

$$\Box\, h_{\mu\nu} = 0,$$

which implies

$$\Box\, F_i = 0$$

Hence we have[13]

$$F_i(x) = c_i + d_i\Delta^+(x),$$
$$\Delta^+(x) = \frac{i}{2(2\pi)^3}\int e^{-ikx}\frac{d^3k}{|k_0|}.$$

In view of the spectral condition, the integral is taken over the cone

$$k^2 = 0, \qquad k_0 \geq 0.$$

As a consequence, we can write

$$\begin{aligned}\|h(f)\Psi_0\|^2 &= a\bar{\hat{f}}^{\rho\sigma}(0)\hat{f}_{\rho\sigma}(0) + b\int\frac{d^3k}{k_0}\bar{\hat{f}}_{\rho\sigma}(k)\hat{f}^{\rho\sigma}(k)\\ &+ c\,|\hat{f}^{\rho}{}_{\rho}(0)|^2 + d\int\frac{d^3k}{k_0}\,|\hat{f}^{\mu}{}_{\mu}(k)|^2\\ &+ e\int\bar{\hat{f}}_{\mu}\ (k)k_\rho k_\sigma\hat{f}^{\rho\sigma}(k)\frac{d^3k}{k_0} + f\int k_\mu k_\nu\bar{\hat{f}}^{\mu\nu}\hat{f}_{\rho}{}^{\rho}\frac{d^3k}{k_0}\\ &+ g\int\hat{f}^{\mu\nu}(k)\bar{\hat{f}}_{\mu}{}^{\sigma}\,k_\nu k_\sigma\frac{d^3k}{k_0} + h\int|k_\mu k_\nu\hat{f}^{\mu\nu}|^2\frac{d^3k}{k_0},\end{aligned}$$

where $a, \ldots, h$ are suitable constants and

$$\hat{f}(k) = (2\pi)^{-2}\int f(x)e^{ikx}d^4x$$

is the Fourier transform of the test function. We may choose a test function with the following properties:

$$\hat{f}_1^{00} = 3e^{-\omega(k_0^2+\mathbf{k}^2)}, \qquad \hat{f}_1^{11} = \hat{f}_1^{22} = \hat{f}_1^{33} = e^{-\omega(k_0^2+\mathbf{k}^2)}, \qquad \omega > 0,$$

whereas all the other components vanish:

$$\hat{f}_1^{ij} = 0, \qquad i \neq j.$$

Then we have

$$\|h(f_1)\Psi_0\|^2 = 12a + 6\pi(b/\omega) + \pi g(1/\omega^2) + \tfrac{1}{2}\pi\, h(1/\omega^3).$$

Hence, if $\eta \geq 0$, $a$ and $h$ must be real and positive. On the other hand, by choosing

$$\hat{f}_2^{01} = \hat{f}_2^{10} = \hat{f}_2^{02} = \hat{f}_2^{20} = \hat{f}_2^{30} = e^{-\omega(k_0^2+\mathbf{k}^2)}, \qquad \omega > 0$$

and the other components equal to zero, we obtain

$$\|h(f_2)\Psi_0\|^2 \leq -6a - 3\pi(b/\omega) - \tfrac{1}{4}\pi g(1/\omega^2) + \tfrac{3}{8}\pi h(1/\omega^3),$$

which requires $a \leq 0$, if $\eta \geq 0$. Thus we must have

$$a = 0$$

and consequently

$$b = g = 0.$$

In conclusion we have

$$W_{\mu\nu\rho\sigma} = g_{\mu\nu}g_{\rho\sigma}F_2 + W'_{\mu\nu\rho\sigma},$$

where $W'_{\mu\nu\rho\sigma}$ does not contribute to the two-point function

$$(\Psi_0, R_{\alpha\beta\gamma\delta}\,R_{\lambda\mu\nu\rho}\Psi_0) = D_{\alpha\beta\gamma\delta}^{\epsilon\eta}\,D_{\lambda\mu\nu\rho}^{\sigma\tau}W_{\epsilon\eta\sigma\tau}.$$

The only contributing part is $g_{\mu\nu}g_{\rho\sigma}\,F_2$; but the part of $h_{\mu\nu}$ proportional to $g_{\mu\nu}$ has no spin-2, and therefore $D_{\lambda\mu\nu\rho}^{\sigma\tau}h_{\sigma\tau}\Psi_0$ cannot be a state containing a physical spin-2 particle.

Thus the request of a positive or semipositive metric forces us to have a two-point function which cannot describe physical gravitons. It follows that a covariant and local description of a spin-2 massless field by means of a potential $h_{\mu\nu}(x)$ can be made only by using an indefinite metric.

## 6. LOCAL AND COVARIANT QUANTIZATIONS OF EINSTEIN EQUATIONS

According to the results of the previous sections any local and covariant theory must involve unphysical states and use an indefinite metric. These are the peculiar features of Gupta formulation, and in fact we will prove in this section that any local and covariant quantization of Einstein equations reduces essentially to Gupta formulation.

To this purpose we start by investigating the characteristic properties of any local and covariant quantization of Einstein equations in terms of the potentials $h_{\mu\nu}(x)$.

(0) From the previous sections, in order to have a nontrivial theory, $h_{\mu\nu}(x)$ may be defined as a local and covariant operator valued distribution only if the Hilbert space $H$ is equipped with an indefinite metric. We denote by $\eta$ the metric operator.

(1) From Sec. 3 one knows that not all the vectors of $H$ may describe physical states.[14] The identification of the *vectors describing physical states* may actually depend on the formulation of the theory, i.e., on the subsidiary conditions one chooses. In any acceptable theory, however, the vectors of the form $\mathcal{P}(R_{\alpha\beta\gamma\delta}(f^{\alpha\beta\gamma\delta}))\Psi_0$, where $\mathcal{P}$ is a polynomial in the

smeared fields $R_{\alpha\beta\gamma\delta}(f^{\alpha\beta\gamma\delta})$ and $\Psi_0$ is the vacuum state, may be given a physical meaning. Thus, independently of the quantization procedure, the vectors belonging to $D_0$,

$$D_0 \equiv \{\text{set of vectors of the form } \Psi = \mathcal{P}(R(f))\Psi_0\}, \quad (\alpha)$$

are candidates to describe physical states. The subsidiary condition must therefore be chosen in such a way that it is satisfied by vectors belonging to $D_0$.

(2) According to Sec. 3 the Einstein equations cannot hold as weak equations (Eq. 1). They should however hold as mean values on the vectors of $D_0$, i.e,

$$(\Psi, R_{\mu\nu}\Phi) = 0,$$

where $\Psi$ and $\Phi$ are vectors of $D_0$.

In particular, by taking $\Psi = R_{\mu\nu}\Phi$ one gets

$$(R_{\mu\nu}\Phi, R_{\mu\nu}\Phi) = 0. \quad (\beta)$$

Therefore, in any local and covariant theory the Einstein equations must yield vectors of zero norm when applied to vectors of $D_0$.

As we will see below the above conditions $(\alpha)$ and $(\beta)$ uniquely fix the possible formulation in a Fock space.

As a first step, we define the Hilbert space as a Fock space

$$H = \sum_{n=0}^{\infty} H_n,$$

where $H_0 = C$ and $H_n$ is the set of the tensors of rank $2n$ defined on the direct product of the momentum space cones and having the following properties:

$$\Phi \cdots_{\mu_i\nu_i} \cdots = \Phi \cdots_{\nu_i\mu_i} \cdots \quad (8)$$

$$\Phi \cdots_{\mu_i\nu_i} \cdots_{\mu_j\nu_j} \cdots (\cdots k_i, \cdots k_j, \cdots) = \Phi \cdots_{\mu_j\nu_j} \cdots_{\mu_i\nu_i} \cdots (\cdots k_j, \cdots k_i, \cdots),$$

$$\int \frac{d^3k_1}{k_0^1} \cdots \frac{d^3k_n}{k_0^n} \, |\Phi_{\mu_i\nu_i \cdots \mu_n\nu_n}|^2 < \infty. \quad (9)$$

The scalar product between two vectors

$$\Phi \equiv (\Phi^0, \Phi^1, \cdots), \qquad \Psi \equiv (\Psi^0, \Psi^1, \cdots)$$

is defined as follows:

$$\langle \Phi, \Psi \rangle = \sum_{n=0}^{\infty} \langle \Phi^n, \Psi^n \rangle = \sum_{n=0}^{\infty} 2\pi \int \frac{d^3k_1}{k_0^1} \cdots \frac{d^3k_n}{k_0^n} \times \sum_{r=1}^{n} \sum_{\mu_r,\nu_r=0}^{3} \overline{\Phi}^n_{\mu_1 \cdots \nu_n} \Psi^n_{\mu_1 \cdots \nu_n}$$

Since the vectors of $H$ have finite norm,

$$\Psi = (\Psi^0, \Psi^1, \cdots) \in H$$

if and only if

$$\langle \Psi, \Psi \rangle = \sum_{n=0}^{\infty} \langle \Psi^n, \Psi^n \rangle < \infty.$$

A representation of the Poincaré group in the Hilbert space is given in the following way:

$$U(a, \Lambda)\Phi^n_{\mu_1 \cdots \nu_n}(k_1, \ldots, k_n) = e^{i\Sigma k_j a} \Lambda_{\mu_1}^{\rho_1} \cdots \Lambda_{\nu_n}^{\sigma_n} \Phi^n_{\rho_1 \cdots \sigma_n}(\Lambda^{-1}k_1, \ldots, \Lambda^{-1}k_n).$$

The potential $h_{\mu\nu}(x)$ is assumed to be an operator valued tempered distribution on $H$.

As proved in the previous sections, the arbitrariness in the quantization of Einstein equations may be only in

(i) the representation of the operator $h_{\mu\nu}$,

(ii) the identification of the physical states by means of a subsidiary condition,

(iii) the choice of the sesquilinear form

$$(\Phi, \Psi) = \langle \eta\Phi, \Psi \rangle$$

in terms of which one has to compute all the physically meaningful quantities like transition probabilities, vacuum expectation values, etc.

As we will see, conditions $(\alpha)$ and $(\beta)$ reduce this arbitrariness to a one-parameter family of subsidiary conditions, and all the corresponding theories are isometrically equivalent.

### A. Representation of $h_{\mu\nu}$

The most general way of representing $h_{\mu\nu}(x)$ as a covariant and local operator is the following

$$(h(f)\Phi) = \Psi^n, \qquad h(f) = \int h_{\mu\nu}(x) f^{\mu\nu}(x) d^4x,$$

$$\Psi^n_{\mu_1 \cdots \nu_n}(k_1, \ldots, k_n) \equiv \sqrt{n} \sqrt{n+1} \int \frac{d^3k}{k_0} \, [\alpha' \hat{f}^{\mu\nu}(k) \times \Phi^{n+1}_{\mu\nu\mu_1\nu_1 \cdots \nu_n} + \alpha \hat{f}_\tau{}^\tau \Phi^{n+1}_{\mu\ \mu_1 \cdots \nu_n}(k, k_1, \ldots, k_n)] + \sqrt{\frac{\pi}{n}} \sum_{j=1}^{n} [\beta' \hat{f}_{\mu_j\nu_j}(-k_j) + \beta g_{\mu_j\nu_j} \hat{f}_\lambda{}^\lambda] \times \Phi^{n-1}_{\mu_1 \cdots \mu_{j-1}\nu_{j-1}\mu_{j+1}\nu_{j+1} \cdots \nu_n}(\cdots k_{j-1}, k_{j+1} \cdots). \quad (10)$$

As a consequence of this definition and of the tensor character of the $\Phi$'s, $h_{\mu\nu}(x)$ transforms covariantly under the Poincaré group

$$U(a, \Lambda)h_{\mu\nu}(x)U(a, \Lambda)^{-1} = \Lambda_\mu^{-1\rho}\Lambda_\nu^{-1\sigma} h_{\rho\sigma}(\Lambda x + a).$$

Furthermore, by using Eq. 10 it is easy to check that the following commutation rules hold:

$$[h_{\mu\nu}(x), h_{\lambda\rho}(y)] = [\alpha'\beta'(g_{\mu\lambda}g_{\nu\rho} + g_{\nu\rho}g_{\mu\lambda}) + 2(\alpha'\beta' + \alpha\beta' + 4\alpha\beta) g_{\mu\nu}g_{\lambda\rho}]\Delta(x - y), \quad (11)$$

$$\Delta(x) = \Delta^+(x) + \Delta^-(x) = \Delta^+(x) - \Delta^+(-x).$$

Thus $h_{\mu\nu}(x)$ is both local and covariant.

### B. Subsidiary Condition

Now we try to characterize the set of physical states $D_0$ by means of a supplementary condition. We note that if

$$\Phi = R_{\alpha\beta\gamma\delta}(\tfrac{1}{4} f^{\alpha\beta\gamma\delta})\Psi_0,$$

then the component of $\Phi$ in the one-particle space is given by

$$\Phi^1_{\mu\nu} = -\beta' k^\lambda k^\rho \hat{f}_{\lambda\mu\nu\rho} - \beta g_{\mu\nu} k^\lambda k^\rho \hat{f}_{\sigma\lambda\rho}{}^\sigma, \quad (12)$$

and $\Phi^1_{\mu\nu}$ satisfies the following condition:

$$k_\mu \Phi^{1\,\mu\nu} + qk^\nu \Phi^{1\,\sigma}_{\sigma} = 0, \tag{13}$$

where $q$ is the solution of the equation

$$\beta' q + 4\beta q + \beta = 0. \tag{14}$$

One may assume $\beta' \neq 0$, since, otherwise, $D_0$ would consist only of vectors describing scalar gravitons. Besides that, this choice is necessary if one wants consistency with the Einstein equations, as will be discussed in Sec. 11.

Furthermore, one may fix the normalization of $h_{\mu\nu}$ in such a way that $\beta' = 1$. Then Eq. (14) reduces to

$$q + 4\beta q + \beta = 0. \tag{15}$$

This equation has no solution for $q$ if $\beta = -\frac{1}{4}$, and, conversely, there is no solution for $\beta$ if $q = -\frac{1}{4}$. The case $q = -\frac{1}{4}(\beta = -\frac{1}{4})$ is equivalent to the case $\beta' = 0$, and will be discussed in Sec. 11.

In a similar way, one may easily verify that each tensor $\Phi^{n+1}$ in the representation

$$\Phi = \mathcal{P}(R(f))\Psi_0 = (\Phi^0, \Phi^1, \cdots)$$

obeys Eq. (13) for each pair of indices $\mu_i\nu_i$. Thus, we have shown that all the physical states are contained in the subspace $H'_q$

$$H'_q \equiv \{\Phi : \Phi = (\Phi^0, \Phi^1, \cdots), \Phi^{n+1} \text{ obeys Eq. (13)}\}$$

The subscript $q$ will sometimes be omitted in the following.

In conclusion, we take the equation

$$k_\mu \Phi^{\mu\nu\cdots} + qk^\nu \Phi_\sigma{}^{\sigma\cdots} = 0$$

as the subsidiary condition, identifying the subspace of "physical" states.

### C. Choice of the Metric Operator

On the "physical" states, the most general form of a covariant metric operator not involving derivatives is the following:

$$(\eta\Phi)^n_{\mu_1\nu_1\cdots\mu_n\nu_n} = \prod_{i=1}^{n} (\lambda' g_{\mu_i\rho_i} g_{\nu_i\sigma_i} - \lambda g_{\mu_i\nu_i} g_{\rho_i\sigma_i}) \Phi^{\cdots\rho_i\sigma_i\cdots}, \tag{16}$$

where $\lambda', \lambda$ are up to now indetermined parameters.

Obviously we have $\eta = \eta^+$. As far as $\lambda'$ is concerned, we can exclude the case $\lambda' = 0$, since then, from the equation

$$(R_{\mu\nu}(f^{\mu\nu})\Psi_0, R_{\mu\nu}(f^{\mu\nu})\Psi_0) = 0, \tag{17}$$

one would get

$$(1 + 4\beta)^2 |k_\rho k_\sigma \hat{f}^{\rho\sigma}|^2 = 0,$$

i.e., $\beta = -\frac{1}{4}$, which is in contradiction with Eq. (15). Then, without loss of generality, we can put $\lambda' = 1$.

Using the definition of $\eta$, it is easy to see that the Hermiticity of the observable fields $R_{\mu\nu\rho\sigma}(f^{\mu\nu\rho\sigma})$, fixes the value of $\alpha'$:

$$\alpha' = \beta' = 1.$$

[Needless to say, Hermiticity as well as unitarity are defined with respect to the metric operator $\eta$,

$$(\Psi, R_{\lambda\mu\nu\rho}\Phi) = (R^+_{\lambda\mu\nu\rho}\Psi, \Phi) = (R_{\lambda\mu\nu\rho}\Psi, \Phi),$$
$$R^+_{\lambda\mu\nu\rho} = \eta^{-1} R^*_{\lambda\mu\nu\rho}\eta = R_{\lambda\mu\nu\rho},$$

$R^*_{\lambda\mu\nu\rho}$ being the adjoint of $R_{\lambda\mu\nu\rho}$ according to the ordinary scalar product in $H$.]

By using condition $(\beta)$, one may show that there is a constraint between $\lambda$ and $q$. One has, in fact,

$$(R^{\lambda\sigma}(f_{\lambda\sigma})\Psi_0)^1_{\mu\nu} \equiv \Phi^1_{\mu\nu} = k^\lambda k_\mu f_{\lambda\nu} + k^\lambda k^\lambda k_\nu f_{\lambda\mu} - (2\beta + 1) g_{\mu\nu} k^\rho k^\sigma f_{\rho\sigma},$$

and condition (17) yields

$$\lambda = \{[4\beta(2\beta + 1) + 1]/[2(4\beta + 1)^2]\} = \tfrac{1}{2}(8q^2 + 4q + 1). \tag{18}$$

The case $\beta = -\frac{1}{4}$ (or $q = -\frac{1}{4}$) is excluded as before. In conclusion we have

*Statement 1:* In any quantization of Einstein equations in terms of a local and covariant operator $h_{\mu\nu}(x)$ satisfying conditions $(\alpha)$ and $(\beta)$, the choice of the metric operator cannot be made independently of the definition of $h_{\mu\nu}$ and the constraint is given by Eq. (18).

Now we want to show an important property of $\eta$ derived from the above equation.

*Statement 2:* If $\eta$ is such that $\|R_{\mu\nu}\Psi\|^2 = 0$, then it is semipositive in the subspace $H'$ defined by Eq. (13).

*Proof:* For the sake of simplicity we restrict ourselves to one-particle states. They obey the equation

$$k_\mu \Phi^{\mu\nu} + qk^\nu \Phi_\sigma{}^\sigma = 0,$$

which is convenient to explicitate in a frame of reference in which $k^\mu = (k, 0, 0, k)$. In that frame $N(\Phi) \equiv \bar{\Phi}^{\mu\nu}\Phi_{\mu\nu} - \lambda |\Phi_\sigma{}^\sigma|^2$, with $\lambda$ obeying Eq. (18), is a quadratic form

$$N(\Phi) = \sum a_{ij} \bar{z}_i z_j,$$

where $z_1 = \Phi^{00}$, $z_2 = \Phi^{33}$, $z_3 = \Phi^{11}$, $z_4 = \Phi^{12}$, and

$$a_{ij} = \begin{pmatrix} \frac{1}{2} - \frac{\lambda}{2q^2} + \left(\frac{1}{2q} + 1\right)^2 & -\frac{1}{2} - \left(\frac{1}{2q} + 1\right)^2 + \frac{\lambda}{4q^2} & -\left(\frac{1}{2q} + 1\right) & 0 \\ -\frac{1}{2} + \frac{\lambda}{2q} - \left(\frac{1}{2q} + 1\right)^2 & \frac{1}{2} + \left(\frac{1}{2q} + 1\right)^2 - \frac{\lambda}{4q^2} & \frac{1}{2q} + 1 & 0 \\ -\left(\frac{1}{2q} + 1\right) & \frac{1}{2q} + 1 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

The eigenvalues of $a_{ij}$ are the following: $x_1 = 0$, $x_2 = 0$, and the roots of the equation

$$x^2 - 2(1+k)x + 4k - 2H = 0,$$
$$H \equiv (1/2q+1)^2, \quad k = \tfrac{1}{2} - \lambda/4q^2 + (1/2q+1)^2.$$

The conditions for the semipositiveness of the roots are

$$\lambda < 10q^2 + 4q + 1, \quad \lambda \leq \tfrac{1}{2}(8q^2 + 4q + 1),$$

which are both satisfied, since $\|R_{\mu\nu}\Psi_0\|^2 = 0$ implies Eq. (18). The conclusion is still valid also for $q = 0$. In that case one has $\lambda = \frac{1}{2}$ and

$$N(\Phi) = 2|\Phi^{12}|^2 + \tfrac{1}{2}|\Phi^{11} - \Phi^{12}|^2 \geq 0,$$
$$\|\Phi\|^2 = 2\pi \int N(\Phi)\frac{d^3k}{k_0} \geq 0.$$

We conclude this section by showing that there is a connection between the parameter $q$(or $\lambda$, or $\beta$) and the parameter $\alpha$ occuring in the definition (10) of $h_{\mu\nu}$. This is a consequence of condition ($\beta$).

*Theorem 5:* If $\|R_{\mu\nu}\Psi_0\| = 0$, the Einstein equations hold as mean values in $D_0$ if

$$q = -\tfrac{1}{2}(1 + 2\alpha) \tag{19}$$

and, conversely, if Eq. (19) holds, the Einstein equations hold as mean values on $H'_q$.

*Proof:* By taking a vector $\Phi \in D_0$ of the following form

$$\Phi = (0, \Phi^1_{\mu\nu}, 0, \cdots),$$

one has

$$(\Psi_0, R_{\mu\nu}(f^{\mu\nu})\Phi) = 0.$$

The above equation implies

$$\int \frac{d^3k}{k_0}\,[(1+2\alpha)k^\rho k^\sigma f_{\rho\sigma}\Phi^1{}_\lambda{}^\lambda - k_\mu k^\rho f_{\rho\nu}\Phi^{\mu\nu} - k_\nu k^\rho f_{\rho\mu}\Phi^{\mu\nu}] = 0.$$

Therefore one must have

$$-\tfrac{1}{2}(1+2\alpha) = q.$$

To prove the second part, as $\eta \geq 0$ in $H'$ by statement 2, it is sufficient to show that $R_{\mu\nu}H' \subset H'' \equiv \{$set of vectors of $H'$ with vanishing norm$\}$. It is easy to see that both the negative and positive frequency part of $R_{\mu\nu}$ maps $H'$ into $H'$. Therefore it suffices to see that

$$\|R^-_{\mu\nu}\Psi\|^2 = 0 = \|R^+_{\mu\nu}\Psi\|, \quad \forall\Psi \in H'.$$

The first of the above equations involving the negative frequency part is easily verified by remembering the definition of $\eta$:

$$(\hat{t}_{\mu\nu} + \beta g_{\mu\nu}\hat{t}_\sigma{}^\sigma)(\hat{t}^{\mu\nu} + \beta g^{\mu\nu}\hat{t}_\sigma{}^\sigma) - \lambda(1+4\beta)|\hat{t}_\sigma{}^\sigma|^2 = 0,$$
$$\hat{t}^{\mu\nu} \equiv k^\mu k_\rho \hat{f}^{\rho\nu} + k^\nu k_\rho \hat{f}^{\rho\mu} - g^{\mu\nu}k_\rho k_\sigma \hat{f}^{\rho\sigma}.$$

For the positive frequency part we note that

$$\hat{t}^{\mu\nu}\Psi_{\mu\nu} + \alpha\hat{t}_\sigma{}^\sigma\Psi_\rho{}^\rho = k^\mu\Psi_{\mu\nu}k_\rho\hat{f}^{\rho\nu} + k^\nu\Psi_{\mu\nu}k_\rho\hat{f}^{\rho\mu} - k_\lambda k_\rho \hat{f}^{\lambda\rho}\Psi_\tau{}^\tau - 2\alpha k_\lambda k_\rho \hat{f}^{\lambda\rho}\Psi_\tau{}^\tau$$
$$= -(1 + 2\alpha + 2q)k_\lambda k_\rho \hat{f}^{\lambda\rho}\Psi_\tau{}^\tau = 0,$$

since $\Psi \in H'$

Thus $R_{\mu\nu}\Psi \in H''$ and this implies

$$(\Phi, R_{\mu\nu}\Psi) = 0, \quad \forall\Phi, \Psi \in H'.$$

## 7. PHYSICAL STATES AND EQUIVALENCE CLASSES

In this section we will further inquire on the structure of $H'_q$ and arrive at a consistent identification of physical states. The first step is to identify those vectors of $H'_q$ which cannot describe physically realizable states. This amounts to characterize those states of $H'_q$ with zero norm. For the sake of simplicity we will discuss the one-particle states. The extension to many particle states is straightforward.

*Statement 3:* The one-particle vectors of $H'_q$ with vanishing norm have the form

$$\Phi_{\mu\nu} = k_\mu F_\nu + k_\nu F_\mu - [(1+2q)/(1+4q)]g_{\mu\nu}k_\sigma F^\sigma. \tag{20}$$

*Proof:* In a frame of reference in which $k = (k, 0, 0, k)$ we have, according to Eqs. (13) and (18),

$$N(\Phi) = \bar{\Phi}^{\mu\nu}\Phi_{\mu\nu} - \lambda|\Phi_\rho{}^\sigma|^2 = |[1/2q) + 1](1/\sqrt{2}) \times (\Phi^{33} - \Phi^{00}) + \sqrt{2}\,\Phi^{11}|^2 + 2|\Phi^{12}|^2.$$

The condition of vanishing norm is equivalent to the following equations:

$$\Phi^{12} = 0, \quad [(1/2q) + 1](1/\sqrt{2})(\Phi^{33} - \Phi^{00}) + \sqrt{2}\,\Phi^{11} = 0.$$

Then $\Phi_{\mu\nu}$ has the following form:

$$\Phi^{\mu\nu} = \begin{pmatrix} \Phi^{00} & \Phi^{01} & \Phi^{02} & \tfrac{1}{2}(\Phi^{00} + \Phi^{33}) \\ \Phi^{01} & \frac{1}{2}\left(\frac{1}{2q} + 1\right)(\Phi^{00} - \Phi^{33}) & 0 & \Phi^{01} \\ \Phi^{02} & 0 & \frac{1}{2}\left(\frac{1}{2q} + 1\right)(\Phi^{00} - \Phi^{33}) & \Phi^{02} \\ \tfrac{1}{2}(\Phi^{00} + \Phi^{33}) & \Phi^{01} & \Phi^{02} & \Phi^{33} \end{pmatrix}$$

and can be written as

$$\Phi^{\mu\nu} = k^\mu F^\nu + k^\nu F^\mu - [(1+2q)/(1+4q)]\,g^{\mu\nu}k_\sigma F^\sigma.$$

Here $F^\mu$ is a tensor with components:

$$F^0 = \frac{1+6q}{8kq}\Phi^{00} - \frac{1+2q}{8kq}\Phi^{33}, \quad F^1 = \frac{\Phi^{01}}{k},$$

$$F^2 = \frac{\Phi^{02}}{k}, \qquad F^3 = -\frac{1+2q}{8kq}\,\Phi^{00} + \frac{1+6q}{8kq}\,\Phi^{33},$$

$$k_\sigma F^\sigma = \frac{1+4q}{4q}(\Phi^{00} - \Phi^{33})$$

in the frame chosen above. The case $q = 0$ is not exceptional, since then $\Phi^{00} = \Phi^{33}$.

In order to formulate a sensible theory of gravitation, we must be able to associate a vector of positive norm to a physical state, and to make the presence of unphysical states irrelevant. In this way we can compute the physically meaningful quantities, according to the general laws of quantum mechanics.

We may not identify physical states with vectors of $H'-H''$, since this splitting is not Lorentz invariant. A state having no component in $H''$ in a given frame of reference may acquire an unphysical component after a Lorentz transformation. Therefore one is led to introduce equivalence classes: All the vectors which differ only by their components in $H''$ lie in the same class. One may then associate the physical states to the equivalence classes of the quotient space $H'/H''$. This definition is Lorentz invariant since $H'$ and $H''$ are separately Lorentz invariant.

One may define the norm of a physical state (i.e., the norm of an equivalence class of $H'/H''$) as the norm of a vector belonging to the given equivalence class. This definition does not depend on the choice of the vector in the equivalence class. In this way the norm of a physical state is clearly positive definite. Moreover, in $H'/H''$ the Einstein equations are satisfied as a consequence of Theorem 5.

## 8. SPIN CONTENT OF THE THEORY

The physical interpretation of the theory given so far may be further justified by a group theoretical approach. One may show, in fact, that the equivalence classes discussed in the previous section yield a representation of the Poincaré group corresponding to massless particles of spin 2.

The analysis of the problem from a group theoretical point of view will moreover strengthen the results of the previous sections by showing that an acceptable representation of the Poincaré group can be obtained only in the quotient space $H'/H''$.

The representations of the Poincaré group corresponding to massless particles are usually characterized by the condition[15]:

$$W^2 = W^\mu W_\mu = 0,$$

where $W_\mu$ is the helicity operator defined by

$$W^\mu = \tfrac{1}{2}\epsilon^{\mu\nu\rho\sigma} M_{\nu\rho} P_\sigma$$

Now, in the space of symmetric tensors $\Phi_{\mu\nu}(x)$, the representation of the generators of the Poincaré group is the following:

$$(P_\mu \Phi)_{\rho\sigma} = i\partial_\mu \Phi_{\rho\sigma}(x),$$

$$i(M_{\mu\nu}\Phi)_{\rho\sigma} = (x_\mu \partial_\nu - x_\nu \partial_\mu)\,\Phi_{\rho\sigma} + g_{\mu\rho}\Phi_{\nu\sigma} - g_{\nu\rho}\Phi_{\mu\sigma} + g_{\mu\sigma}\Phi_{\nu\rho} - g_{\nu\sigma}\Phi_{\mu\rho}.$$

Therefore, in momentum space, in the case of vanishing mass, the operators $W_\mu$ and $W^2$ act in the following way:

$$(W^\mu \Phi)^{\rho\sigma}(k) = -i(\epsilon^\mu{}_\rho{}^{\beta\lambda} k_\lambda \Phi_{\beta\sigma} + \epsilon^\mu{}_\sigma{}^{\beta\lambda} k_\lambda \Phi_{\beta\rho}), \tag{21}$$

$$(W^2\Phi)^{\rho\sigma} = 2k^\rho k_\beta \Phi^{\beta\sigma} + 2k^\sigma k_\beta \Phi^{\beta\rho} - g^{\rho\sigma} k^\alpha k^\beta \Phi_{\alpha\beta} - k^\rho k^\sigma \Phi_\tau{}^\tau. \tag{22}$$

The condition $W^2 = 0$ becomes

$$2k^\rho k_\beta \Phi^{\beta\sigma} + 2k^\sigma k_\beta \Phi^{\beta\rho} - g^{\rho\sigma} k^\alpha k^\beta \Phi_{\alpha\beta} - k^\rho k^\sigma \Phi_\tau{}^\tau = 0. \tag{23}$$

By multiplying the above equation by $k_\rho$ one has

$$k_\alpha k_\beta \Phi^{\alpha\beta} = 0,$$

and therefore Eq. (23) implies

$$k_\beta \Phi^{\beta\sigma} - \tfrac{1}{4} k^\sigma \Phi_\tau{}^\tau = 0.$$

In conclusion, the subspace of $H$ on which $W^2 = 0$ coincides with the set of vectors satisfying the Hilbert Lorentz condition with $q = -\frac{1}{4}$. As it has been remarked (see also Sec. 6) these vectors cannot correspond to physical states and therefore one cannot identify $H'_{q=-1/4}$ with the subspace $H'$ of "physical" states. This difficulty has no counterpart in quantum electrodynamics where the condition $W^2 = 0$ does identify the subspace $H'$ of "physical" states.

*Statement 4:* In the Hilbert space $H$ of symmetric tensors defined in Sec. 6 the condition $W^2 = 0$, can be required only in the weak sense:

$$W^2 H' \subset H''. \tag{24}$$

Equation (24) is indeed satisfied for $\Phi_{\mu\nu} \in H'_q (q \neq -\frac{1}{4})$.

Equation (24) guarantees that the representation of the Poincaré group in $H'/H''$ corresponds to massless particles. In order to complete the group theoretical analysis, one must discuss the eigenvalues of the helicity operator in $H'/H''$, i.e., the spin content of the theory.

The eigenvalue equation is the following:

$$\epsilon_{\mu\rho\beta\gamma} k^\gamma \Phi_\sigma^\beta + \epsilon_{\mu\sigma\beta\gamma} k^\gamma \Phi_\rho^\beta = i\lambda k_\mu \Phi_{\rho\sigma} + k_\rho T_{\mu\sigma} + k_\sigma T_{\mu\rho} - [(1+2q)/(1+4q)]\, g_{\rho\sigma} k^\tau T_{\mu\tau}. \tag{25}$$

The second term on the right-hand side is a vector of $H''(q)$, whose general form has been already discussed in Sec. 7. The eigenvalue equation must in fact be solved in $H'/H''$, i.e., up to vectors of $H''$. A detailed analysis of Eq. (25) gives the following.

*Theorem 6:* The eigenvalue of the helicity operator in $H'/H''$ are only 2 and $-2$.

*Proof:* The proof consists in showing that any tensor satisfying Eq. (25) with $\lambda^2 \neq 4$ belongs to $H''$, i.e., the only eigenvector in $H'/H''$ corresponding to $\lambda^2 \neq 4$ is the null vector.

Contracting Eq. (25) with $g^{\rho\sigma}$ gives

$$k^\rho T_{\mu\rho} = \tfrac{1}{2} i\lambda k_\mu (1+4q)\Phi_\rho{}^\rho.$$

Substituting this result back in Eq. (25) and summing over the permutations $\mu \to \rho \to \sigma \to \mu$ and $\sigma \to \rho \to \mu \to \sigma$ yields

$$k_\rho\{T_{\mu\sigma} + T_{\sigma\mu} + i\lambda[\Phi_{\mu\sigma} - \tfrac{1}{2}(1+2q)\,g_{\mu\sigma}\Phi_\tau{}^\tau]\} + k_\mu\{T_{\sigma\rho} + T_{\rho\sigma} + i\lambda[\Phi_{\rho\sigma} - \tfrac{1}{2}(1+2q)\,g_{\rho\sigma}\Phi_\tau{}^\tau]\} + k_\mu\{T_{\rho\mu} + T_{\mu\rho} + i\lambda[\Phi_{\mu\rho} - \tfrac{1}{2}(1+2q)\,g_{\mu\rho}\Phi_\tau{}^\tau]\} = 0.$$

This implies

$$T_{\rho\sigma} + T_{\sigma\rho} + i\lambda[\Phi_{\rho\sigma} - \tfrac{1}{2}(1+2q)\,g_{\rho\sigma}\Phi_\tau{}^\tau] = 0. \tag{26}$$

It is convenient to distinguish the following cases:

(i) Case $\lambda = 0$: By using the antisymmetry of $T_{\rho\sigma}$, one obtains

$$N(\Phi) = \Phi_{\lambda\rho}\overline{\Phi}^{\lambda\rho} - \tfrac{1}{2}(8q^2 + 4q + 1)|\,\Phi_\mu{}^\mu\,|^2 = 0.$$

Therefore $\Phi_{\mu\nu} \in H_q''$

(ii) Case $\lambda \neq 0$:

One may define a new tensor

$$\Psi_{\rho\sigma} = \Phi_{\rho\sigma} - \tfrac{1}{2}(1+2q)\,g_{\rho\sigma}\Phi_\mu{}^\mu, \tag{27}$$

which satisfies the following equation

$$k^\rho\Psi_{\rho\sigma} - \tfrac{1}{2}k_\sigma\Phi_\tau{}^\tau = 0.$$

Equation (25) can then be written in the form

$$\epsilon_{\mu\rho\beta\gamma}k^\gamma\Psi_\sigma^\beta + \epsilon_{\mu\sigma\beta\gamma}k^\gamma\Psi_\rho^\beta = i\lambda k_\mu\Psi_{\rho\sigma} + k_\rho T_{\mu\sigma} + k_\sigma T_{\mu\rho}. \tag{28}$$

[Note that $W^\mu(g_{\rho\sigma}A) = 0$].

Splitting $T_{\rho\sigma}$ in its antisymmetric and symmetric part [this last is determined by Eq. (26)], one has

$$\tfrac{1}{2}k^\rho(T_{\rho\sigma} - T_{\sigma\rho}) \equiv k^\rho A_{\rho\sigma} = \tfrac{1}{4}i\lambda\,k_\sigma\Psi_\tau{}^\tau.$$

After some calculations one finds

$$K_\rho A_{\rho\sigma} = 0 = \Psi_\tau{}^\tau$$

and

$$\lambda(\tfrac{1}{4}\lambda^2 - 1)\Psi_{\beta\tau}\overline{\Psi}^{\beta\tau} = 0.$$

If $\lambda \neq 0$, $\lambda^2 \neq 4$, then one can conclude

$$\Psi_{\beta\tau}\Psi^{\beta\tau} = \Phi_{\beta\tau}\overline{\Phi}^{\beta\tau} = N(\Phi) = 0.$$

Therefore $\Phi_{\mu\nu} \in H_q''$ and the theorem is proved. For the details see Appendix A.

## 9. EQUIVALENCE OF ANY LOCAL AND COVARIANT QUANTIZATION OF EINSTEIN EQUATIONS TO GUPTA FORMULATION

In Sec. 6 we proved that all the possible quantizations of the Einstein equations by means of a local and covariant operator $h_{\mu\nu}(x)$ can be classified according to the parameter $q$ entering in the subsidiary condition

$$k^\mu\Phi_{\mu\nu}\ldots + qk_\nu\Phi^\mu{}_\mu\ldots = 0.$$

Thus the arbitrariness in the definition of $h_{\mu\nu}(x)$, in the choice of the metric operator $\eta$ and in the subsidiary condition reduces to a one-parameter family of possible subsidiary conditions characterizing the "physical" states.

From a Hilbert space point of view the theories corresponding to different values of $q$ are substantially different. For example the manifold of "physical states" as well as the definition of the fields $R_{\lambda\mu\nu\rho}$ are different for different choices of $q$.

This arbitrariness has been a source of discussion[4] in the literature mainly because different values of $q$ lead to different propagators.

In this section we will eliminate this arbitrariness by showing that all the theories with $q \neq -\frac{1}{4}$ are equivalent, in a sense which will be made precise in the following. Before proving this statement we need a definition and a lemma.

*Definition 1:* Let $\eta_1$ and $\eta_2$ be two Hermitian sesquilinear forms defined in the Hilbert spaces $H_1$ and $H_2$. An operator $V: H_1 \to H_2$ is called *isometric with respect to* the metric operators $\eta_1$ *and* $\eta_2$ if

(1) The domain of $V$ is the whole Hilbert space $H_1$, and the range of $V$ is the whole Hilbert space $H_2$

$$D_V = H_1, \qquad \Delta_V = H_2;$$

(2) $$(V\Phi, V\Psi)_{\eta_2} = \langle\eta_2 V\Phi, V\Psi\rangle = (\Phi, \Psi)_{\eta_1} = \langle\eta_1\Phi, \Psi\rangle.$$

If $\eta_1 = \eta_2 = \eta$ and $H_1 = H_2$, the above definition coincides with the definition of unitarity of $V$ with respect to the metric $\eta$.

*Lemma 1:* Let $\phi(x)$ and $\psi(x)$ be two Wightman fields defined in the Hilbert spaces $H_1$ and $H_2$, with cyclic vectors $\Psi_{01}$ and $\Psi_{02}$, and let the corresponding Wightman functions be defined in terms of the metric operators $\eta_1$ and $\eta_2$, respectively:

$$W_n^1 = \langle\eta_1\Psi_{01}, \phi(x_1)\cdots\phi(x_n)\Psi_{01}\rangle,$$
$$W_n^2 = \langle\eta_2\Psi_{02}, \psi(x_1)\cdots\psi(x_n)\Psi_{02}\rangle.$$

If all the Wightman functions coincide

$$W_n^1 = W_n^2, \quad \forall n, \tag{29}$$

then there exists an operator $V: H_1 \to H_2$ which is isometric in the sense of Def. 1.

*Proof:* One may define the following mapping $V$:

$$\Psi = \mathcal{P}(\phi_1, \ldots, \phi_n)\Psi_{01} \to \Psi' = \mathcal{P}(\psi_1, \ldots, \psi_n)\Psi_{02}.$$

Since the vacuum states $\Psi_{01}$ and $\Psi_{02}$ are cyclic vectors, the operator $V$ so defined has domain and range in the whole spaces $H_1$ and $H_2$. Moreover, it is easy to see that $V$ acts linearly, and therefore defines a linear operator: $H_1 \to H_2$. Finally, $V$ is isometric according to Def. 1, as a consequence of Eq. (29).

*Theorem 7:* The Wightman theories of the Einstein equations defined for different values of $q (q \neq -\frac{1}{4})$ are all equivalent, i.e., there exists an operator $V$ relating the different theories, which is isometric according to Def. 1.

*Proof:* Let $h_{\mu\nu}(x)$ be an operator valued distribution in $H$ and let

$$\overline{\mathcal{P}(R(f)\Psi_0)} \equiv H_q'$$

[$q$ depends on the definition of $h(f)$ via Eq. (18)]. Clearly $H'_q$ is a subspace of $H$ and, therefore, is a Hilbert space.

One can compute the two point function

$$(\Psi_0, h_{\mu\nu}(f^{\mu\nu})h_{\rho\sigma}(g^{\rho\sigma})\Psi_0) = 2\pi\int[\hat{f}^{\mu\nu}(k)g_{\mu\nu}(k) - \tfrac{1}{2}\hat{f}_\rho{}^\rho(k)\hat{g}_\lambda{}^\lambda(k)]\frac{d^3k}{k_\nu}.$$

The right-hand side is independent of $q$ and therefore the two-point function is the same whatever the subsidiary condition one chooses. Since we are working on a free field theory this result guarantees that all the Wightman functions are independent of $q$.

Therefore, given two theories defined by the values $q$ and $q'$, all the Wightman functions coincide, [16] and, by Lemma 1 there exists an isometric operator $V$ relating the two theories.

It may be interesting to show explicitly how the various theories are related by the isometric operator $V$. In particular it is worthwhile to see how a theory defined by $q \neq -\frac{1}{2}$ is related to the theory corresponding to $q = -\frac{1}{2}$ (Gupta formulation, see Sec. 10).

If $h_{\mu\nu}(x)$ is the potential in the $q$ theory, one may define a local and covariant field $h'_{\mu\nu}(x)$ in the following way:

$$h'_{\mu\nu}(x) = h'^{+}_{\mu\nu} + h'^{-}_{\mu\nu},$$
$$h'^{+}_{\mu\nu} = h^{+}_{\mu\nu} - \{(1+2q)/[2(1+4q)]\}\, g_{\mu\nu}h^{+\lambda}_{\lambda},$$
$$h'^{-}_{\mu\nu} = h^{-}_{\mu\nu} - \tfrac{1}{2}(1+2q)\, g_{\mu\nu}h^{-\lambda}_{\lambda}.$$

It is immediate to verify that $h'_{\mu\nu}$ actually coincides with $h_{\mu\nu}$ ($q = -\frac{1}{2}$), and the Hilbert space $H'_{-1/2}$ is given by

$$H'_{-1/2} = \mathcal{P}(R_{h'}(f)\Psi_0).$$

In conclusion all the theories with $q \neq -\frac{1}{2}$ are isometrically equivalent to the theory defined by $q = -\frac{1}{2}$ corresponding to the choice made by Gupta.

## 10. GUPTA FORMULATION

Since all the theories with $q \neq -\frac{1}{4}$ are isometrically equivalent, it may be worthwhile to discuss the case $q = -\frac{1}{2}$ in some detail, in connection with Gupta formulation.

For the case $q = -\frac{1}{2}$ the definition of $h_{\mu\nu}(x)$ is the following

$$h_{\mu\nu}(f^{\mu\nu})\Psi = (\Phi^0, \Phi^1, \cdots),$$

$$\Phi^n_{\mu_1\cdots\nu_n} = \sqrt{2\pi}\sqrt{n+1}\int\frac{d^3k}{k_0}\hat{f}^{\mu\nu}(k)\Psi^{n+1}_{\mu\nu\mu_1\cdots\nu_n}(k, k_1, \ldots, k_n)$$
$$+\sqrt{\frac{2\pi}{n}}\sum_{j=1}^{n}[\hat{f}_{\mu_j\nu_j}(-k_j) - \tfrac{1}{2}g_{\mu_j\nu_j}\hat{f}_\lambda{}^\lambda]$$
$$\times\Psi^{n-1}_{\mu_1\cdots\underbrace{\mu_i\nu_i}_{j}\cdots\mu_n\nu_n}(k_1, \cdots\underbrace{k_j}\cdots). \qquad (30)$$

According to the discussion of Sec. 9 the symmetric tensor $h_{\mu\nu}(x)$ cannot describe only physical (spin-2) particles. In the classical theory the lower (0, 1) spin part of $h_{\mu\nu}$ is eliminated by the subsidiary condition[5]

$$\partial^\mu h_{\mu\nu} - \tfrac{1}{2}\partial_\nu h_\lambda{}^\lambda = 0. \qquad (31)$$

In the quantized theory this equation cannot be required to hold. In fact, if Eq. (31) is added to

$$\Box h_{\mu\nu} = 0,$$

we obtain the following operator equation

$$R_{\mu\nu} = 0.$$

As shown in Ref. 1 this is inconsistent with the properties of locality and/or covariance. Then one may require that Eq. (31) hold only as mean value on the "physical" states: a way to realize that is to require that Eq. 31) hold for the positive frequency part. More precisely, if $H'$ denotes the set of "physical" states, one has

$$(\partial_\mu h^{\mu\nu} - \tfrac{1}{2}\partial^\nu h_\lambda{}^\lambda)^+\Psi = 0, \qquad \forall\Psi \in H'.$$

This equation may be regarded as the condition which characterizes the "physical" states. It is not difficult to see that $H'$, so defined, is the set of vectors $\Phi = (\Phi^0, \Phi^1, \cdots)$ for which

$$k^\mu\Phi^{n+1}_{\mu\nu\cdots} - \tfrac{1}{2}k_\nu\Phi^{n+1}{}_{\mu}{}^{\mu}{}_{\cdots} = 0.$$

Thus $H'$ coincides with the space $H'_{-1/2}$ discussed in Sec. 6, as one could have anticipated, since $h_{\mu\nu}(x)$ defined by Eq. (30) corresponds to the case $q = -\frac{1}{2}$ of Sec. 6. Accordingly, the only possible choice for the metric $\eta$ is the following one:

$$(\Phi, \Psi) = \sum\langle\eta\Phi^\eta, \Psi^\eta\rangle$$
$$\eta\Phi^n_{\mu_1\cdots\nu_\eta} = \prod_{i=1}^{n}(g^{\mu_i\rho_i}g^{\nu_i\sigma_i} - \tfrac{1}{2}g^{\mu_i\nu_i}g^{\rho_i\sigma_i})\Phi^n_{\cdots}$$

(see the discussion in Sec. 6). The above definition of $\eta$ coincides with that given by Gupta.

As a last check, we can verify that the commutation rules and propagator are the same as the Gupta formulation if evaluated in terms of $h_{\mu\nu}$:

$$[h_{\mu\nu}(x), h_{\lambda\rho}(y)] = i(g_{\mu\nu}g_{\nu\rho} + g_{\mu\rho}g_{\nu\lambda} - g_{\mu\nu}g_{\lambda\rho})\,\Delta(x-y).$$

In conclusion, there is no arbitrariness in Gupta formulation except for the choice of $q$. All the other parameters of the theory, like the definition of $h_{\mu\nu}$ or the choice of the metric operator, are uniquely fixed once $q$ is fixed.

Before closing on Gupta formulation, it is worthwhile to see how this local and covariant theory escapes the difficulties discussed in Ref. 1. The representation of the two-point function derived in Refs. 1 and 8 for any local and covariant theory is indeed satisfied by Gupta formulation:

$$(\Psi_0, h_{\mu\nu}(x)R_{\alpha\beta\gamma\delta}(y)\Psi_0) = \tfrac{1}{2}(g_{\mu\rho}g_{\nu\sigma} + g_{\mu\sigma}g_{\nu\rho} - g_{\mu\nu}g_{\rho\sigma})[\partial_\gamma\partial_\beta\delta^\rho_\alpha\delta^\sigma_\delta + \partial_\alpha\partial_\delta\delta^\rho_\beta\delta^\sigma_\gamma - \partial_\alpha\partial_\gamma\delta^\rho_\beta\delta^\sigma_\delta - \partial_\beta\partial_\delta\delta^\rho_\alpha\delta^\sigma_\gamma]\Delta^+(x-y).$$

Then one has

$$(\Psi_0, h_{\mu\nu}(x)R_{\beta\gamma}(y)\Psi_0) = -\tfrac{1}{2}(\partial_\beta\partial_\mu g_{\nu\gamma} + \partial_\beta\partial_\nu g_{\mu\gamma} + \partial_\gamma\partial_\nu g_{\mu\beta} + \partial_\gamma\partial_\mu g_{\nu\beta})\Delta^+ \neq 0.$$

The essential point is that in Gupta formulation the Einstein equations do not hold as weak equations

$$(\Psi, R_{\mu\nu}\Psi_0) = 0, \quad \forall \Psi \in H$$

(see Sec. 5 of Ref. 1), and therefore one cannot get the conclusions of Refs. 1 and 9. As a matter of fact the Einstein equations do not hold when applied to vectors of $H'$, but only as mean values on $H'$. This may be verified explicitly. Indeed, $h_{\mu\nu}(f^{\mu\nu})\Psi_0 \in H'$ only if $\partial_\mu f^{\mu\nu} = 0$. In this case one has

$$(\Psi_0, h(f)R_{\mu\nu}(y)\Psi_0) = 0$$

in agreement with Theorem 5 of Sec. 6.

## 11. CASE $q = -\frac{1}{4}$

In this section we will see why the case $q = -\frac{1}{4}$, corresponding to $\beta' = 0$, must be excluded. The main reason is that it does not satisfy conditions $(\alpha)$ and $(\beta)$. In fact, if we want to identify the "physical" states with the vectors belonging to $H_{-1/4}$, one must define the negative frequency part of $h_{\mu\nu}(x)$ in such a way that

$$(R_{\alpha\beta\gamma\delta}(f^{\alpha\beta\gamma\delta})\Psi_0)_{\mu\nu} = -\tfrac{1}{2}\beta g_{\mu\nu}k_\lambda k_\rho \hat{f}^{\tau\lambda\rho}{}_\tau.$$

Only if this condition is satisfied, the one-particle vectors of $D_0$ belong to $H_{-1/4}$, i.e., correspond to "physical" one-particle states. In this case however one cannot have condition $(\beta)$ satisfied. As a matter of fact, condition $(\beta)$ is equivalent to require that the one-particle vectors of the form

$$(R_{\rho\sigma}\Psi_0)_{\mu\nu} = -2\beta g_{\mu\nu}k_\rho k_\sigma f^{\rho\sigma}$$

have zero norm. This is possible only if the metric operator $\eta$ is so chosen that all the one-particle vectors of the form

$$\phi_{\mu\nu} = g_{\mu\nu}\Psi$$

have zero norm, and this in turn gives

$$\| R_{\alpha\beta\gamma\delta}(f^{\alpha\beta\gamma\delta})\|^2 = 0 \quad \forall f.$$

Therefore all the on-particle vectors of $D_0$ would have zero norm, a result which is clearly not acceptable. In particular the above result shows that one cannot define a scalar theory of the Einstein equations by naively putting

$$h_{\mu\nu}(x) = g_{\mu\nu}\varphi(x).$$

There is also another way of seeing that such a scalar theory of gravitation cannot be based on the Einstein equations. In fact, in such a theory one should have

$$R_{\mu\nu} = (\Box g_{\mu\nu} + 2\partial_\mu\partial_\nu)\varphi(x). \tag{32}$$

If we impose that the Einstein equations hold as mean values on $D_0$ we obtain

$$(\Box g_{\mu\nu} + 2\partial_\mu\partial_\nu)(\Box g_{\rho\sigma} + 2\partial_\rho\partial_\sigma)(\Psi_0, \varphi(x)\varphi(y)\Psi_0) = 0. \tag{33}$$

The Wightman function

$$W(x,y) = (\Psi_0, \varphi(x)\varphi(y)\Psi_0)$$

is obviously translation and Lorentz invariant:

$$W(x,y) = W(x-y) + W(\Lambda(x-y)).$$

Then Eq. (33) reads

$$(\Box g_{\mu\nu} + 2\partial_\mu\partial_\nu)(\Box g_{\rho\sigma} + 2\partial_\rho\partial_\sigma)W = 0. \tag{34}$$

Contracting with $g_{\rho\sigma}$ we obtain

$$(\Box g_{\mu\nu} + 2\partial_\mu\partial_\nu)\Box W = 0.$$

The Lorentz invariant solutions of this equation are[17]

$$\Box W = \text{const.}$$

Then Eq. (34) implies

$$\partial_\mu\partial_\nu\partial_\rho\partial_\sigma W = 0$$

and, consequently,

$$W(x) = ax^2 + b.$$

This leads to

$$(\Psi_0, R_{\alpha\beta\gamma\delta}R_{\mu\nu\rho\sigma}\Psi_0) = 0.$$

Therefore the resulting theory is trivial, and one cannot hope to get a scalar theory of the Einstein equations.

## ACKNOWLEDGMENT

One of us (FS) would like to thank Professor A. S. Wightman for making available a Research Associateship at Princeton University and for his interest in this work.

## APPENDIX A

In this appendix we will give the details of the proof of Theorem 6. The equation to be discussed is the following:

$$\epsilon_{\mu\rho\beta\gamma}k^\gamma\phi^\beta{}_\sigma + \epsilon_{\mu\sigma\beta\gamma}k^\gamma\phi^\beta{}_\rho = i\lambda k_\mu\phi_{\rho\sigma} + k_\rho T_{\mu\sigma} + k_\sigma T_{\mu\rho} - [(1+2q)/(1+4q)]g_{\rho\alpha}k^\tau T_{\mu\tau}, \tag{A1}$$

where $T_{\rho\sigma}$ was found to obey the equations

$$T_{\rho\sigma} + T_{\sigma\rho} = i\lambda[\phi_{\rho\sigma} - \tfrac{1}{2}(1+2q)g_{\rho\sigma}\phi^\tau{}_\tau] \tag{A2}$$

and

$$k^\rho T_{\mu\rho} = i\lambda k_\mu \tfrac{1}{2}(1+4q)\phi^\rho{}_\rho. \tag{A3}$$

### 1. $\lambda = 0$

Since $T_{\rho\sigma}$ is antisymmetric, one can define a tensor $\hat{T}^{\lambda\tau}$ such that

$$T_{\mu\nu} = \epsilon_{\mu\nu\lambda\tau}\hat{T}^{\lambda\tau}.$$

Then Eq. (A1) becomes

$$\epsilon_{\mu\rho\beta\gamma}|k^\gamma\phi^\beta{}_\sigma - k_\sigma\hat{T}^{\beta\gamma}| + \epsilon_{\mu\sigma\beta\gamma}|k^\gamma\phi^\beta{}_\rho - k_\rho\hat{T}^{\beta\gamma}| = 0.$$

By contracting with $\epsilon^{\mu\alpha\lambda\tau}$, one gets

$$3(k^\tau\phi^{\lambda\rho} - k^\lambda\phi^{\tau\rho}) - 6k^\rho\hat{T}^{\lambda\tau} + (1+q)(k^\lambda g^{\tau\rho} - k^\tau g^{\lambda\rho})\phi^\mu{}_\mu + 2g^{\tau\rho}k_\gamma\hat{T}^{\lambda\gamma} - 2g^{\lambda\rho}k_\gamma\hat{T}^{\tau\gamma} = 0, \tag{A4}$$

and by further multiplying by $k_\tau$ one obtains

$$K_\lambda \hat{T}^{\lambda\tau} = \tfrac{1}{4}(1 + 4q)k^\lambda \phi^\mu{}_{\mu\cdot}$$

Finally, substituting this result in Eq. (A4) and contracting with $\bar{\phi}^{\lambda\rho}$ one has

$$\bar{\phi}^{\lambda\rho}\phi_{\lambda\rho} - \tfrac{1}{2}(8q^2 + 4q + 1)\,|\,\phi^\mu{}_\mu\,|^2 = N(\phi) = 0$$

as anticipated in Sec. 8.

2. $\lambda \neq 0$

In terms of the tensor

$$\psi_{\rho\sigma} = \phi_{\rho\sigma} - \tfrac{1}{2}(1 + 2q)g_{\rho\sigma}\phi^\mu{}_\mu.$$

Eq. (A1) becomes

$$\epsilon_{\mu\rho\beta\gamma}k^\gamma\psi^\beta{}_\sigma + \epsilon_{\mu\sigma\beta\gamma}k^\gamma\psi^\beta{}_\rho = i\lambda k_\mu\psi_{\rho\sigma} + k_\rho T_{\mu\sigma} + k_\sigma T_{\mu\rho}. \quad \text{(A5)}$$

Contracting Eq. (A5) with $k_\mu$ one gets

$$k^\mu T_{\mu\sigma} = 0.$$

If $T_{\rho\sigma}$ is split into its symmetric and antisymmetric part

$$T_{\rho\sigma} = \tfrac{1}{2}(T_{\rho\sigma} + T_{\sigma\rho}) + \tfrac{1}{2}(T_{\rho\sigma} - T_{\sigma\rho}) = -\tfrac{1}{2}i\lambda\psi_{\rho\sigma} + A_{\rho\sigma}, \quad \text{(A6)}$$

the antisymmetric part $A_{\rho\sigma}$ satisfies

$$k^\rho A_{\rho\sigma} = \tfrac{1}{4}i\lambda k_\sigma\psi^\tau{}_\tau. \quad \text{(A7)}$$

Substituting Eq. (A6) in Eq. (A5) and contracting with $\epsilon^{\mu\rho\lambda\tau}$ yields

$$\begin{aligned} &-3(k^\tau\psi^{\lambda\sigma} - k^\lambda\psi^{\sigma\tau}) - \tfrac{1}{2}\,|\,g^{\sigma\tau}k^\lambda - g^{\lambda\sigma}k^\tau\,|\,\psi^\mu{}_\mu \\ &\quad = i\lambda\epsilon^{\mu\rho\lambda\tau}k_\mu\psi_\rho{}^\sigma - \tfrac{1}{2}i\lambda\epsilon^{\mu\rho\lambda\tau}k_\rho\psi_\mu{}^\sigma \\ &\qquad + \epsilon^{\mu\rho\lambda\tau}(k_\rho A_\mu{}^\sigma + k^\sigma A_{\mu\rho}). \end{aligned} \quad \text{(A8)}$$

By exchanging $\sigma$ and $\tau$ and summing one has

$$\begin{aligned} &3(\tfrac{1}{4}\lambda^2 - 1)(k^\tau\psi^{\lambda\sigma} + k^\sigma\psi^{\lambda\tau} - 2k^{\lambda\sigma}\psi^{\sigma\tau}) \\ &\quad = \tfrac{1}{2}(2g^{\sigma\tau}k^\lambda - g^{\lambda\sigma}k^\tau - g^{\lambda\tau}k^\sigma)\psi^\mu \\ &\qquad + \epsilon^{\mu\rho\lambda\tau}(k_\rho A_\mu{}^\sigma + k^\sigma A_{\mu\rho}) + \epsilon^{\mu\rho\lambda\sigma}(k_\rho A_\mu{}^\tau + k^\tau A_{\mu\rho}), \end{aligned} \quad \text{(A9)}$$

where Eq. (A7) has been taken into account.

Contracting with $\epsilon_{\lambda\sigma\alpha\beta}k^\alpha$ one gets

$$3k^\alpha[\delta^\tau{}_\beta k^\sigma A_{\alpha\sigma} - \delta^\tau{}_\alpha k^\sigma A_{\beta\sigma} + 2k^\tau A_{\beta\alpha} + k_\alpha A_\beta{}^\tau - k_\beta A_\alpha{}^\tau] = 0$$

from which

$$k^\alpha A_{\beta\alpha} = 0.$$

This implies

$$\psi^\tau{}_\tau = 0.$$

Then by contracting Eq. (A9) with $\epsilon_{\lambda\sigma\alpha\beta}$ one obtains

$$-3(\tfrac{1}{4}\lambda^2 - 1)\epsilon_{\lambda\sigma\alpha\beta}k^\lambda\psi^\sigma{}_\tau = 2k_\tau A_{\beta\alpha} + k_\alpha A_{\beta\tau} - k_\beta A_{\alpha\tau}. \quad \text{(A10)}$$

Subtracting Eq. (A9) from that obtained with the permutation $\alpha \to \tau \to \beta \to \alpha$ we have, taking into account Eqs. (A5) and (A6),

$$\begin{aligned} &k_\tau A_{\beta\alpha} - k_\beta A_{\alpha\tau} \\ &\quad = (\tfrac{1}{4}\lambda^2 - 1)(i\lambda k_\alpha\psi_{\beta\tau} - \tfrac{1}{2}i\lambda k_\beta\psi_{\alpha\tau} \\ &\qquad - \tfrac{1}{2}i\lambda k_\tau\psi_{\alpha\beta} + k_\beta A_{\alpha\tau} + k_\tau A_{\alpha\beta}). \end{aligned}$$

Finally, by contraction with $\bar{\psi}^{\beta\tau}$ one has

$$\lambda(\tfrac{1}{4}\lambda^2 - 1)\psi_{\beta\tau}\bar{\psi}^{\beta\tau} = 0,$$

and the conclusion of Theorem 6 follows.

## APPENDIX B

In this Appendix we will discuss the role played by Lorentz transformations in the theory. For the sake of definiteness, we will refer to the case $q = -\tfrac{1}{2}$.

As a matter of fact, the role of Lorentz transformations is a bit different than in quantum electrodynamics.

There, by a Lorentz transformation, one can always eliminate the unphysical (i.e., belonging to $H''$) part from a vector of $H'$. The analog for gravitation would be as follows.

In a frame of reference in which $K^\mu = (K\,0\,0\,K)$, a vector of $H'$ can be written in this way:

$$\phi^{\mu\nu} = \begin{pmatrix} \phi^{00} & \phi^{01} & \phi^{02} & \tfrac{1}{2}(\phi^{00} + \phi^{33}) \\ \phi^{01} & \phi^{11} & \phi^{12} & \phi^{01} \\ \phi^{02} & \phi^{12} & -\phi^{11} & \phi^{02} \\ \tfrac{1}{2}(\phi^{00} + \phi^{33}) & \phi^{01} & \phi^{02} & \phi^{33} \end{pmatrix} = \phi_1^{\mu\nu} + \phi_2^{\mu\nu},$$

$$\phi_1^{\mu\nu} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \phi^{11} & \phi^{12} & 0 \\ 0 & \phi^{12} & -\phi^{11} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\phi_2^{\mu\nu} = \begin{pmatrix} \phi^{00} & \phi^{01} & \phi^{02} & \tfrac{1}{2}(\phi^{00} + \phi^{33}) \\ \phi^{01} & 0 & 0 & \phi^{01} \\ \phi^{02} & 0 & 0 & \phi^{02} \\ \tfrac{1}{2}(\phi^{00} + \phi^{33}) & \phi^{01} & \phi^{02} & \phi^{33} \end{pmatrix}.$$

Both $\phi_1$ and $\phi_2$ belong to $H'$, and $\phi_2$ has zero norm. The physical part of $\phi^{\mu\nu}$ is contained in $\phi_1^{\mu\nu}$ whose form makes it clear that there is no contribution from a vector $\psi^{\mu\nu} \in H''$,

$$\psi^{\mu\nu} = k^\mu F^\nu + k^\nu F^\mu$$

About the possibility of eliminating the unphysical part of $\phi^{\mu\nu}$ by means of a Lorentz transformation, we have the following.

*Statement 5:* Given a vector $\phi^{\mu\nu} \in H'$, it is in general not true that it can be reduced to the form of $\phi_1^{\mu\nu}$. However, in each equivalence class ($\neq H''$) there is always a vector which can be put into the form of $\phi_1^{\mu\nu}$ by means of a Lorentz transformation.

*Proof:* To find a frame of reference in which $\phi^{\mu\mu}$ has the form of $\phi_1^{\mu\nu}$ is equivalent to look for a timelike solution of the equation

$$\phi^{\mu\nu}v_\nu = 0. \tag{B1}$$

Indeed, if such a frame exists, $v = (t\ 0\ 0\ 0)$ solves the problem, and conversely, if the solution of Eq. (B1) is timelike, in the rest system of $v$ Eq. (B1) is

$$\phi^{\mu 0} = 0,$$

and then Eq. (13) of Sec. 6 with $q = -\frac{1}{2}$ implies that $\phi^{\mu\nu}$ has the form of $\phi_1^{\mu\nu}$. It is easy to see that Eq. (B1) has in general no solution. For example, if $\phi^{\mu\nu}$ is such that

$$\phi^{01} = \phi^{02} = \phi^{13} = \phi^{23} = \phi^{32} = 0, \qquad \phi^{00} = \phi^{33} \neq 0,$$

it has no timelike eigenvector with zero eigenvalue, and therefore cannot be transformed into the form of $\phi_1^{\mu\nu}$.

The second part of the statement is obvious, since in the same class of equivalence of $\phi^{\mu\nu}$ one has also

$$\phi'^{\mu\nu} = \phi^{\mu\nu} + k^\mu F^\nu + k^\nu F^\mu,$$
$$F^\mu = (-\phi^{00}/2k, 0, -\phi^{02}/k, -\phi^{33}/k),$$

and $\phi'^{\mu\nu}$ has the form of $\phi_1^{\mu\nu}$.

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4 For a discussion of the different subsidiary conditions and their connection with the spin of the virtual particles see V. I. Ogievetsky and I. V. Polubarinov, Ann. Phys. (N.Y.) **35**, 167 (1965).

5 L. Landau et E. Lifchitz, *Théorie du champ* (Editions Mir, Moscou, 1966).

6 The choice of tempered distributions is not strictly necessary. On this point see Ref. 1. Also the spectral condition (d) below is here assumed only for simplicity. The discussion can be carried through without assuming it.

7 Unitarity is intended with respect to the metric operator $\eta$ of the Hilbert space, on which no hypothesis is made. In this general case $U$ is unitary if

$$U^*\eta U = \eta.$$

8 J. Schwinger, Phys. Rev. **130**, 1253 (1963); R. Arnowitt, S. Deser, and C. W. Misner, Phys. Rev. **113**, 745 (1959); **116**, 1322 (1959); **117**, 1595 (1960).

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13 S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1964).

14 By vector describing a physical state we mean a vector having a physical meaning. Here and in the following we will call them "physical" states.

15 E. P. Wigner, *Theoretical Physics* (International Atomic Energy Agency, Vienna, 1963).

16 Perhaps it is worthwhile noticing that, even if the two-point function can be calculated simply knowing the definition of the negative frequency part of $h_{\mu\nu}$, the definition of the positive frequency part is by no means arbitrary. Indeed the request of locality and Hermiticity for the field $h_{\mu\nu}$ uniquely fixes the definition of $h^+_{\mu\nu}$.

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# On the Reduction of the Generalized RPA Eigenvalue Problem


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The $2n$-dimensional eigenvalue problem, which arises when the random phase approximation (RPA) matrix is not real, is reduced to an $n$-dimensional eigenvalue problem. Some properties of the reduced eigenvalue problem are studied. A numerical example is considered for illustrative purposes.

## I. INTRODUCTION

The random phase approximation (RPA) and the equations of motion method have been widely used[1] for calculating the vibrational collective states of nuclei. Because of the presence of both the particle–hole creation and destruction operators, one arrives at $2n \times 2n$ non-Hermitian matrix of the general form

$$C = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}, \tag{1}$$

where the $n \times n$ matrices $A$ and $B$ are Hermitian and symmetric, respectively.

From the early days of the RPA calculations,[2] there has been considerable interest in reducing the $2n \times 2n$ eigenvalue problem

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} Y \\ Z \end{pmatrix} = \omega \begin{pmatrix} Y \\ Z \end{pmatrix}, \tag{2}$$

to an $n \times n$ eigenvalue problem. If the matrices $A$ and $B$ are real symmetric and the combination matrices $A + B, A - B$ are at least positive semidefinite, then such a reduction can be achieved by a method proposed by Chi,[3] in which one constructs a lower triangular matrix. Due to the approximations which go into setting up the matrix $C$, the positive semidefinite condition imposed on the matrices $A + B$, $A - B$ may not be satisfied in practice. A more general approach for the case of real symmetric matrices $A$ and $B$ has been given by Ullah and Rowe.[4] In this approach no condition has to be imposed on the combination matrices $A + B, A - B$ and only a symmetric matrix diagonalization is needed to reduce the $2n \times 2n$ eigenvalue problem given by Eq. (2) to the following $n \times n$ eigenvalue problem:

$$RX = \omega^2 X, \tag{3}$$

where $R$ is an $n \times n$ symmetric matrix. It will be real if one of the combination matrices $A + B$ or

*Proof:* To find a frame of reference in which $\phi^{\mu\mu}$ has the form of $\phi_1^{\mu\nu}$ is equivalent to look for a timelike solution of the equation

$$\phi^{\mu\nu}v_\nu = 0. \tag{B1}$$

Indeed, if such a frame exists, $v = (t\ 0\ 0\ 0)$ solves the problem, and conversely, if the solution of Eq. (B1) is timelike, in the rest system of $v$ Eq. (B1) is

$$\phi^{\mu 0} = 0,$$

and then Eq. (13) of Sec. 6 with $q = -\frac{1}{2}$ implies that $\phi^{\mu\nu}$ has the form of $\phi_1^{\mu\nu}$. It is easy to see that Eq. (B1) has in general no solution. For example, if $\phi^{\mu\nu}$ is such that

$$\phi^{01} = \phi^{02} = \phi^{13} = \phi^{23} = \phi^{32} = 0, \qquad \phi^{00} = \phi^{33} \neq 0,$$

it has no timelike eigenvector with zero eigenvalue, and therefore cannot be transformed into the form of $\phi_1^{\mu\nu}$.

The second part of the statement is obvious, since in the same class of equivalence of $\phi^{\mu\nu}$ one has also

$$\phi'^{\mu\nu} = \phi^{\mu\nu} + k^\mu F^\nu + k^\nu F^\mu,$$
$$F^\mu = (-\phi^{00}/2k, 0, -\phi^{02}/k, -\phi^{33}/k),$$

and $\phi'^{\mu\nu}$ has the form of $\phi_1^{\mu\nu}$.

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$$U^*\eta U = \eta.$$

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10 R. Jost, *The General Theory of Quantized Fields* (Amer. Math. Soc., Providence, R.I., 1965).

11 K. Hepp, Helv. Phys. Acta **36**, 355 (1963).

12 For example when the indices $\mu, \nu, \rho, \sigma$, are all different only $\partial_\mu\partial_\nu\partial_\rho\partial_\sigma F_6$ survives. This implies that $F_6$ must be analytic in $\mathcal{T}'$. Similarly one can see that all the other invariant functions $F_j$ must be analytic in $\mathcal{T}'$.

13 S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1964).

14 By vector describing a physical state we mean a vector having a physical meaning. Here and in the following we will call them "physical" states.

15 E. P. Wigner, *Theoretical Physics* (International Atomic Energy Agency, Vienna, 1963).

16 Perhaps it is worthwhile noticing that, even if the two-point function can be calculated simply knowing the definition of the negative frequency part of $h_{\mu\nu}$, the definition of the positive frequency part is by no means arbitrary. Indeed the request of locality and Hermiticity for the field $h_{\mu\nu}$ uniquely fixes the definition of $h^+_{\mu\nu}$.

17 F. Strocchi, Phys. Rev. **162**, 1429 (1967).


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# On the Reduction of the Generalized RPA Eigenvalue Problem


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The $2n$-dimensional eigenvalue problem, which arises when the random phase approximation (RPA) matrix is not real, is reduced to an $n$-dimensional eigenvalue problem. Some properties of the reduced eigenvalue problem are studied. A numerical example is considered for illustrative purposes.

## I. INTRODUCTION

The random phase approximation (RPA) and the equations of motion method have been widely used[1] for calculating the vibrational collective states of nuclei. Because of the presence of both the particle–hole creation and destruction operators, one arrives at $2n \times 2n$ non-Hermitian matrix of the general form

$$C = \begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}, \tag{1}$$

where the $n \times n$ matrices $A$ and $B$ are Hermitian and symmetric, respectively.

From the early days of the RPA calculations,[2] there has been considerable interest in reducing the $2n \times 2n$ eigenvalue problem

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} Y \\ Z \end{pmatrix} = \omega \begin{pmatrix} Y \\ Z \end{pmatrix}, \tag{2}$$

to an $n \times n$ eigenvalue problem. If the matrices $A$ and $B$ are real symmetric and the combination matrices $A + B, A - B$ are at least positive semidefinite, then such a reduction can be achieved by a method proposed by Chi,[3] in which one constructs a lower triangular matrix. Due to the approximations which go into setting up the matrix $C$, the positive semidefinite condition imposed on the matrices $A + B$, $A - B$ may not be satisfied in practice. A more general approach for the case of real symmetric matrices $A$ and $B$ has been given by Ullah and Rowe.[4] In this approach no condition has to be imposed on the combination matrices $A + B, A - B$ and only a symmetric matrix diagonalization is needed to reduce the $2n \times 2n$ eigenvalue problem given by Eq. (2) to the following $n \times n$ eigenvalue problem:

$$RX = \omega^2 X, \tag{3}$$

where $R$ is an $n \times n$ symmetric matrix. It will be real if one of the combination matrices $A + B$ or

$A - B$ have all positive or zero roots and complex if both of them have negative roots.

In the usual RPA and equations of motion calculations, the matrices $A$ and $B$ are almost invariably real and the above methods suffice to reduce the $2n \times 2n$ eigenvalue problem to an $n \times n$ eigenvalue problem. However, recently it has been shown[5] that, due to the long range correlations of the residual two-body interaction, one has to construct an intrinsically correlated RPA state from a given deformed Hartree–Fock state. The projected states from an RPA correlated state are shown to be in much better agreement with their experimental values than the ones which are obtained with no RPA correlations present. In such calculations one has to deal with the generalized RPA eigenvalue problem given by Eq. (2). The purpose of the present note is to show how to reduce the generalized $2n \times 2n$ eigenvalue problem to an $n \times n$ eigenvalue problem. In Sec. II we carry out this reduction and pass on a couple of remarks on the reduced eigenvalue problem in Sec. III. For illustrative purposes a numerical example is presented in Sec. IV.

## II. DERIVATION OF THE REDUCED EIGENVALUE EQUATION

We follow the method of Ref. 4 and introduce two new vectors $x$ and $y$ which are related to the vectors $Y$ and $Z$ in the following way:

$$x = Y + Z, \tag{4a}$$

$$y = Y - Z. \tag{4b}$$

From Eq. (2) it is easy to see that these vectors satisfy the following set of coupled equations:

$$Mx + i\eta y = \omega y, \tag{5a}$$

$$Ny - i\tilde{\eta}x = \omega x, \tag{5b}$$

where the matrices $M, N, \eta$ are given by

$$M = \tfrac{1}{2}[(A + A^*) + (B + B^*)], \tag{6a}$$

$$N = \tfrac{1}{2}[(A + A^*) - (B + B^*)], \tag{6b}$$

$$\eta = (1/2i)[(A - A^*) - (B - B^*)]. \tag{6c}$$

Since $A$ is Hermitian and $B$ symmetric, it is easy to see from relations (6a), (6b), and (6c) that the matrices $M$ and $N$ are real symmetric and that the matrix $\eta$ is real. Further, if $A$ and $B$ would have been real, the matrix $\eta$ will be zero and the set of equations given by (5) is the same as the one given in Ref. 4 for the real case.

Since the matrices $M$ and $N$ are real symmetric, we can diagonalize them by a real orthogonal transformation. If one of these matrices, say $M$, has all positive roots, we diagonalize it first by a real orthogonal matrix $T$,

$$TM\tilde{T} = M_d, \tag{7}$$

where $M_d$ are the eigenvalues of $M$, which are all positive. No such preference between $M$ and $N$ has to be made if both of them have negative eigenvalues and we can choose any one of them, say $M$ again, for diagonalization. Applying this transformation to Eq. (5), we get

$$M_d x' + i\eta' y' = \omega y', \tag{8a}$$

$$N' y' - i\tilde{\eta}' x' = \omega x', \tag{8b}$$

where

$$N' = TN\tilde{T}, \quad \eta' = T\eta\tilde{T}, \quad x' = Tx, \quad y' = Ty. \tag{9}$$

Eliminating $x', y'$ between Eqs. (8a), (8b), we arrive at the following reduced $n$-dimensional eigenvalue problem:

$$[R - i\xi\omega - \omega^2]y'' = 0, \tag{10}$$

where

$$R = M_d^{1/2}[N' - \tilde{\eta}' M_d^{-1}\eta']M_d^{1/2}, \tag{11a}$$

$$\xi = M_d^{1/2}[\tilde{\eta}' M_d^{-1} - M_d^{-1}\eta']M_d^{1/2}, \tag{11b}$$

$$y'' = M_d^{-1/2} y'. \tag{11c}$$

It is easy to see from Eqs. (11) that if all $M_d$ are positive, then the $n \times n$ matrix $R$ is real symmetric and $\xi$ is real antisymmetric. If all $M_d$ are not positive, i.e., if both $M$ and $N$ have negative eigenvalues, then the matrices $R$ and $\xi$ will be complex symmetric and complex antisymmetric, respectively. For the case where both the matrices $A$ and $B$ are real symmetric, the reduced eigenvalue equation (10) becomes the same as Eq. (3), as it should be.

In arriving at Eq. (10), we have assumed that none of the $M_d$'s are zero. If some of the $M_d$'s are zero, the dimensionality of Eq. (10) is further reduced, but its structure becomes more complicated. This does not happen in case of real symmetric matrices $A$ and $B$, since the matrix $\eta$ is then zero.

## III. REMARKS ON THE REDUCED EIGENVALUE EQUATION

We would first like to show that the coefficient of $\omega$ in the reduced eigenvalue equation (10) cannot be eliminated by a nonsingular linear transformation of the vectors $y''$. To see this, let us write

$$y'' = Sx'', \tag{12}$$

in Eq. (10) and multiply it from the left by $S^{-1}$. This gives us

$$[S^{-1}RS - iS^{-1}\xi S\omega - \omega^2]x'' = 0. \tag{13}$$

The condition

$$S^{-1}\xi S = 0 \tag{14}$$

will be satisfied only if the antisymmetric matrix $\xi$ is zero. This shows that the coefficient of $\omega$ cannot be eliminated by a nonsingular linear transformation of the vectors $y''$.

Since the matrix $R$ is symmetric and $\xi$ antisymmetric, we can also write the eigenvalue equation (10) in the following form:

$$(P - \omega)(\tilde{P} + \omega)y'' = 0, \tag{15}$$

where the matrix $P$ satisfies the relations

$$\tilde{P} - P = i\xi, \tag{16a}$$

$$P\tilde{P} = R. \tag{16b}$$

Since any nonsingular complex matrix can be written as a product of a complex symmetric matrix $S$ and an orthogonal matrix $Q$,[6] we write $P$ as

$$P = SQ. \tag{17}$$

Equation (16b) immediately determines $S$,

$$S^2 = R. \tag{18}$$

If the dimensions of $Q$ are not very large, then, using the parametrized form of the complex orthogonal matrix, we can determine it from Eq. (16a). We shall construct the matrix $P$ for the numerical example, which we consider in Sec. IV.

Since the eigenvalues $\omega$ occur in pairs $(\omega, -\omega)$, we can find them by determining the eigenvalues of the matrix $P$, for the lower dimensions where this matrix can be easily constructed.

## IV. NUMERICAL EXAMPLE

We would now like to consider a numerical example. Let us take the Hermitian matrix $A$ to be

$$A = \begin{pmatrix} 2 & i \\ -i & 2 \end{pmatrix},$$

and the symmetric matrix $B$ to be

$$B = \begin{pmatrix} -1 & i \\ i & -1 \end{pmatrix}.$$

The $4 \times 4$ eigenvalue equation (2) gives the following eigenvalues:

$$\omega_1 = (\tfrac{3}{4})^{1/4}(\sqrt{3}+1), \quad \omega_2 = -i(\tfrac{3}{4})^{1/4}(\sqrt{3}-1),$$
$$\omega_3 = -\omega_1, \quad \omega_4 = -\omega_2.$$

The matrices $M, N, \eta$ can be easily calculated and are given by

$$M = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad N = \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}, \quad \eta = \begin{pmatrix} 0 & 0 \\ -2 & 0 \end{pmatrix}.$$

The reduced $2 \times 2$ eigenvalue equation is given by

$$\begin{pmatrix} -1-\omega^2 & 2i\omega \\ -2i\omega & 3-\omega^2 \end{pmatrix} \begin{pmatrix} y_1'' \\ y_2'' \end{pmatrix} = 0.$$

As can be easily seen, it gives the same four eigenvalues, which were obtained from the $4 \times 4$ eigenvalue equation. The matrix $P$ can be easily constructed in this case using Eqs. (16), (17), and (18), and is given by

$$P = \begin{pmatrix} (\frac{3}{64})^{1/4}[(\sqrt{3}-1) - i(\sqrt{3}+1)] & \frac{1}{2}(\sqrt{3}+i) \\ (\frac{3}{4})^{1/2}(1 - i\sqrt{3}) & (\frac{27}{64})^{1/4}[(\sqrt{3}+1) + i(\sqrt{3}-1)] \end{pmatrix}.$$

The eigenvalues of $P$ are $\omega_1, \omega_2$.

In our example all the eigenvalues $\omega$ of the RPA matrix $C$ are not real. This is obvious if we use Thouless' theorem,[7] which says that if the eigenvalues of the associated Hermitian matrix

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$$

are not all positive, then all the $\omega$'s cannot be real.

We remark at the end that if the antisymmetric matrix $\xi$ is small compared to the symmetric matrix $R$ in the reduced eigenvalue equation (10), then the effect of $\xi$ can be calculated by perturbation approximation.


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# Conservation of Kinks and Spin in Nonlinear Quantum Field Theories


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Certain nonlinear field theories exhibit particlelike structures called "kinks" that have fermionlike properties. This paper uses a Feynman path integral approach to show that, in the quantum theory, the number of kinks and the spin associated with them are both conserved quantities.

## 1. INTRODUCTION

It has been pointed out by a number of authors[1,2] that certain nonlinear classical field theories possess particlelike structures that are strictly conserved in number for topological reasons, irrespective of the particular dynamics of the system. Such structures are called "kinks." An example of a one-dimensional theory that "admits" kinks is found by considering the set of all mappings[3] $\alpha$ from the real line $R^1$ into the circle $S^1$,

$$\alpha : R^1 \to S^1,$$

subject to the boundary conditions

$$\alpha(x) \to 0 (\mathrm{mod} 2\pi) \quad \text{as } x \to \pm\infty,$$

where $x \in R^1$. The field $\alpha$ can be represented by a narrow strip stretching from $x = -\infty$ to $x = +\infty$, and a kink may then be pictured intuitively as a $2\pi$ twist in the strip. As a result of the boundary conditions the number of kinks is strictly conserved in time. Skyrme[1] has generalized this theory to three dimensions by considering the set of mappings from three-dimensional space $R^3$ into a 3-sphere $S^3$. Thus

$$\tilde{P} - P = i\xi, \tag{16a}$$

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## 1. INTRODUCTION

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where $x \in R^1$. The field $\alpha$ can be represented by a narrow strip stretching from $x = -\infty$ to $x = +\infty$, and a kink may then be pictured intuitively as a $2\pi$ twist in the strip. As a result of the boundary conditions the number of kinks is strictly conserved in time. Skyrme[1] has generalized this theory to three dimensions by considering the set of mappings from three-dimensional space $R^3$ into a 3-sphere $S^3$. Thus

three angular variables, $\alpha_1, \alpha_2, \alpha_3$, are involved. Alternatively, $S^3$ can be parametrized by four real variables $\phi_\rho$, $\rho = 1, 2, 3, 4$, whose squares sum to unity. Another three-dimensional example is provided by considering the set of mappings from $R^3$ into the space $S_{4,1}$ of general relativity.[4] (This is the set of all $4 \times 4$ real, symmetric matrices of signature 1). Both of these three-dimensional theories have appropriate boundary conditions so that the number of kinks is conserved. Furthermore, it has been shown[5] for both these theories that it is possible to define wavefunctionals on the space of mappings that are doublevalued under $2\pi$ rotations. Following Finkelstein,[2] such theories will be said to "admit spin" (or admit half-integer spin).

Suppose that a field theory is given involving mappings $\varphi$ from $R^3$ into any manifold $Y$,

$$\varphi : R^3 \to Y$$

and that appropriate boundary conditions are also supplied. We denote the set of such mappings by $M(R^3, Y)$. Furthermore, we assume that the theory admits both kinks and spin. Although the kink number is conserved in the classical theory, one might imagine that when the theory is quantized that quantum jumps would be permissible from an $n$-kink state to an $m$-kink state, $n \neq m$. Also, bearing in mind the way in which spin is described in such theories, one might imagine that in the quantized theory a state of half-integer spin might evolve into a state of integer spin. It is the purpose of this paper to point out that neither of these occurs and that both the kink number and the spin are conserved in the quantum theory.

The proof of conservation given in this paper is stronger than that of Finkelstein and Rubinstein,[2] which applies for the case of classical fields.

## 2. CONSERVATION OF KINKS

Consider the field theory defined by the mappings $\varphi \in M(R^3, Y)$. Thus $\varphi(\mathbf{x}) \in Y$, where $\mathbf{x}$ is any point of $R^3$. In quantizing such a theory, let us suppose that the evolution of the system from an initial field configuration $\varphi_a$ at a time $t = t_a$ to a later field configuration $\varphi_b$ at a time $t = t_b$ is given by a Feynman integral over all possible paths[6] joining $\varphi_a$ and $\varphi_b$. We use $t$ to label the different mappings that occur along a path, and write $\varphi(t)$:

$$\begin{aligned} \varphi(t_a) &= \varphi_a, \\ \varphi(t_b) &= \varphi_b. \end{aligned} \tag{1}$$

We shall use $\varphi(\mathbf{x}; t)$ to denote the point of $Y$ onto which $\mathbf{x} \in R^3$ is mapped by the mapping $\varphi(t) \in M(R^3, Y)$.

An infinitesimal volume in $M(R^3, Y)$ will be represented symbolically by

$$\mathfrak{D}(\varphi) = N \prod_{\text{all } \mathbf{x}} d\varphi(\mathbf{x}), \tag{2}$$

where $N$ is a normalization constant, independent of $\varphi$. In terms of a sufficiently accurate finite-dimensional approximation to the space of the $\varphi(\mathbf{x})$, the infinitesimal volume element of Eq. (2) is a displacement-invariant Haar measure.[7] As an example consider the three-dimensional theory of Skyrme in which three angular variables $\alpha_1, \alpha_2, \alpha_3$ are involved. Writing $|\alpha| = [\alpha_1^2(\mathbf{x}) + \alpha_2^2(\mathbf{x}) + \alpha_3^2(\mathbf{x})]^{1/2}$, the infinitesimal volume element is given by

$$\mathfrak{D}(\alpha_1, \alpha_2, \alpha_3) = N \prod_{\text{all } \mathbf{x}} [2(\sin \tfrac{1}{2}|\alpha|)/|\alpha|]^2 d\alpha_1(\mathbf{x}) \times d\alpha_2(\mathbf{x})\, d\alpha_3(\mathbf{x}).$$

Let us now consider the kernel $K(\varphi_b, \varphi_a; t_b - t_a)$ for the propagation from a field configuration $\varphi_a$ at a time $t_a$ to a field configuration $\varphi_b$ at a time $t_b$. $K$ must satisfy the following composition law:

$$K(\varphi_b, \varphi_a; t_b - t_a) = \int K(\varphi_b, \varphi; t_b - t) K(\varphi, \varphi_a; t - t_a)\, \mathfrak{D}(\varphi).$$

This can be expressed as an iteration of the propagation kernel for infinitesimal time differences $\Delta t$:

$$\begin{aligned} K(\varphi_b, \varphi_a; t_b - t_a) &= \int \prod_{m=1}^{M} K[\varphi(\mathbf{x}; t_a + m\Delta t), \varphi(\mathbf{x}; t_a + (m-1)\Delta t); \Delta t] \\ &\quad \times \prod_{m=1}^{M} \mathfrak{D}(\varphi(\mathbf{x}; t_a + m\Delta t)). \end{aligned} \tag{3}$$

As $\Delta t \equiv (t_b - t_a)/M \to 0$, time assumes the role of a continuous parameter.

Let $D$ denote the metric on the manifold $Y$. Then a metric $d$ on the space $M(R^3, Y)$ can be defined by writing

$$d[\varphi_1, \varphi_2] = \max_{\mathbf{x} \in R^3} D[\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})],$$

where $\varphi_1, \varphi_2 \in M(R^3, Y)$. This is a natural definition, for then the metric topology on $M(R^3, Y)$ coincides with the compact-open topology. Let $\varphi_a$ be a field with $n_a$ kinks and $\varphi_b$ be a field with $n_b$ kinks, $n_a \neq n_b$. Because such fields are not homotopic, $\varphi_a$ cannot be joined to $\varphi_b$ by a continuous path. Since Eq. (1) is true, the path defined by $\varphi(t)$ must have at least one discontinuity. It follows that there must be at least one value of $t$, call it $t_k$, such that

$$d[\varphi(t_k + \Delta t) - \varphi(t_k)] \geq B > 0$$

for any time interval $\Delta t$, no matter how small. To show that such a lower bound exists, let us suppose that it does not. Thus by letting $\Delta t$ tend to zero, $d[\varphi(t_k + t) - \varphi(t_k)]$ can be made as small as possible. Hence

$$\max_{\mathbf{x} \in R^3} D[\varphi(\mathbf{x}; t_k + \Delta t) - \varphi(\mathbf{x}; t_k)] \to 0 \quad \text{as } \Delta t \to 0,$$

$$\therefore\ D[\varphi(\mathbf{x}; t_k + \Delta t) - \varphi(\mathbf{x}; t_k)] \to 0 \quad \text{as } \Delta t \to 0 \text{ for all } \mathbf{x},$$

$$\therefore\ \varphi(\mathbf{x}; t_k + \Delta t) \to \varphi(\mathbf{x}; t_k) \quad \text{as } \Delta t \to 0 \text{ for all } \mathbf{x}.$$

However, $\varphi(\mathbf{x}; t_k)$ is an $n_a$-kink field and $\varphi(\mathbf{x}; t_k + \Delta t)$ is an $n_b$-kink field, and such fields cannot be continuously deformed into each other. Hence contradiction. Hence the metric $d$ between two fields of different kink number has a lower bound.

Consider the factors making up the product in Eq. (3). According to Feynman's prescription, the infinitesimal propagation kernel has the form

$$K[\varphi(\mathbf{x}; t_a + m\Delta t), \varphi(\mathbf{x}; t_a + (m-1)\Delta t); \Delta t] = A^{-1} \exp(iL[\tilde{\varphi}, \dot{\tilde{\varphi}}]\Delta t), \tag{4}$$

where $L$ is the Lagrangian of the system. For nonlinear field theories there is some difficulty in interpreting $\tilde{\varphi}$ and $\dot{\tilde{\varphi}}$. Symbolically, we "define"

$$\tilde{\varphi} = \tfrac{1}{2}[\varphi(\mathbf{x}; t_a + m\Delta t) + \varphi(\mathbf{x}; t_a + (m-1)\Delta t)],$$

$$\dot{\tilde{\varphi}} = (\Delta t)^{-1}[\varphi(\mathbf{x}; t_a + m\Delta t) - \varphi(\mathbf{x}; t_a + (m-1)\Delta t)].$$

For Skyrme's theory $\dot{\tilde{\varphi}}$ would involve terms like

$$(\Delta t)^{-1}[\phi_\rho(\mathbf{x}; t_a + m\Delta t) - \phi_\rho(\mathbf{x}; t_a + (m-1)\Delta t)]\cdot C(\phi_\rho).$$

$C(\phi_\rho)$ is a function of the fields at time $t_a + m\Delta t$. For a physical field theory, the Lagrangian should contain a term quadratic in $\dot{\tilde{\varphi}}$, and thus the infinitesimal propagator of Eq. (4) will contain terms like

$$\exp\{i[\varphi(\mathbf{x}; t_a + m\Delta t) - \varphi(\mathbf{x}; t_a + (m-1)\Delta t)]^2/\Delta t\},$$

and in particular it will contain a term for which

$$t_a + (m-1)\Delta t < t_k < t_a + m\Delta t.$$

As $\Delta t \to 0$ there will always be such a term, and, since the metric connecting fields across the discontinuity has a nonzero lower bound, the argument of the exponential will tend to infinity, thus giving a rapidly oscillating term that will cancel out any contributions to the propagator of Eq. (3). Thus if the fields $\varphi_a, \varphi_b$ contain a different number of kinks,

$$K(\varphi_b, \varphi_a; t_b - t_a) = 0.$$

## 3. CONSERVATION OF SPIN

Schulman[8] has pointed out that the path integral in a multiply connected space has complications owing to the fact that paths in different homotopy classes cannot be continuously deformed into each other. He showed that while the partial probability amplitude $K^\beta$ for a transition involving only paths in homotopy class $\beta$ may be obtained by performing the path integration over all paths belonging to this class, the total probability amplitude $K$ involves a sum of the $K^\beta$ with unknown weight factors:

$$K = \sum_\beta \lambda(\beta) K^\beta. \tag{5}$$

It has been shown by Laidlaw and DeWitt[9] that the $\lambda(\beta)$ must form a scalar unitary representation of the fundamental group of the space. The space that we are considering is $M(R^3, Y)$. The fact that we are assuming $M(R^3, Y)$ to admit spin means that the fundamental group $\pi_1(M(R^3, Y))$ equals $Z_2$, the group of integers modulo 2:

$$\pi_1(M(R^3, Y)) = Z_2. \tag{6}$$

Thus $\lambda(\beta)$ takes on only the values $\pm 1$.

Let $\varphi_b, \varphi_a \in M(R^3, Y)$ be 1-kink mappings. Denote the total amplitude for transition between $\varphi_a$ at time $t_a$ and $\varphi_b$ at time $t_b$ by $K(\varphi_b, \varphi_a; t_b - t_a)$. Now for the theory to admit spin we need more than Eq. (6). Let us suppose that a path from $\varphi_a$ to $\varphi_b$, labeled by time running from $t_a$ to $t_b$, belongs to homotopy class 1. We shall write the partial probability amplitude corresponding to such paths as $K(\varphi_b, \varphi_a^1; t_b - t_a)$. Using Eq. (6), we can rewrite Eq. (5) as

$$K(\varphi_b, \varphi_a; t_b - t_a) = K(\varphi_b, \varphi_a^1; t_b - t_a) - K(\varphi_b, \varphi_a^2; t_b - t_a).$$

Similarly, if $\varphi_b$ is reached by a path which involves rotating $\varphi_a$ through $2\pi$ and then following a path of homotopy class 1, then we shall write $R_{2\pi}\varphi_a^1$ in the partial probability amplitude. For the theory to admit spin, it must be shown that

$$R_{2\pi}\varphi_a^1 = \varphi_a^2$$

for *all* $\varphi_a \in M(R^3, Y)$. Of course, if this is true, it follows that

$$R_{2\pi}\varphi_a^2 = \varphi_a^1$$

and

$$K(\varphi_b, R_{2\pi}\varphi_a; t_b - t_a) = -K(\varphi_b, \varphi_a; t_b - t_a). \tag{7}$$

We wish to show that if Eq. (7) holds for a particular state $K(\varphi_b, \varphi_a; t_b - t_a)$ of the system, then it holds for any state $K(\varphi_c, \varphi_a, t_c - t_a)$ into which the system may evolve. That is to say, we wish to show that spin is conserved. (Clearly, $\varphi_b$ and $\varphi_c$ must be fields corresponding to an equal number of kinks.)

Let Eq. (7) be true for a particular $\varphi_b \in M(R^3, Y)$ and let $\varphi_c$ be any member of $M(R^3, Y)$ containing the same number of kinks as $\varphi_b$. First of all, consider an infinitesimal time change $t_b \to t_b + \delta t$. Since this cannot bring about a flip in sign, Eq. (7) implies

$$K(\varphi_b, R_{2\pi}\varphi_a; t_b + \delta t - t_a) = -K(\varphi_b, \varphi_a; t_b + \delta t - t_a).$$

By constructing a continuous sequence of such small time differences, a finite time difference can be built up, and it follows that

$$K(\varphi_b, R_{2\pi}\varphi_a; t_0 - t_a) = -K(\varphi_b, \varphi_a; t_0 - t_a).$$

Suppose that an amplitude $K(\varphi_c, \varphi_a; t_c - t_a)$ is given. We can choose $t_0$ such that $t_0 < t_c$. By the composition law for Feynman integrals

$$K(\varphi_c, \varphi_a; t_c - t_a) = \int K(\varphi_c, \varphi_b; t_c - t_0) K(\varphi_b, \varphi_a, t_0 - t_a)\, \mathfrak{D}(\varphi_b);$$

$$\therefore\ K(\varphi_c, R_{2\pi}\varphi_a; t_c - t_a) = \int K(\varphi_c, \varphi_b, t_c - t_0) K(\varphi_b, R_{2\pi}\varphi_a, t_0 - t_a)\mathfrak{D}(\varphi_b) = -\int K(\varphi_c, \varphi_b, t_c - t_0) K(\varphi_b, \varphi_a, t_0 - t_a)\mathfrak{D}(\varphi_b) = -K(\varphi_c, \varphi_a, t_c - t_a),$$

which is the desired result.

## 4. SUMMARY

This paper has explained how, in a nonlinear quantum field theory, the number of kinks and the associated spin must both be conserved quantities. Conservation of kinks was proved by showing that the transition amplitude between states of different kink number involved only discontinuous paths whose contribution was zero. The conservation of spin was shown to be a natural consequence of the composition law for Feynman integrals.

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# Rigorous Statistical Mechanics for Nonuniform Systems*

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The thermodynamic limit of a classical system with many-body interactions and under the influence of an external potential is investigated for the canonical ensemble. By scaling the external potential to a sequence of domains which are isotropic expansions of an initial domain confining the system, it is shown that the canonical free energy per particle has an infinite system limit. Moreover, by restricting consideration to internal interactions which have the property that separated groups of particles have negligible mutual attractive energy as the system becomes infinite, it is proven that the free energy per particle limit is precisely the free energy per particle obtained by minimizing the integral $\int[\phi\rho + f(\rho, \beta)]$ with respect to all properly normalized functions $\rho(r)$. $\phi$ is the external potential; $f(\rho, \beta)$ is the free energy per unit volume for a uniform system of density $\rho$ and inverse temperature $\beta$. The only technical complication is the above-mentioned restriction on the allowed internal interactions. It is demonstrated that there exists a wide class of many-body interactions which have the required separation properties. The simplest example is a two-body interaction which includes a hard core.

## 1. INTRODUCTION

We shall consider a classical system specified by a Hamiltonian of the form

$$H_n = \sum_{i=1}^{n} \frac{p_i^2}{2m} + \sum_{i=1}^{n} \phi(x_i) + U_n(x_1, \ldots, x_n), \qquad (1.1)$$

where $U_n(x_1, \ldots, x_n)$ is an $n$-particle interaction potential and $\phi(x)$ is a single-particle external potential dependent on a position variable $x$. Let $\phi(x)$ be defined on a bounded domain $\Lambda$ contained in Euclidean space. The interaction and external potentials may depend on other internal coordinates having a fixed bounded range, but these coordinates will make no essential change in our analysis. We assume that the potential $U_n(x_1, \ldots, x_n)$ is symmetric in the variables $x_i$ and that $U_n$ is translationally invariant.

For $n$ particles confined to the domain $\Lambda$, the canonical partition function is

$$Z(\Lambda, n, \beta, \phi) = (2\pi m/\beta)^{3n/2} Q(\Lambda, n, \beta, \phi), \qquad (1.2)$$

where $Q(\Lambda, n, \beta, \phi)$ is the configurational partition function given by

$$Q(\Lambda, n, \beta, \phi) = \frac{1}{n!} \int_{\Lambda^n} dx_1 \cdots dx_n \times \exp\left[-\beta\left(\sum_{i=1}^{n} \phi(x_i) + U_n(x_1, \ldots, x_n)\right)\right]. \qquad (1.3)$$

The free energy per particle is given by

$$-(\beta^{-1}/n) \ln Z(\Lambda, n, \beta, \phi). \qquad (1.4)$$

In order to obtain a well-defined infinite system free energy per particle for a nonuniform system given by (1.1), it is necessary that we consider a sequence of external potentials $\{(\Lambda, \phi)\}$ where each potential is paired with one member of an expanding sequence of domains $\{\Lambda\}$. We shall define the thermodynamic limit as follows. Let $\phi_0$ be defined on a domain $\Lambda_0$. Then for each $n \geq n_0$ for some positive integer $n_0$, we define a sequence $\{(\Lambda, \phi)\}$ by

$$\Lambda = \{x \mid x = (n/n_0)^{1/3} y,\ y \in \Lambda_0\} \qquad (1.5)$$

and

$$\phi(x) = \phi_0(y) \text{ where } y = (n_0/n)^{1/3} x, \quad \text{all } x \in \Lambda.$$

The domains of the sequence defined by (1.5) satisfy the constraint

$$nV(\Lambda)^{-1} = n_0 V(\Lambda_0)^{-1} = \rho_0, \qquad (1.6)$$

where $V(\Lambda)$ denotes the volume (Lebesque measure) of $\Lambda$. The configurational free energy per particle is given by

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and we shall say that the thermodynamic limit exists if the sequence $\{\mathfrak{F}(\Lambda, n, \beta, \phi)\}$ converges for the sequence $\{(\Lambda, \phi)\}$ defined by (1.5).

As required for the existence of the thermodynamic limit of uniform systems, we assume that the interaction $U_n$ is stable and tempered.[1] Then $\phi \equiv 0$ on $\Lambda$ gives that

$$\lim_n \mathfrak{F} = \rho_0^{-1} f(\rho_0), \qquad (1.8)$$

where $f(\rho)$ is a convex function defined on an interval $0 \leq \rho \leq \rho_{cp}$.[2] The function $f$ is also a concave function of $\beta^{-1}$, but we will not be concerned with this dependence. For the sequence (1.5), we have the result

$$V(\Lambda)^{-1} \int_{\Lambda} e^{-\beta\phi(x)} dx = V(\Lambda_0)^{-1} \int_{\Lambda_0} e^{-\beta\phi_0(x)} dx \qquad (1.9)$$

for all $n \geq n_0$ if the integral on the right exists. Then for the case that $U_n \equiv 0$ for all $n$, the sequence $\{\mathfrak{F}\}$ converges. In the general case, we can show that the sequence $\{\mathfrak{F}\}$ is bounded since the stability condition

$$U_n(x_1, \ldots, x_n) \geq -bn \quad (b > 0) \qquad (1.10)$$

which holds for all $(x_1, \ldots, x_n)$ and all $n$ gives

$$\liminf_n \mathfrak{F} \geq -\beta^{-1}[1 - \ln\rho_0 + \beta b + \ln(V(\Lambda)^{-1} \int_{\Lambda} e^{-\beta\phi(x)} dx)]. \qquad (1.11)$$

With the restriction $0 < \rho_0 < \rho_{cp}$, we obtain

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$$\liminf_n \mathfrak{F} \geq -\beta^{-1}[1 - \ln\rho_0 + \beta b + \ln(V(\Lambda)^{-1} \int_{\Lambda} e^{-\beta\phi(x)} dx)]. \qquad (1.11)$$

With the restriction $0 < \rho_0 < \rho_{cp}$, we obtain

$$\lim_n \sup \mathfrak{F} \le \rho_0^{-1} f(\rho_0) - \beta^{-1} \ln(V(\Lambda)^{-1} \int_\Lambda e^{-\beta \phi(x)} dx). \tag{1.12}$$

## 2. THE THERMODYNAMIC LIMIT

In this section, we shall establish three main theorems. We begin with some terminology. A step potential $\phi_r$ (simple function) of $r$ steps defined on $\Lambda$ is a function of the form

$$\phi_r(x) = \sum_{i=1}^{r} a_i C_{\Lambda i}, \tag{2.1}$$

where the $a_i$ are real constants, $\{\Lambda_i\}_{i=1}^r$ is a partition of $\Lambda$ into $r$ disjoint subdomains such that their union equals $\Lambda$, and $C_{\Lambda i}$ is the characteristic function of each $\Lambda_i$. We also require that each $\Lambda_i$ has a connected interior and that $V(\Lambda_i) \to \infty$ in the Fisher sense for each $i = 1, \ldots, r$ as $n \to \infty$.[3] A sequence $\{(\Lambda, \phi_r)\}$ of step potentials is obtained from some initial step potential as defined by (1.5) so that

$$V(\Lambda_i)/V(\Lambda) = \omega_i \quad (i = 1, \ldots, r) \tag{2.2}$$

holds for all $n \ge n_0$, where each $\omega_i$ is a fixed constant. On each $\Lambda$ the supremum norm of $\phi$ is defined by

$$\|\phi\| = \sup_\Lambda |\phi(x)| = \|\phi_0\|. \tag{2.3}$$

Now, if $\phi_0$ is the uniform limit of a sequence of step potentials defined on $\Lambda_0$, then $\phi_r \to \phi$ equiuniformly on each $\Lambda$ as $r \to \infty$. Then for each $r$ the norm $\|\phi - \phi_r\|$ defined over $\Lambda$ by (2.3) is a constant for all $n \ge n_0$.

We obtain an important property:

*Lemma 2.1:* Let $\phi_r \to \phi$ uniformly on $\Lambda$. Then, for every $\epsilon > 0$, there exists an $s$ such that

$$|\mathfrak{F}(\Lambda, n, \beta, \phi) - \mathfrak{F}(\Lambda, n, \beta, \phi_r)| \le \epsilon \tag{2.4}$$

holds for all $n \ge n_0$ whenever $r > s$.

*Proof:* Given $\epsilon > 0$ there exists an $s$ such that

$$\|\phi - \phi_r\| < \epsilon \tag{2.5}$$

holds for all $n \ge n_0$ whenever $r > s$. Hence

$$e^{-\beta\epsilon n} Q(\Lambda, n, \beta, \phi) \le Q(\Lambda, n, \beta, \phi_r) \le e^{\beta\epsilon n} Q(\Lambda, n, \beta, \phi) \tag{2.6}$$

holds for all $n$ and gives (2.4).

We continue by defining a class of interactions $U_n$ which yield the result that the thermodynamic limit exists for step potentials. Let $E$ donote three-dimensional Euclidean space. The domains $\Lambda$ are bounded subsets of $E$. For $i = 1, \ldots, r$ let $X_i = (x_1, \ldots, x_{n_i})$, where $X_i \in E^{n_i}$. We denote $X = (X_1, \ldots, X_r)$, where $X \in E^n$ and $\sum_{i=1}^r n_i = n$. With $X = (x_1, \ldots, x_n)$ the interaction potential can be decomposed as follows:

$$U_n(X) = \sum_{i=1}^{r} U_{n_i}(X_i) + \Psi_n(X_1, \ldots, X_r), \tag{2.7}$$

where $\sum_{i=1}^r n_i = n$ and where $\Psi_n(X_1, \ldots, X_r)$ represents the mutual potential energy of $r$ collections of particles having $n_i$ particles in the collection $X_i$. For $X = (x_1, \ldots, x_n)$ the notation $x \in X_i$ with $n_i \ge 1$ will mean that $x$ is one of the components $x_1, \ldots, x_n$. In case $n_i = 0$, then $X_i$ is a null point and has no components. We shall say that an interaction is asymptotically additive if the following holds.

*Definition 2.1:* For each integer $r \ge 2$:

(i) Temperedness: There exist positive constants, $w$, $\lambda$, and $R_0$ independent of $r$ such that

$$|\Psi_n(X_1, \ldots, X_r)| \le w n^2 / d^{3+\lambda} \tag{2.8}$$

for all $n$ whenever $d > R_0$, where $d = \min\{D(X_i, X_j) | n_i, n_j \ge 1, i \ne j\}$ and where $D(X_i, X_j) = \inf\{|x - x'| | x \in X_i, x' \in X_j\}$, $i, j = 1, \ldots, r$.

(ii) Let $\{\Lambda_i\}_{i=1}^r$ be a disjoint partition of $\Lambda$ satisfying (2.2) such that each $\Lambda_i$ has a connected interior and $V(\Lambda_i) \to \infty$ in the Fisher sense as $n \to \infty$. Define for each $R \ge 0$ a sequence of sets

$$\Omega_R = \{(x_1, \ldots, x_n) \in \Lambda^n \,|\, |x_i - x_j| \ge R \text{ if } i \ne j; \quad i, j = 1, \ldots, r\}. \tag{2.9}$$

For every $\epsilon > 0$, there exists an $N(\epsilon)$ and sequences $\{R\}$ and $\{A\}$ (as functions of $n$) with $\lim A = +\infty$ such that

$$U_n(X) \ge -nb + nA \quad \text{if} \quad X \in \Lambda^n - \Omega_R$$

and

$$\Psi_n(X_1, \ldots, X_r) \ge -\epsilon n \quad \text{if} \quad X \in \Omega_R$$

whenever $n > N(\epsilon)$ and $X_i \in \Lambda_i^{n_i}$, $i = 1, \ldots, r$, with $\sum_{i=1}^r n_i = n$. Part (ii) of Definition 2.1 can be stated in another form without reference to the sets $\{\Omega_R\}$. For every $(X_1, \ldots, X_r) = X$

$$\Psi_n(X_1, \ldots, X_r) < -\epsilon n \quad \text{implies} \quad U_n(X) \ge -nb + nA \tag{2.10}$$

whenever $n > N(\epsilon)$ and $X_i \in \Lambda_i^{n_i} (i = 1, \ldots, r)$ with $\sum_{i=1}^r n_i = n$.

The condition (2.10) has the effect that groups of particles confined by different wall-less containers (the subdomains $\Lambda_i$) in contact will have negligible mutual attractive energy as the containers become infinitely large. Asymptotic additivity will give the result that the free energy per particle associated with accumulations of particles near the boundaries of the subdomains $\Lambda_i$ is negligible in the thermodynamic limit. For positive and tempered interactions we can take $\Omega_R = \Lambda^n$ for all $n$ and satisfy Definition 2.1. Hence the class of asymptotically additive interactions is nonempty.

*Theorem 2.1:* Let $U_n(x_1, \ldots, x_n)$ be stable and asymptotically additive. Then the sequence $\{\mathfrak{F}(\Lambda, n, \beta, \phi_r)\}$ converges for a step potential $\phi_r$. Furthermore, if $\phi$ is the uniform limit of a sequence of step potentials defined on $\Lambda$, then the thermodynamic limit exists for $\phi$.

If $\phi$ is the uniform limit of a sequence $\{\phi_r\}$ of step potentials, the convergence of $\{\mathfrak{F}\}$ is an immediate consequence of Lemma 2.1. After stating our second main theorem, we shall return to the proof of Theorem 2.1 in Sec. 4.

Let $f(\rho_0)$ be the free energy per unit volume associated with the thermodynamic limit of a uniform system determined by an asymptotically additive interaction $U_n(x_1, \ldots, x_n)$. The function $f(\rho_0)$ is continuous and convex on an interval $0 \le \rho_0 < \rho_{cp}$. We define a convex functional

$$F(\rho) = \frac{1}{n} \int_\Lambda f(\rho(x)) dx \tag{2.11}$$

on all density distributions $\rho(x)$ defined and integrable on $\Lambda$. For $\phi$ integrable on $\Lambda$ we let

$$(\phi, \rho) = \frac{1}{n}\int_\Lambda \phi(x)\rho(x)dx. \tag{2.12}$$

Two norms we will use are

$$\|\rho\| = \sup_\Lambda |\rho(x)| \quad \text{and} \quad \|\rho\|_1 = \frac{1}{n}\int_\Lambda |\rho(x)|dx. \tag{2.13}$$

Let $\phi$ be the uniform limit of a sequence $\{\phi_r\}$ of step potentials of form (2.1). We will write

$$\rho_r(x) = \sum_{i=1}^{r} \rho_i C_{\Lambda_i} \tag{2.14}$$

for the same partition $\{\Lambda_i\}_{i=1}^r$ which determines $\phi_r$ on $\Lambda$. For each $r$ we define a special set of density distributions on $\Lambda$:

$$D_r = \{\rho_r \geq 0 \mid \|\rho_r\|_1 = 1\}. \tag{2.15}$$

Let $L$ denote the real normed linear space of all bounded Lebesque measurable functions on $\Lambda$ with uniform norm $\|\cdot\|$. The space $L$ is a Banach space. Let

$$S = \{\rho \in L \mid \|\rho\| < \rho_{cp}\} \tag{2.16}$$

and

$$D = \overline{\bigcup_r D_r} \tag{2.17}$$

be the closure of $\cup_r D_r$ in $L$. With these definitions we obtain

*Lemma 2.2:* The convex functional $F$ is continuous in $S \cap \text{dom}F$ with respect to the uniform norm.

The proof of Lemma 2.2 follows directly from the uniform continuity of $f$ on every closed subinterval of $[0, \rho_{cp})$. The next two theorems identify the thermodynamic limit.

*Theorem 2.2:* Let $\phi$ be a uniform limit of step potentials on $\Lambda$. Then

$$\lim_n \mathcal{F}(\Lambda, n, \beta, \phi) = \inf_{D\cap S}\{(\phi, \rho) + F(\rho)\} \tag{2.18}$$

when $nV(\Lambda)^{-1} = \rho_0 < \rho_{cp}$.

One should note that if $\phi$ is a step potential $\phi_r$, then the infimum in (2.18) is taken over $D_r \cap S$. Our last main theorem is

*Theorem 2.3:* Let the interaction $U_n(x_1, \ldots, x_n)$ be stable and asymptotically additive. Let $\phi$ defined on $\Lambda$ be a step potential or the uniform limit of a sequence of step potentials defined on $\Lambda$. Then

$$\lim_n \mathcal{F}(\Lambda, n, \beta, \phi) = \inf\{(\phi, \rho) + F(\rho) \mid \|\rho\|_1 = 1\} \tag{2.19}$$

when $nV(\Lambda)^{-1} = \rho_0 < \rho_{cp}$.

In the next section we give some examples of asymptotically additive interactions and in the following sections prove the main theorems.

## 3. ASYMPTOTICALLY ADDITIVE INTERACTIONS

We indicate now criteria under which interactions constructed from pair potentials are asymptotically additive. A pair potential $\Phi(x)$ is a symmetric and bound below measurable function. The interaction is given by

$$U_n(x_1, \ldots, x_n) = \tfrac{1}{2}\sum_{i\neq j} \Phi(x_i - x_j). \tag{3.1}$$

Interactions for which $\Psi_n(X_1, \ldots, X_r)$ is always nonnegative are the first examples of asymptotically additive interactions.

*Proposition 3.1:* (a) If $\Phi(x) \geq 0$ all $x$ and (b) there exist positive constants $w$, $\lambda$, and $R_0$ such that

$$|\Phi(x)| \leq w/|x|^{3+\lambda} \tag{3.2}$$

if $|x| \geq R_0$, then $U_n$ is stable and asymptotically additive.

For pair potentials we shall always assume that part (b) of Proposition 3.1 holds. Then the interaction (3.1) will be tempered.

*Proposition 3.2:* (a) Hard core: There exists $R_1 > 0$ such that $\Phi(x) = +\infty$ if $|x| < R_1$ and (b) there exists $b > 0$ such that

$$\sum_{i=1}^{n} \Phi(x_i) \geq -\frac{b}{R_1^3} \tag{3.3}$$

holds for all $n$ and all $(x_1, \ldots, x_n)$ with $|x_i - x_j| \geq R_1$ for $i \neq j$, then (3.1) is stable and asymptotically additive. The proof of Proposition 3.2 will be delayed and given as a special case of the following.

*Proposition 3.3:* (a) Let $\alpha$, $c$, and $R_1$ be positive constants such that

$$\Phi(x) \geq c/|x|^\alpha \tag{3.4}$$

if $|x| < R_1$.

(b) Suppose there exists a constant $b > 0$ such that for every $R > 0$

$$\sum_{i=1}^{n} \Phi(x_i) \geq -\frac{b}{R^3} \tag{3.5}$$

holds for all $n$ and all $(x_1, \ldots, x_n)$ with $|x_i - x_j| \geq R$ for $i \neq j$. Then there exists sufficiently large $\alpha$ such that the interaction (3.1) is stable and asymptotically additive.

In particular, condition (3.5) will hold if there exists a positive decreasing function $\Phi_0(t)$ on $[0, \infty)$ such that

$$\int_0^\infty \Phi_0(t)t^2dt < \infty \quad \text{and} \quad \Phi(x) \geq -\Phi_0(|x|) \quad \text{for all } x. \tag{3.6}$$

Ruelle has shown that interactions satisfying (3.6) and (3.4) with $\alpha > 3$ are superstable. He has also shown that interactions satisfying (3.3) are stable. We shall now prove asymptotic additivity for the Propositions 3.2 and 3.3.

*Proof:* Temperedness is assumed so that we need only show that part (ii) of Definition 2.1 holds. Observe that there is a largest constant $b > 0$ such that $\Phi(x) \geq -b$ and $U_n(x_1, \ldots, x_n) \geq -nb$ as well as (3.3) and (3.5) hold. Let $r$ be a fixed positive integer and let $\{\Lambda_i\}_{i=1}^r$ be a disjoint partition of $\Lambda$ with $V(\Lambda_i) \to +\infty$ in the Fisher sense as $n \to \infty$, $i = 1, \ldots, r$. Let $\partial\Lambda_i$ denote the boundary of $\Lambda_i$. Then, by the regularity of each $\Lambda_i$, there exists a boundary region $B_i \subset \Lambda_i$ each $i$ and a divergent sequence $\{d\}$ such that

$$V(B)V(\Lambda)^{-1} \to 0 \quad \text{and} \quad n/d^{3+\lambda} \to 0 \quad \text{as } n \to \infty$$

where

$$B = \bigcup_{i=1}^{r} B_i \quad \text{and} \quad B_i = \{x \in \Lambda_i | D(x, \partial\Lambda_i) \le d\}$$

for $i = 1, \ldots, r$.

Here $D(x, \partial\Lambda_i)$ is the distance between $x$ and the boundary $\partial\Lambda_i$. For Proposition 3.3 we restrict consideration to partitions of $\Lambda$ which satisfy

$$V(\Lambda)^{\alpha-6}/V(B)^{\alpha} \to \infty \quad \text{as } n \to \infty \tag{3.7}$$

for some $\alpha$. If $V(B) = V(\Lambda)^{\delta}$ with $0 < \delta < 1$, then the condition (3.7) will occur. We define

$$\Omega_R = \{(x_1, \ldots, x_n) \in \Lambda^n \mid |x_i - x_j| \ge R \text{ if } i \ne j\}. \tag{3.8}$$

Given $\epsilon > 0$, we shall construct sequences $\{R\}$ and $\{A\}$ with $\lim_n A = \infty$ such that

$$U_n(X) \ge -nb + nA \quad \text{if } X \in \Lambda^n - \Omega_R$$

and

$$\Psi_n(X_1, \ldots, X_r) \ge -n\epsilon \quad \text{if } X \in \Omega_R$$

where

$$X = (X_1, \ldots, X_r) \text{ with } X_i \in \Lambda_i^{n_i} (i = 1, \ldots, r),$$

$$\sum_{i=1}^{r} n_i = n \quad \text{whenever } n \text{ is sufficiently large.}$$

Let $X_i = (X_i - Y_i, Y_i)$ where $Y_i \in B_i^{k_i}$ for $0 \le k_i \le n_i$, $i = 1, \ldots, r$. The points of $X_i$ not in $B_i$ are $X_i - Y_i$. Now the mutual potential can be decomposed as follows:

$$\Psi_n(X_1, \ldots, X_r) = \sum_{j=1}^{r-1} \sum_{y \in X_j} \sum_{i=j+1}^{r} \sum_{x \in X_i} \Phi(x - y). \tag{3.9}$$

For $X \in \Omega_R$, we have

$$\sum_{i=j+1}^{r} \sum_{x \in X_i} \Phi(x) \ge -\frac{b}{R^3}, \tag{3.10}$$

which gives

$$\sum_{y \in Y_j} \sum_{i=j+1}^{r} \sum_{x \in X_i} \Phi(x - y) \ge -k_j \frac{b}{R^3} \tag{3.11}$$

for $(j = 1, \ldots, r-1)$. Temperedness gives that

$$\sum_{j=1}^{r-1} \sum_{y \in (X_j - Y_j)} \sum_{i=j+1}^{r} \sum_{x \in X_i} \Phi(x - y) \ge -w\frac{n^2}{d^{3+\lambda}}. \tag{3.12}$$

From (3.11) and (3.12) we obtain

$$\Psi_n(X_1, \ldots, X_r) \ge -w\frac{n^2}{d^{3+\lambda}} - k\frac{b}{R^3}, \tag{3.13}$$

where $k = \sum_{i=1}^{r} k_i$.

If $X \in \Lambda^n - \Omega_R$ for $R \le R_1$, then $|x_j - x_l| < R$ for some $j$ and $l$ with $j \ne l$; and

$$U_n(X) \ge -2bn + c/R^{\alpha} \tag{3.14}$$

since

$$\sum_{i=1, i \ne l}^{n} \Phi(x_l - x_i) \ge -(n-2)b + \Phi(x_l - x_j). \tag{3.15}$$

If $R_1$ is the hard core distance, then $X \in \Lambda^n - \Omega_R$ with $R \le R_1$ implies $U_n(X) = +\infty$. Now there exists a constant $c_1 > 0$ such that $c_1/R^3$ is an upper bound for the maximum packing density of spheres of radius $R/2$. Let $c_1 > 0$ be such that for all $R > 0$

$$k/V(B) > c_1/R^3 \text{ implies } X \notin \Omega_R.$$

Let the sequences $\{R\}$ and $\{A\}$ be determined by

$$R^{-6} = (bc_1)^{-1}(\epsilon - wn/d^{3+\lambda})[n/V(B)] \tag{3.16}$$

and

$$c/R^{\alpha} = n(A + b). \tag{3.17}$$

Note that $\lim A = +\infty$ by condition (3.7).

Now suppose that

$$\Psi_n(X_1, \ldots, X_r) < -\epsilon n$$

for $X \in \Omega_R$. Then (3.13) implies that

$$k/V(B) > (R^3/b)[\epsilon - wn/d^{3+\lambda}][n/V(B)] = c_1/R^3, \tag{3.18}$$

which implies $X \notin \Omega_R$ (if $n$ sufficiently large) a contradiction. For hard cores we can take the sequence $\{R\}$ to be a constant sequence $R = R_1$ all $n$ and $\{A\}$ can be any divergent sequence of positive numbers. Let $N(\epsilon)$ be such that

$$\epsilon > wn/d^{3+\lambda} \tag{3.19}$$

if $n > N(\epsilon)$; then (3.16), (3.17), and (3.18) hold. This completes the proof of the propositions.

## 4. THERMODYNAMIC LIMIT FOR STEP POTENTIALS

In this section we shall prove Theorem 2.1. Let $\phi_r$ be a step potential defined on $\Lambda$ as given by (2.1). The associated disjoint partition of $\Lambda$ is $\{\Lambda_i\}_{i=1}^{r}$. The configurational partition function (1.3) defined for $\phi_r$ has the following expansion:

$$Q(\Lambda, n, \beta, \phi_r) = \sum_{\substack{n_1 = 0 \\ n_1 + \cdots + n_r = n}}^{n} \cdots \sum_{n_r = 0}^{n} \prod_{i=1}^{r} \frac{e^{-\beta a_i n_i}}{n_i!} \times \int_{\prod_{i=1}^{r} \Lambda_i^{n_i}} e^{-\beta U_n(X)} dX_1 \cdots dX_r \tag{4.1}$$

with notation $X = (X_1, \ldots, X_r)$. We now define a sequence of functions $F_{r,n}$ of an $r$-dimensional vector variable by

$$F_{r,n}(\rho_r) = -\beta^{-1}\frac{1}{n} \ln\left(\prod_{i=1}^{r} \frac{1}{n_i!} \int_{\prod_{i=1}^{r} \Lambda_i^{n_i}} e^{-\beta U_n(X)} dX_1 \cdots dX_r\right), \tag{4.2}$$

where for each $n$ the domain $D_{r,n}$ of $F_{r,n}$ is the finite set of all

$$\rho_r = (\rho_1, \ldots, \rho_r)$$

such that

$$\rho_i = n_i/V(\Lambda_i) \quad \text{for } 0 \le n_i \le n, \quad i = 1, \ldots, r, \tag{4.3}$$

and such that

$$\sum_i^r \omega_i \rho_i = \rho_0. \tag{4.4}$$

With $\phi_r = (a_1, \ldots, a_r)$ and $\boldsymbol{\rho}_r = (\rho_1, \ldots, \rho_r)$ we define

$$(\phi_r, \boldsymbol{\rho}_r) = \rho_0^{-1} \sum_{i=1}^r \omega_i a_i \rho_i. \tag{4.5}$$

We further define

$$\mathfrak{F}^*_{r,n} = \inf_{D_{r,n}} \{(\phi_r, \boldsymbol{\rho}_r) + F_{r,n}(\boldsymbol{\rho}_r)\}. \tag{4.6}$$

Since $D_{r,n}$ is a finite set, there exists, for each $n$, a $\boldsymbol{\rho}^*_{r,n} \in D_{r,n}$ at which (4.6) assumes its minimum. Then

$$\mathfrak{F}^*_{r,n} = (\phi_r, \boldsymbol{\rho}^*_{r,n}) + F_{r,n}(\boldsymbol{\rho}^*_{r,n}). \tag{4.7}$$

Now the sum (4.1) is comprised of less than $(n+1)^r$ distinct nonnegative terms so that by factoring out a largest term from this sum we obtain the inequality

$$0 \le \mathfrak{F}^*_{r,n} - \mathfrak{F}(\Lambda, n, \beta, \phi_r) \le \beta^{-1}(r/n) \ln(n+1). \tag{4.8}$$

Therefore, the thermodynamic limit for an external step potential $\phi_r$ exists if and only if the sequence $\{\mathfrak{F}^*_{r,n}\}$ of minima converges. To prove that the sequence (4.7) converges, we shall need the next proposition which will utilize the properties of asymptotically additive interactions. We first give some definitions.

We define another convex function of an $r$-dimensional vector variable by

$$F_r(\boldsymbol{\rho}_r) = \rho_0^{-1} \sum_{i=1}^r \omega_i f(\rho_i) \tag{4.9}$$

where the domain of this function is all $\boldsymbol{\rho}_r = (\rho_1, \ldots, \rho_r)$ with $0 \le \rho_i < \rho_{cp}$, $i = 1, \ldots, r$. For the norm

$$\|\boldsymbol{\rho}_r\| = \sup_{i=1,\ldots,r} |\rho_i| \tag{4.10}$$

the closure of the union $\cup_n D_{r,n}$ is the set

$$\{(\rho_1, \ldots, \rho_r) \Big| \sum_{i=1}^r \omega_i \rho_i = \rho_0,\ \rho_i \ge 0,\ i = 1, \ldots, r\}. \tag{4.11}$$

The set (4.11) is a compact subset of $r$-dimensional Euclidean space and is identical to $D_r$ except for representation (isometrically isomorphic to $D_r$).

We shall further restrict the interaction $U_n$ by requiring that the uniform free energy per volume $f(\rho)$ which is a continous function on the interval $[0, \rho_{cp})$ be lower semi-continuous on the closed interval $[0, \rho_{cp}]$. If $\rho_{cp} = +\infty$, then stability of the interaction gives

$$\liminf_{\rho \to \rho_{cp}} f(\rho) = +\infty \tag{4.12}$$

since

$$f(\rho) \ge \rho(\ln \rho - 1 - \beta b)/\beta. \tag{4.13}$$

Then $f$ is lower semicontinuous as required. When the interaction has a finite hard core packing density $\rho_{cp}$, the free energy $f$ may not satisfy the condition (4.12). However, if $\beta > 0$ and $\rho_{cp} > 0$ are finite, then we can define $f(\rho) = +\infty$ for $\rho > \rho_{cp}^2$. In the case that the interaction has a finite hard core packing density, we shall restrict our considerations to those which have a free energy function $f$ satisfying (4.12). By defining $F_r(\boldsymbol{\rho}_r) = +\infty$ if $\|\boldsymbol{\rho}_r\| \ge \rho_{cp}$, then $F_r$ is lower semicontinuous. The importance of the condition (4.12) will become clear in what follows.

*Proposition 4.1:* Let $U_n(x_1, \ldots, x_n)$ be asymptotically additive. Let $\{\boldsymbol{\rho}_{r,n}\}$ be a sequence with $\boldsymbol{\rho}_{r,n} \in D_{r,n}$ for each $n$ such that

$$\boldsymbol{\rho}_{r,n} \to \boldsymbol{\rho}_r \quad \text{as } n \to \infty.$$

Then

$$\lim_n F_{r,n}(\boldsymbol{\rho}_{r,n}) = F_r(\boldsymbol{\rho}_r). \tag{4.14}$$

*Proof:* Let the disjoint partition $\{\Lambda_i\}_{i=1}^r$ of $\Lambda$, the boundary regions $B_i \subset \Lambda_i$, and the sequence $\{d\}$ be as previously defined. We define

$$f_n(\rho_{i,n}; \Lambda_i) = -\beta^{-1} V(\Lambda_i)^{-1} \ln\left(\frac{1}{n_i!} \int_{\Lambda_i^{n_i}} e^{-\beta U_{n_i}(X_i)} dX_i\right) \tag{4.15}$$

for each $n$, where $\boldsymbol{\rho}_{r,n} = (\rho_{1,n}, \ldots, \rho_{r,n})$ and $\rho_{i,n} = n_i / V(\Lambda_i)$ for $i = 1, \ldots, r$. So that by applying temperedness we obtain

$$F_{r,n}(\boldsymbol{\rho}_{r,n}) \le \rho_0^{-1} \sum_{i=1}^r \omega_i' f_n(\rho'_{i,n}; \Lambda_i - B_i) + wn/d^{3+\lambda}, \tag{4.16}$$

where

$$\omega_i' = \omega_i - V(B_i)/V(\Lambda) \quad \text{and}$$
$$\rho'_{i,n} = \rho_{i,n}(1 - V(B_i)/V(\Lambda_i))^{-1} \tag{4.17}$$

for $i = 1, \ldots, r$. From the thermodynamic limit for uniform systems we have

$$\lim_n f_n(\rho'_{i,n}; \Lambda_i - B_i) = \lim_n f_n(\rho_{i,n}; \Lambda_i) = f(\rho_i) \tag{4.18}$$

for each $i = 1, \ldots, r$, where $\boldsymbol{\rho}_r = (\rho_1, \ldots, \rho_r)$. Now, if $\rho_i \ge \rho_{cp}$ for some $i$, then

$$\lim \inf_n f_n(\rho_{i,n}; \Lambda_i) \ge \lim_{\rho' \to \rho_i} \inf f(\rho') = +\infty \tag{4.19}$$

follows by applying condition (4.12). Therefore,

$$\lim \sup_n F_{r,n}(\boldsymbol{\rho}_{r,n}) \le F_r(\boldsymbol{\rho}_r) \tag{4.20}$$

follows from (4.16) and (4.9). Note that if $\|\boldsymbol{\rho}_r\| \ge \rho_{cp}$ and

$$\lim \inf_n F_{r,n}(\boldsymbol{\rho}_{r,n}) = +\infty$$

then the result (4.14) holds. We now show that asymptotic additivity will imply the inequality

$$\lim \inf_n F_{r,n}(\boldsymbol{\rho}_{r,n}) \ge F_r(\boldsymbol{\rho}_r). \tag{4.21}$$

Let $\epsilon > 0$ be given; and let the sequences $\{A\}, \{R\}$, and $\{\Omega_R\}$ satisfy the conditions which define an asymptotically additive interaction. Then there exists an $N(\epsilon)$ such that

$$X = \{(X_1, \ldots, X_r) | X_i \in \Lambda_i^{n_i}\ (i = 1, \ldots, r), \Psi_n(X_1, \ldots, X_r) < -\epsilon n\} \subset \Lambda^n - \Omega_R$$

whenever $n > N(\epsilon)$. Now

$$\lim_n \frac{1}{n} \ln\left(\frac{1}{n!} \int_{\Lambda^n - \Omega_R} e^{-\beta U_n(X)} dX\right) = -\infty \tag{4.22}$$

since

$$\frac{1}{n} \ln\left\{\frac{1}{n!} \int_{\Lambda^n - \Omega_R} e^{-\beta U_n(X)} dX\right\} \le \beta(b - A) + \frac{1}{n} \ln\left(\frac{V(\Lambda)^n}{n!}\right) \tag{4.23}$$

holds for $n > N(\epsilon)$. We can write

$$\int_{\prod_{i=1}^{r}\Lambda_i^{n_i}} e^{-\beta U_n(X)}\,dX_1\cdots dX_r$$

$$= \int_{\prod_{i=1}^{r}\Lambda_i^{n_i}\cap\Omega_R} e^{-\beta U_n(X)}dX_1\cdots dX_r$$

$$+ \int_{\prod_{i=1}^{r}\Lambda_i^{n_i}\cap(\Lambda^n-\Omega_R)} e^{-\beta U_n(X)}dX_1,\ldots,X_r \qquad (4.24)$$

for each $n$. Now if $\limsup F_{r,n}(\boldsymbol{\rho}_{r,n}) < +\infty$, then

$$-\beta F_{r,n}(\boldsymbol{\rho}_{r,n})$$

$$\le \frac{1}{n}\ln\left(\prod_{i=1}^{r}\frac{1}{n_i!}\int_{\prod_{i=1}^{r}\Lambda_i^{n_i}\cap\Omega_R} e^{-\beta U_n(X)}dX_1\ldots dX_r\right)$$

$$+\frac{1}{n}\ln 2 \qquad (4.25)$$

holds for all $n$ sufficiently large. The inequality (4.25) gives that

$$-\beta F_{r,n}(\boldsymbol{\rho}_{r,n})$$

$$\le \frac{1}{n}\ln\left[\prod_{i=1}^{r}\left(\frac{1}{n_i!}\int_{\Lambda_i^{n_i}} e^{-\beta U_{n_i}(X_i)}dX_i\right)e^{\beta\epsilon n}\right]+\frac{1}{n}\ln 2$$

$$\le -\beta\rho_0^{-1}\sum_{i=1}^{r}\omega_i f_n(\rho_{i,n};\Lambda_i)+\beta\epsilon+\frac{1}{n}\ln 2 \qquad (4.26)$$

holds for $n$ sufficiently large since

$$U_n(X) \ge \sum_{i=1}^{r} U_{n_i}(X_i) - \epsilon n$$

if $(X_1,\ldots,X_r)\in\prod_{i=1}^{r}\Lambda_i^{n_i}\cap\Omega_R$ and $n > N(\epsilon)$.

We conclude that

$$\liminf_n F_{r,n}(\boldsymbol{\rho}_{r,n}) \ge F_r(\boldsymbol{\rho}_r) - \epsilon. \qquad (4.27)$$

If $\|\boldsymbol{\rho}_r\| < \rho_{cp}$, then the original assumption that $\limsup F_{r,n}(\boldsymbol{\rho}_{r,n}) < \infty$ which implied (4.27) will hold. Now if $\|\boldsymbol{\rho}_r\| \ge \rho_{cp}$ and $\liminf F_{r,n}(\boldsymbol{\rho}_{r,n}) < \infty$, then

$$\limsup_n -\beta F_{r,n}(\boldsymbol{\rho}_{r,n}) \le \limsup_n \frac{1}{n}\ln$$

$$\times\left(\prod_{i=1}^{r}\frac{1}{n_i!}\int_{\prod_{i=1}^{r}\Lambda_i^{n_i}\cap\Omega_R} e^{-\beta U_n(X)}dX_1\cdots dX_r\right) \qquad (4.28)$$

holds and (4.27) follows giving a contradiction. Thus we conclude that $\liminf F_{r,n}(\boldsymbol{\rho}_r) = +\infty$ if $\|\boldsymbol{\rho}_r\| \ge \rho_{cp}$ and the conclusion (4.14) holds. Since $\epsilon > 0$ is arbitrary, (4.27) implies (4.21) if $\|\boldsymbol{\rho}_r\| < \rho_{cp}$ and completes the proof.

The next lemma will complete the proof that the thermodynamic limit exists for step potentials of type (2.1) if the interaction is asymptotically additive. We define for any $n \ge n_0$

$$\mathfrak{F}_r^* = \inf_{D_r}\{(\phi_r,\rho_r)+F(\rho_r)\}. \qquad (4.29)$$

Now for each $\rho_r \in D_r$ of form (2.13) we have

$$F(\rho_r) = F_r(\boldsymbol{\rho}_r) \quad\text{and}\quad (\phi_r,\rho_r) = (\boldsymbol{\phi}_r,\boldsymbol{\rho}_r), \qquad (4.30)$$

where $\boldsymbol{\rho}_r = (\rho_1,\ldots,\rho_r)$, and conversely for each $\boldsymbol{\rho}_r$ in the set (4.11). Since $F_r$ is lower semicontinuous on the compact set (4.11), there exists a $\boldsymbol{\rho}_r^*$ in the set (4.11) such that

$$\mathfrak{F}_r^* = (\boldsymbol{\phi}_r,\boldsymbol{\rho}_r^*)+F_r(\boldsymbol{\rho}_r^*) = (\phi_r,\rho_r^*)+F(\rho_r^*), \qquad (4.31)$$

where $\rho_r^* \in D_r$ is the step density distribution corresponding to $\boldsymbol{\rho}_r^* = (\rho_1^*,\ldots,\rho_r^*)$.

*Lemma 4.1:* For the step potential $\phi_r$ let $\{\mathfrak{F}_{r,n}^*\}$ be the sequence defined by (4.7). Then

$$\lim_n \mathfrak{F}_{r,n}^* = \mathfrak{F}_r^*. \qquad (4.32)$$

*Proof:* First we observe that $\mathfrak{F}_r^*$ exists and is finite since

$$|(\boldsymbol{\phi}_r,\boldsymbol{\rho}_r)| \le \|\boldsymbol{\phi}_r\| \qquad (4.33)$$

for all $\boldsymbol{\rho}_r$ in set (4.11). Moreover, the point $\boldsymbol{\rho}_r^*$ must satisfy $\|\boldsymbol{\rho}_r^*\| < \rho_{cp}$ by the lower semicontinuity of $F_r$.

Now there exists a sequence $\{\boldsymbol{\rho}_{r,n}\}$ with $\boldsymbol{\rho}_{r,n}\in D_{r,n}$ such that $\boldsymbol{\rho}_{r,n}\to\boldsymbol{\rho}_r^*$ and

$$\lim_n[(\boldsymbol{\phi}_r,\boldsymbol{\rho}_{r,n})+F_{r,n}(\boldsymbol{\rho}_{r,n})] = \mathfrak{F}_r^* \qquad (4.34)$$

since

$$(\boldsymbol{\phi}_r,\boldsymbol{\rho}_{r,n})\to(\boldsymbol{\phi}_r,\boldsymbol{\rho}_r^*) \quad\text{and}\quad F_{r,n}(\boldsymbol{\rho}_{r,n})\to F_r(\boldsymbol{\rho}_r^*)$$

as $n\to\infty$. But we have

$$\mathfrak{F}_{r,n}^* \le (\boldsymbol{\phi}_r,\boldsymbol{\rho}_{r,n})+F_{r,n}(\boldsymbol{\rho}_{r,n}) \qquad (4.35)$$

for all $n$. Hence

$$\limsup_n \mathfrak{F}_{r,n}^* \le \mathfrak{F}_r^*. \qquad (4.36)$$

Also since the set (4.11) is sequentially compact there exists a subsequence $\{\boldsymbol{\rho}_{r,K}^*\}$ of $\{\boldsymbol{\rho}_{r,n}^*\}$ and a point $\boldsymbol{\rho}_r$ such that $\boldsymbol{\rho}_{r,K}\to\boldsymbol{\rho}_r$ as $K\to\infty$ and

$$\lim_K[(\boldsymbol{\phi}_r,\boldsymbol{\rho}_{r,K}^*)+F_{r,K}(\boldsymbol{\rho}_{r,K}^*)] = \liminf_n \mathfrak{F}_{r,n}^*. \qquad (4.37)$$

Then

$$\lim_K[(\boldsymbol{\phi}_r,\boldsymbol{\rho}_{r,K}^*)+F_{r,K}(\boldsymbol{\rho}_{r,K}^*)] = (\boldsymbol{\phi}_r,\boldsymbol{\rho}_r)+F_r(\boldsymbol{\rho}_r), \qquad (4.38)$$

and

$$\mathfrak{F}_r^* \le (\boldsymbol{\phi}_r,\boldsymbol{\rho}_r)+F_r(\boldsymbol{\rho}_r) = \liminf_n \mathfrak{F}_{r,n}^* \qquad (4.39)$$

follows. This ends the proof.

Applying inequality (4.8) and Lemma 4.1 we find that

$$\lim_n \mathfrak{F}(\Lambda,n,\beta,\phi_r) = \mathfrak{F}_r^*. \qquad (4.40)$$

To complete the proof of Theorem 2.1 suppose that $\phi$ is the uniform limit of step potentials $\phi_r$ defined on $\Lambda$. Then the sequence $\{\phi_r\}$ is a Cauchy sequence in the norm (2.3) and by Lemma 2.1 the bounded sequence $\{\mathfrak{F}_r^*\}$ of real numbers is also Cauchy. Hence the sequence $\{\mathfrak{F}_r^*\}$ has a finite limit which we shall call $\mathfrak{F}^*$. Again by Lemma 2.1 it follows that

$$\lim_n \mathfrak{F}(\Lambda,n,\beta,\phi) = \mathfrak{F}^*. \qquad (4.41)$$

The finiteness of $\mathfrak{F}^*$ is guaranteed by the bounds (1.11) and (1.12). The proof of Theorem 2.1 is now complete.

The final section will be concerned with the proof of Theorems 2.2 and 2.3. One should observe that in the proof of Theorem 2.1 we have established Theorem 2.2 in the special case that the external potential is a step potential.

## 5. THE THERMODYNAMIC LIMIT

In the section let $n \geq n_0$ be a fixed integer and $\Lambda$ a fixed domain satisfying the restriction $nV(\Lambda)^{-1} = \rho_0$ with $\rho_0 < \rho_{cp}$. The external potential $\phi$ is defined on $\Lambda$ and is the uniform limit of a sequence $\{\phi_\nu\}$ of step potentials also defined on $\Lambda$. The sets of density distributions $D_\nu$, $S$, and $D$ are defined by (2.14), (2.15), and (2.16), respectively. The convex functional $F$ defined by (2.10) has an effective domain

$$\operatorname{dom} F = \{\rho \geq 0 \mid F(\rho) < +\infty\}, \tag{5.1}$$

where $\rho$ is a bounded Lebesque measurable function defined on $\Lambda$. One should note that for most cases Riemann measure and integration will be enough. We begin the proof of Theorem 2.2 with a lower bound on $F$. Using Jensen's inequality, which is

$$f(V(\Lambda)^{-1}\textstyle\int_\Lambda \rho(x)dx) \leq V(\Lambda)^{-1}\int_\Lambda f(\rho(x))dx, \tag{5.2}$$

we obtain

$$F(\rho_0) \leq F(\rho) \tag{5.3}$$

for $\|\rho\|_1 = 1$, where $\rho_0$ is the constant function on $\Lambda$. Since $\|\phi\|$ and $\|\phi\|_1$ are assumed to be finite, we have

$$|(\phi, \rho)| \leq \|\phi\| \tag{5.4}$$

for all $\rho \in D$ since $\|\rho\|_1 = 1$, and

$$|(\phi, \rho)| \leq \|\phi\|_1 \|\rho\| < \infty \tag{5.5}$$

for $\rho \in L$. Then

$$-\|\phi\| + F(\rho_0) \leq \inf_{D\cap S}\{(\phi, \rho) + F(\rho)\} \leq \rho_0\|\phi\|_1 + F(\rho_0) \tag{5.6}$$

holds and the infimum indicated exists and is finite. We shall show that

$$\mathfrak{F}^* = \lim_\nu[(\phi_\nu, \rho_\nu^*) + F(\rho_\nu^*)] = \inf_{D\cap S}\{(\phi, \rho) + F(\rho)\}, \tag{5.7}$$

where $\{\rho_\nu^*\}$ is the sequence defined by (4.31). Now $(\phi_\nu, \rho) \to (\phi, \rho)$ uniformly for $\rho \in D$ by (5.4), and

$$\inf_{D\cap S}\{(\phi, \rho) + F(\rho)\} \leq (\phi, \rho_\nu^*) + F(\rho_\nu^*) \tag{5.8}$$

for all $\nu$ since $\{\rho_\nu^*\} \subset D \cap S$. Thus

$$\inf_{D\cap S}\{(\phi, \rho) + F(\rho)\} \leq \mathfrak{F}^*. \tag{5.9}$$

It remains to show that

$$\inf_{D\cap S}\{(\phi, \rho) + F(\rho)\} \geq \mathfrak{F}^*. \tag{5.10}$$

Suppose $\rho \in D \cap S$, then there exists a sequence $\{\rho_s\}$ with $\rho_s \in D_s \cap S$ such that $\rho_s \to \rho$ as $s \to \infty$ since $D$ is the closure of $\cup_\nu D_\nu$ and $S$ is open. Furthermore, $(\phi, \rho_s) \to (\phi, \rho)$ and $F(\rho_s) \to F(\rho)$ as $s \to \infty$ since

$$|(\phi, \rho) - (\phi, \rho_s)| \leq \|\phi\|_1\|\rho - \rho_s\|, \tag{5.11}$$

and $F$ is continuous in $D \cap S$. Therefore, there exists a sequence $\{\rho_\lambda\}$ with $\rho_\lambda \in D_\lambda \cap S$ such that

$$\lim_\lambda[(\phi, \rho_\lambda) + F(\rho_\lambda)] = \inf_{D\cap S}\{(\phi, \rho) + F(\rho)\}. \tag{5.12}$$

Now $\{\rho_\lambda^*\} \subset \{\rho_\nu^*\}$ is a subsequence with

$$(\phi_\lambda, \rho_\lambda^*) + F(\rho_\lambda^*) \leq (\phi_\lambda, \rho_\lambda) + F(\rho_\lambda). \tag{5.13}$$

Hence

$$\mathfrak{F}^* \leq \lim_\lambda[(\phi_\lambda, \rho_\lambda) + F(\rho_\lambda)] = \inf_{D\cap S}\{(\phi, \rho) + F(\rho)\} \tag{5.14}$$

follows since every subsequence of a convergent sequence has the same limit. This completes the proof of Theorem 2.2.

Our final result is the proof of Theorem 2.3. It will be convenient to define

$$\mathfrak{F}_*(\phi) = \inf\{(\phi, \rho) + F(\rho) \mid \|\rho\|_1 = 1\}, \tag{5.15}$$

where $\rho \in \operatorname{dom} F$. It is easy to see that

$$\lim_\nu \mathfrak{F}_*(\phi_\nu) = \mathfrak{F}_*(\phi) \tag{5.16}$$

since

$$|(\phi, \rho) - (\phi_\nu, \rho)| \leq \|\phi - \phi_\nu\| \tag{5.17}$$

for all integrable $\rho(x)$ defined on $\Lambda$ with $\|\rho\|_1 = 1$.

We shall first show that

$$\mathfrak{F}_\nu^* = \mathfrak{F}_*(\phi_\nu) \tag{5.18}$$

for every $\nu$. Clearly we have

$$\mathfrak{F}_\nu^* \geq \mathfrak{F}_*(\phi_\nu). \tag{5.19}$$

Now for each fixed $\nu$ every $\epsilon > 0$ there is a $\rho(x)$ defined on $\Lambda$ with $\|\rho\|_1 = 1$ such that

$$(\phi_\nu, \rho) + F(\rho) \leq \mathfrak{F}_*(\phi_\nu) + \epsilon. \tag{5.20}$$

To the $\rho(x)$ satisfying (5.20) there corresponds a step density distribution given by

$$\rho_\nu(x) = \sum_{i=1}^{\nu} \rho_i C_{\Lambda i}, \tag{5.21}$$

where

$$\rho_i = V(\Lambda_i)^{-1}\int_{\Lambda_i} \rho(x)dx \qquad (i = 1, \ldots, \nu). \tag{5.22}$$

By Jensen's inequality

$$f(V(\Lambda_i)^{-1}\textstyle\int_{\Lambda_i} \rho(x)dx) \leq V(\Lambda_i)^{-1}\int_{\Lambda_i} f(\rho(x))dx \tag{5.23}$$

for $i = 1, \ldots, \nu$, we have that

$$F(\rho_\nu) \leq F(\rho). \tag{5.24}$$

But we also have

$$(\phi_\nu, \rho_\nu) = (\phi_\nu, \rho) \tag{5.25}$$

so that

$$(\phi_\nu, \rho_\nu) + F(\rho_\nu) \leq \mathfrak{F}_*(\phi_\nu) + \epsilon. \tag{5.26}$$

However, $\rho_\nu \in D_\nu$ implies that

$$\mathfrak{F}_\nu^* \leq (\phi_\nu, \rho_\nu) + F(\rho_\nu) \leq \mathfrak{F}_*(\phi_\nu) + \epsilon, \tag{5.27}$$

and this proves (5.18) since $\epsilon > 0$ is arbitrary. The conclusion (2.19) follows immediately from (5.16) and (5.18) since

$$\mathfrak{F}^* = \lim_{\gamma} \mathfrak{F}_\gamma^* = \lim_{\gamma} \mathfrak{F}_*(\phi_\gamma) = \mathfrak{F}_*(\phi). \tag{5.28}$$

The proof of Theorem 2.3 is now complete.

Our results for the infinite system free energy can be applied to show that the infinite system average pressure exists for a nonuniform system. Before considering the grand canonical ensemble we shall need to restate the preceding Theorem 2.3 in terms of the free energy per unit volume. We redefine the following. Let

$$(\phi, \rho) = V(\Lambda)^{-1} \int_\Lambda \phi(x)\rho(x)dx, \tag{5.29}$$

$$F(\rho) = V(\Lambda)^{-1} \int_\Lambda f(\rho(x))dx \tag{5.30}$$

and

$$\|\rho\|_1 = V(\Lambda)^{-1} \int_\Lambda |\rho(x)|dx. \tag{5.31}$$

Using the above new definitions (5.29), (5.30), and (5.31), we define

$$F^*(\rho_0) = \inf\{(\phi, \rho) + F(\rho) \mid \|\rho\|_1 = \rho_0\} \tag{5.32}$$

for $0 \le \rho_0 \le \rho_{cp}$. The functions $F$ and $F^*$ also depend on $\beta$, which we do not explicitly indicate. Both $\beta F$ and $\beta F^*$ are concave functions of $\beta$. Furthermore, $F^*$ is a concave functional of the external potential $\phi$ and a convex function of $\rho_0$. Let $\rho_0 = \lambda'\rho_0' + \lambda''\rho_0''$, where $\lambda' + \lambda'' = 1$. Now for every $\epsilon > 0$ there exist $\rho'(x)$ and $\rho''(x)$ on $\Lambda$ with $\|\rho'\|_1 = \rho_0'$ and $\|\rho''\| = \rho_0''$ such that

$$\epsilon + \lambda' F^*(\rho_0') + \lambda'' F^*(\rho_0'') \ge (\phi, \lambda'\rho' + \lambda''\rho'') + \lambda' F(\rho') + \lambda'' F(\rho''). \tag{5.33}$$

But

$$F(\rho) \le \lambda' F(\rho') + \lambda'' F(\rho''), \tag{5.34}$$

where $\rho(x) = \lambda'\rho'(x) + \lambda''\rho''(x)$ by the convexity of $F$. Hence

$$\epsilon + \lambda' F^*(\rho_0') + \lambda'' F^*(\rho_0'') \ge (\phi, \rho) + F(\rho) \ge F^*(\rho_0) \tag{5.35}$$

since $\|\rho\|_1 = \rho_0$. Because $\epsilon > 0$ is arbitrary, this proves that $F^*$ is a convex function of $\rho_0$. We find that $F^*(\rho_0)$ is continuous in $[0, \rho_{cp})$ since it is bounded and convex in every closed subinterval of $[0, \rho_{cp})$.

Let $\Lambda_0$ be a bounded subset of $\nu$-dimensional Euclidean space. Let $\{(\Lambda, \phi)\}$ be a sequence obtained from the initial pair $(\Lambda_0, \phi_0)$ by means of any isotropic expansion. That is

$$\Lambda = \alpha^{1/\nu}\Lambda_0, \tag{5.36}$$

where $\lim\alpha = +\infty$, and

$$\phi(x) = \phi_0(x_0) \quad \text{for } x \in \Lambda, \tag{5.37}$$

where $x = \alpha^{1/\nu}x_0$ and $x_0 \in \Lambda_0$. Then $V(\Lambda) = \alpha V(\Lambda_0)$ and $V(\Lambda) \to \infty$ in the Fisher sense as $\alpha \to \infty$. Under the hypothesis of Theorem 2.3 we have

*Corollary 5.1:* Let $\{n(\Lambda)\}$ by any sequence of positive integers such that $nV(\Lambda)^{-1} \to \rho_0$ as $V(\Lambda) \to \infty$ in the Fisher sense. Then

$$\lim_{\Lambda\to\infty} V(\Lambda)^{-1} \ln Q(\Lambda, n, \beta, \phi) = -\beta F^*(\rho_0) \tag{5.38}$$

if $0 \le \rho_0 \le \rho_{cp}$.

The proof of Corollary 5.1 is essentially a repetition of the proof of Theorem 2.3. To obtain (5.38), we need only redefine the sets $D_{r,n}$ to be all $\boldsymbol{\rho}_r = (\rho_1, \ldots, \rho_r)$ such that

$$\rho_i = n_i V(\Lambda_i)^{-1} \quad \text{for } 0 \le n_i \le n \quad (i = 1, \ldots, r) \tag{5.39}$$

and satisfying

$$\sum_{i=1}^{r} \omega_i \rho_i = nV(\Lambda)^{-1},$$

where the $\omega_i = V(\Lambda_i)/V(\Lambda)$ $(i = 1, \ldots, r)$ are constants. If $nV(\Lambda)^{-1} \to \rho_0$, then for every $\boldsymbol{\rho}_r$ satisfying

$$\sum_{i=1}^{r} \omega_i \rho_i = \rho_0 \tag{5.40}$$

there exists a sequence $\boldsymbol{\rho}_{r,n} \in D_{r,n}$ with $\boldsymbol{\rho}_{r,n} \to \boldsymbol{\rho}_r$ as $V(\Lambda) \to \infty$. With this new definition of the sets $D_{r,n}$ and with replacement of particle number normalization by volume normalization, all previous results remain valid and Corollary 5.1 follows. Indeed, Corollary 5.1 amounts to multiplying the free energy per particle by $\rho_0$ to obtain the free energy per unit volume.

## 6. GRAND CANONICAL ENSEMBLE

In this final section we shall demonstrate that the grand canonical thermodynamic limit exists whenever the canonical limit (5.38) exists. We redefine the sequence $\{\mathfrak{F}\}$ by

$$-\beta\mathfrak{F}(\Lambda, n, \beta, \phi) = V(\Lambda)^{-1} \ln Q(\Lambda, n, \beta, \phi), \tag{6.1}$$

and assume that

$$\lim\mathfrak{F}(\Lambda, n, \beta, \phi) = F^*(\rho_0) \tag{6.2}$$

whenever $nV(\Lambda)^{-1} \to \rho_0$ where $0 \le \rho_0 \le \rho_{cp}$.

The grand partition function is

$$\Xi(\Lambda, z, \beta, \phi) = \sum_{n=0}^{\infty} z^n Q(\Lambda, n, \beta, \phi), \tag{6.3}$$

where $z > 0$ is the activity and $Q(\Lambda, 0, \beta, \phi) = 1$. With the definition

$$\beta P(z, \beta) = \sup_{0\le\rho_0\le\rho_{cp}} \{\rho_0 \ln z - \beta F^*(\rho_0)\} \tag{6.4}$$

for $\beta > 0$ and $z > 0$ we have

*Theorem 6.1:* Let $\Lambda \to \infty$ in the Fisher sense. Under the assumption (6.2) we have that

$$\lim_{\Lambda\to\infty} V(\Lambda)^{-1} \ln\Xi(\Lambda, z, \beta, \phi) = \beta P(z, \beta), \tag{6.5}$$

where $\beta P(z, \beta)$ given by (6.4) is a convex function of $\ln z$ and $\beta$ and $P(z, \beta) \ge 0$ is an increasing function of $z$.

The proof of Theorem 6.1 is a copy of Ruelle's or Fisher's proof for uniform systems, and we will not repeat the details here. However, we shall give a lemma which allows Ruelle's proof for uniform systems to be applied.

*Definition 6.1:* We say that $\{\mathfrak{F}(\Lambda, n, \beta, \phi)\}$ converges uniformly to $F^*$ on a subset $K \subset [0, \rho_{cp})$ if for every $\epsilon > 0$ there exists an $M(\epsilon)$ such that

$$|\mathfrak{F}(\Lambda, n, \beta, \phi) - F^*(nV(\Lambda)^{-1})| < \epsilon \tag{6.6}$$

whenever $nV(\Lambda)^{-1} \in K$ and $V(\Lambda) > M(\epsilon)$.

*Lemma 6.1:* Let $K \subset [0, \rho_{cp})$ be compact. Then under the assumption (6.2) the sequence $\{\mathfrak{F}(\Lambda,n,\beta,\phi)\}$ converges uniformly to $F^*$ on $K$.

*Proof:* Suppose that $\{\mathfrak{F}\}$ does not satisfy Definition 6.1. Then there exists a sequence $\{\rho_k\} \subset K, \rho_k = n_k V(\Lambda_k)^{-1}$, such that

$$|\mathfrak{F}(\Lambda_k, n_k, \beta, \phi) - F^*(\rho_k)| \geq \epsilon > 0 \tag{6.7}$$

holds for all $k$. Since $K$ is compact, it is closed and bounded and does not include the point $\rho_{cp}$. Further there exists a subsequence $\{\rho_j\}$ of $\{\rho_k\}$ such that $\rho_j \to \rho_0$ where $\rho_0 \in K$.

But $F^*(\rho_j) \to F^*(\rho_0)$ by continuity of $F^*$, and $\mathfrak{F}(\Lambda_j, n_j, \beta, \phi) \to F^*(\rho_0)$, which is a contradiction. Hence $\{\mathfrak{F}\}$ must satisfy Definition 6.1 on $K$, and the lemma is proven.

Via lemma 6.1 and the assumption that $\|\phi\|$ is a finite constant for all $\Lambda$, Theorem 6.1 follows directly by applying Ruelle's proof for a uniform system.[4]

We indicate another representation of the average pressure $p(z, \beta)$,[5] which is

$$P(z, \beta) = -\inf\{(\phi - \mu, \rho) + F(\rho) \,\big|\, \|\rho\|_1 \leq \rho_{cp}\}, \tag{6.8}$$

where we write $\mu = \beta^{-1} \ln z$. The representation (6.8) follows from

$$P(z, \beta) = \sup_{0 \leq \rho_0 \leq \rho_{cp}} \{ \sup_{\|\rho\|_1 = \rho_0} \{-(\phi - \mu, \rho) - F(\rho)\}\}. \tag{6.9}$$

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* Work supported in part by the U.S. Atomic Energy Commission.

1 M. E. Fisher, Arch. Ratl. Mech. Anal. 17, 377 (1964).
2 D. Ruelle, *Statistical Mechanics. Rigorous Results* (Benjamin, New York, 1969).
3 D. Ruelle, Commun. Math. Phys. 18, 127 (1970).
4 See Ref. 2, Sec. 3. 4. 5, p. 56.
5 O. Penrose and D. J. Gates, Commun. Math. Phys. 15, 255 (1969).

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# Stability of Finite-Sized Radiating Plasmas

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(Received 4 April 1972)

It is shown that the onset of instabilities in a finite-sized, optically thin, radiating plasma coincides with the loss of uniqueness of solutions to the governing nonlinear differential equations. Furthermore, conditions on the luminosity function are derived for the existence of metastable states of such plasmas with dimensions smaller than the critical maximum size derived from conventional normal mode stability analysis. The results are applied to a simple configuration modelling free–free emission from a confined radiating, high-temperature plasma.

## 1. INTRODUCTION

The question of stability of optically thin, radiating high temperature plasmas arises in many contexts, notably controlled fusion research, astrophysics, plasma diagnostics, and the like. In this paper the stability of a particularly simple configuration is re-examined from the point of view of existence and uniqueness of nontrivial solutions to the differential equations governing the steady state temperature distribution within the plasmas. In addition to recovering the results of conventional normal mode stability analysis, we find the conditions necessary for the existence of metastable solutions which are not discernible from a conventional approach.

Before continuing, it is important to say something about physical conditions under which radiation losses from the plasma are significant. Often physical conditions of interest, be it on the laboratory scale or the astronomical scale, are such that the collisionless regime prevails. That is, the size of the object under observation is smaller than the collision mean free path. However, the radiative collision cross section is much smaller than the elastic collision cross section, being in the ratio of $\alpha kT/mc^2$ in hydrogen at a nonrelativistic temperature $T$—here $\alpha$ is the fine structure constant, $k$ is the Boltzman constant, and $mc^2$ is the electron rest mass. Therefore, on the time scale in which radiation is observed, the system must have undergone many nonradiative collisions, either with the containing walls (i.e., laboratory plasma) or among the particles themselves, as, say, in a solar flare. This suggests that whenever nonequilibrium radiative losses are observed, the time scale is such that phenomena dependent on collisions, e,g., thermal and electrical conductivities, must be explicitly accounted for.[1]

In our search for macroscopic description of systems far from equilibrium we have inquired into the criteria necessary for the existence of stable steady states and/or stable quasi-steady states. Of special significance seems to be the role played by the characteristic dimensions of the radiating plasma: It appears that if the object is too large it tends to break up into smaller plasma aggregates–some at lower mean temperatures and some at higher mean temperatures–such that the largest aggregate does not exceed, in size, a critical dimension determined by the plasma parameters. This conjecture is supported by the following considerations.[2–4]

First, studies of the stability of radiating plasmas of indefinite extent show that under certain conditions small perturbations with wavelengths exceeding a critical length grow in amplitude.[3,4] The existence of such lower bounds on the wavelengths of unstable modes suggests an analogy with the relationship between onset of turbulence and onset of instabilities

*Definition 6.1:* We say that $\{\mathfrak{F}(\Lambda, n, \beta, \phi)\}$ converges uniformly to $F^*$ on a subset $K \subset [0, \rho_{cp})$ if for every $\epsilon > 0$ there exists an $M(\epsilon)$ such that

$$|\mathfrak{F}(\Lambda, n, \beta, \phi) - F^*(nV(\Lambda)^{-1})| < \epsilon \tag{6.6}$$

whenever $nV(\Lambda)^{-1} \in K$ and $V(\Lambda) > M(\epsilon)$.

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*Proof:* Suppose that $\{\mathfrak{F}\}$ does not satisfy Definition 6.1. Then there exists a sequence $\{\rho_k\} \subset K, \rho_k = n_k V(\Lambda_k)^{-1}$, such that

$$|\mathfrak{F}(\Lambda_k, n_k, \beta, \phi) - F^*(\rho_k)| \geq \epsilon > 0 \tag{6.7}$$

holds for all $k$. Since $K$ is compact, it is closed and bounded and does not include the point $\rho_{cp}$. Further there exists a subsequence $\{\rho_j\}$ of $\{\rho_k\}$ such that $\rho_j \to \rho_0$ where $\rho_0 \in K$.

But $F^*(\rho_j) \to F^*(\rho_0)$ by continuity of $F^*$, and $\mathfrak{F}(\Lambda_j, n_j, \beta, \phi) \to F^*(\rho_0)$, which is a contradiction. Hence $\{\mathfrak{F}\}$ must satisfy Definition 6.1 on $K$, and the lemma is proven.

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## 1. INTRODUCTION

The question of stability of optically thin, radiating high temperature plasmas arises in many contexts, notably controlled fusion research, astrophysics, plasma diagnostics, and the like. In this paper the stability of a particularly simple configuration is re-examined from the point of view of existence and uniqueness of nontrivial solutions to the differential equations governing the steady state temperature distribution within the plasmas. In addition to recovering the results of conventional normal mode stability analysis, we find the conditions necessary for the existence of metastable solutions which are not discernible from a conventional approach.

Before continuing, it is important to say something about physical conditions under which radiation losses from the plasma are significant. Often physical conditions of interest, be it on the laboratory scale or the astronomical scale, are such that the collisionless regime prevails. That is, the size of the object under observation is smaller than the collision mean free path. However, the radiative collision cross section is much smaller than the elastic collision cross section, being in the ratio of $\alpha kT/mc^2$ in hydrogen at a nonrelativistic temperature $T$—here $\alpha$ is the fine structure constant, $k$ is the Boltzman constant, and $mc^2$ is the electron rest mass. Therefore, on the time scale in which radiation is observed, the system must have undergone many nonradiative collisions, either with the containing walls (i.e., laboratory plasma) or among the particles themselves, as, say, in a solar flare. This suggests that whenever nonequilibrium radiative losses are observed, the time scale is such that phenomena dependent on collisions, e,g., thermal and electrical conductivities, must be explicitly accounted for.[1]

In our search for macroscopic description of systems far from equilibrium we have inquired into the criteria necessary for the existence of stable steady states and/or stable quasi-steady states. Of special significance seems to be the role played by the characteristic dimensions of the radiating plasma: It appears that if the object is too large it tends to break up into smaller plasma aggregates–some at lower mean temperatures and some at higher mean temperatures–such that the largest aggregate does not exceed, in size, a critical dimension determined by the plasma parameters. This conjecture is supported by the following considerations.[2–4]

First, studies of the stability of radiating plasmas of indefinite extent show that under certain conditions small perturbations with wavelengths exceeding a critical length grow in amplitude.[3,4] The existence of such lower bounds on the wavelengths of unstable modes suggests an analogy with the relationship between onset of turbulence and onset of instabilities

in certain types of laminar flow at large Reynolds numbers.[5] Another analogy which comes to mind seems to be the problem of buckling of beams under axial compression: For a given stress, buckling occurs when the beam exceeds a critical length.

Second, an inspection of the entropy equation for a fluid suggests the existence of a characteristic length. Thus, for instance, we have the conduction equation for a fluid at rest:

$$q\frac{\partial s}{\partial t} = \frac{\nabla\cdot\kappa\nabla T}{T}, \tag{1.1}$$

where $s$ is entropy per unit mass, $\kappa$ is the thermal conductivity, $q$ is the fluid density, and $T$ is the temperature. From dimensional analysis it follows that the characteristic length $L$ is given here by

$$L^2 \sim \kappa/\left(q\frac{\partial s}{\partial t}\right). \tag{1.2}$$

It is known that inasmuch as the realm of validity of Eq. (1.1) coincides with that in which the Chapman–Enskog method is applicable (for that method serves as the rational basis for Fick's law and, consequently, as the basis for evaluating $\kappa$), the process must be consistent with the principle of least entropy production.[6] This is because the Chapman–Enskog method and the principle of least entropy production apply to systems close to thermal equilibrium. Therefore, it follows from Eq. (1.2) that in the steady state the characteristic length must be maximum subject to whatever external constraints apply. In particular, if such constraint are of a purely geometric nature, $L$ is simply given by the size of the heat conductor within which the temperature drop occurs.

In Sec. 2 we formulate the mathematical model which is the object of our study and recover the standard results of normal mode stability analysis. In Sec. 3 theorems on existence and uniqueness of the solutions for our model are established. In Sec. 4 we apply the results to the effects of free–free emission on the stability of a plasma sphere.

## 2. THE MODEL

We consider a spherical region $V(r_0)$ of radius $r_0$ (cm) in which hydrogenic plasma of mean density $n_0$ ($cm^{-3}$) is maintained at a high temperature $T$. The size of the region, the temperature, and the density distributions are taken to be such that the plasma is transparent to its own radiation. The outer boundary of the region is assumed to be adiabatically insulated from the surroundings in the conventional sense of this concept; that is,

$$\kappa\nabla T = 0 \quad \text{at} \quad r = r_0, \tag{2.1}$$

where $\kappa$ is the thermal conductivity, here assumed to be some given function of $T$. This outer boundary condition is picked for the sake of simplicity. Most of the results obtained hereunder can easily be generalized to the case of a finite temperature gradient at $r_0$. The enclosure (i.e., the adiabatic insulation) is assumed to be diathermanous, i.e., it is transparent to the plasma radiation. Furthermore, the enclosure admits to the interior some form of energy input which balances the radiation losses, thereby achieving a steady state. For instance, the form of input energy could be microwaves, cosmic rays, or any other form consistent with the properties of the enclosure.

Let $Q(n, T)$ denote the volume emissivity (energy/unit volume-unit time) of the plasma and $S(n, T)$ the rate at which the energy from external sources is deposited in a unit volume of the plasma ($n$ is the particle density).

Then, in general, for a steady state to exist we have

$$\nabla\cdot\kappa\nabla T = Q(P, T) - S(P, T), \tag{2.2}$$

where we have eliminated $n$ by using the ideal gas law $nT \propto P$ ($P$ is the pressure). Integration of Eq. (2.2) over the region $V(r_0)$ together with Eq. (2.1) gives

$$-\kappa r^2\nabla T|_{r=0} = \int_{V(r_0)} dV[Q(T) - S(T)], \tag{2.3}$$

where $T$ is the solution to Eq. (22.). In the absence of internal sources of energy, the condition of steady state requires that the total energy emitted per unit time from the region under discussion be equal to the total energy deposited in that volume in a unit time. This implies that the right-hand side of Eq. (2.3) must vanish, from which it follows that the inner boundary condition is

$$\kappa r^2\nabla T = 0 \quad \text{at} \quad r = 0. \tag{2.4}$$

Because the plasma is in a quiescent state, implicit in Eq. (2.2) is the isobaric condition. Therefore, to the extent that the plasma may be approximately treated as an ideal gas, there follows

$$nT = \text{const} \tag{2.5}$$

throughout the region within radius $r_0$. Note that unless otherwise indicated we assume throughout the discussion spherical symmetry; therefore,

$$\nabla \to \frac{\partial}{\partial r} \quad \text{and} \quad \nabla^2 \to \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}.$$

It follows immediately from Eq. (2.2) that $T = T_c$, a constant for $0 \leq r \leq r_0$, is a solution satisfying the given boundary conditions as long as the equation

$$Q(T_c) = S(T_c) \tag{2.6}$$

is satisfied.

It is our purpose to investigate the uniqueness of this solution and its relationship to the problem of stability of the radiating plasma as described by our model. The importance of this question lies in the possibility that the onset of instability may, in fact, be an aspect of the lack of uniqueness of solutions to the differential equations representing the given system. This is somewhat analogous to the bifurcation of the solution of the Navier–Stokes equations at sufficiently high Reynolds numbers where onset of turbulence is expected.[7] Furthermore, there is the distinct possibility that there is more than one solution satisfying the given differential equations and the associated boundary conditions, which are stable with respect to infinitesimal perturbations, but not necessarily with respect to finite amplitude perturbations (metastable states).

Conventionally, the stability of the uniform temperature distribution is determined as follows. Consider the time-dependent counterpart of Eq. (2.2):

$$\frac{PC_p}{T}\frac{\partial T}{\partial t} = \nabla\cdot\kappa\nabla T - f(T), \tag{2.7}$$

where $P$ is the pressure, $C_p$ is the specific heat at constant pressure, and we have let $f(T) \equiv Q(T) - S(T)$. Let

$$T = T_c + \delta T(r,t), \tag{2.8}$$

where $\delta T$ is a small amplitude time and space dependent perturbation of the temperature $T_c$ given by Eq. (2.6). We take $\delta T$ to be subject to the same boundary conditions as are implicit in Eq. (2.2), i.e.,

$$\kappa(T_c)r^2\nabla\delta T(r,t)\big|_{r=0} = \kappa(T_c)\nabla\delta T(r,t)\big|_{r=r_0} = 0. \tag{2.9}$$

Substitution of Eq. (2.8) in Eq. (2.7) gives

$$\frac{PC_p}{T_c}\frac{\partial\delta T}{\partial t} = \kappa(T_c)\nabla^2\delta T - f'(T_c)\delta T \tag{2.10}$$

to first order in $\delta T$. Here, $f'(T_c) \equiv (\partial f/\partial T)_{T=T_c}$ (the derivative is taken at constant pressure). Let $\delta T$ be an eigenfunction of the operator $\nabla^2$ satisfying the given boundary conditions, i.e.,

$$\nabla^2\delta T = -\lambda^2\delta T. \tag{2.11}$$

Of course, because of the linearity of Eq. (2.10) an arbitrary $\delta T$ may be made up from a superposition of solutions to Eq. (2.11) for various values of $\lambda$. Here, it suffices to look at one of these eigensolutions. Thus, it follows that

$$\frac{PC_p}{T_c}\frac{\partial\delta T}{\partial t} = -[\lambda^2\kappa(T_c) + f'(T_c)]\delta T. \tag{2.12}$$

For luminosity functions $f(T)$ such that $f'(T_c) > 0$, Eq. (2.12) indicates that small perturbations will decay in time for all eigenvalues $\lambda$. On the other hand, if $f'(T_c) < 0$ there is a smallest value of $\lambda$, say $\lambda_c$, defined as

$$\lambda_c^2 \equiv -f'(T_c)/\kappa(T_c) \tag{2.13}$$

below which the coefficient of $\delta T$ on the right-hand side of Eq. (2.12) is positive, thereby indicating the growth of $\delta T$ with time. Now, in a spherical enclosure of radius $r_0$ the lowest eigenvalue for the set of eigenfunctions satisfying the given boundary conditions is of the order of $1/r_0$. Therefore, Eq. (21.3) may be regarded as the condition on the maximum value of $r_0$ (say $r_c$) for which the isothermal sphere at $T = T_c$ is stable with respect to small perturbations given the plasma parameters and the heating/cooling mechanism. We have thus established a connection between the smallest wavenumber for the growth of thermal instability[2] and the largest possible uniform spherical radiating plasma aggregate, as determined by normal mode stability analysis.

It should be stressed here that the preceding analysis is only valid for small perturbations from the assumed isothermal solution. The form of the space dependent part of $\delta T$, say $\theta(r)$, is

$$\theta(r) \propto \frac{\sin r\lambda}{r}, \tag{2.14}$$

where $\lambda$ is given by the solution of the transcendental equation

$$r_0\lambda = \tan r_0\lambda, \tag{2.15}$$

which follows from the condition of Eq. (2.1). Therefore in the present context, the smallest value of $\lambda$ is

$$\lambda_{min} \simeq 4.49/r_c. \tag{2.16}$$

It is useful to compare the characteristic length of Eq. (2.2) with that of Eq. (1.1). To begin with when $r_0$ is sufficiently small, minute gradients in temperature decay in time. They are effectively smoothed out by the finite thermal conductivity, a result reminiscent of the corresponding well-known results in Field's theory of thermal instability in which large wavenumber (large $\lambda$) disturbances are quenched by the finite thermal conductivity.[2,3] Thus, $r_0$ may be identified with $L$ of Eq. (1.2). But here $r_0$ has an upper bound $r_c$ One is then tempted to identify formally $-f'(T_c)$ with the entropy production rate, since it takes the place of $q\partial S/\partial t$ in the definition of $L$ [Eq. (1.2)]. This identification seems permissible as long as $f'(T_c) < 0$. It is as if the emission of radiation tended to decrease the entropy production rate of the system increased by the finite heating rate by external sources. Conventional thermodynamic concepts, if used here indiscriminately, would lead one to conclude that the heating-emission process is at least partially reversible. Intuitively, this conclusion seems to be quite wrong, and it appears that the resolution of this apparent paradox rests with the relationship between irreversibility and entropy production, under conditions when both heating and cooling of a system occur far from thermal equilibrium.[6]

We proceed now with the study of the existence and uniqueness of solutions of Eq. (2.2) subject to the boundary conditions (2.1) and (2.3). In particular, we will demonstrate in the next section that for spherical configurations with radii $r_0$ larger than the critical radius, given by Eqs. (2.13) and (2.16) there is no unique solution to our problem. We shall also demonstrate that, for $r_0$ smaller than the critical radius, there is range of radii for which metastable states exist.

## 3. PROPERTIES TO SOLUTIONS OF EQ. (2.2)

We will investigate the existence, uniqueness, and qualitative behavior of the solutions over $r \geq 0$ of the differential equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\kappa(T)\frac{dT}{dr}\right) = f(T), \tag{3.1}$$

where

$$f(T) \equiv Q(T) - S(T) \tag{3.2}$$

subject to the initial conditions

$$T\big|_{r=0} = T_0 > 0, \qquad \kappa(T)\frac{dT}{dr}\Big|_{r=0} = 0 \tag{3.3}$$

and under the following assumptions regarding the functions $\kappa(T)$ and $f(T)$:

(i) $f(T)$ is defined and bounded analytic in a closed finite interval $I_T = [T_1, T_2]$, $0 < T_1 < T_2$;

(ii) $f(T)$ is strictly monotonic in $I_T$, i.e., $f'(T) \neq 0$ there;

(iii) $f(T)$ vanishes for $T = T_c, T_1 < T_c < T_2$;

(iv) $\kappa(T)$ is a positive function defined over the interval $0 \leq T \leq T_2$ where it is analytic except perhaps at the origin and such that its integral over any closed interval $[0,T]$, $T \leq T_2$ exists.

Note that the second of the initial conditions (3.3) is less general than condition (2.4). There may be other solutions for which condition (2.4) is satisfied with $\kappa dT/dr|_{r=0} \neq 0$. However, we have excluded them from our analysis, because initial conditions (3.3) suffice to establish criteria for nonuniqueness of the trivial solution $T(r) = T_c$.

Assumption (iv) allows us to simplify notation by using the function

$$X(T) = \left(\int_0^T \kappa(T')dT'\right) \Big/ \left(\int_0^{T_c} \kappa(T')dT'\right)$$

as a new scale of temperature. Clearly, $X(T_c) = 1$ and $X(T)$ has an inverse $T(X)$ which is analytic over the range $I_X = [X_1, X_2]$, where $X_1 = X(T_1), X_2 = X(T_2)$.

In terms of $X$, Eq. (3.1) becomes

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dX}{dr}\right) = F(X), \tag{3.4}$$

where

$$F(X) \equiv \frac{f(T(X))}{\int_0^{T_c} \kappa(T')dT'},$$

and the initial conditions (3.3) are now

$$X\Big|_{r=0} = X_0 \quad \text{and} \quad \frac{dX}{dr}\Big|_{r=0} = 0. \tag{3.5}$$

From assumptions (i)–(iii) and the definition of $F(X)$, we see that this function is analytic and strictly monotonic in $I_X$ and that $F(1) = 0$, with $X_1 < 1 < X_2$.

It is immediately recognized that Eq. (3.4) is of the Emden type.[8]

*Theorem I:* Equation (3.4) has a unique solution $X(r, X_0)$ satisfying the initial conditions (3.5) for all $X_0$ in the open interval $(X_1, X_2)$ which is analytic in $r$ for $0 \leq r' < \bar{r}, \bar{r} > 0$.

*Proof:* Set $u = dX/dr$ and introduce a new independent variable $\xi = \ln r$ so that $-\infty \leq \xi \leq \infty$ for $0 \leq r \leq \infty$. Then, the autonomous system

$$\frac{dr}{d\xi} = r, \tag{3.6a}$$

$$\frac{du}{d\xi} = -2u + rF(X), \tag{3.6b}$$

$$\frac{dX}{d\xi} = ur \tag{3.6c}$$

is equivalent to Eq. (3.4).

Note that the right-hand sides of these three equations vanish for $r = u = 0$. Hence, in the associated phase-space the $X$-axis is a line of singular points.

Poincaré has shown[9] that the nature of each of these singular points $(0, 0, X_0)$ can be determined from the nature of the eigenvalues of the linear approximation to Eqs. (3.6a) and (3.6b) in the vicinity of the point, namely,

$$\frac{dr}{d\xi} = r,$$
$$\frac{du}{d\xi} = F(X_0)r - 2u. \tag{3.7}$$

These eigenvalues are roots of the characteristic equation

$$s^2 + s - 2 = 0,$$

i.e., $s_1 = 1, s_2 = -2$. Poincaré's results then assert that since these eigenvalues are real with opposite signs there exist only two trajectories of system (3.6) going through the point under consideration. Along one of them the point is approached as $\xi \to \infty$; it is, therefore, of no interest to us since this corresponds to $r \to \infty$. It is easily seen by setting $r = 0$ in system (3.6) that this trajectory is a straight line lying in the plane $r = 0$ which is an integral surface.

Along the other trajectory the singular point is approached as $\xi \to -\infty$, i.e., as $r \to 0$ in agreement with the requirement of the problem. More precisely, as shown by Poincaré, the corresponding solution $X(r, X_0)$ can be expressed in the form of a series of powers of $e^{s_1\xi} = e^{\xi} = r$ which has a positive radius of convergence $\bar{r}$. The theorem is thus established.

The determination of the coefficients of the power series representation of $X(r, X_0)$ is most easily obtained through the application of the method of undetermined coefficients to Eq. (3.4) where $F$ itself is represented by its Taylor expansion about $X = X_0$.

The result is

$$X(r, X_0) = X_0 + \tfrac{1}{6}F_0 r^2 + \tfrac{1}{120}F_0 F_0' r^4 + \cdots, \tag{3.8}$$

where the subscript "0" refers to the value of the function at $X = X_0$.

Next, we study the boundedness of the solution $X(r, X_0)$ just obtained.

*Theorem II:* (1) If $F'(X) < 0$, then a closed interval $J = [X'_1, X'_2] \subseteq I_X$ can be found such that for all $X_0 \in J$: (a) $X(r, X_0) \in J$ for $r \geq 0$ and (b) $\lim_{r\to\infty} X(r, X_0) = 1$; moreover, $dX(r, X_0)/dr$ is bounded for $r \geq 0$.

(2) If $F'(X) > 0$, then $dX/dr \neq 0$ for all values of $r$ for which $X(r, X_0)$ is defined.

*Proof:* We will use the fact that the trajectory derivative of the function

$$\varphi(u, X) \equiv H(X) - \tfrac{1}{2}u^2 \tag{3.9}$$

where

$$H(X) = \int_1^X F(X)dX \tag{3.10}$$

is never negative along the solutions of system (3.6). Indeed, we easily find

$$\frac{d\varphi}{d\xi} = 2u^2 \geq 0. \tag{3.11}$$

We determine the configuration of the family of curves $\Gamma(\varphi_0)$ defined by the equation $\varphi(u, X) = \varphi_0 = \text{const}$. It

is readily seen that the curve $\Gamma(0)$ reduces to the point $u = 0$, $X = 1$. The shape of the curves in the neighborhood of this point is obtained from the approximation

$$\tfrac{1}{2}[F_1'(X-1)^2 - u^2] = \varphi_0 \tag{3.12}$$

valid for $|X-1|$ and $|u|$ small, where, as in the following, the subscript "1" refers to the value of the function at $X = 1$.

First assume that $F'(X) < 0$ so that in particular $F_1' < 0$. Then, Eq. (3.12) defines concentric ellipses for negative values of $\varphi_0$. In fact, we now show that all curves $\Gamma$ are closed as long as they lie in the strip $X \subseteq I_X$. Consider the function $H(X)$ as defined by Eq. (3.10). Since $F(X)$ decreases monotonically from $F(X_1) > 0$ to $F(X_2) < 0$, we see that $H(X)$ increases from $H(X_1) < 0$ to its single maximum $H(1) = 0$ and decreases down to $H(X_2) < 0$ as $X$ goes from $X_1$ to $X_2$. It follows (see Fig. 1) that we can always find an interval $J = [X_1', X_2'] \subseteq I_X$ such that

$$H(X_1') = H(X_2') \geq \max(H(X_1), H(X_2)) = \bar{\varphi}_0$$

and that the equation

$$\varphi(0,X) = H(X) = \varphi_0$$

has exactly two roots $X_m \leq X_M$ in $J$ for $\bar{\varphi}_0 \leq \varphi_0 \leq 0$ where $X_m = X_M (= 1)$ only for $\varphi_0 = 0$. If we now write

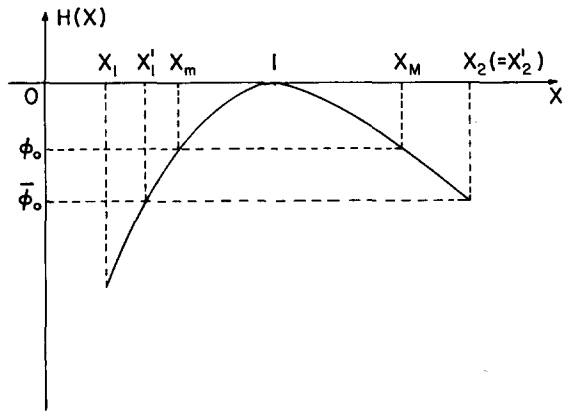


FIG. 1. Graph of the function $H(X)$.

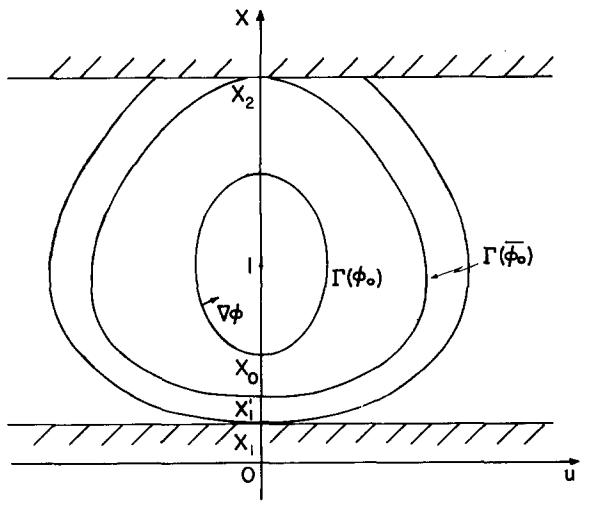


FIG. 2. Configuration of the curves $\Gamma$ for $F' < 0$.

the equation of the curves $\Gamma$ in the form

$$u = \pm\{2[H(X) - \varphi_0]\}^{1/2},$$

we conclude from the form of the right-hand side that the corresponding curve $\Gamma$ is closed for all values of $\varphi_0$ such that $\bar{\varphi}_0 \leq \varphi_0 < 0$ (see Fig. 2).

Now consider the solution $X(r, X_0)$ of the problem with $X_0 \subseteq J$ and choose $\varphi_0 = \varphi(0, X_0)$. With this particular choice of $\varphi_0$ the equation $\varphi(u,X) = \varphi_0$ actually represents a closed cylinder $C(\varphi_0)$ in the phase space of system (3.6) within which the trajectory corresponding to the solution $X(r, X_0)$ is confined for $r > 0$. More precisely, if we designate the set of the $r, u, X$ space where $\varphi(u,X) > \varphi_0$ and $r \geq 0$ by $E(\varphi_0)$, every point of the boundary $C(\varphi_0)$ of this set is a point of ingress[10] of $E(\varphi_0)$ with respect to system (3.6). This is obvious from inequality (3.11) at points where $u \neq 0$ since from the foregoing the gradient of $\varphi$ at such a point is directed towards the inside of $C(\varphi_0)$, i.e., into $E(\varphi_0)$. Points where $u = 0$ are also points of ingress. Indeed, the series representation of $\varphi$ in the vicinity of one of these points, $(\bar{r}, 0, X)$ say, is of the form

$$\varphi = \varphi(0,\bar{X}) + \tfrac{2}{3}\bar{r}^2 F^2(\bar{X})(\xi - \bar{\xi})^3 + \cdots,$$

where $\bar{\xi} = \ln\bar{r}$. Clearly, $\varphi$ increases as $\xi$ increases from $\xi = \bar{\xi}$.

It follows that $X(r, X_0)$ as well as its derivative $dX/dr = u$ are bounded for $r \geq 0$.

Also, since system (3.6) does not have any singular points inside the cylinder $C(\varphi_0)$ for $0 < r < \infty$ as is easily verified, the solution can be continued over this whole interval. Moreover from (3.11) we must have

$$\lim_{r\to\infty} u = 0$$

for otherwise, according to (3.11), $\varphi$ would increase without bound which is impossible since $\varphi \leq 0$ for all points within $C(\varphi_0)$. Finally, looking at Eq. (3.6) we see that we must have

$$\lim_{r\to\infty} f(X(r, X_0)) = 0$$

in order for $du/d\xi$ to remain finite. Hence,

$$\lim_{r\to\infty} X(r, X_0) = 1,$$

and the first part of the theorem is proved.

We now treat the second part of the theorem, namely, the case where $F'(X) > 0$.

Going back to the approximate equation (3.12) of the curves $\Gamma$ in the vicinity of the point $u = 0$, $X = 1$, we see that it now represents a family of hyperbolas centered at this point. Proceeding as in the proof of part 1 of the theorem it is possible to show that the curves $\Gamma$ are as sketched in Fig. 3 where the arrows indicate the direction of $\nabla\varphi$.

First, assume that $X_0 = X_0'$ with $X_1 < X_0' < 1$. Referring to Fig. 3 we see that the trajectory solution of (3.8) corresponding to $X(r, X_0)$ will be confined within the cylinder with generatrices parallel to the $r$ axis whose trace on any $r$ = constant plane is made

up of the arc $AB$ of the curve $\Gamma_0'$ and of the segment $AB$ of the line $X = X_1$. Now consider the set of points of the $u = 0$ plane where $r > 0$ and $X_1 \leq X \leq X_0'$. From Eq. (3.6) $du/d\xi = rF(X) < 0$ on this set which means that once the solution trajectory has entered the region $u < 0$ it cannot come back into $u > 0$ through the plane $u = 0$. But from Eq. (3.7) we see that the solution leaves the initial point $u = r = 0$, $X = X_0'$ in the region $u < 0$ since $F(X_0') < 0$. Hence, we necessarily have $dX/dr < 0$ along this solution.

A similar reasoning applied to the case where $1 < X_0 = X_0'' < X_2$ shows that $dX/dr$ is then positive.

The theorem is thus proved.

We now turn our attention to the qualitative behavior of the solution $X(r,X_0)$ assuming that $F'(X) < 0$ for $X \in I_X$.

*Theorem III:* When $F'(X) < 0$, the solution $X(r,X_0)$ to Eq. (3.4) subject to the initial conditions (3.5) is oscillatory, i.e., has an infinity of zeros over the whole interval $r \geq 0$ as long as $X_0 \subseteq J$ (cf. Theorem II).

*Proof:* We introduce the function

$$Z(r,X_0) = r[X(r,X_0) - 1]. \tag{3.13}$$

We then readily find that the function $Z$ is a solution of the differential equation

$$\frac{d^2Z}{dr^2} + p(r,X_0)\, Z = 0, \tag{3.14}$$

where

$$p(r,X_0) \equiv -\frac{F(X(r,X_0))}{X(r,X_0) - 1}$$

subject to the initial conditions

$$Z(0,X_0) = 0, \quad Z'(0,X_0) = X_0 - 1,$$

where the prime means differentiation with respect to $r$.

Equation (3.13) is a linear second-order differential equation to which we will apply Sturm's fundamental theorem[11] using the fact that the function $p(r,X_0)$ has a positive lower bound over the interval $r \geq 0$.

Indeed let

$$P(X) \equiv -\frac{F(X)}{X - 1},$$

and note that under the assumptions made [i.e., $F'(X) < 0$ for $X \subseteq I_X$ and $F(1) = 0$]:

(a) $F(X) > 0$ for $X_1 \leq X < 1$;

(b) $\lim_{X \to 1} P(X) = -F'(1) >$ by $l'$ Hospital's rule;

(c) $F(X) < 0$ for $1 < X \leq X_2$.

Hence, $P(X) > 0$ for $X \subseteq I_X$ and its minimum value over this closed interval is certainly positive since the ratio $F(X)/(X - 1)$ does not vanish here. If we denote this minimum value by $\omega^2$, we, therefore, have

$$p(r,X_0) = P[X(r,X_0)] > \omega^2$$

for $r \geq 0$, since by Theorem II

$$X(r,X_0) \in J \subseteq I_X = [X_1,X_2].$$

The solution $Z(r,X_0)$ of Eq. (3.13) can, therefore, be compared to those of

$$\frac{d^2v}{dr^2} + \omega^2 v = 0 \tag{3.15}$$

which are known to be oscillatory. Sturm's theorem indicates that $Z(r,X_0)$ is more oscillatory than any solution $v(r)$ of Eq. (3.15). More precisely, if $v(r)$ has $n$ zeros within a certain interval $r_1 < r < r_2$, then $Z(r,X_0)$ has at least $n$ zeros in the same interval. Looking back at the definition of $Z$ [Eq. (3.13)] this result implies that $X(r,X_0)$ has the same property and oscillates about $X = 1$. This completes the proof of Theorem III. Now we prove

*Theorem IV:* The solution of Eq. (3.4) subject to the boundary conditions $dX/dr|_{r=0} = dX/dr|_{r=r_0} = 0$ is not unique for $r_0$ sufficiently large and $F(X) < 0$.

The proof of this theorem follows from the boundedness of $X(r,X_0)$ as well as its oscillating behavior which implies the existence of minima and maxima of this function between its successive zeros. Whenever $r_0$ coincides with an extremum of some $X(r,X_0)$, the boundary conditions are satisfied by a solution of Eq. (3.4) other than $X = 1$. But as $X_0$ varies, the manifold $X(r,X_0)$ generates a continuum of locations along $r$ at which $dX/dr = 0$. This continuum must start at a value of $r$ (say $r_c$) no less than that for which the solution of Eq. (3.15) satisfies the boundary conditions of this theorem. This must be so because of $|X_0 - 1|$ small enough, the linear approximation to Eq. (3.4) must be valid. Thus, for any $r_0 > r_c$, Eq. (3.4) with the boundary conditions has no unique solution.

It can be shown that this lack of uniqueness extends to more general boundary conditions; namely, for a given $r_0 > r_c$ there exist well-defined ranges of $dX/dr|_{r=r_0} \neq 0$ for which Eq. (3.4) has more than one solution.

It is immediately recognized that the critical radius $r_c$ obtained above is identical with that (see Sec. 2) at which the constant solution $X = 1$ to Eq. (2.2) becomes

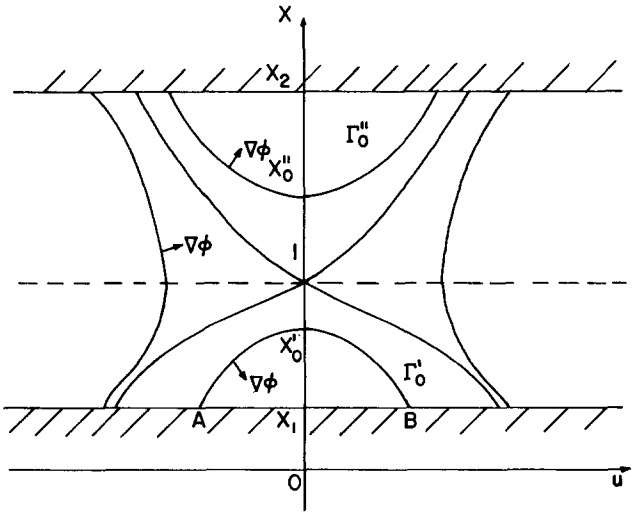


FIG. 3. Configuration of the curves $\Gamma$ for $F' > 0$.

unstable with respect to small perturbations. That is the onset of instability as a function of the size of the radiating plasma sphere coincides with the presence of multiplicity of temperature profiles satisfying the given physical constraints.

We shall now find the conditions for the existence of a nontrivial solution to Eq. (3.4) satisfying the boundary conditions of Theorem IV with $r_0 < r_c$. We restrict ourselves to the case $|X_0 - 1| \ll 1$, but not vanishing.

*Theorem V:* For $|X_0 - 1| \ll 1$, the sign of $dX/dr|_{r=r_c}$ is opposite of the sign of $F''(1) \equiv d^2F/dX^2|_{X=1}$.

*Proof:* Let $y \equiv X - 1$, $y_0 \equiv X_0 - 1$, and $g(y) \equiv F(X)$. Then

$$\frac{d^2(ry)}{dr^2} + \lambda^2 ry = H(y), \quad y(0) = y_0, \quad \frac{dy}{dr}\Big|_{r=0} = 0, \tag{3.16}$$

where $\lambda^2 \equiv -dg/dy|_{y=0}$, and $H(y) = r(g + \lambda^2 y)$.

A formal solution of Eq. (3.16) is

$$y = y_0 \frac{\sin\lambda r}{\lambda r} + \frac{\sin\lambda r}{\lambda r}\int_0^r dr' \cos\lambda r' H(y) - \frac{\cos\lambda r}{\lambda r}\int_0^r dr' \sin\lambda r' H(y) \tag{3.17}$$

Now to determine the slope of $y(r)$ at $r = r_c$, recall that at that point

$$\frac{d}{dr}\left(\frac{\sin\lambda r}{r}\right)\Big|_{r=r_c} = 0.$$

Hence,

$$\frac{dy}{dr}\Big|_{r=r_c} = -K\int_0^{r_c} dr\, rH(y)\sin\lambda r, \tag{3.18}$$

where $K = [(1 + \lambda^2 r_c)^{1/2}/\lambda r_c^2]$.

But since $g(y)$ is an analytic function of $y$ near $y = 0$,

$$g(y) = -\lambda^2 y + \tfrac{1}{2} y^2 g_0'' + \cdots,$$

where

$$g_0'' \equiv \frac{d^2g}{dy^2}\Big| y = 0.$$

Therefore,

$$H(y) = \tfrac{1}{2} y^2 g_0'' + \cdots$$

and up to terms in $y^2$

$$\frac{dy}{dr}\Big|_{r=r_c} \simeq -\tfrac{1}{2} g_0'' K \int_0^{r_c} dr\, ry^2 \sin\lambda r. \tag{3.19}$$

Now consider the differential equation

$$\frac{d^2(ry)}{dr^2} + \lambda^2 ry = ary^2 \tag{3.20}$$

with

$$y(0) = y_0 \quad \text{and} \quad \frac{dy}{dr}\Big|_{r=0} = 0.$$

The solution of Eq. (3.20) $y = y(r, a)$, belonging to the manifold discussed in Theorems II–IV is an analytic function of the parameter $a$. Hence, it can be shown that for $|y_0|$ small enough an approximate solution $y$ is found if in Eq. (3.17) we set

$$H(y) = H\ [y_0(\sin\lambda r/\lambda r)] \tag{3.21}$$

On substituting into Eq. (3.19), we obtain

$$\frac{dy}{dr}\Big|_{r=r_c} = \frac{-y_0^2 g_0'' K}{2\lambda^2}\int_0^{r_c} dr\, \frac{\sin^3\lambda r}{r} = -\frac{y_0^2 g_0'' K}{8\lambda^2}\left(3\int_0^{\lambda r_c} dr\, \frac{\sin r}{r} - \int_0^{3\lambda r_c} dr \frac{\sin r}{r}\right) \tag{3.22}$$

But it follows from the well-known properties of the function $\int_0^r dr(\sin r)/r$ that

$$\left|\int_{\lambda r_c}^{3\lambda r_c} dr\, \frac{\sin r}{r}\right| < \int_0^{\lambda r_c} dr\, \frac{\sin r}{r},$$

where we have taken into account that

$$\pi < \lambda r_c < 3\pi/2.$$

Hence,

$$\int_0^{r_c} dr\, \frac{\sin^3\lambda r}{r} > 0$$

and

$$\frac{dy}{dr}\Big|_{r=r_c} \begin{cases} < 0 & \text{if} \quad g_0'' > 0, \\ > 0 & \text{if} \quad g_0'' < 0, \end{cases}$$

which concludes the proof of this theorem.

An important consequence of Theorem V is that for $F''(1) > 0$ and $X_0 < 1$, if $X - 1$ has only one zero within the interval $(0, r_c)$, $X$ has an extremum at some $r_0 < r_c$. That is, under these conditions there exists a nontrivial solution of Eq. (3.4) satisfying the boundary conditions (3.5) with $r_0 < r_c$. It is important to note that the existence and properties of this solution cannot be established from the linearized differential equation.

Finally, we establish an important property of the solutions of Eq. (3.4) satisfying the boundary conditions (3.5) at $r_0 < r_c$.

*Theorem VI:* For $X$ satisfying the conditions of Theorem V and $F''(1) > 0$,

$$\int_0^{r_0} dr\, r^2 \ln X > 0 \quad \text{if} \quad F''(1)/\lambda^2 > 1.$$

*Proof:* Note that near $X = 1$, $F(X)$ is an analytic function of $\ln X$. Thus

$$F(X) = -\lambda^2 \ln X + \tfrac{1}{2}[F''(1) - \lambda^2](\ln X)^2 + O[(\ln X)^3].$$

Further, recall that

$$\int_0^{r_0} dr\, r^2 F(X) = 0.$$

Hence,

$$\int_0^{r_0} dr\, r^2 \ln X = \int_0^{r_0} dr\, r^2 [\ln X + F(X)/\lambda^2] = -\tfrac{1}{2}[1 - F''(1)/\lambda^2]\int_0^{r_0} dr\, r^2 (\ln X)^2 > 0$$

up to terms in $(\ln X)^2$ if

$$F''(1)/\lambda^2 > 1.$$

Implicit in the results of this section is the conclusion that when $F'(X) > 0$ the uniqueness of the trivial solutions to Eq. (3.4) is guaranteed. This finds its

correspondence in the stability of the uniform temperature solution for arbitrary size of the plasma (see Sec. 2), when the luminosity increases with temperature at constant pressure.

## 4. THE MODEL—A SPECIAL CASE

The discussion of the preceding section concerned itself with proving that for a certain type of luminosity function there are no uniquely determined temperature profiles for radiating plasma spheres exceeding a critical size. This critical size was found to coincide with that beyond which the isothermal plasma sphere becomes unstable with respect to small perturbations. Further, we have established under certain conditions the existence of nontrivial solutions for spheres with radii smaller than the critical radius $r_c$. We have not been able, as yet, to establish analytically the minimum radius $r_0$ above which these solutions exist. However, in special cases we can establish this limiting value of $r_0$ by numerical integration of the given differential equation for a sufficiently broad range of initial conditions.

For the purpose of this investigation we have assumed that $T_c$ is sufficiently high so that in the interval $I_T = [T_1, T_2]$ radiation is principally due to free-free emission, i.e.,

$$Q(T) = An^2 T^{1/2} = AP^2/T^{3/2}, \tag{4.1}$$

where $A$ is a constant. Energy deposition per unit volume at a given point was taken to be proportional to the density at that point, i.e.,

$$S(T) = Bn = BP/T, \tag{4.2}$$

where $B$ is a constant. Further, we have assumed that the thermal conductivity is approximately that for a quiescent plasma, i.e.,

$$\kappa(T) = \kappa_0 T^{5/2} \tag{4.3}$$

with $\kappa_0$ a constant (we ignore here the logarithmic temperature dependence of $\kappa_0$). The constant temperature solution $T_c$ is found to be

$$T_c = (B/An)^2 = (AP^2/B). \tag{4.4}$$

The luminosity function $f(T)$ is

$$f(T) = (AP^2/T^{3/2}) - (BP/T) \tag{4.5}$$

and

$$f'(T) = \frac{\partial f}{\partial T} = -\frac{3}{2}\frac{AP^2}{T^{5/2}} + \frac{BP}{T^2} < 0 \quad \text{for} \quad T < \left(\frac{3}{2}\frac{AP}{B}\right)^2. \tag{4.6}$$

At $T = T_c$, we have

$$f'(T_c) = -\tfrac{1}{2}(AP^2/T_c^{5/2}) = -Q(T_c)/2T_c. \tag{4.7}$$

The critical eigenvalue $\lambda_c$ at which instabilities arise is then

$$\lambda_c^2 = -\frac{f'(T_c)}{\kappa(T_c)} = \frac{AP^2}{2\kappa_0 T_c^5} = \frac{Q(T_c)}{2T_c\kappa(T_c)}. \tag{4.8}$$

In terms of the following nondimensional variables,

$$X = (T/T_c)^{7/2}, \tag{4.9a}$$

$$\rho = r\lambda_c\sqrt{7}. \tag{4.9b}$$

Equation (2.2) becomes

$$\rho^{-2}\frac{d}{d\rho}\rho^2\frac{dX}{d\rho} = X^{-3/7} - X^{-2/7} \equiv F(X), \tag{4.10}$$

and boundary conditions (2.1) and (2.4) become

$$\left.\frac{dX}{d\rho}\right|_{\rho=0} = \left.\frac{dX}{d\rho}\right|_{\rho=\rho_0} = 0,$$

where $\rho_0 = r_0\lambda_c\sqrt{7}$. We note that $F'(1) = 12/49 > 0$. We have integrated numerically this equation starting from a point $X(\rho = 0) < 1$ and found that as expected from Theorem V of the previous section $dX/d\rho = 0$ at some $\rho_0 < \rho_c$, where $\rho_c$ is the nondimensional distance variable corresponding to the smallest root of Eq. (2.15) (see Fig. 4). It is noteworthy that the internal energy of the nontrivial solution is identical to that for the uniform temperature (trivial) solution. This follows immediately from the isobaric conditions satisfied by both solutions and the fact that at one point inside the sphere of radius $r_0 < r_c$, the nonuniform temperature profile crosses the value $T = T_c$ (or $X = 1$).

From the definition of free energy[12] in a differential volume $dV$, the incremental free energy $d\mathfrak{F}$ is given by

$$d\mathfrak{F} = \epsilon_0 dN + [P(\ln P - 1 - \xi) - C_p P \ln T]\, dV,$$

where $\epsilon_0$ and $\xi$ are constants, and $dN$ is the number of particles within the volume $dV$. Hence, the free energy within the volume of a sphere with radius $r_0$ is

$$\mathfrak{F} = C_p P \int_{V(r_0)} \ln T dV + \epsilon_0 N + PV(\ln P - 1 - \xi).$$

For the special case where $T = T_c$ for all $r$, $0 \le r \le r_0$ [i.e., the trivial solution for Eq. (2.2)], we have

$$\mathfrak{F}_c \equiv \mathfrak{F}(T = T_c) = [-C_p P \ln T_c + P(\ln P - 1 - \xi)] \times V + \epsilon_0 N,$$

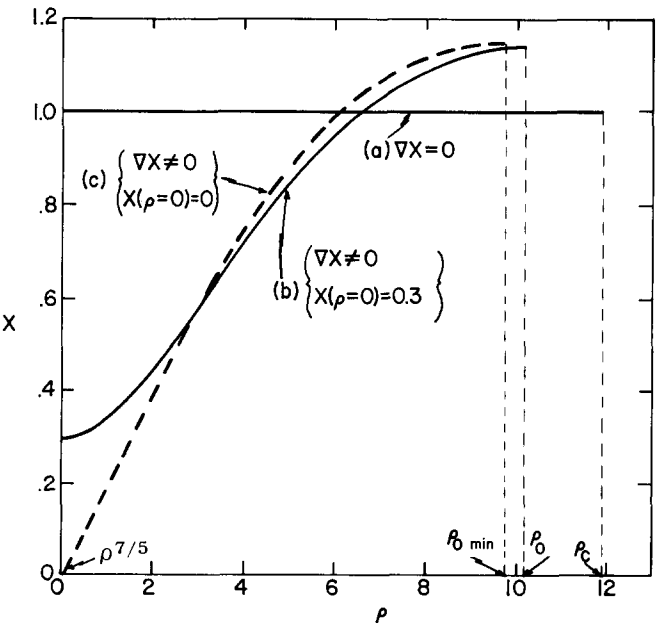


FIG. 4. Typical solutions of Eq. (4.10); a) the trivial solution, b) nontrivial solution $X_0 = 0.3$, and c) nontrivial solution $X_0 = 0$.

where we have taken into account that the total number of particles $N$ and the pressure $P$ within the volume $V$ are the same for the trivial and nontrivial solutions of Eq. (2.2). The difference between the free energies of the two configurations is

$$\Delta\mathfrak{F} = \mathfrak{F} - \mathfrak{F}_c = -C_p P \int_{V(r_0)} dV \ln T/T_c. \qquad (4.11)$$

Hence, for the model under discussion

$$\Delta\mathfrak{F} < 0$$

if

$$\int_0^{\rho_0} d\rho\, \rho^2 \ln X > 0.$$

But by Theorem VI of the previous section, this integral is indeed positive because in the present case

$$-F''(1)/F'(1) = \tfrac{12}{7} > 1.$$

(Note this integral is positive for all luminosity functions of the form $F(X) = X^{-\alpha} - X^{-\beta}$, $\alpha, \beta > 0$.)

It follows from the preceding that if we take a decrease in free energy as evidence of increase in relative stability of a given configuration, especially with respect to finite disturbances, then the nontrivial (nonuniform) solution to Eq. (2.2) subject to given boundary conditions, is more stable than the uniform solution. The latter solution may then be viewed as a metastable state.

On the other hand if $\Delta\mathfrak{F} > 0$, then it is the nonuniform solution which may be viewed as a metastable state. This follows from the observation that, as shown below, granting the existence of nonuniform temperature profiles for $r_0 < r_c$, those profiles are stable with respect to small perturbations.

Let the nondimensional time variable be

$$\tau \equiv [7Q(T_c)/2PC_p]\, t.$$

[The characteristic time $PC_p/Q(T_c)$ may be regarded as the time during which a significant amount of the internal plasma energy is lost by radiation.] Then Eq. (2.7) becomes

$$\frac{1}{X}\frac{\partial X}{\partial \tau} = \nabla^2 X - F(X), \qquad (4.12)$$

where now

$$\nabla^2 = \rho^{-2}\frac{d}{d\rho}\,\rho^2\,\frac{d}{d\rho};$$

$X$, $\rho$, and $F$ have previously been defined. Let $\overline{X}$ be a nonuniform solution of the problem

$$\nabla^2\overline{X} - F(\overline{X}) = 0 \qquad \nabla\overline{X}\Big|_{\rho=0} = \nabla\overline{X}\Big|_{\rho=\rho_0} = 0.$$

Consider a perturbed solution

$$X = \overline{X} + \delta X,$$

where

$$\delta X = \sin\lambda\rho/\rho \quad \text{for} \quad n\pi/\lambda < \rho < \{[(n+1)\pi]/\lambda\},$$
$$n = \text{some integer}, \ = 0 \quad \text{elsewhere.}$$

For the purpose of the present discussion we shall consider the profile $\overline{X}$ to be stable if for the selected $\delta X$, the right-hand side of Eq. (4.12) is negative given $\delta X > 0$ (and positive given $\delta X < 0$) for it indicates that at least initially the perturbation decreases (increases) with time. To first order in $\delta X$ we obtain

$$\frac{\partial X}{\partial t} = -\overline{X}[\lambda^2 + F'(\overline{X})]\delta X. \qquad (4.13)$$

This will satisfy our stability criterion if

$$\lambda^2 = F'(\overline{X}) > 0.$$

Now we note that

$$\overline{X}(0) < \overline{X}(\rho) \quad \text{for} \quad 0 \leq \rho \leq \rho_0$$

and, therefore,

$$\lambda^2 + F'(\overline{X}) \geq \lambda^2 + F'[X(0)]$$

as long as $\overline{X} < (3/2)$ [cf. Eq. (4.6)]; hence, the inequality will be satisfied if

$$\lambda^2 > -F'[X(0)] > -F'(1) \sim 1/\rho_c^2,$$

where $\rho_c$ is the nondimensional critical radius. Therefore, we require that the wavelength of the perturbation be smaller than $\rho_c$. But, since the largest wavelength excitable in a cavity of radius $\rho_0$ is comparable to $\rho_0$, and by hypothesis $\rho_0 < \rho_c$, the inequality always appears to be satisfied. Hence, the nonuniform solutions appear to be stable with respect to small perturbations.

It is of some interest that the free–free emission from a plasma with the nonuniform temperature profile is somewhat harder than would be the case with a uniform temperature profile. This follows from the fact that the former profile has a region with $T > T_c (X > 1)$.

The proof of Theorem VI is restricted to initial values of $T$ only a little less than $T_c$. We have numerically investigated the behavior of the solution of Eq. (4.10) in the limit of very small initial temperatures ($X_0 \ll 1$). The limiting behavior for $X_0 = 0$ is shown in Fig. 4. It can be shown that near the origin $X \sim \rho^{7/5}$. It should be noted that the minimum value of $\rho_0$, $\rho_{0\min} = 9.687$, is about 80% of the value of $\rho_c$. Moreover, numerical integration shows that even in this limiting case the integral

$$\int_0^{r_0} d\rho\, \rho^2 \ln X > 0$$

as it appears to be for all the cases intermediate between $X_0 = 1$ and $X_0 = 0$.

We recognize that the physical significance of our model is lost before $X_0$ reaches zero; however, it must be borne in mind that only one order of magnitude change in the temperature $T$ corresponds to three and a half orders of magnitude change in the variable $X$, so that a physically realistic range of temperatures may correspond to most of the values of $X$ in the interval (0, 1). It should perhaps be mentioned here that because of the isobaric assumption, if the drop in temperature in the interior of the radiating sphere is large enough, the particle density may rise to the point where the underlying assumption of optical thinness is no longer valid. In addition, on an astronomical scale, the density may rise to the

point where self-gravitation effects can no longer be neglected.

Finally, we point out the similarity between phase transitions, in general, and the possibility of transitions from the uniform to the nonuniform solutions. When the radius of the radiating plasma sphere is close to that corresponding to $\rho_{0\min}$, small variations in the flux of the incoming radiation may cause that radius to be actually larger (or smaller) than the corresponding $r_{0\min}$, thus inducing transitions from the nonuniform (uniform) temperature profile to the uniform (nonuniform) one.

## 5. CONCLUDING REMARKS

We have shown that under certain physically realizable conditions for finite-sized radiating plasmas, there may exist alternative stable and metastable configurations satisfying the given boundary conditions. Their existence cannot be established from the linearized differential equations. We have presented some simple tests for the presence and relative stability of such solutions. Applications of these results to a simple model of uniformly heated confined plasma show that for a range of parameters the emitted radiation by a configuration stable to finite disturbances is harder than would be predicted on the basis of normal mode analysis. To the extent that for a given total energy emitted, the emission of fewer photons with higher energies represents a lower entropy production rate, it is possible that the lower free-energy configurations discovered by us belong to the category of "dissipative structures" discussed by Glansdorff and Prigogine.[6] This point of view will be explored elsewhere.

## ACKNOWLEDGMENTS

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# Exactly Soluble Model of Interacting Electrons*

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(Received 9 March 1972)

We diagonalize a many-fermion Hamiltonian consisting of terms quadratic as well as quartic in the field operators. A dual spectrum of eigenstates is an interesting result. We also derive a formula for obtaining the free energy at finite temperature.

## I. INTRODUCTION

The Hubbard model of interacting electrons on a linear chain,

$$\mathcal{H}_{\text{Hub}} = -\epsilon \sum_{\substack{j=1 \\ \sigma=\pm 1/2}}^{N-1} (c_{j\sigma}^* c_{j+1\sigma} + c_{j+1\sigma}^* c_{j\sigma}) + U \sum_{j=1}^{N} (n_{j\uparrow} - \tfrac{1}{2})(n_{j\downarrow} - \tfrac{1}{2}), \quad \text{where } n_{j\sigma} = c_{j\sigma}^* c_{j\sigma}, \tag{1}$$

was given an ingenious solution by Lieb and Wu[1] who obtained the ground state, and later by others[2] who found the elementary excitations. The complete set of eigenstates has not yet been determined nor has the statistical mechanics, although numerical calculations[3,4] on finite systems ($N = 6$) has revealed many interesting features such as level crossings and dual excitation spectra. These are totally absent in the approximate RPA solution of (1), and such structure is lacking in the exactly soluble, relativistic model of interacting electrons.[5] It is therefore of interest to discuss the predictions of a new model, a modification of (1), which we have been able to solve exactly for arbitrary $N$, $\epsilon$, and $U$. We obtain and classify the eigenstates and eigenvalues, and reduce the calculation of the free energy to the solution of an implicit equation. One of our results is a two-fold degeneracy of the ground state, which is antiferromagnetically ordered. A dual excitation spectrum is also a feature of this model.

## II. MODEL HAMILTONIAN

Like (1), the exactly soluble Hamiltonian is a combination of quadratic and quartic terms:

$$\mathcal{H} = \frac{\epsilon}{4} \sum_{\substack{j=1 \\ \sigma=\pm}}^{N-1} (c_{j\sigma} - c_{j\sigma}^*)(c_{j+1\sigma} + c_{j+1\sigma}^*) + U \sum_{j=1}^{N} (n_{j\uparrow} - \tfrac{1}{2})(n_{j\downarrow} - \tfrac{1}{2}). \tag{2}$$

The $c$'s are a complete set of anticommuting operators.

An important (and anomalous) operator in the above is

$$\sum (c_{j\sigma} c_{j+1\sigma} - c_{j\sigma}^* c_{j+1\sigma}^*), \tag{3}$$

which causes charges to be created or destroyed in pairs (as in the BCS theory of superconductivity). It

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The $c$'s are a complete set of anticommuting operators.

An important (and anomalous) operator in the above is

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which causes charges to be created or destroyed in pairs (as in the BCS theory of superconductivity). It

is evident that the current density operator j has to be suitably modified to take this into account in order to satisfy an equation of continuity. These considerations have also suggested to us that one should seek an analogous modification of the current operator in the BCS theory, as we discuss elsewhere.[6] In the present work the anomalous terms (3) are introduced merely as a convenience to allow a solution of the problem. This device first proved useful in the exact solution of one and two "magnetic" impurity atoms in a three-dimensional nonmagnetic metal host,[7] although the subsequent calculations and results, in these problems, have little in common with the present work.

Our first step in the manipulation of $\mathcal{H}$ is a Jordan–Wigner transformation to pseudospin matrices $T_i$ and $S_i$, defined via

$$S_j^- = c_{j\uparrow} e^{\pi i \sum_{m<j} n_{m\uparrow}}, \quad T_j^- = c_{j\downarrow} e^{\pi i \left(\sum_{\text{all } m} n_{m\uparrow} + \sum_{m<j} n_{m\downarrow}\right)}, \tag{4}$$

with similar equations relating $S^+$ and $T^+$ to the $c^*$'s. Insertion into (2) yields

$$\mathcal{H} = -\epsilon \sum_j (S_j^x S_{j+1}^x + T_j^x T_{j+1}^x) + U \sum_j S_j^z T_j^z. \tag{5}$$

It is now advantageous to introduce a new set of spin matrices, the $P_j^\alpha$ and $J_j^\alpha$, in terms of which the original spin vectors are

$$\begin{aligned} (S_j^x, S_j^y, S_j^z) &= (J_j^x, 2J_j^y P_j^x, 2J_j^z P_j^x), \\ (T_j^x, T_j^y, T_j^z) &= (-2P_j^z J_j^x, 2P_j^y J_j^x, P_j^x). \end{aligned} \tag{6a}$$

The inverse of these relations is useful to record:

$$\begin{aligned} (J_j^x, J_j^y, J_j^z) &= (S_j^x, 2S_j^y T_j^z, 2S_j^z T_j^z), \\ (P_j^x, P_j^y, P_j^z) &= (T_j^z, 2S_j^x T_j^y, -2S_j^x T_j^x). \end{aligned} \tag{6b}$$

[Note that our matrices are all normalized to spin $\frac{1}{2}$, such that, e.g., $(P_j^x)^2 = \frac{1}{4}$.] When this is substituted into $\mathcal{H}$, there results

$$\mathcal{H} = -\epsilon \sum_j J_j^x J_{j+1}^x (4P_j^z P_{j+1}^z + 1) + \tfrac{1}{2} U \sum_j J_j^z. \tag{7}$$

## III. EIGENVALUES

Now we note that the $P_j^z$ are the constants of the motion and can therefore each be taken to be either $+\frac{1}{2}$ or $-\frac{1}{2}$. We denote this the "$P$-eigenvalue."

Inspection of (7) shows that if neighboring sites have opposite $P$-eigenvalues, the connection via the $J_j^x J_{j+1}^x$ bond becomes broken. Conversely, if they have similar $P$-eigenvalues, the bond strength is

$$-2\epsilon J_j^x J_{j+1}^x$$

regardless of whether the $P$-eigenvalue is $\pm\frac{1}{2}$. Thus in any eigenstate the chain of $N$ atoms is partioned into a number of noninteracting "molecules" of alternating $P$-eigenvalue. The number of such molecules can be as small as 1, which is indeed the case of the ground state, consisting of a single molecule of $N$ atoms all of which belong to a common eigenvalue of $P_j^z$. As, however, this eigenvalue can be $\pm\frac{1}{2}$, the ground state is a doublet regardless of the relative magnitudes of $\epsilon$ and $U$. At the opposite extreme, the largest number of molecules is $N$, each consisting of a single site.

We now solve for the eigenvalue spectrum of any one such molecule, which, we shall assume, extends from a site $A$ ($A \geq 1$) to a site $B$ ($A < B \leq N$). The applicable part of $\mathcal{H}$ is

$$\mathcal{H}_{AB} = -2\epsilon \sum_A^{B+1} J_j^x J_{j+1}^x + \tfrac{1}{2} U \sum_A^B J_j^z. \tag{8}$$

The eigenvalues are symmetric in $\epsilon$, therefore we restrict the following to $\epsilon \geq 0$. This $\mathcal{H}$ is reduced to quadrature by a transformation to fermions, the inverse of (4). Define the set of anticommuting operators $a_j$:

$$a_j = J_j^- e^{\pi i \sum_{i<j} J_i^+ J_i^-} \tag{9}$$

and similar Hermitian conjugates, such that

$$\begin{aligned} \mathcal{H}_{AB} = \tfrac{1}{2}\epsilon \sum_A^{B-1} (a_j - a_j^*)(a_{j+1} + a_{j+1}^*) \\ + \tfrac{1}{2} U \sum_A^B (a_j^* a_j - \tfrac{1}{2}). \end{aligned} \tag{10}$$

The diagonalization of precisely this quadratic form has been previously studied in connection with the "Heisenberg–Ising model",[8] and it is straightforward to "plagiarize" these old results:

The diagonal form of $\mathcal{H}_{AB}$ becomes

$$\mathcal{H}_{AB} = \sum_A \Lambda_k (a_k^* a_k - \tfrac{1}{2}), \tag{11}$$

where

$$\Lambda_k = [(U/2 - \epsilon)^2 + 2U\epsilon \sin^2 k/2]^{1/2} \tag{12a}$$

and the $k$'s are the roots of

$$\sin k(B - A + 2)/\sin k(B - A + 1) = 2\epsilon/U, \tag{12b}$$

i.e.,

$$\Lambda_k = |\sin k/\sin k(B - A + 1)|(U/2). \tag{12c}$$

By (11), the ground-state energy is

$$E_{AB}^0 = -\tfrac{1}{2} \sum_k \Lambda_k. \tag{12d}$$

Because of obvious symmetry in $\mathcal{H}$, we have taken $\epsilon \geq 0$ in these relations without loss of generality. For $0 < \epsilon < U/2$ there are $B - A + 1$ real roots, exhausting the normal modes. For $\epsilon > U/2$, however, there are only $B - A$ real roots but, in addition, an imaginary one representing a "surface" state. Denoting it $k_0 \equiv iv$, one finds.[8]

$$\begin{aligned} \sinh(B - A + 2)v/\sinh(B - A + 1)v &= 2\epsilon/U, \\ \Lambda_0 = |\sinh v/\sinh v(B - A + 1)|(U/2). \end{aligned} \tag{13}$$

It is interesting to note that when $B - A \to \infty$, $\Lambda_0 \to 0$ for all $U < 2|\epsilon|$.

## IV. THERMODYNAMICS

The partition function of an $\mathcal{L}$-atom molecule is

$$z(\mathcal{L}) = \prod_k 2 \cosh \tfrac{1}{2} \beta \Lambda_k, \quad \beta = 1/kT, \tag{14}$$

where the set of $\mathcal{L}$ $k$'s and $\Lambda_k$'s are given in the preceding equations, with $\mathcal{L} \equiv B - A + 1$. If we decompose the chain of $N$ atoms into molecules of lengths

$\ell_1, \ell_2, \cdots$, subject to the constraint

$$\sum \ell_i = N, \tag{15}$$

then the grand partition function is $Z = \exp(-\beta F)$, where $F$ = free energy. This is given in terms of the individual molecules as

$$Z = \sum \prod_i z(\ell_i). \tag{16}$$

The sum is over all possible decompositions. We now discuss a method for calculating this in the thermodynamic limit ($N \to \infty$).

Let

$$z(\ell) \equiv \lambda^\ell \, e^{\phi(\ell)}, \tag{17}$$

where $\lambda$ includes the extensive contribution, and $\phi(\ell)$ the influence of finite ends, of a molecule $\ell$ units in length. Thus, we define $\lambda$ by

$$\log\lambda = \lim_{\ell\to\infty} \ell^{-1} \log z(\ell) = \pi^{-1} \int_0^\pi d\theta \log \times \{2 \cosh \tfrac{1}{2}\beta[(U/2 - \epsilon)^2 + 2U\epsilon \sin^2\theta/2]^{1/2}\}. \tag{17'a}$$

We have

$$\phi(\ell) \equiv \log[z(\ell)\lambda^{-\ell}] \tag{17'b}$$

an intensive quantity, i.e.,

$$\lim_{\ell\to\infty} \ell^{-1}\phi(\ell) = 0. \tag{17'c}$$

The calculation of $Z$ reduces to that of an auxiliary quantity $G$, defined via:

$$Z = \lambda^N \sum e^{\sum_i \phi(\ell_i)} \equiv \lambda^N G(N), \tag{18}$$

$G$ obeys an iterative equation:

$$G(N) = e^{\phi(1)}G(N-1) + e^{\phi(2)}G(N-2) + \cdots. \tag{19}$$

In the thermodynamic limit ($N \to \infty$) we set $G(N) = g^{-N}$, with $g > 1$, and

$$1 = \sum_{\ell=1}^{\infty} e^{\phi(\ell)} g^{-\ell} \tag{20}$$

follows from (19), and is the implicit equation determining $Z$.

If $\phi(\ell)$ were constant for $\ell \geq 1$, then (20) is solved by

$$1 = e^\phi \sum_{\ell=1}^{\infty} g^{-\ell} = e^\phi/(g-1),$$

i.e.,

$$g = 1 + e^\phi. \tag{21a}$$

If $\phi(\ell) = \phi(1)$ for $\ell = 1$ and $\phi(2)$ for $\ell \geq 2$, then

$$1 = e^{\phi(1)}g^{-1} + e^{\phi(2)}g^{-1} \sum_{\ell=1}^{\infty} g^{-\ell} = e^{\phi(1)}g^{-1} + e^{\phi(2)}/g(g-1),$$

i.e., $$g = \tfrac{1}{2}(1 + e^{\phi(1)}) + [\tfrac{1}{4}(1 + e^{\phi(1)})^2 + (e^{\phi(2)} - e^{\phi(1)})]^{1/2}. \tag{21b}$$

It is easy to see if $\phi(\ell)$ becomes constant after $r$ steps, the solution of an $r$th degree equation yields $g$, and hence $G$ and $Z$. If $\phi$ is not really constant at $\ell > r$, corrections may be obtained by iteration. It is believed that because the $\phi(\ell)$ are analytic functions of the temperature, the solution $g$ and hence $Z$ must be analytic as well, so that there is no phase transition at finite $T$.

## V. ELEMENTARY EXCITATION

Assuming the ground state to be a single molecule of length $N$, belonging to either $P$-eigenvalue $\pm\frac{1}{2}$, the spectra of elementary excitations are twofold: (A) the set of internal excitations, of energy $\Lambda_k$, and (B) the (quite distinct) breaking up of the chain into smaller molecules which must, of course, belong to alternating $P$-eigenvalues. Both type excitations are counted in the calculation of $Z$ in the previous chapter. They must be treated distinctly in a study of the dynamics of our model.

### A. Internal Excitations

Consider Eqs. (11) and (12) with $B - A = N - 1 \to \infty$. We observe that for $|\epsilon| \leq \frac{1}{2}U$ the spectrum of elementary excitations represents the addition of a quasiparticle of energy:

$$\Lambda_k = [(U/2 - \epsilon)^2 + 2U\epsilon \sin^2 k/2]^{1/2} \tag{22}$$

with $k$ ranging over closely spaced eigenvalues from 0 to $\pi$.

When $|\epsilon| > \frac{1}{2}U$ then is also a bound state of energy $\Lambda_0 = 0$.

### B. External Excitations

For lack of a better name we denote "external excitations" the process of creating an additional molecule.

As we are principally concerned with excitations connecting to the ground state, the problem reduces to consideration of the energy to break up the original ground state molecule extending from (1 to $N$) into three: (1 to $A-1$), ($A$ to $B$), and ($B+1$ to $N$). It may be assumed that $A$ and $N - B$ both $\gg 1$ and that $B - A \equiv \ell - 1 \ll N$. We define the ground state energy of a molecule of length $L$ to be $E_0(L)$, and the ground state of the same molecule with the two ends connected (periodic boundary conditions[9]) $E_{0p}(L)$, with $E_{0p}(L) \leq E_0(L)$ and $E_0(L) - E_{0p}(L) = O(1)$ for obvious reasons. Then the energy $\Delta(\ell)$ to break the initial molecule into 3 is calculable as follows:

$$\Delta(\ell) = E_0(\ell) + [E_{0p}(N-\ell) - E_{0p}(N)] + [E_0(N-\ell) - E_{0p}(N-\ell)], \tag{23}$$

where ($N \to \infty$),

$$E_{0p}(N-\ell) - E_{0p}(N) = (\ell/2\pi) \int_0^\pi d\theta \, \Lambda_\theta = (\ell/\pi)(U/2 + |\epsilon|)E(2U|\epsilon|/[U/2 + |\epsilon|]^2). \tag{24}$$

Here $E(x)$ is the complete elliptic integral. Also,

$$E_0(N-\ell) - E_{0p}(N-\ell) = \tfrac{1}{4}[|U/2 + |\epsilon|| - |U/2 - |\epsilon|| ] + (1/2\pi)\int_0^\pi d\theta \, \Phi(\theta) \frac{\partial \Lambda_\theta}{\partial \theta}, \tag{25}$$

where $\Phi$ is defined through $k = \theta + (1/L)\Phi(\theta)$, where $k$ satisfied Eq. (12) with $B - A + 1 \equiv L$ and $\theta =$

$(\pi n/L)$, $(n = 0, 1, \cdots, L-1)$, and $L \to \infty$. Thus

$$\frac{\sin\left[\left(\theta + \frac{1}{L}\Phi\right)(L+1)\right]}{\sin\left[\left(\theta + \frac{1}{L}\Phi\right)L\right]} = \frac{\sin(\theta+\Phi)}{\sin\Phi} = \frac{2\epsilon}{U}, \quad (26)$$

which has the solution

$$\Phi(\theta) = \cot^{-1}[(2\epsilon/U - \cos\theta)/\sin\theta]. \quad (27)$$

In the special limit, $2\epsilon = U$, the $\Delta(\ell)$ becomes

$$\Delta(\ell) = U[\tfrac{1}{2} - 1/\pi - \tfrac{1}{4}(\csc x - 1/x)],$$

where $x = \pi/(4\ell + 2)$. For $2\epsilon > U$, using $\theta = \pi n/(L+1)$ in Eq. (2b), we get $\Phi(\theta)$ for Eq. (25) by replacing $2\epsilon/U$ by $U/2\epsilon$ in Eq. (27).

## VI. MATRIX ELEMENTS AND CORRELATION FUNCTIONS

Here we are concerned with some typical ground state correlations and some matrix elements to excited states. The ground state of a linear chain (length $N \to \infty$) is at least twofold degenerate: Aside from the two choices of $P$-eigenvalue there exists, for $U < 2|\epsilon|$, the option of exciting or not exciting the surface state of Eq. (13) which has energy $\Lambda_0 = 0$. Let us label the set of possible ground states by $|\alpha\rangle$. Then

$$\langle\alpha|n_{j\uparrow}|\alpha\rangle = \tfrac{1}{2} + 2\langle\alpha|J_j^z P_j^x|\alpha\rangle = \tfrac{1}{2}$$
and
$$\langle\alpha|n_{j\downarrow}|\alpha\rangle = \tfrac{1}{2} + \langle\alpha|P_j^x|\alpha\rangle = \tfrac{1}{2}. \quad (28)$$

Thus $\sigma_j^z \sigma_{j+p}^z$ correlations are nonexistent for all $p \neq 0$:

$$\langle\alpha|(n_{j\uparrow} - n_{j\downarrow})(n_{j+p\uparrow} - n_{j+p\downarrow})|\alpha\rangle = 0. \quad (29)$$

However, the nearest-neighbor transverse correlations are

$$\begin{aligned}\langle\alpha|c_{j\uparrow}^* c_{j\downarrow} c_{j+1\downarrow}^* c_{j+1\uparrow}|\alpha\rangle &= -\langle\alpha|[(J_j^z - \tfrac{1}{2})(P_j^z + iP_j^y)] \\ &\quad \times [(J_{j+1}^z - \tfrac{1}{2})(P_{j+1}^z + iP_{j+1}^y)]|\alpha\rangle \\ &= -\tfrac{1}{4}\langle\alpha|(J_j^z - \tfrac{1}{2})(J_{j+1}^z - \tfrac{1}{2})|\alpha\rangle. \end{aligned} \quad (30)$$

This can easily be calculated by (9), (10) and a plane wave expansion related to use of periodic boundary conditions ($a_j = 1/N^{-1/2}\sum_k e^{ik\cdot R_j} c_k$). One can see that (30) is negative, and concludes that nearest-neighbor sites within a molecule are antiferromagnetically correlated.

This also allows us to estimate the spin correlation of adjacent ends of two molecules. If $j$ is at the end of one molecule (has $P$-eigenvalue $P_j^z$) and $j+1$ at the beginning of the next $P$-eigenvalue $P_{j+1}^z = -P_j^z$), then the expectation value (30) becomes intrinsically positive. It is therefore tempting to interpret the molecules as antiferromagnetic domains, and the break in $P$-eigenvalue between $j$ and $j+1$ as the domain wall. However, the true picture must be somewhat more complex than this, as we see when examining matrix elements to excited states. The fundamental charge density operator $n_{i\uparrow} + n_{i\downarrow}$ has matrix element:

$$\langle\gamma|n_{i\uparrow} + n_{i\downarrow}|\alpha\rangle = 2\langle\gamma|(J_i^z + \tfrac{1}{2})P_i^x|\alpha\rangle, \quad (31)$$

where $|\alpha\rangle$ is one of the ground states. This vanishes unless $\langle\gamma|$ is an "external" elementary excited state, having the same $P$-eigenvalue as $|\alpha\rangle$ for $j \neq i$ and opposite $P$-eigenvalue at $i$. The energy of such a state relative to the ground state, $\Delta(1)$, has already been calculated in a previous chapter.

Similarly, a magnetic field (in the $z$ direction) involves matrix elements

$$\langle\gamma|n_{i\uparrow} - n_{i\downarrow}|\alpha\rangle = 2\langle\gamma|J_i^z - \tfrac{1}{2})P_i^x|\alpha\rangle \quad (32)$$

which connect to the same "external" excited states $\langle\gamma|$ as the above.

## VII. CONCLUSION

We have reduced to quadrature a many-body problem of fermions with spin, constrained to a linear chain. The problem was first brought to the form, Eq. (7), in which the nonlinear terms (with $P_j^z$) could be characterized by quantum numbers $\pm\frac{1}{2}$. The remainder, Eq. (8), could be solved by transforming to a quadratic form in spinless fermions.

We found the ground state to be a single molecule. For $U > 2|\epsilon|$ the ground state is twofold degenerate, such as an antiferromagnetic Ising chain, and has two Néel ground states (differing by one atomic translation). However, when $U < 2|\epsilon|$ the ground state is fourfold degenerate. There is a "phase transition" for $T = 0$ at $U = 2|\epsilon|$. We obtain an implicit expression for the partition function and estimate for fixed $U$ and $\epsilon$, that there is no phase transition when the temperature $T$ is varied.

Finally, we find that external perturbations (magnetic or electric fields) connect only to that part of the excitation spectrum we have labelled "external" excitations. Internal excitations ($\Lambda_k$), in which all $P_j^z$-eigenvalues are conserved, are therefore not accessible to probing by external forces even though they contribute to the thermodynamic properties. Thus at $U = 2|\epsilon|$ the model has an absorption threshold at finite energy, i.e., an "optical" gap, even though the continuous spectrum of internal elementary excitations extends down to $\Lambda_k = 0$.

The dual excitation spectrum suggests that a solution of the free energy equations (14)–(21) will yield *two* maxima in the specific heat, a feature which has already been discovered in numerical computation[4] of the properties of finite Hubbard-model chains ($N \leq 6$).

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# Unbounded Solutions of Coupled Mode Equations*

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A number of sufficient conditions for the existence of unbounded solutions of two and three coupled mode equations are obtained when some modes are linearly unstable and all initial amplitudes are arbitrarily small. The difficulty of obtaining sufficient conditions for boundedness of all solutions is discussed, and only two such conditions are obtained. In certain cases it is proved that the unbounded solutions are not more rapid than exponential, whereas they can be shown to be singular ("explosive") in other cases.

## 1. INTRODUCTION

In recent years there has been increasing interest in the properties of the solutions of nonlinear equations which describe the coupling of linear modes[1-3] particularly in those cases where the linear modes are unstable. A question of primary interest is whether the nonlinear mode coupling can produce bounded solutions when the linear modes are unstable. The mathematical problem of establishing the boundedness of all solutions of a system of ordinary differential equation is one of great difficulty. At present there is apparently very few known methods for establishing boundedness of all solutions[4], the most common methods relying on extensions of Liapunov's method used in establishing stability. The complimentary problem of establishing sufficient conditions under which some solutions are unbounded is, at least in principle, considerably simpler. While this information does not indicate when there may be only bounded solutions, it at least establishes conditions under which the mode coupling cannot stabilize the linear instability. It should be emphasized that the sufficient conditions of interest are those which hold for initial states arbitrarily near the stationary point [e.g., $\sum|x_k(0)|^2 < \epsilon$ in Eq. (1) below].

To investigate this problem, we will first consider a system of equations describing the interactions between three linear modes. Another system involving two coupled modes will be discussed in Sec. 4. The three-mode equations are

$$\begin{aligned} \dot{x}_1 &= \alpha_1 x_1 + \beta_1 x_3 x_2^*, \\ \dot{x}_2 &= \alpha_2 x_2 + \beta_2 x_3 x_1^*, \\ \dot{x}_3 &= \alpha_3 x_3 + \beta_3^* x_1 x_2, \end{aligned} \tag{1}$$

where all quantities are complex, the dot refers to a time derivative, and the asterisk indicates the complex conjugate. These equations have been widely studied[1,3] under a variety of special assumptions concerning the complex coefficients $(\alpha_k, \beta_k)$. In Sec. 2 we will also make use of one of the common assumptions concerning the coefficients $\beta_k$ in order to obtain certain sufficient conditions for the existence of unbounded solutions. [Solutions of (1) are called bounded if, for all $t \geq 0$, $\sum|x_k(t)|^2 \geq M < \infty$ for some $M$.] In this case it will be shown that there is an interesting geometric interpretation which also clearly indicates the difficulty involved in establishing the boundedness of all solutions. The general case of arbitrary $(\alpha_k, \beta_k)$ will be taken up in Sec. 3, where a number of more abstract conditions for unbounded solutions will be obtained. In Sec. 4 these results will be compared with those obtained for two coupled modes. In addition the existence of singular solutions will be established under certain conditions.

As mentioned above, the primary interest in Eq. (1) is when the linear modes are unstable. If we set

$$\alpha_k = i\omega_k + \gamma_k \quad (\omega_k, \gamma_k: \text{real}), \tag{2}$$

then this means that at least one of the $\gamma_k$ is positive. Unless noted otherwise, it will be assumed in the following that this is the case.

## 2. THE CASE $\beta_k = \rho_k e^{i\phi}$

In this section we will assume that the coefficients $\beta_k$ in Eq. (1) are of the form

$$\beta_k = \rho_k e^{i\phi} \quad (\rho_k, \phi: \text{real}). \tag{3}$$

Note that all $\phi$ are the same, but the sign of $\rho_k$ is not restricted to being positive. In this case one readily obtains from Eq. (1)

$$\frac{d}{dt}(\rho_j n_k - \rho_k n_j) = 2(\gamma_k \rho_j n_k - \gamma_j \rho_k n_j), \quad j,k = 1, 2, 3, \tag{4}$$

where $n_k = |x_k|^2$. A simple but useful lemma which can be applied here, and to other cases with various generalizations, is the following:

*Lemma:* Consider the equation

$$\frac{d}{dt}[F(t) + G^2(t)] = aF(t) + bG^2(t), \tag{5}$$

where $a > 0$ and $b$ are constants and $F(t)$, $G(t)$ are arbitrary functions. If there exists initial states such that

$$(b - a)[F(0) + G^2(0)] > 0$$

then, for these states,

$$|F(t) + G^2(t)| \geq |F(0) + G^2(0)|e^{at}, \qquad t \geq 0.$$

The proof is elementary. If $b > a$, then $aF + bG^2 > a(F + G^2)$, and the result follows for the indicated initial states. If $b < a$, then the same reasoning holds for $-F - G^2$. Note that if $F(0)$ can have arbitrary sign, then the condition $(b - a)[F(0) + G^2(0)] > 0$ can always be satisfied. In this case the conclusion holds for any constant $b$ (not necessarily positive).

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To investigate this problem, we will first consider a system of equations describing the interactions between three linear modes. Another system involving two coupled modes will be discussed in Sec. 4. The three-mode equations are

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where $n_k = |x_k|^2$. A simple but useful lemma which can be applied here, and to other cases with various generalizations, is the following:

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From Eq. (4) one can now establish:

Eq. (1) has unbounded solutions if (3) holds and either of the following conditions hold:

$$\text{(a) } \gamma_j > 0 \quad \text{and} \quad \gamma_k > 0, \qquad (6)$$
$$\text{(b) } \gamma_j\gamma_k < 0 \quad \text{and} \quad \rho_j\rho_k > 0.$$

These results follow simply from (5) by multiplying (4) by either $\rho_j$ or $-\rho_k$. It will be noted that conditions (6) do not depend on the magnitudes of the $\omega_k$ or $\gamma_k$ (the magnitudes of the $\rho_k$ are never of importance, since they can be eliminated by renormalizing the $n_k$). It is of some interest to note that Eq. (4) can be written in terms of determinants, namely

$$\frac{d}{dt}\begin{vmatrix} n_j & \rho_j \\ n_k & \rho_k \end{vmatrix} = 2\begin{vmatrix} n_j & \gamma_k\rho_j \\ n_k & \gamma_j\rho_k \end{vmatrix}. \qquad (4')$$

The determinants equal (plus or minus) the area of the parallelograms generated by their two respective column vectors, only one of which is a function of time (and which is constrained to remain in the first quadrant). Thus (4) can be interpreted as the time rate of change of one area being equal to another area both generated by a common vector $(n_j, n_k)$ in the first quadrant. (The relative signs of the two determinants must, of course, be considered.) The problem with establishing boundedness [at least from Eq. (4)] is related to the fact that, even if the area decreases monotonically, it does not prove that the vector $(n_j, n_k)$ remains bounded. In only one case can this be established: If $\gamma_j < 0$, $\gamma_k < 0$, and $\rho_j\rho_k < 0$ then, for all initial states, $x_j$ and $x_k$ asymptotically approach zero. This result is obvious for small $x_k$, but not entirely trivial if the $x_k$ is initially large. However, even in this case, the remaining $x_l$ (for which $\gamma_l > 0$) becomes unbounded, so one again has no demonstrably bounded situation [however, see (17)].

To obtain further results, dependent on the magnitudes of the $(\omega_k, \gamma_k)$, one introduces the action-angle variables

$$x_k(t) = A_k(t)\exp\{i[\omega_k t + \theta_k(t)]\}, \qquad (7)$$

where $A_k(t)$ and $\theta_k(t)$ are real function. Substituting (7) into (1) yields

$$\dot{A}_k = \gamma_k A_k + \rho_k A_{k'} A_{k''}\cos\theta, \qquad (8)$$

where $k \neq k' \neq k''$, and $\theta = \theta_3 - \theta_2 - \theta_1 + \phi$ satisfies

$$\dot{\theta} = \Delta\omega - (\rho_1 A_1^{-1}A_2A_3 + \rho_2 A_2^{-1}A_1A_3 + \rho_3 A_3^{-1}A_1A_2) \times \sin\theta. \qquad (9)$$

From Eqs. (8) and (9) one can obtain

$$\frac{d}{dt}(A_1A_2A_3\sin\theta) = \Delta\omega A_1A_2A_3\cos\theta + \Gamma A_1A_2A_3\sin\theta,$$

which can be put in the form [using (8)]

$$\frac{d}{dt}\left(A_1A_2A_3\sin\theta - \frac{\Delta\omega}{2\rho_k}A_k^2\right) = \Gamma A_1A_2A_3\sin\theta - 2\gamma_k\left(\frac{\Delta\omega}{2\rho_k}\right)A_k^2 \qquad (10)$$

for any $k$. In these equations

$$\Delta\omega = \omega_3 - \omega_2 - \omega_1, \qquad \Gamma = \gamma_1 + \gamma_2 + \gamma_3. \qquad (11)$$

From (10) one can conclude the following:

Eq. (1) has unbounded solutions if (3) holds and either

$$\text{(a) } \Gamma > 0, \qquad (12)$$
$$\text{(b) } \Gamma = 0, \quad \Delta\omega \neq 0 \quad (\text{some } \gamma_k > 0).$$

(12a) clearly holds if $\Delta\omega = 0$. Note that, if $\Delta\omega \neq 0$ and $\Gamma \leq 0$, one cannot conclude from (10) that all solutions are bounded. If $\Delta\omega \neq 0$, then, by taking $G = A_k$ and $F = -(2\rho_k/\Delta\omega)A_1A_2A_3\sin\theta$, one can again apply (5). Since $F(0)$ can have arbitrary sign, only the condition (12a) is required. Part (b) is based on the fact that if $d(FG)/dt = cF^2 (c > 0)$, then either $FG$ is unbounded, or $F$ tends to zero and $FG$ may remain finite—in which case $G$ is unbounded. In either case one has unbounded functions. If (12b) holds, one will also have a constant of the motion if one of the $\gamma_l = 0$. It is noteworthy that conditions (12) do not depend on the signs of the nonlinear coefficients $\rho_k$.

The results of this section show that if (3) holds and there is linearly unstable mode (say $\gamma_1 > 0$), then all solutions of (1) can be bounded only if

$$\gamma_2 \leq 0,\ \gamma_3 \leq 0, \quad \rho_1\rho_2 < 0,\ \rho_1\rho_3 < 0, \qquad (13)$$
$$\gamma_1 + \gamma_2 + \gamma_3 \leq 0 \text{ (and } \Delta\omega = 0 \text{ in the case of equality).}$$

That even these conditions are not sufficient to guarantee the boundedness of all solutions is illustrated by the following case. Assume that (13) holds, $\Delta\omega = 0$, and $\gamma_2 = \gamma_3$. In that case $\theta = (0, \pi)$ are solutions of (9), and Eqs. (8) for $k = 2, 3$ are redundant if $A_2 = (\rho_2/\rho_3)^{1/2}A_3$. One can then easily show that $A_1$ can have unbounded solutions. An important feature of this last unbounded solution is that it is related to a set of initial conditions which have measure zero [namely $\theta(0)$ is restricted and $(A_2, A_3)$ are related]. This is one of the characteristic problems which arise in trying to establish boundedness—namely one must deal with all solutions, including groups of measure zero.

## 3. GENERAL CASE

We now consider the general case where

$$\beta_k = \rho_k e^{i\phi_k} \quad (\rho_k > 0), \qquad (14)$$

where $(\rho_k, \phi_k)$ are real and the $\rho_k$ are now positive quantities. Unless noted otherwise, we will assume $\sin(\phi_k - \phi_l) \neq 0$. Substituting

$$x_k = \rho_k^{-1/2}A_k(t)\exp\{i[\omega_k t + \theta_k(t)]\}$$

into (1) yields, in place of (8) and (9),

$$\dot{A}_k = \gamma_k A_k + VA_{k'}A_{k''}\cos(\theta + \phi_k),$$
$$\dot{\theta} = \Delta\omega - V[A_3^{-1}A_1A_2\sin(\theta + \phi_3) + A_2^{-1}A_1A_3 \times \sin(\theta + \phi_2) + A_1^{-1}A_2A_3\sin(\theta + \phi_1)], \qquad (15)$$

where $V = (\rho_1\rho_2\rho_3)^{1/2}$, $\theta = \theta_3 - \theta_2 - \theta_1$ and $\Delta\omega = \omega_3 - \omega_2 - \omega_1$. In the present case, with arbitrary phases $\phi_k$, it is only possible to obtain one equation

which involves only the square on the amplitudes $N_k = A_k^2$. From the first equation of (15) one obtains

$$\sin(\phi_3 - \phi_2)\dot{N}_1 + \sin(\phi_1 - \phi_3)\dot{N}_2 + \sin(\phi_2 - \phi_1)\dot{N}_3 = 2\gamma_1 \sin(\phi_3 - \phi_2)N_1 + 2\gamma_2 \sin(\phi_1 - \phi_3)N_2 + 2\gamma_3 \sin(\phi_2 - \phi_1)N_3. \quad (16)$$

From (16) we can establish a number of conclusions:

> If the three complex vectors $\beta_k$ do not lie in the same half plane, then the solutions of (1) are unbounded, bounded, asympotically tend to zero if all $\gamma_k > 0, \gamma_k = 0, \gamma_k < 0$, respectively. (17)

This result comes from the fact that, if the $\beta_k$ do not lie in the same half plane, all the sine functions in (16) have the same sign, and (17) follows trivially. It was concluded by Wilhelmsson, Stenflo, and Engelmann[3] that a necessary condition for singular ("explosive") solutions of (1) is that the complex vectors $\beta_k$ must lie in the same half plane. This is confirmed by (16), because otherwise the magnitude of $\sin(\phi_3 - \phi_2)N_1 + \sin(\phi_1 - \phi_3)N_2 + \sin(\phi_2 - \phi_1)N_3$ cannot increase faster than $\exp[2\max(\gamma_1, \gamma_2, \gamma_3)t]$, and hence there is no singular solution. It might be noted that the existence of singular solutions can never be established from linear equations such as (16). Next:

> If $\sin(\phi_k - \phi_l) = 0$, and if either $\gamma_k$ or $\gamma_l$ is positive, then (1) has unbounded solutions. (18)

This is similar to (6) except that the third vector $\beta_j$ now is not colinear with the other two. Another conclusion one can draw from (16) is the following:

> Assume that the three vectors $\beta_k$ lie in the same half plane. If the $\gamma_k$ corresponding to the vector $\beta_k$ which lies between the other two vectors satisfies $\gamma_k\gamma_l < 0$ (for both $l \neq k$), then there are solutions of (1) which are unbounded in time. (19)

Under the assumption of (19), all sine functions in (16) do not have the same sign. Label the vectors such that $\phi_3 > \phi_2 > \phi_1 (\phi_3 - \phi_1 < \pi)$. If $\gamma_1, \gamma_3 > 0$, $\gamma_2 < 0$, then the function on the right side of (16) is positive, and not less than $2\min(\gamma_1, \gamma_3)$ times $\sin(\phi_3 - \phi_2)N_1 + \sin(\phi_1 - \phi_3)N_2 + \sin(\phi_2 - \phi_1)N_3 \equiv M(t)$. Hence for the initial state $M(0) > 0$, one has unbounded solutions. On the other hand, if $\gamma_1, \gamma_3 < 0$, and $\gamma_2 > 0$, the right side of (16) is negative, and hence $d(-M)/dt$ is not less than $2\gamma_2(-M)$ and there are unbounded solutions if $M(0) < 0$. This establishes (19). By an analogous argument one can establish:

> If the three vectors $\beta_k$ lie in the same half plane, and $\gamma_2 > (\gamma_1, \gamma_3) > 0$ or $(\gamma_1, \gamma_3) > \gamma_2 > 0$ labeled as above), then there are solutions at least exponentially unbounded with growth rates of at least $2\gamma_2$ or $2\min(\gamma_1, \gamma_3)$, respectively. (20)

What is curious is that one cannot establish unboundedness from (16) when the $\beta_k$ are in the same half-plane and $\gamma_2$ lies between $\gamma_1$ and $\gamma_3$—even if they are all positive. This will be partially remedied below.

To obtain sufficient conditions involving $\Delta\omega$ and $\Gamma$, one can proceed by obtaining a generalization of Eq. (10). From (15) one finds that, for any $k$,

$$\frac{d}{dt}\left(A_1A_2A_3 \sin(\theta + \phi_k) - \frac{\Delta\omega}{2V}A_k^2\right) = \Gamma A_1A_2A_3 \sin(\theta + \phi_k) - 2\gamma_k\left(\frac{\Delta\omega}{2V}\right)A_k^2 + VA_k^2A_{k'}^2 \sin(\phi_k - \phi_{k''}) + VA_k^2A_{k''}^2 \sin(\phi_k - \phi_{k'}), \quad (21)$$

where $k \neq k' \neq k''$. The appearance of the last two terms, which are of highest order in the unknown functions, complicates the sufficient conditions which are most readily obtainable. The most general condition which has been found from (21) is

> Eq. (1) has unbounded solutions if, for some $k$, $\sin(\phi_k - \phi_{k'}) \sin(\phi_k - \phi_{k''}) > 0$, $(\Gamma - 2\gamma_k)\Delta\omega \sin(\phi_k - \phi_{k'}) \geq 0$ and $\Gamma \geq 0$, (22)

which may be compared with (12). The first proviso of (22) can only be satisfied if all three vectors $\beta_k$ lie in the same half-plane. Even then it is not satisfied for one $k$. The second proviso is clearly the strangest in that the sign of $\Delta\omega$ and $(\Gamma - 2\gamma_k)$ enters the picture. While it seems doubtful that this is a necessary condition, it is required to establish unbounded solutions from (21) by our present elementary methods.

The proof of (22), which is more tedious than profound, consists of examining each of the many special cases satisfying (22) and using arguments similar to (5) or the one applied to (12b). These will not be given since they are fairly straightforward. One effect of the last two terms of (21) is to produce unbounded solutions even if $\Gamma = 0 = \Delta\omega$ [compare with (12)]. Indeed, if $\Delta\omega = 0$, one can obtain from (21)

$$\frac{d}{dt}\ln[A_1A_2A_3 \sin(\theta + \phi_k)] \geq \Gamma + 2[\sin(\phi_k - \phi_{k'}) \times \sin(\phi_k - \phi_{k''})]^{1/2}A_k \quad (23)$$

for those $k$'s satisfying (22), and for those initial states for which $\sin(\theta + \phi_k) > 0$ (see Sec. 4 for an analogous analysis). This proves that there are unbounded solutions even if $\Gamma = 0$. Moreover, (23) strongly suggests[3] that these unbounded solutions will also be singular, but unfortunately no proof of this has yet been found. However, in the case of two coupled modes it is fairly easy to prove that some solutions have singularities if $\Delta\omega = 0$ (Sec. 4).

## 4. TWO MODE EQUATIONS

Another system of equations, which is not frequently considered despite its physical importance, involves the coupling of only two modes (e.g., an unstable mode and its harmonic). In this case the equations have the form

$$\dot{x}_1 = \alpha_1x_1 + \beta_1x_2x_1^*, \qquad \dot{x}_2 = \alpha_2x_2 + \beta_2^*x_1^2, \quad (24)$$

where normally one would be interested in the case $\gamma_1 > 0$. If the $\beta_k$ are of the form (3), one can again obtain (4) and hence the results (6) (with $j = 1$, $k = 2$). Moreover, in place of (10), one now obtains

$$\frac{d}{dt}\left(A_1^2A_2 \sin\theta - \frac{\Delta\omega}{2\rho_k}A_k^2\right) = \Gamma A_1^2 \sin\theta - 2\gamma_k\left(\frac{\Delta\omega}{2\rho_k}\right)A_k^2, \quad (25)$$

where now $\theta = \theta_2 - 2\theta_1 + \phi$, $\Delta\omega = \omega_2 - 2\omega_1$, and $\Gamma = 2\gamma_1 + \gamma_2$. With these revised definitions the results (12) again follow. Thus when (3) holds, the proofs of unbounded solutions are very similar.

However, in the more general case when (14) applies, it is no longer possible to obtain an equation analogous to (16). On the other hand, the equation analogous to (21) is somewhat simpler. Using the variables introduced in Sec. 3, one can obtain from (24)

$$\frac{d}{dt}\left(A_1^2A_2\sin(\theta+\phi_k) - \frac{\Delta\omega}{2V}A_k^2\right) = \Gamma A_1^2A_2\sin(\theta+\phi_k) - 2\gamma_k\left(\frac{\Delta\omega}{2V}\right)A_k^2 + kVA_k^{(6-2k)}A_{k'}^{2(k-1)}\sin(\phi_k-\phi_{k'}), \tag{26}$$

where $k' \neq k$, $V = (\rho_1^2\rho_2)^{1/2}$, $\theta = \theta_2 - 2\theta_1$, and $(\Delta\omega, \Gamma)$ are defined as in (25). The most general sufficient condition obtained from (26) is, in analogy with (22):

> Eq. (24) has unbounded solutions if, for some $k$, $(\Gamma - 2\gamma_k)\Delta\omega\sin(\phi_k - \phi_{k'}) \geq 0$ and $\Gamma \geq 0$, (27)

where again the signs of $\Delta\omega$ and $(\Gamma - 2\gamma_k)$ enter.

The new feature which arises in the present case is that one can prove the following result concerning the existence of solutions which are singular ("explosive").

> If $\Delta\omega = 0$ and $\Gamma \geq 0$, then there are solutions of (24), with arbitrarily small $|x_k(0)| > 0$, which have movable singularities.[5] (28)

That is, there are solutions which become infinite at finite $t$, the value of which depends on the initial conditions.

To prove this, subtract Eq. (26) with $k = 1$ from the one with $k = 2$ ($\Delta\omega = 0$). One readily obtains

$$\frac{d}{dt}(A_1^2A_2\cos\theta') = \Gamma A_1^2A_2\cos\theta' + V(2A_1^2A_2^2 + A_1^4)\times\cos\tfrac{1}{2}(\phi_2-\phi_1),$$

where $\theta' = \theta + \frac{1}{2}(\phi_1 + \phi_2)$. Assume that $\cos\frac{1}{2}(\phi_2 - \phi_1) > 0$ (if negative, then multiply by minus one, and replace $\cos\theta'$ by $-\cos\theta'$ in all that follows), and note that $2A_1^2A_2^2 + A_1^4 \geq (A_1^2A_2)^{4/3}$. Then

$$\frac{d}{dt}(A_1^2A_2\cos\theta') \geq \Gamma A_1^2A_2\cos\theta' + V(A_1^2A_2)^{4/3}\cos\tfrac{1}{2}(\phi_2-\phi_1)\cos\theta'.$$

We consider those initial states for which $\cos\theta'(0) > 0$, then for all $t \geq 0$ for which $|A_1^2A_2| < \infty$; the last equation implies that $\cos\theta'(t) > 0$. Dividing by $A_1^2A_2\cos\theta'$ and integrating yields

$$\ln(A_1^2A_2) \geq \ln(A_1^2A_2\cos\theta') \geq 3a + \Gamma t + V\cos\tfrac{1}{2}(\phi_2-\phi_1)\int_0^t (A_1^2A_2)^{1/3}dt',$$

where the constant $a$ is related to the initial conditions. We now neglect ($\Gamma \geq 0$) and write this in the form

$$\ln F \geq a + b\int_0^t F(t')dt',$$

where $a = \frac{1}{3}V\cos\frac{1}{2}(\phi_2 - \phi_1)$. The function $G(t) = [e^{-c} - bt]^{-1}$ satisfies the equation

$$\ln G = c + b\int_0^t G(t')dt'.$$

Subtracting this from the last equation yields

$$\ln(F/G) \geq a - c + b\int_0^t [F(t') - G(t)dt',$$

and choosing $c$ such that $a - c > 0$ proves that $F(t) \geq G(t)$ for all $t > 0$ such that $|F(t)| < \infty$. Thus $A_1^2A_2$ has a singularity which is not less than $[t_0 - t]^{-3}$, for these initial states. The above analysis is easily generalized (by retaining $\Gamma t$) to show that if the initial states satisfy $V|\cos\frac{1}{2}(\phi_2 - \phi_1)|(A_1^2A_2)^{1/3} + \Gamma > 0$, then there are solutions which are singular (even if $\Gamma < 0$). In other words, for finite initial states there are singular solutions if $\Gamma$ is not negative too.

## 5. CONCLUSION

It has been shown that under a number of conditions the solutions of (1) and (24), in which one linear mode is unstable, are unbounded. In certain cases it was possible to show that the unbounded solutions are not more rapid than exponential, whereas in other cases they have movable singularities.[5] The fact that the mode coupling does not produce bounded solutions under more general conditions is undoubtedly due to the particular form of the couplings which appear in these equations. This convolution form of coupling, with its off-diagonal character, allows for a number of possible "leaks" in the phase plan $(x_1, x_1^*, \cdots)$. Indeed, only the last two cases in (17) give any assurance that there are cases for which (1) [but not (24)] has only bounded solutions, and these do not refer to the situation where some $\gamma_k > 0$. What would be of greater physical interest are the properties of the solutions of systems with the combined couplings in both (1) and (24). Clearly more sophisticated methods of analysis must be developed before these interesting questions can be answered.

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1 A great deal of literature concerning mode coupling has been published. See, e.g., V. N. Tsytovich, *Nonlinear Effects in Plasma* (Plenum, New York, 1970); R. Z. Sagdeev and A. A. Galeev, *Nonlinear Plasma Theory* (Benjamin, New York, 1969); A. S. Bakai, Nuclear Fusion **10**, 53 (1970). Instabilities induced by nonlinear mode coupling of definite phases have been studied by R. C. Davidson and A. N. Kaufman, J. Plasma Phys. **3**, 97 (1968); F. Engelmann and H. Wilhelmsson, Z. Naturforsch. **24a**, 206 (1969); A. Jarmen, L. Stenflo, and H. Wilhelmsson, Phys. Letters **29A**, 217 (1969).

2 Instabilities induced by nonlinear mode coupling, assuming random phases, have also been extensively studied. See, e.g., R. E. Aamodt and M. L. Sloan, Phys. Letters **19**, 1227 (1967); Phys. Fluids 11, 2218 (1968). M. N. Rosenbluth, B. Coppi, and R. N. Sudan, Plasma Phys. Controlled Nucl. Fusion Res. 1, 771 (1968); Ann. Phys. (N.Y.) 55, 207, 248 (1969).

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# Study of Differential Equations of Physics in the Hardy-Lebesgue Space

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The problem of polynomial solutions of differential equations which are of interest in physics is studied by the Hardy–Lebesgue space technique.

## INTRODUCTION

The Hardy–Lebesgue space $\mathcal{H}_2(D)$ which is a Hilbert space consisting of analytic functions in the unit disc $D$ of the complex plane is particularly suitable for the study of the problem of "polynomial solutions" of differential equations. Such solutions have led to the classical orthogonal polynomials which are of particular interest in physics.

In a recent paper[1] one of us (E.K.I.) has presented a uniform technique for the study of differential and difference equations in the Hardy–Lebesgue space. The approach is based on the representation of the Hardy–Lebesgue space by means of the unilateral shift operator and the reduction of the problem of solution of differential and difference equations in $\mathcal{H}_2(D)$ to a perturbation problem of nonself-adjoint operators in an abstract separable Hilbert space $\mathcal{H}$.

In the present work we extend this approach to the study of differential equations of physics and examine the conditions under which these equations have polynomial solutions.

## I. THE REPRESENTATION OF THE HARDY–LEBESGUE SPACE BY MEANS OF THE SHIFT OPERATOR

Denote by $\mathcal{H}$ an abstract separable Hilbert space over the complex field, by $\mathcal{H}_2(D)$ the Hardy–Lebesgue space consisting of all analytic functions $f(z) = \sum_{n=1}^{\infty} \overline{\alpha(n)} z^{n-1}$, $|z| < 1$ with the additional property $\sum_{n=1}^{\infty} |\alpha(n)|^2 < \infty$, by $\{e_n\}_{n=1}^{\infty}$ an orthonormal basis in $\mathcal{H}$ and by $V$ the unilateral shift operator ($V : Ve_n = e_{n+1}$). We can easily see that the following statements hold[1,2]:

(1) Every value $z$ in the unit disc ($|z| < 1$) is an eigenvalue of $V^*$, the adjoint of $V$, and the set of eigenelements $f_z = \sum_{n=1}^{\infty} z^{n-1} e_n$ forms a complete system in $\mathcal{H}$, in the sense that if $f$ is orthogonal to $f_z$ for every $z : |z| < 1$, then $f = 0$.

(2) The mapping $f(z) = (f_z, f), f \in \mathcal{H}$ is an isomorphism from $\mathcal{H}$ onto $\mathcal{H}_2(D)$.

(3) If $C_0$ is the diagonal operator, $C_0 : C_0 e_n = n e_n$, $n = 1, 2 \cdots$, and $f(z) = (f_z, f)$, then

$$zf(z) = (f_z, Vf), \tag{1}$$

$$f'(z) = (f_z, C_0 V^* f), \tag{2}$$

$$f''(z) = (f_z, (C_0 V^*)^2 f), \tag{3}$$

$$f^{(n)}(z) = (f_z, (C_0 V^*)^n f), \tag{4}$$

$$zf'(z) = (f_z, (C_0 - I) f), \tag{5}$$

$$z^2 f''(z) = (f_z, (C_0 - I)(C_0 - 2I) f), \tag{6}$$

$$z^n f^{(n)}(z) = (f_z, (C_0 - I)(C_0 - 2I) \cdots (C_0 - nI) f), \tag{7}$$

$$zf''(z) = (zf'(z))' - f' = (f_z, (C_0 V^* C_0 - 2C_0 V^*) f), \tag{8}$$

$$z^2 f'''(z) = (z^2 f''(z))' - 2zf''(z) = (f_z, (C_0 V^* C_0^2 - 5C_0 V^* C_0 + 6C_0 V^*) f), \tag{9}$$

$$zf'''(z) = (zf''(z))' - f''(z) = (f_z, (C_0 V^* C_0 V^* C_0 - 3C_0 V^* C_0 V^*) f) \text{ etc.} \tag{10}$$

## II. DIFFERENTIAL EQUATIONS WITH POLYNOMIAL SOLUTIONS

Consider the general differential equation leading to the classical orthogonal polynomials

$$(a + a_0 z + \beta z^2) f''(z) + (\mu + \gamma z) f'(z) + bf(z) = 0. \tag{11}$$

Due to (2), (3), (5), (6), and (8) the corresponding operator[1] in $\mathcal{H}$ is

$$T = a(C_0 V^*)^2 + \mu C_0 V^* + a_0 (C_0 V^* C_0 - 2C_0 V^*) + \beta (C_0 - I)(C_0 - 2I) + \gamma (C_0 - I)$$

or in virtue of $[V^*, C_0]_- = V^*$:

$$T = aC_0(C_0 + I) V^{*2} + [a_0 C_0 (C_0 + I) + (\mu - 2a_0) C_0] V^* + \beta (C_0 - I)(C_0 + 2I) + \gamma (C_0 - I). \tag{12}$$

This operator is of the general form

$$T_2 = A_2 V^{*2} + A_1 V^* + A_0, \tag{13}$$

where $A_i$, $i = 0, 1, 2$, are diagonal operators $A_i : A_i e_n = \alpha_i(n) e_n$, $i = 0, 1, 2$, $n = 1, 2, \cdots$.

The operator (13) leaves, obviously, invariant every finite-dimensional subspace $\mathcal{H}_n$, spanned by the elements $\{e_1, e_2, \ldots, e_n\}$. $T_2$ has, therefore, restricted in the subspace $\mathcal{H}_n$, a nonempty purely point spectrum.

*Proposition 1:* The eigenvalues of $T_2$ restricted on the subspace $\mathcal{H}_n$ are precisely the values $\alpha_0(m)$, $m = 1, 2, \ldots, n$.

*Proof:* Let

$$T_2 f = \lambda f \tag{14}$$

with $\lambda \neq \alpha_0(m)$, $m = 1, 2, \ldots, n$ and $f \in \mathcal{H}_n$. Then scalar multiplication of (14) by $e_n$ gives $(f, e_n) = 0$; consequently, scalar multiplication by $e_{n-1}$ gives $(f, e_{n-1}) = 0$ etc, i.e., $f = 0$. Hence $\lambda \subseteq \alpha_0(m)$, $m = 1, 2, \ldots, n$. Conversely, given an $\alpha_0(m)$, $m \leq n$, it is possible to determine the coefficients $x_1, x_2, \ldots, x_m$ of the element $f = \sum_{i=1}^{m} x_i e_i$, where $x_i, i = 1, 2, \ldots, m$ not all zero in such a way that (14) is satisfied for $\lambda = \alpha_0(m)$. In fact, for $\lambda = \alpha_0(m)$ we are led to a linear homogeneous system of $m - 1$ equations with $m$ unknowns. We can normalize $f$ by taking $x_m = 1$ and determine recursively the other components. Of course, without loss of generality we assume that $\alpha_0(i) \neq \alpha_0(m)$, $i < m$ because if $\alpha_0(i) = \alpha_0(m)$ for $i < m$ then instead of $\lambda = \alpha_0(m)$, we consider $\lambda = \alpha_0(i)$ and instead

of the element $\sum_{j=1}^{m} x_j e_j$, the element $\sum_{j=1}^{i} x_j e_j$.

Proposition 1 holds in general for every operator $T_k$ of the form $T = A_k V^{*k} + A_{k-1} V^{*k-1} + \cdots + A_1 V^* + A_0$. It also holds for the operator

$$T_1 = A_1 V^* + A_0, \tag{15}$$

which is of particular interest.

*Remark:* In Ref. 1 the typical example of the ordinary Schrödinger equation for a class of meromorphic potentials of the form $U(z) = a_n z^{-n} + \cdots + a_2 z^{-2} + a_1 z^{-1} + w(z)$ was studied, where $w(z) \in \mathcal{K}_2(\bar{D})$ i.e., $w(z)f(z) \in \mathcal{K}_2(D)$ for every $f(z) \in \mathcal{K}_2(D)$.

The condition $w(z)f(z) \in \mathcal{K}_2(D)$ for every $f(z) \in \mathcal{K}_2(D)$ was used for the boundedness of the operator $W(V)$.

For $a_i = 0$, $i = 3, 4, \ldots, n$ it has been proven that the Schrödinger equation has solutions in $\mathcal{K}_2(D)$ for $a_2 \subseteq \alpha(n) = (n-1)(n-2), n = 1, 2, \cdots$. However, Proposition 4 of Ref. 1, which refers to a counter example for the exclusion of the case

$$a_2 = \alpha(n), \quad n = 1, 2, \cdots, \tag{16}$$

for some $n$, is false. Obviously, the element $f = \frac{1}{2}e_2 + e_3$ is an eigenelement of $T = A + V^* - \frac{1}{2}V^{*2}$ [operator (12) of Ref. 1]; with eigenvalue $\alpha(3) = 2$. This is also an eigenvalue of $T = A + V - \frac{1}{2}V^2$. According to Proposition 1, which can be easily generalized, and due to the fact that $Sp(T) = \overline{Sp(T^*)}$, (16) always holds.

*Proposition 2:* For the operator (15) restricted on the subspace $\mathcal{K}_n$ if one of the values $\alpha_1(n)$ vanishes, say $\alpha_1(k) = 0$, then the eigenvalues are also the values $\alpha_0(m)$; but the corresponding eigenelements for $m > k$ have the form

$$f = \sum_{i=k+1}^{m} x_i e_i, \quad x_i \neq 0.$$

The proof is similar to that of Proposition 1.

*Proposition 3:* For $A_0 = 0$ the only possible eigenvalue of $T_k$, restricted on the subspace $\mathcal{K}_n$ is the point zero.

*Proof:* Let $\lambda \neq 0$ be an eigenvalue of $T_k$ with the eigenelement $f \neq 0$. Then scalar multiplication of the eigenequation by $e_n, e_{n-1}, \cdots$ leads to $f = 0$ which contradicts the hypothesis.

The above propositions cover the cases of hypergeometric equations and the equations leading to the Bessel, Laguerre, Hermite, Legendre, Gegenbauer, and Jacobi polynomials.

## III. APPLICATIONS

### A. The Hypergeometric Equation $z(1-z)f''(z) + [\gamma - (a+\beta+1)z]f'(z) - a\beta f(z) = 0$

The corresponding operator is of the form (15) where $A_1 = C_0(C_0 - I + \gamma)$, $A_0 = -(C_0 - I)(C_0 - 2I) - (a+\beta+1)(C_0 - I)$ and $\lambda = a\beta$ are the eigenvalues. Hence

$$\alpha_0(n) = -(n-1)(n-2) - (a+\beta+1)(n-1),$$
$$\alpha_1(n) = n(n-1+\gamma).$$

According to Proposition 1 for $\alpha_1(n) \neq 0$, $n = 1, 2, \cdots$ i.e., $\gamma \neq -n, n = 0, 1, 2, \ldots$, we have polynomial solutions if and only if

$$a\beta = -(n-1)(n-2) - (a+\beta+1)(n-1), \quad n = 1, 2, \ldots,$$

or

$$a\beta = -n(a+\beta+n), \quad n = 0, 1, 2, \cdots,$$

or

$$\beta(a+n) = -n(a+n), \text{ i.e., if and only if}$$

either

$$a = -n, \ n = 0, 1, 2, \cdots, \quad \text{or } \beta = -n, \ n = 0, 1, 2, \cdots.$$

In the case that $\gamma$ = negative integer or zero, it follows from Proposition 2 that we again have polynomial solutions if $a$ or $\beta = -n$, $n = 0, 1, 2, \cdots$.

The polynomials in this case [$\gamma = -m, \alpha_1(m+1) = 0$, $m < n$] are of the form

$$f(z) = \sum_{i=m+1}^{n} C_{i+1} z^i.$$

### B. The Kummer-Laplace (Confluent Hypergeometric) Equation $zf''(z) + (a+1-z)f'(z) + bf(z) = 0$

In this particular case we have from (2), (5), and (8)

$$T_1 = C_0(C_0 + aI)V^* - (C_0 - I).$$

Hence

$$A_1 = C_0(C_0 + aI), \quad A_0 = -(C_0 - I),$$

and

$$\alpha_1(n) = n(n+a), \quad \alpha_0(n) = -(n-1).$$

Thus, for $a \neq -n, n = 1, 2, \ldots$, we have polynomial solutions if and only if $b = n-1$, $n = 1, 2, \cdots$, or $b = n$, $n = 0, 1, 2, \cdots$. These solutions are the well-known generalized Laguerre polynomials $L_n^{\alpha}(z)$.

If $\alpha_1(k) = k(k+a) = 0$, i.e., $a = -k$, then $e_{k+1}$ is an eigenelement of $T_1$ with eigenvalue $b = k$ and the corresponding to $n = k+1$ solution is of the form $f(z) = cz^k$.

### C. The $S$-Wave Schrödinger Equation

Consider the equation

$$f''(z) + \frac{d}{z} f(z) = 0, \quad d \neq 0,$$

i.e., the $S$-wave Schrödinger equation for Coulomb potential at zero energy. From (8) we have

$$T_1 = C_0(C_0 - I)V^*$$

and $\lambda = -d \neq 0$. From Proposition 3 it follows that the above equation for $d \neq 0$ does not accept a polynomial solution.

### D. The Bessel Polynomials

These orthogonal polynomials were encountered by Burchnall and Chaundy[3] and studied by Krall and Frink[4] and Burchnall.[5] They are related to the Hankel functions of imaginary argument. The differential equation is

$$z^2 f''(z) + (az + a_1) f'(z) + bf(z) = 0.$$

In that case from (2), (5), and (6) we have

$$T_1 = a_1 C_0 V^* + (C_0 - I)(C_0 + aI - 2I).$$

For $a_1 \neq 0$ we have polynomial solutions if and only if $b = -n(a+n-1), n = 0,1,2,\cdots$. These are the Bessel polynomials. In the special case $z^2 f''(z) + (2z+2)f'(z) + bf(z) = 0$ considered also by Krall and Frink in connection with certain solutions of the wave equation we have $a = a_1 = 2$ and $b = -n(n+1)$, $n = 0,1,2,\cdots$. For $a_1 = 0$ the operator $T_1$ is diagonal with eigenelements the basis $\{e_n\}_1^\infty$, i.e., the solutions in this case are the polynomials $z^n, n = 0,1,2,\cdots$.

### E. The Hermite Polynomials

In the $\{q\}$ representation the equation of the one-dimensional harmonic oscillator is[6]

$$f''(z) - 2zf'(z) + bf(z) = 0.$$

The corresponding operator is

$$T_2 = C_0(C_0 + I)V^{*2} - 2(C_0 - I).$$

Here $\alpha_2(n) = n(n+1) \neq 0$ for $n = 1,2,\cdots$. From Proposition 1 it follows that the above equation has polynomial solutions if and only if $b = 2(n-1), n = 1, 2,\cdots$ or $b = 2n$, $n = 0,1,2,\cdots$. These are the well-known Hermite polynomials.

### F. The Legendre Polynomials

Consider the equation

$$(1 - z^2)f''(z) - 2zf'(z) + bf(z) = 0.$$

In this case we have

$$T_2 = C_0(C_0 + I)V^{*2} - (C_0 - I)^2,$$

where $\alpha_2(n) = n(n+1) \neq 0$ for $n = 1,2,\cdots$. We have polynomial solutions if and only if $b = (n-1)^2$, $n = 1,2,\cdots$ or $b = n^2$, $n = 0,1,2,\cdots$. These are the well-known Legendre spherical polynomials.

### G. The Gegenbauer Polynomials

Consider the equation

$$(1 - z^2)f''(z) - (2a+1)zf'(z) + bf(z) = 0;$$

we have

$$T_2 = C_0(C_0 + I)V^{*2} - (C_0 - I)(C_0 + 2aI - I).$$

Here again $\alpha_2(n) = n(n+1) \neq 0$ for $n = 1,2,\cdots$. We have polynomial solutions if and only if $b = n(n+2a)$, $n = 0,1,2,\cdots$. These are the so-called Gegenbauer or ultraspherical polynomials.

### H. The Chebyshev Polynomials

Consider the equation

$$(1 - z^2)f''(z) - zf'(z) + bf(z) = 0.$$

In that case

$$T_2 = C_0(C_0 + I)V^{*2} - (C_0 - I)^2.$$

We obtain the so-called Chebyshev polynomials if and only if $b = n^2$, $n = 0,1,2,\cdots$.

Note that in examples E–H, $A_1 = 0$. This means that $\alpha_1(n) = 0$, $\forall n$ and we are led to even or odd polynomials.

### I. The Jacobi or Hypergeometric Polynomials

For the hypergeometric differential equation

$$(1 - z^2)f''(z) + [\beta_1 - a_1 - (a_1 + \beta_1 + 2)z]f'(z) + bf(z) = 0,$$

we have

$$T_2 = C_0(C_0 + I)V^{*2} + (\beta_1 - a_1)C_0 V^* - (C_0 - I)(C_0 + a_1 + \beta_1).$$

Proposition 1 holds for both cases $\beta_1 - a_1 \neq 0$ or $\beta_1 - a_1 = 0$. Thus, we obtain polynomial solutions if and only if $b = n(a_1 + \beta_1 + n + 1), n = 0,1,2,\cdots$. These polynomials are the well-known Jacobi or hypergeometric polynomials.

## IV. GENERALIZATION

Consider the $n$-order differential equation

$$[P_{n-1}(z) + a_n z_n]y^{(n)} + [P_{n-2}(z) + a_{n-1}z^{n-1}]y^{(n-1)} + \cdots + [P_0(z) + a_1 z]y' + by = 0, \quad (17)$$

where $P_n$ are polynomials of degree $n$.

Denote by $\Omega$ the operator in $\mathcal{K}$, which corresponds to the above differential operator in $\mathcal{K}_2(D)$ and by $Op(\Omega)$ the diagonal operator, which corresponds to the Euler-type part $a_n z^n y^{(n)} + a_{n-1}z^{n-1}y^{(n-1)} + \cdots a_1 z y'$. Then according to the generalization of the Proposition 1 we conclude that the necessary and sufficient condition for Eq. (17) to have a polynomial solution is

$$-b = \text{spectrum of } Op(\Omega).$$

$Op(\Omega)$ is given by (5)–(7).

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# Contributions to the Theory of Multiplicative Stochastic Processes

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The theory of multiplicative stochastic processes is contrasted with the theory of additive stochastic processes. The case of multiplicative factors which are purely random, Gaussian, stochastic processes is treated in detail. In a spirit originally introduced by theoretical work in nuclear magnetic resonance and greatly extended by Kubo, dissipative behavior is demonstrated, on the average, for dynamical equations which do not show dissipative behavior without averaging. It is suggested that multiplicative stochastic processes lead to a conceptual foundation for nonequilibrium thermodynamics and nonequilibrium statistical mechanics, of marked generality.

## 1. INTRODUCTION

The purpose of this paper is to present results in the theory of "multiplicative stochastic processes." The physical applications of this theory will be presented in a sequel to this paper.

Effective use of stochastic processes in physics was first achieved in the theory of Brownian motion.[1] The basic ideas were generalized by Onsager and Machlup in their theory of fluctuations and irreversible processes.[2] Further generalizations, which resulted in a general stochastic theory for the linear dynamical behavior of classical thermodynamical systems, close to but not yet in full equilibrium, were presented by Fox and Uhlenbeck.[3,4] The theory of Fox and Uhlenbeck includes the Langevin theory of Brownian motion and the Onsager and Machlup theory for irreversible processes as special cases. In addition, it includes the linearized fluctuating hydrodynamical equations of Landau and Lifshitz[5] and the linearized fluctuating Boltzmann equation as special cases.

In each of these special cases, and in the general theory, the mathematical description used involves either linear partial integro-differential equations or linear matrix equations which are inhomogeneous. The inhomogeneity is the stochastic "driving force" of the process. Consequently, we shall refer to these processes as "additive stochastic processes." The processes to be presented in this paper will be seen to involve homogeneous equations in which the stochastic "driving force" enters in a multiplicative way. These processes will, consequently, be called "multiplicative stochastic processes."

Multiplicative stochastic processes arise in a natural way in the field of nuclear magnetic resonance. The nature and history of this development may be found in a paper by Redfield.[6] Major generalizations of these ideas for other areas of physics have been presented by Kubo.[7-9] Kubo has also pursued the mathematical foundations for a theory of multiplicative stochastic processes in his work. The special attention paid to purely random, Gaussian, stochastic processes in this paper will serve to further clarify and support the spirit of Kubo's earlier work.

## 2. MATHEMATICAL PRELIMINARIES

The fundamental stochastic process to be considered here is the purely random, stationary, Gaussian process.[10] Let $\tilde{\varphi}(t)$ denote such a process. Processes with an average value of zero will be considered throughout. This is denoted by

$$\langle\tilde{\varphi}(t)\rangle = 0. \tag{1}$$

The mean square correlation is given by

$$\langle\tilde{\varphi}(t)\,\tilde{\varphi}(s)\rangle = 2\lambda\delta(t-s), \tag{2}$$

where $\lambda$ is a constant. The purely random quality of the process is reflected in the presence of $\delta(t-s)$. The dependence upon time differences only, in (2), reflects the condition of stationarity. The Gaussian property may be introduced in terms of the higher order averaged products. All odd order averaged products are zero:

$$\langle\tilde{\varphi}(t_1)\cdots\tilde{\varphi}(t_{2n-1})\rangle = 0, \quad n = 1, 2, \cdots. \tag{3}$$

All even order averaged products are given by

$$\langle\tilde{\varphi}(t_1)\cdots\tilde{\varphi}(t_{2n})\rangle = \frac{1}{2^n n!}\sum_{p\in S_{2n}}\prod_{j=1}^{n}\langle\tilde{\varphi}(t_{p(2j)})\tilde{\varphi}(t_{p(2j-1)})\rangle$$
$$= \frac{1}{2^n n!}\sum_{p\in S_{2n}} 2^n\lambda^n\prod_{j=1}^{n}\delta(t_{p(2j)} - t_{p(2j-1)}). \tag{4}$$

$\sum_{p\in S_{2n}}$ denotes the sum over all permutations $p$ of the symmetric group of order $(2n)!$, $S_{2n}$. Because the two orders of the arguments of a delta function give the same value and because each arrangement of factors in a product of delta functions gives the same value, each distinct term in (4) is $(2^n n!)$-fold redundant. Since $S_{2n}$ is of order $(2n)!$ the expression in (4) has $[(2n)!/2^n n!] = 1\cdot3\cdot5\cdots(2n-1)$ distinct terms.[11]

## 3. ADDITIVE STOCHASTIC PROCESSES

The prototype for the application of stochastic processes to physical phenomena is found in the theory of Brownian motion.[1,3,10,12,13] The velocity $u(t)$ of a heavy particle with mass $M$ in a fluid which is in thermal equilibrium obeys the Langevin equation

$$M\frac{du(t)}{dt} = -\alpha u(t) + \tilde{F}(t), \tag{5}$$

where $\alpha$ is the dissipative, friction coefficient, and $\tilde{F}(t)$ is a purely random, stationary, Gaussian driving force. It is thought that $\tilde{F}(t)$ corresponds with the true microscopic force on the heavy particle which is produced by a great quantity of collisions in rapid succession, between the heavy particle and the molecules constituting the fluid. From a point of view which considers time on a much longer scale than the scale determined by the time between collisions, the true force may be replaced by $\tilde{F}(t)$. This means that $M/\alpha \gg \tau_c$, where $\tau_c$ measures the microscopic collision correlation time, and $M/\alpha$ measures the relaxation time from the macroscopic viewpoint.

By assuming that $\tilde{F}(t)$ is purely random we have that

$$\langle\tilde{F}(t)\tilde{F}(s)\rangle = 2D\delta(t-s), \tag{6}$$

which means that microscopic collision correlations last effectively "no time" in the macroscopic time scale. In this way, a purely random process is used to describe a situation involving two distinct time scales: a microscopic time scale and a macroscopic

time scale. Because the fluid remains in thermal equilibrium throughout the relaxation process, $\tilde{F}(t)$ is also stationary. The Gaussian property for $\tilde{F}(t)$ may be thought to be a consequence of the central limit theorem of probability theory since $\tilde{F}(t)$ results from the collective effect of large numbers of thermally randomized collisions. Using the equipartition of energy theorem leads one to the Einstein relation

$$D = K_B T\alpha \tag{7}$$

in which $T$ is the temperature, and $K_B$ is Boltzmann's constant. Equation (7) is the prototype of so-called fluctuation-dissipation theorems.[3,4]

Equation (5) is manifestly inhomogeneous and exhibits the "additive" quality of this stochastic process. The process described by (5) is a one-component stationary, Gaussian, Markov process. The generalization to $N$-component stationary, Gaussian, Markov processes has the form[3]

$$\frac{d}{dt}a_i(t) = \sum_j A_{ij}a_j(t) + \sum_j S_{ij}a_j(t) + \tilde{F}_i(t), \tag{8}$$

where $i = 1, 2, \ldots, N$, $A_{ij}$ is an $N \times N$ antisymmetric, real matrix, $S_{ij}$ is an $N \times N$ symmetric, real matrix with nonpositive eigenvalues, and $\tilde{F}_i(t)$ is an $N$-component purely random, stationary, Gaussian "driving force". The analog to (6) is

$$\langle \tilde{F}_i(t)\tilde{F}_j(s)\rangle = 2Q_{ij}\delta(t-s), \tag{9}$$

where $Q_{ij}$ is a symmetric matrix with nonnegative eigenvalues. Corresponding with (7) is the general fluctuation-dissipation theorem

$$Q_{ij} = \tfrac{1}{2}\sum_k (G_{ik}E^{-1}_{kj} + E^{-1}_{ik}G_{jk}), \tag{10}$$

where $G_{ij} = A_{ij} + S_{ij}$, and $E_{ij}$ is the entropy matrix which appears in the second-order formula for the entropy

$$S(t) = S_0 - \tfrac{1}{2}K_B\sum_i\sum_j a_i(t)E_{ij}a_j(t). \tag{11}$$

$E_{ij}$ is symmetric and positive definite. Note that (8) is also manifestly an "additive" stochastic process, with $N$ components. The general physical applicability of (8)–(11) suggests that the interactions generated by a macroscopic system which is fluctuating about its equilibrium state may be characterized as purely random, stationary, Gaussian "forces."

## 4. MULTIPLICATIVE STOCHASTIC PROCESSES

An alternative usage for stochastic processes in the description of nonequilibrium processes is possible. The prototype for this alternative method will be called "frequency fluctuation dissipation." In Kubo's work this is the example of a harmonic oscillator with a randomly modulated frequency.[7]

Consider a harmonic oscillator described by the complex variable $a(t)$. The equation of motion is

$$\frac{d}{dt}a(t) = i\omega_0 a(t), \tag{12}$$

where $i = \sqrt{-1}$, and $\omega_0$ is the frequency of oscillation. The solution is (12), is trivial, and is

$$a(t) = e^{i\omega_0 t}a(0). \tag{13}$$

Suppose that the oscillator is at temperature $T$, so that those physical properties which determine $\omega_0$ exhibit thermal fluctuations. For instance, the length of a pendulum or the spring constant of a Hooke's law spring are such properties. As a consequence, the frequency of the oscillator will fluctuate. We will assume that this frequency fluctuation may be characterized by a purely random, stationary, Gaussian process $\tilde{\varphi}(t)$ with mean value zero. The properties of $\tilde{\varphi}(t)$ are given by (1)–(4). Equation (12) becomes

$$\frac{d}{dt}a(t) = i[\omega_0 + \tilde{\varphi}(t)]a(t). \tag{14}$$

The homogeneity of (14) is manifest, and the "multiplicative" nature of the stochastic process is evident. It will be proved that the average value of (14) is

$$\frac{d}{dt}\langle a(t)\rangle = (i\omega_0 - \lambda)\langle a(t)\rangle. \tag{15}$$

The solution to (15) is clearly a damped oscillation, whereas the solution to (14), without averaging, is oscillatory. This example must be distinguished from an example of damped oscillations which arises from the Brownian motion of a harmonic oscillator.[3]

*Proof of Eq. (15):* The formal solution to (14) is

$$a(t) = e^{i\omega_0 t}\exp\left(i\int_0^t \tilde{\varphi}(s)\,ds\right)a(0). \tag{16}$$

Therefore,

$$\langle a(t)\rangle = e^{i\omega_0 t}\left\langle \exp\, i\left(\int_0^t \tilde{\varphi}(s)\,ds\right)\right\rangle a(0). \tag{17}$$

However,

$$\left\langle \exp\left(i\int_0^t \tilde{\varphi}(s)\,ds\right)\right\rangle = \sum_{n=0}^{\infty}\frac{(i)^n}{n!}\left\langle\left(\int_0^t \tilde{\varphi}(s)\,ds\right)^n\right\rangle. \tag{18}$$

Using (3) gives, for odd $n = 2m-1$,

$$\left\langle\left(\int_0^t \tilde{\varphi}(s)\,ds\right)^n\right\rangle = \int_0^t\cdots\int_0^t \langle\tilde{\varphi}(s_1)\cdots \times \tilde{\varphi}(s_{2m-1})\rangle\, ds_1\cdots ds_{2m-1} = 0. \tag{19}$$

Using (4) gives, for even $n = 2m$,

$$\begin{aligned}
&\left\langle\left(\int_0^t \tilde{\varphi}(s)\,ds\right)^n\right\rangle \\
&= \int_0^t\cdots\int_0^t \langle\tilde{\varphi}(s_1)\cdots\tilde{\varphi}(s_{2m})\rangle\, ds_1\cdots ds_{2m} \\
&= \int_0^t\cdots\int_0^t \frac{1}{2^m m!}\sum_{p\in S_{2m}} 2^m\lambda^m \\
&\quad\times \prod_{j=1}^{m}\delta(s_{p(2j)} - s_{p(2j-1)})\, ds_1\cdots ds_{2m} \\
&= \frac{\lambda^m}{m!}\sum_{p\in S_{2m}}\int_0^t\cdots \\
&\quad\times\int_0^t\prod_{j=1}^{m}\delta(s_{p(2j)} - s_{p(2j-1)})\, ds_1\cdots ds_{2m} \\
&= \frac{\lambda^m}{m!}\sum_{p\in S_{2m}}\left(\int_0^t\int_0^t \delta(s_1 - s_2)\,ds_1 ds_2\right)^m \\
&= \frac{\lambda^m}{m!}(2m)!\,t^m.
\end{aligned} \tag{20}$$

Putting (20) and (19) into (18) gives

$$\left\langle \exp\left( i \int_0^t \tilde{\varphi}(s)\, ds \right) \right\rangle = \sum_{m=0}^{\infty} \frac{(i)^{2m}}{(2m)!} \frac{\lambda^m}{m!} (2m)!\, t^m = \sum_{m=0}^{\infty} \frac{(-\lambda t)^m}{m!} = e^{-\lambda t}. \quad (21)$$

Therefore, putting (21) into (17) gives (15). This completes the proof.

Because of (15), it is clear why (14) is called frequency fluctuation dissipation. This is an example of a one-complex-component situation. There is also an $N$-complex-component generalization for multiplicative stochastic processes. However, it will later be shown that a multicomponent-complex situation is a special case of a multicomponent real variable generalization. Therefore, the multicomponent generalization will be given for the real variable case. The multicomponent case is proved using the purely random character of the stochastic "force" and the Gaussian property of its higher order averages.

Let $a_\alpha(t)$ for $\alpha = 1, 2, \ldots, N$ be an $N$-component real process which satisfies the equation

$$\frac{d}{dt} a_\alpha(t) = \sum_{\alpha'} [A_{\alpha\alpha'} + \tilde{A}_{\alpha\alpha'}(t)]\, a_{\alpha'}(t), \quad (22)$$

where $A_{\alpha\alpha'} = -A_{\alpha'\alpha}$ and $\tilde{A}_{\alpha\alpha'}(t) = -\tilde{A}_{\alpha'\alpha}(t)$. The matrix components of $\tilde{A}_{\alpha\alpha'}(t)$ will be assumed to be purely random, stationary, Gaussian processes with average values of zero, and therefore, we have

$$\langle \tilde{A}_{\alpha\alpha'}(t) \rangle = 0 \quad \text{for all } \alpha \text{ and } \alpha', \quad (23)$$

$$\langle \tilde{A}_{\alpha\beta}(t) \tilde{A}_{\mu\nu}(s) \rangle = 2 Q_{\alpha\beta\mu\nu} \delta(t-s), \quad (24)$$

$$\langle \tilde{A}_{\mu_{2n-1}\nu_{2n-1}}(s_{2n-1}) \cdots A_{\mu_1\nu_1}(s_1) \rangle = 0, \quad (25)$$

$$\begin{aligned} &\langle \tilde{A}_{\mu_{2n}\nu_{2n}}(s_{2n}) \cdots \tilde{A}_{\mu_1\nu_1}(s_1) \rangle \\ &= \frac{1}{2^n n!} \sum_{p \in S_{2n}} \prod_{j=1}^{n} \langle \tilde{A}_{\mu_{p(2j)}\nu_{p(2j)}}(s_{p(2j)}) \\ &\quad \times \tilde{A}_{\mu_{p(2j-1)}\nu_{p(2j-1)}}(s_{p(2j-1)}) \rangle \\ &= \frac{1}{2^n n!} \sum_{p \in S_{2n}} 2^n \prod_{j=1}^{n} Q_{\mu_{p(2j)}\nu_{p(2j)}\mu_{p(2j-1)}\nu_{p(2j-1)}} \\ &\quad \times \delta(s_{p(2j)} - s_{p(2j-1)}). \end{aligned} \quad (26)$$

The average value of (22) is

$$\frac{d}{dt} \langle a_\alpha(t) \rangle = \sum_{\alpha'} A_{\alpha\alpha'} \langle a_{\alpha'}(t) \rangle + \sum_{\alpha'} \sum_{\theta} Q_{\alpha\theta\theta\alpha'} \langle a_{\alpha'}(t) \rangle. \quad (27)$$

This is the generalization of (15).

The proof to (27) is found in the Appendix. Here, we will give a plausibility argument for (27) which is made rigorous by the more lengthy, rigorous, proof in the Appendix. The irreversibility implicit in (27) will be demonstrated following the plausibility argument.

From (22), by averaging, we get

$$\frac{d}{dt} \langle a_\alpha(t) \rangle = \sum_{\alpha'} A_{\alpha\alpha'} \langle a_{\alpha'}(t) \rangle + \sum_{\alpha'} \langle \tilde{A}_{\alpha\alpha'}(t) a_{\alpha'}(t) \rangle. \quad (28)$$

It is the second term on the right-hand side of (28) which needs simplification. Integrating (22) with respect to time between $t - \tau$ and $t$ gives

$$a_\alpha(t) - a_\alpha(t-\tau) = \sum_{\alpha'} A_{\alpha\alpha'} \int_{t-\tau}^{t} a_{\alpha'}(s)\, ds + \sum_{\alpha'} \int_{t-\tau}^{t} \tilde{A}_{\alpha\alpha'}(s) a_{\alpha'}(s)\, ds. \quad (29)$$

Multiplying (29) by $\tilde{A}_{\beta\alpha}(t)$, and summing over $\alpha$ gives, upon averaging the sum,

$$\begin{aligned} &\sum_{\alpha} \langle \tilde{A}_{\beta\alpha}(t) a_\alpha(t) \rangle - \sum_{\alpha} \langle \tilde{A}_{\beta\alpha}(t) a_\alpha(t-\tau) \rangle \\ &= \sum_{\alpha} \sum_{\alpha'} A_{\alpha\alpha'} \int_{t-\tau}^{t} \langle \tilde{A}_{\beta\alpha}(t) a_{\alpha'}(s) \rangle\, ds \\ &\quad + \sum_{\alpha} \sum_{\alpha'} \int_{t-\tau}^{t} \langle \tilde{A}_{\beta\alpha}(t) \tilde{A}_{\alpha\alpha'}(s) a_{\alpha'}(s) \rangle\, ds. \end{aligned} \quad (30)$$

Now, it seems plausible that because of (24) and (26) that

$$\langle \tilde{A}_{\beta\alpha}(t) a_\alpha(t-\tau) \rangle = 0 \quad (31)$$

and

$$\int_{t-\tau}^{t} \langle \tilde{A}_{\beta\alpha}(t) a_{\alpha'}(s) \rangle\, ds = 0. \quad (32)$$

Using (31) and (32) in (30) will give

$$\sum_{\alpha} \langle \tilde{A}_{\beta\alpha}(t) a_\alpha(t) \rangle = \sum_{\alpha} \sum_{\alpha'} \int_{t-\tau}^{t} \langle \tilde{A}_{\beta\alpha}(t) \tilde{A}_{\alpha\alpha'}(s) a_{\alpha'}(s) \rangle\, ds. \quad (33)$$

Using the Gaussian property of $\tilde{A}_{\mu\nu}(t)$ and (23) makes it plausible that

$$\sum_{\alpha} \sum_{\alpha'} \int_{t-\tau}^{t} \langle \tilde{A}_{\beta\alpha}(t) \tilde{A}_{\alpha\alpha'}(s) a_{\alpha'}(s) \rangle\, ds = \sum_{\alpha} \sum_{\alpha'} \int_{t-\tau}^{t} \langle \tilde{A}_{\beta\alpha}(t) \tilde{A}_{\alpha\alpha'}(s) \rangle \langle a_{\alpha'}(s) \rangle\, ds. \quad (34)$$

For the right-hand side of (34) we use (24) and get

$$\begin{aligned} &\sum_{\alpha} \sum_{\alpha'} \int_{t-\tau}^{t} \langle \tilde{A}_{\beta\alpha}(t) \tilde{A}_{\alpha\alpha'}(s) \rangle \langle a_{\alpha'}(s) \rangle\, ds \\ &= \sum_{\alpha} \sum_{\alpha'} \int_{t-\tau}^{t} 2 Q_{\beta\alpha\alpha\alpha'} \delta(t-s) \langle a_{\alpha'}(s) \rangle\, ds \\ &= \sum_{\alpha} \sum_{\alpha'} Q_{\beta\alpha\alpha\alpha'} \langle a_{\alpha'}(t) \rangle. \end{aligned} \quad (35)$$

Putting (35) with (34) into (33) gives

$$\sum_{\alpha} \langle \tilde{A}_{\beta\alpha}(t) a_\alpha(t) \rangle = \sum_{\alpha'} \sum_{\alpha} Q_{\beta\alpha\alpha\alpha'} \langle a_{\alpha'}(t) \rangle. \quad (36)$$

Returning to (28) with (36) gives (27), if we simply rename indices. This plausibility argument depends upon the truth of (31), (32), and (34). In the Appendix it is shown that the result obtained in (27) is rigorously achieved.

## 5. IRREVERSIBILITY

The irreversibility in (15) is obvious. That of (27) is less easily seen. To see that irreversibility arises from averaging, we will consider both $\sum_\alpha a_\alpha(t) a_\alpha(t)$ and $\sum_\alpha \langle a_\alpha(t) \rangle \langle a_\alpha(t) \rangle$ using both (22) and (27).

Using (22) and the antisymmetry of both $A_{\alpha\alpha'}$ and $\tilde{A}_{\alpha\alpha'}(t)$ gives

$$\frac{d}{dt} \sum_{\alpha} a_\alpha(t) a_\alpha(t) = 2 \sum_{\alpha} \sum_{\alpha'} a_\alpha(t) A_{\alpha\alpha'} a_{\alpha'}(t) + 2 \sum_{\alpha} \sum_{\alpha'} a_\alpha(t) \tilde{A}_{\alpha\alpha'}(t) a_{\alpha'}(t) = 0. \quad (37)$$

Therefore $\sum_\alpha a_\alpha(t)a_\alpha(t)$ is a conserved quantity during the unaveraged time evolution. Using (27) and the antisymmetry of $A_{\alpha\alpha'}$ gives

$$\frac{d}{dt}\sum_\alpha \langle a_\alpha(t)\rangle\langle a_\alpha(t)\rangle = 2\sum_\alpha\sum_{\alpha'}\langle a_\alpha(t)\rangle A_{\alpha\alpha'}\langle a_{\alpha'}(t)\rangle + 2\sum_\alpha\sum_{\alpha'}\sum_\theta \langle a_\alpha(t)\rangle Q_{\alpha\theta\theta\alpha'}\langle a_{\alpha'}(t)\rangle = 2\sum_\alpha\sum_{\alpha'}\sum_\theta \langle a_\alpha(t)\rangle Q_{\alpha\theta\theta\alpha'}\langle a_{\alpha'}(t)\rangle. \tag{38}$$

From (24) it follows that

$$\sum_\theta \langle \tilde{A}_{\alpha\theta}(t)A_{\theta\alpha'}(s)\rangle = 2\sum_\theta Q_{\alpha\theta\theta\alpha'}\delta(t-s). \tag{39}$$

Let $y_\alpha$ be an arbitrary $N$-component vector. Using (39) gives

$$\begin{aligned}\sum_\alpha\sum_{\alpha'}\sum_\theta y_\alpha Q_{\alpha\theta\theta\alpha'}y_{\alpha'} &= \sum_\alpha\sum_{\alpha'}\sum_\theta 2y_\alpha Q_{\alpha\theta\theta\alpha'}y_{\alpha'}\int_0^t\delta(t-s)ds\\ &= \sum_\alpha\sum_{\alpha'}\sum_\theta\int_0^t y_\alpha\langle\tilde{A}_{\alpha\theta}(t)\tilde{A}_{\theta\alpha'}(s)\rangle y_{\alpha'}ds\\ &= -\sum_\theta\int_0^t\left\langle\left(\sum_\alpha\tilde{A}_{\theta\alpha}(t)y_\alpha\right)\left(\sum_{\alpha'}\tilde{A}_{\theta\alpha'}(s)y_{\alpha'}\right)\right\rangle ds\\ &\le 0.\end{aligned} \tag{40}$$

The last equality in (40) follows from the antisymmetry of the matrix $\tilde{A}_{\mu\nu}(t)$, and the inequality follows from the form of the integral. Putting the results expressed by (40) into (38) gives

$$\frac{d}{dt}\sum_\alpha\langle a_\alpha(t)\rangle\langle a_\alpha(t)\rangle = +2\sum_\alpha\sum_{\alpha'}\sum_\theta\langle a_\alpha(t)\rangle \times Q_{\alpha\theta\theta\alpha'}\langle a_{\alpha'}(t)\rangle \le 0. \tag{41}$$

Therefore the quantity $\sum_\alpha\langle a_\alpha(t)\rangle\langle a_\alpha(t)\rangle$ shows a monotonic decrease to its equilibrium value. The inequality in (40) shows that the matrix $\sum_\theta Q_{\alpha\theta\theta\alpha'}$ is a symmetric matrix with nonpositive eigenvalues. If all the eigenvalues of $\sum_\theta Q_{\alpha\theta\theta\alpha'}$ are also nonzero, then the equilibrium state corresponds with $\langle a_\alpha\rangle = 0$ for all $\alpha = 1, 2, \ldots, N$. The possibility of zero value eigenvalues of $\sum_\theta Q_{\alpha\theta\theta\alpha'}$ corresponds with the possibility of certain linear combinations of the $\langle a_\alpha(t)\rangle$'s being conserved quantities during the overall approach to equilibrium. In this case equilibrium is not characterized by $\langle a_\alpha\rangle = 0$ for all $\alpha = 1, 2, \ldots, N$; for some $\alpha$, $\langle a_\alpha\rangle \neq 0$.

## 6. COMPLEX COMPONENT CASE

A problem closely related to the real case just described involves $N$ complex components $C_\alpha(t)$ for $\alpha = 1, 2, \ldots, N$ satisfying the equation

$$i\frac{d}{dt}C_\alpha(t) = \sum_{\alpha'}M_{\alpha\alpha'}C_{\alpha'}(t) + \sum_{\alpha'}\tilde{M}_{\alpha\alpha'}(t)C_{\alpha'}(t). \tag{42}$$

Both $M_{\alpha\alpha'}$ and $\tilde{M}_{\alpha\alpha'}(t)$ are complex Hermitian matrices. Therefore

$$M^*_{\alpha\alpha'} = M_{\alpha'\alpha} \quad \text{and} \quad \tilde{M}^*_{\alpha\alpha'}(t) = \tilde{M}_{\alpha'\alpha}(t). \tag{43}$$

$\tilde{M}_{\alpha\alpha'}(t)$ is also a purely random, stationary, Gaussian process with average zero. This implies, in analogy with (23)–(26) that

$$\langle\tilde{M}_{\alpha\alpha'}(t)\rangle = 0, \tag{44}$$

$$\langle\tilde{M}_{\alpha\beta}(t)\tilde{M}_{\mu\nu}(s)\rangle = 2Q'_{\alpha\beta\mu\nu}\delta(t-s), \tag{45}$$

$$\langle\tilde{M}_{\mu_{2n-1}\nu_{2n-1}}(s_{2n-1})\cdots\tilde{M}_{\mu_1\nu_1}(s_1)\rangle = 0, \tag{46}$$

$$\begin{aligned}&\langle\tilde{M}_{\mu_{2n}\nu_{2n}}(s_{2n})\cdots\tilde{M}_{\mu_1\nu_1}(s_1)\rangle\\ &= \frac{1}{2^n n!}\sum_{p\in S_{2n}}\prod_{j=1}^n\langle\tilde{M}_{\mu_{p(2j)}\nu_{p(2j)}}(s_{p(2j)})\\ &\quad\times\tilde{M}_{\mu_{p(2j-1)}\nu_{p(2j-1)}}(s_{p(2j-1)})\rangle\\ &= \frac{1}{2^n n!}\sum_{p\in S_{2n}}2^n\prod_{j=1}^n Q'_{\mu_{p(2j)}\nu_{p(2j)}\mu_{p(2j-1)}\nu_{p(2j-1)}}\\ &\quad\times\delta(s_{p(2j)}-s_{p(2j-1)}).\end{aligned} \tag{47}$$

It will now be shown that the analog to (27) is

$$\frac{d}{dt}\langle C_\alpha(t)\rangle = -i\sum_{\alpha'}M_{\alpha\alpha'}\langle C_{\alpha'}(t)\rangle - \sum_{\alpha'}\sum_\theta Q'_{\alpha\theta\theta\alpha'}\langle C_{\alpha'}(t)\rangle \tag{48}$$

and that $\sum_\theta Q'_{\alpha\theta\theta\alpha'}$ is Hermitian with nonnegative eigenvalues.

Each complex component $C_\alpha(t)$ may be written as

$$C_\alpha(t) = a_\alpha(t) + ib_\alpha(t), \tag{49}$$

wherein $a_\alpha(t)$ and $b_\alpha(t)$ are both real. $M_{\alpha\alpha'}$ and $\tilde{M}_{\alpha\alpha'}(t)$ may be written as

$$M_{\alpha\alpha'} = S_{\alpha\alpha'} + iA_{\alpha\alpha'}, \tag{50}$$

$$\tilde{M}_{\alpha\alpha'}(t) = \tilde{S}_{\alpha\alpha'}(t) + i\tilde{A}_{\alpha\alpha'}(t), \tag{51}$$

wherein $S_{\alpha\alpha'}, A_{\alpha\alpha'}, \tilde{S}_{\alpha\alpha'}(t)$, and $\tilde{A}_{\alpha\alpha'}(t)$ are defined by

$$S_{\alpha\alpha'} = \tfrac{1}{2}(M_{\alpha\alpha'} + M^*_{\alpha\alpha'}), \tag{52}$$

$$A_{\alpha\alpha'} = -\tfrac{1}{2}(M_{\alpha\alpha'} - M^*_{\alpha\alpha'}), \tag{53}$$

$$\tilde{S}_{\alpha\alpha'}(t) = \tfrac{1}{2}[\tilde{M}_{\alpha\alpha'}(t) + \tilde{M}^*_{\alpha\alpha'}(t)], \tag{54}$$

$$\tilde{A}_{\alpha\alpha'}(t) = -\tfrac{1}{2}[\tilde{M}_{\alpha\alpha'}(t) - \tilde{M}^*_{\alpha\alpha'}(t)]. \tag{55}$$

With (43) it is seen that $S_{\alpha\alpha'}, A_{\alpha\alpha'}, \tilde{S}_{\alpha\alpha'}(t)$, and $\tilde{A}_{\alpha\alpha'}(t)$ are real matrices and that $S_{\alpha\alpha'}$, and $\tilde{S}_{\alpha\alpha'}(t)$ are symmetric, while $A_{\alpha\alpha'}$ and $\tilde{A}_{\alpha\alpha'}(t)$ are antisymmetric. Using (49)–(51), (42) can be rewritten as

$$\frac{d}{dt}\begin{pmatrix}a_\alpha(t)\\ b_\alpha(t)\end{pmatrix} = \sum_{\alpha'=1}\begin{pmatrix}A_{\alpha\alpha'} & S_{\alpha\alpha'}\\ -S_{\alpha\alpha'} & A_{\alpha\alpha'}\end{pmatrix}\begin{pmatrix}a_{\alpha'}(t)\\ b_{\alpha'}(t)\end{pmatrix} + \sum_{\alpha'=1}^N\begin{pmatrix}\tilde{A}_{\alpha\alpha'}(t) & \tilde{S}_{\alpha\alpha'}(t)\\ -\tilde{S}_{\alpha\alpha'}(t) & \tilde{A}_{\alpha\alpha'}(t)\end{pmatrix}\begin{pmatrix}a_{\alpha'}(t)\\ b_{\alpha'}(t)\end{pmatrix}. \tag{56}$$

Note that $\binom{a_\alpha(t)}{b_\alpha(t)}$ is a column vector with $2N$ real-valued components. Denote it by $a'_\beta(t)$, where

$$a'_\beta(t) \equiv a_\beta(t) \text{ for } \beta = 1, 2, \ldots, N \tag{57}$$

and

$$a'_\beta(t) \equiv b_{\beta-N}(t) \quad \text{for } \beta = N+1, N+2, \ldots, 2N.$$

In the same spirit, $A'_{\beta\beta'}$ will denote the antisymmetric matrix

$$\begin{pmatrix} A_{\alpha\alpha'} & S_{\alpha\alpha'} \\ -S_{\alpha\alpha'} & A_{\alpha\alpha'} \end{pmatrix},$$

where

$$A'_{\beta\beta'} \equiv A_{\beta\beta'} \quad \text{for } \beta = 1,2,\ldots,N \text{ and } \beta' = 1,2,\ldots,N,$$
$$A'_{\beta\beta'} \equiv S_{\beta\beta'-N} \quad \text{for } \beta = 1,2,\ldots,N \text{ and } \beta' = N+1, N+2,\ldots,2N,$$
$$A'_{\beta\beta'} \equiv S_{\beta-N\beta'} \quad \text{for } \beta = N+1, N+2,\ldots,2N \text{ and } \beta' = 1,2,\ldots,N,$$

and

$$A'_{\beta\beta'} \equiv A_{\beta-N\beta'-N} \quad \text{for } \beta = N+1, N+2,\ldots,2N \text{ and } \beta' = N+1, N+2,\ldots,2N. \tag{58}$$

In a similar manner, define the $2N \times 2N$ real antisymmetric matrix $\tilde{A}'_{\beta\beta'}(t)$ in terms of $\tilde{S}_{\alpha\alpha'}(t)$ and $\tilde{A}_{\alpha\alpha'}(t)$. With these definitions (56) becomes

$$\frac{d}{dt} a'_\beta(t) = \sum_{\beta'=1}^{2N} A'_{\beta\beta'} a'_{\beta'}(t) + \sum_{\beta'=1}^{2N} \tilde{A}'_{\beta\beta'}(t) a'_{\beta'}(t), \tag{59}$$

which is a special case of (22).

In order to get the analogue of (27) for (59) it is necessary to determine the matrix $\sum_{\theta=1}^{2N} Q''_{\beta\theta\theta\beta'}$ defined by

$$\sum_{\theta=1}^{2N} \langle \tilde{A}'_{\beta\theta}(t) \tilde{A}'_{\theta\beta'}(s) \rangle \equiv 2 \sum_{\theta=1}^{2N} Q''_{\beta\theta\theta\beta'} \delta(t-s). \tag{60}$$

The left-hand side of (60) is computed by using the definition of $\tilde{A}'_{\beta\beta'}(t)$, (54), (55), and (45), in that order. The computation is straightforward and somewhat long. The results are

$$\sum_{\theta=1}^{2N} Q''_{\beta\theta\theta\beta'} = -\frac{1}{2}\left( \sum_{\theta=1}^{N} Q'_{\beta\theta\theta\beta'} + \sum_{\theta=1}^{N} Q'^{*}_{\beta\theta\theta\beta'} \right)$$
$$\text{for } \beta = 1,2,\ldots,N \text{ and } \beta' = 1,2,\ldots,N;$$

$$\sum_{\theta=1}^{2N} Q''_{\beta\theta\theta\beta'} = -\frac{i}{2}\left( \sum_{\theta=1}^{N} Q'_{\beta\theta\theta\beta'-N} - \sum_{\theta=1}^{N} Q'^{*}_{\beta\theta\theta\beta'-N} \right)$$
$$\text{for } \beta = 1,2,\ldots,N \text{ and } \beta' = N+1, N+2,\ldots,2N;$$

$$\sum_{\theta=1}^{2N} Q''_{\beta\theta\theta\beta'} = -\frac{i}{2}\left( \sum_{\theta=1}^{N} Q'_{\beta-N\theta\theta\beta'} - \sum_{\theta=1}^{N} Q'^{*}_{\beta-N\theta\theta\beta'} \right) \tag{61}$$
$$\text{for } \beta = N+1, N+2,\ldots,2N \text{ and } \beta' = 1,2,\ldots,N;$$

$$\sum_{\theta=1}^{2N} Q''_{\beta\theta\theta\beta'} = -\frac{1}{2}\left( \sum_{\theta=1}^{N} Q'_{\beta-N\theta\theta\beta'-N} - \sum_{\theta=1}^{N} Q'^{*}_{\beta-N\theta\theta\beta'-N} \right)$$
$$\text{for } \beta = N+1, N+2,\ldots,2N \text{ and } \beta' = N+1, N+2,\ldots,2N.$$

At this point, the use of (49)–(51) and (61) leads to (48) if one notices that

$$\sum_{\theta=1}^{N} Q'_{\alpha\theta\theta\alpha'} = \frac{1}{2}\left( \sum_{\theta=1}^{N} Q'_{\alpha\theta\theta\alpha'} + \sum_{\theta=1}^{N} Q'^{*}_{\alpha\theta\theta\alpha'} \right) - i\,\frac{i}{2}\left( \sum_{\theta=1}^{N} Q'_{\alpha\theta\theta\alpha'} - \sum_{\theta=1}^{N} Q'^{*}_{\alpha\theta\theta\alpha'} \right), \tag{62}$$

where

$$\frac{1}{2}\left( \sum_{\theta=1}^{N} Q'_{\alpha\theta\theta\alpha'} + \sum_{\theta=1}^{N} Q'^{*}_{\alpha\theta\theta\alpha'} \right)$$

and

$$\frac{i}{2}\left( \sum_{\theta=1}^{N} Q'_{\alpha\theta\theta\alpha'} - \sum_{\theta=1}^{N} Q'^{*}_{\alpha\theta\theta\alpha'} \right)$$

are both real matrices. Therefore, it has been justified that (42) and (48) are a special case of (22) and (27).

Via (45) it is seen that

$$\begin{aligned} &\sum_{\alpha}\sum_{\alpha'}\sum_{\theta} y^*_\alpha Q'_{\alpha\theta\theta\alpha'} y_{\alpha'} \\ &= \sum_{\alpha}\sum_{\alpha'}\sum_{\theta} 2 y^*_\alpha Q'_{\alpha\theta\theta\alpha'} y_{\alpha'} \int_0^t \delta(t-s)\,ds \\ &= \sum_{\alpha}\sum_{\alpha'}\sum_{\theta} \int_0^t y^*_\alpha \langle \tilde{M}_{\alpha\theta}(t) \tilde{M}_{\theta\alpha'}(s) \rangle y_{\alpha'} ds \\ &= \sum_{\theta} \int_0^t \left\langle \left( \sum_{\alpha} \tilde{M}^*_{\theta\alpha}(t) y^*_\alpha \right) \left( \sum_{\alpha'} \tilde{M}_{\theta\alpha'}(s) y_{\alpha'} \right) \right\rangle ds \\ &\geq 0. \end{aligned} \tag{63}$$

Therefore, $\sum_\theta Q'_{\alpha\theta\theta\alpha'}$ has nonnegative eigenvalues, and with (48) it is seen that the quantity $\sum_\alpha \langle C^*_\alpha(t) \rangle \langle C_\alpha(t) \rangle$ shows a monotonic decrease to equilibrium; whereas from (42) it is seen that the quantity $\sum_\alpha C^*_\alpha(t) C_\alpha(t)$ is a time invariant. These results are analogs of (41) and (37), respectively.

## 7. COMPLEX BILINEAR FORMS

Starting with Eq. (42), it is possible to define the matrix $\rho_{\alpha\beta}(t)$ by

$$\rho_{\alpha\beta}(t) \equiv C^*_\alpha(t) C_\beta(t) \tag{64}$$

and to ask what the time dependence equations for $\rho_{\alpha\beta}(t)$ and $\langle \rho_{\alpha\beta}(t) \rangle$ are. One gets from (42)

$$i \frac{d}{dt} \rho_{\alpha\beta}(t) = \sum_{\alpha'}\sum_{\beta'} (L_{\alpha\beta\alpha'\beta'} + \tilde{L}_{\alpha\beta\alpha'\beta'}(t)) \rho_{\alpha'\beta'}(t), \tag{65}$$

wherein $L_{\alpha\beta\alpha'\beta'}$ and $\tilde{L}_{\alpha\beta\alpha'\beta'}(t)$ are defined by

$$L_{\alpha\beta\alpha'\beta'} \equiv \delta_{\alpha\alpha'} M_{\beta\beta'} - \delta_{\beta\beta'} M^*_{\alpha\alpha'}, \tag{66}$$

$$\tilde{L}_{\alpha\beta\alpha'\beta'}(t) \equiv \delta_{\alpha\alpha'} \tilde{M}_{\beta\beta'}(t) - \delta_{\beta\beta'} \tilde{M}^*_{\alpha\alpha'}(t). \tag{67}$$

Note that (43) implies that

$$L^*_{\alpha\beta\alpha'\beta'} = L_{\alpha'\beta'\alpha\beta} \quad \text{and} \quad \tilde{L}^*_{\alpha\beta\alpha'\beta'}(t) = \tilde{L}_{\alpha'\beta'\alpha\beta}(t). \tag{68}$$

Both indices $\alpha$ and $\beta$ range over $1,2,\ldots,N$. Therefore it is possible to think of $\rho_{\alpha\beta}(t)$ as an $N^2$ component "vector," and to think of $L_{\alpha\beta\alpha'\beta'}$ and $\tilde{L}_{\alpha\beta\alpha'\beta'}(t)$ as $N^2 \times N^2$ "matrices." Equation (68) suggests that these two "matrices" are Hermitian. Equation (67) shows that $\tilde{L}_{\alpha\beta\alpha'\beta'}(t)$ is a linear combination of two purely random, stationary, Gaussian processes and is, therefore, itself a purely random, stationary, Gaussian process. Consequently, in this way of viewing (65) it is seen that (65) is a special case of (42), as well as being derived from (42). Therefore, $\langle \rho_{\alpha\beta}(t) \rangle$ will obey an equation which is the analog to (48).

In order to get the equation for $\langle \rho_{\alpha\beta}(t) \rangle$ it is necessary to obtain the analog of $\sum_\theta Q'_{\alpha\theta\theta\alpha'}$ which appears

in (48). Comparing (65) with (42) it is seen that one needs the analog of (45) which is

$$\langle \tilde{L}_{\alpha\beta\alpha'\beta'}(t)\tilde{L}_{\mu\nu\mu'\nu'}(s)\rangle = 2Q'_{\alpha\beta\alpha'\beta'\mu\nu\mu'\nu'}\delta(t-s). \quad (69)$$

In order to explicitly determine $Q'_{\alpha\beta\alpha'\beta'\mu\nu\mu'\nu'}$, one uses (67) and also (45). The exercise of a little algebra yields

$$Q'_{\alpha\beta\alpha'\beta'\mu\nu\mu'\nu'} = \delta_{\alpha\alpha'}\delta_{\mu\mu'}Q'_{\beta\beta'\nu\nu'} + \delta_{\beta\beta'}\delta_{\nu\nu'}Q'^{*}_{\alpha\alpha'\mu\mu'} - \delta_{\alpha\alpha'}\delta_{\nu\nu'}Q'_{\beta\beta'\mu'\mu} - \delta_{\beta\beta'}\delta_{\mu\mu'}Q'_{\alpha'\alpha\nu\nu'}. \quad (70)$$

Therefore, renaming indices leads to the analog of $\sum_\theta Q'_{\alpha\theta\theta\alpha'}$ which is

$$\sum_\theta \sum_{\theta'} Q'_{\alpha\beta\theta\theta'\theta\theta'\alpha'\beta'} = \delta_{\alpha\alpha'}\sum_{\theta'} Q'_{\beta\theta'\theta'\beta'} + \delta_{\beta\beta'}\sum_\theta Q'^{*}_{\alpha\theta\theta\alpha'} - Q'_{\beta\beta'\alpha'\alpha} - Q'_{\alpha'\alpha\beta\beta'}. \quad (71)$$

Use of (45) shows that

$$Q'^{*}_{\alpha\theta\theta\alpha'} = Q'_{\theta\alpha\alpha'\theta}. \quad (72)$$

If the left-hand side of (71) is defined to be $R_{\alpha\beta\alpha'\beta'}$, then (71) and (72) give

$$R_{\alpha\beta\alpha'\beta'} = \delta_{\alpha\alpha'}\sum_\theta Q'_{\beta\theta\theta\beta'} + \delta_{\beta\beta'}\sum_\theta Q'_{\theta\alpha\alpha'\theta} - Q'_{\beta\beta'\alpha'\alpha} - Q'_{\alpha'\alpha\beta\beta'}. \quad (73)$$

Consequently, the analog to (48) is

$$\frac{d}{dt}\langle \rho_{\alpha\beta}(t)\rangle = -i\sum_{\alpha'}\sum_{\beta'} L_{\alpha\beta\alpha'\beta'}\langle \rho_{\alpha'\beta'}(t)\rangle - \sum_{\alpha'}\sum_{\beta'} R_{\alpha\beta\alpha'\beta'}\langle \rho_{\alpha'\beta'}(t)\rangle \quad (74)$$

The analog to the proof to (63) may be applied to $R_{\alpha\beta\alpha'\beta'}$ by using (69). Therefore, for an arbitrary matrix $X_{\alpha\beta}$, which is thought of as an $N^2$ component "vector," it follows that

$$\sum_\alpha\sum_\beta\sum_{\alpha'}\sum_{\beta'} X^{*}_{\alpha\beta}R_{\alpha\beta\alpha'\beta'}X_{\alpha'\beta'} \geq 0. \quad (75)$$

Thus the eigen-"vectors" of $R_{\alpha\beta\alpha'\beta'}$ are really the eigenmatrices of a tetratic, and the eigenvalues are nonnegative. The case of a zero eigenmatrix, or eigen-"vector," is realized by using (69) and (67) which show that the identity matrix $\delta_{\alpha'\beta'}$ is an eigen-"vector" eigenmatrix with eigenvalue zero:

$$\sum_{\alpha'}\sum_{\beta'}\tilde{L}_{\alpha\beta\alpha'\beta'}(t)\delta_{\alpha'\beta'} = \sum_{\alpha'}\sum_{\beta'}[\delta_{\alpha\alpha'}\tilde{M}_{\beta\beta'}(t) - \delta_{\beta\beta'}\tilde{M}^{*}_{\alpha\alpha'}(t)]\delta_{\alpha'\beta'} = \tilde{M}_{\beta\alpha}(t) - \tilde{M}^{*}_{\alpha\beta}(t) = 0. \quad (76)$$

Therefore, it also follows that

$$\sum_{\alpha'}\sum_{\beta'} R_{\alpha\beta\alpha'\beta'}\delta_{\alpha'\beta'} = \sum_\theta R_{\alpha\beta\theta\theta} = 0. \quad (77)$$

The symmetry of $R_{\alpha\beta\alpha'\beta'}$, which follows from (69), implies

$$\sum_\theta R_{\theta\theta\alpha'\beta'} = 0. \quad (78)$$

Therefore,

$$\frac{d}{dt}\sum_\alpha\langle \rho_{\alpha\alpha}(t)\rangle = -i\sum_\alpha\sum_{\alpha'}\sum_{\beta'} L_{\alpha\alpha\alpha'\beta'}\langle \rho_{\alpha'\beta'}(t)\rangle - \sum_\alpha\sum_{\alpha'}\sum_{\beta'} R_{\alpha\alpha\alpha'\beta'}\langle \rho_{\alpha'\beta'}(t)\rangle = 0 \quad (79)$$

because of (78) and a result like (76) which follows from (66):

$$\sum_\alpha L_{\alpha\alpha\alpha'\beta'} = \sum_\alpha(\delta_{\alpha\alpha'}M_{\alpha\beta'} - \delta_{\alpha\beta'}M^{*}_{\alpha\alpha'}) = M_{\alpha'\beta'} - M^{*}_{\beta'\alpha'} = 0. \quad (80)$$

Therefore, $\sum_\alpha\langle \rho_{\alpha\alpha}(t)\rangle$ is a conserved quantity. Nevertheless, (75) guarantees that (74) shows irreversible behavior.

## 8. PURELY DIAGONAL BILINEAR BEHAVIOR

Again starting with (42), it is always possible to perform a unitary similarity transformation which diagonalizes $M_{\alpha\alpha'}$ since $M_{\alpha\alpha'}$ is Hermitian. $\tilde{M}_{\alpha\alpha'}(t)$ in the new representation will not necessarily be diagonal, but it will still be Hermitian and a purely random, stationary, Gaussian process. Therefore, without loss of generality, (42) can always be transformed into the form

$$i\frac{d}{dt}c_\alpha(t) = d_\alpha c_\alpha(t) + \sum_{\alpha'}\tilde{M}_{\alpha\alpha'}(t)c_{\alpha'}(t), \quad (81)$$

wherein the $d_\alpha$ are real numbers. This is equivalent with saying that $M_{\alpha\alpha'}$ is diagonal and is given by

$$M_{\alpha\alpha'} = d_\alpha\delta_{\alpha\alpha'}. \quad (82)$$

The program of Sec. 7 can again be carried through with the simple modification that

$$L_{\alpha\beta\alpha'\beta'} \equiv \delta_{\alpha\alpha'}M_{\beta\beta'} - \delta_{\beta\beta'}M^{*}_{\alpha\alpha'} = \delta_{\alpha\alpha'}\delta_{\beta\beta'}d_\beta - \delta_{\beta\beta'}\delta_{\alpha\alpha'}d_\alpha = (d_\beta - d_\alpha)\delta_{\alpha\alpha'}\delta_{\beta\beta'}. \quad (83)$$

Therefore, (74) becomes

$$\frac{d}{dt}\langle \rho_{\alpha\beta}(t)\rangle = -i(d_\beta - d_\alpha)\langle \rho_{\alpha\beta}(t)\rangle - \sum_{\alpha'}\sum_{\beta'} R_{\alpha\beta\alpha'\beta'}\langle \rho_{\alpha'\beta'}(t)\rangle. \quad (84)$$

Using this diagonal $-M_{\alpha\alpha'}$ representation,

$$\langle \tilde{M}_{\alpha\beta}(t)\tilde{M}_{\mu\nu}(s)\rangle = 2Q'_{\alpha\beta\mu\nu}[\delta_{\alpha\nu}\delta_{\beta\mu} + \delta_{\alpha\mu}\delta_{\beta\nu} + (1-\delta_{\alpha\nu})(1-\delta_{\beta\mu})(1-\delta_{\alpha\mu})(1-\delta_{\beta\nu})]\delta(t-s) \quad (85)$$

is a sufficient condition for the reduction of (84) into an equation involving only the diagonal elements of $\langle \rho_{\alpha\beta}(t)\rangle$. The Kronecker delta factors in (85) require that either $\alpha, \beta, \mu$, and $\nu$ are all different, or that either $\alpha = \beta$ *or* $\mu = \nu$, *or* $\alpha = \nu$ *and* $\beta = \mu$, *or* $\alpha = \mu$ *and* $\beta = \nu$, in order that the over-all quantity be nonzero.

Sufficiency is demonstrated by using (85) in place of (45) in the calculation of $R_{\alpha\beta\alpha'\beta'}$ as determined by (73). This is equivalent with replacing the occurrence of $Q'_{\alpha\beta\mu\nu}$ in (73) with $Q'_{\alpha\beta\mu\nu}[\delta_{\alpha\nu}\delta_{\beta\mu} + \delta_{\alpha\mu}\delta_{\beta\mu} + (1-\delta_{\alpha\nu})(1-\delta_{\beta\mu}) \times (1-\delta_{\alpha\mu})(1-\delta_{\beta\nu})]$. The result, after a modicum of computation, is

$$R_{\alpha\beta\alpha'\beta'} = \delta_{\alpha\alpha'}\delta_{\beta\beta'}\Big(\sum_\theta Q'_{\beta\theta\theta\beta'} + \sum_\theta Q'_{\theta\alpha\alpha'\theta} + Q'_{\beta\beta\beta\beta} + Q'_{\alpha\alpha\alpha\alpha}\Big) - 2Q'_{\alpha'\alpha\beta\beta'}[\delta_{\alpha'\beta}\delta_{\alpha\beta'} + \delta_{\alpha\beta}\delta_{\alpha'\beta'} + (1-\delta_{\alpha'\beta})(1-\delta_{\alpha\beta'}) \times (1-\delta_{\alpha\beta})(1-\delta_{\alpha'\beta'})]. \quad (86)$$

Note that (86) implies that in order for $R_{\alpha\beta\alpha'\beta'} \neq 0$, then

$$\alpha = \beta \quad \text{if and only if} \quad \alpha' = \beta'. \quad (87)$$

Consequently, the expression for $R_{\alpha\beta\alpha'\beta'}$ given by (86) will reduce (84) to an equation for the diagonal elements of $\langle \rho_{\alpha\beta}(t)\rangle$ only. Define $P_\alpha(t)$ by

$$P_\alpha(t) \equiv \langle \rho_{\alpha\alpha}(t)\rangle. \quad (88)$$

By using (88), the diagonal equation resulting from (84) is

$$\frac{d}{dt}P_\alpha(t) = \sum_{\alpha'}[W_{\alpha\alpha'}P_{\alpha'}(t) - W_{\alpha'\alpha}P_\alpha(t)], \quad (89)$$

where $W_{\alpha\alpha'}$ is defined by

$$W_{\alpha\alpha'} \equiv 2Q'_{\alpha'\alpha\alpha\alpha'}. \quad (90)$$

Equation (90) holds because (86) leads to the result

$$R_{\alpha\alpha\alpha'\alpha'} = \delta_{\alpha\alpha'}\sum_\theta 2Q'_{\alpha\theta\theta\alpha} - 2Q'_{\alpha'\alpha\alpha\alpha'}. \quad (91)$$

Returning to (45) it is seen that

$$W_{\alpha\alpha'} \geq 0. \quad (92)$$

In addition, (79) may be rewritten using (88) to yield

$$\frac{d}{dt}\sum_\alpha P_\alpha(t) = 0. \quad (93)$$

## 9. FOKKER–PLANCK EQUATION

Because the stochastic "driving force" for the multiplicative stochastic processes presented here is always characterized as a purely random process, as well as a stationary, Gaussian process, the resulting over-all stochastic process is a Markov process. In this section, the Fokker–Planck equation which follows from the Markov property will be presented for the real $N$-component case. As was demonstrated in Secs. 6 and 7, the complex $N$-component case and the complex bilinear case are special cases of the real component case. Therefore, the Fokker–Planck equation presented below for the real component case is sufficiently general to cover all of these cases.

The Markov property alone does not necessarily lead to a Fokker–Planck equation. The following conditions are also necessary[14]:

$$\begin{aligned}
&\lim_{\Delta t\to 0}(1/\Delta t)\langle a_\alpha(\Delta t) - a_\alpha(0)\rangle \equiv A_\alpha[a_1(0)\cdots a_N(0)];\\
&\lim_{\Delta t\to 0}(1/\Delta t)\langle [a_\alpha(\Delta t) - a(0)][a_\beta(\Delta t) - a_\beta(0)]\rangle \equiv B_{\alpha\beta}[a_1(0)\cdots a_N(0)];\\
&\lim_{\Delta t\to 0}\frac{1}{\Delta t}\prod_{j=1}^{n}[a_{\alpha_j}(\Delta t) - a_{\alpha_j}(0)] = 0 \quad \text{for } n \geq 3.
\end{aligned} \quad (94)$$

These conditions do indeed hold for the real $N$-component case as may be rigorously verified by application of the techniques developed in the Appendix for the solution to Eq. (22). Moreover, $A_\alpha$ and $B_{\alpha\beta}$ are explicitly found to be

$$A_\alpha(a_1\cdots a_N) = \sum_{\alpha'=1}^{N}\Big(A_{\alpha\alpha'} + \sum_{\theta=1}^{N}Q_{\alpha\theta\theta\alpha'}\Big)a_{\alpha'}, \quad (95)$$

$$B_{\alpha\beta}(a_1\cdots a_N) = \sum_{\alpha'=1}^{N}\sum_{\beta'=1}^{N}2Q_{\alpha\alpha'\beta\beta'}a_{\alpha'}a_{\beta'}. \quad (96)$$

Using (95) and (96) when (94) is true for a Markov process leads to the Fokker–Planck equation[14]:

$$\begin{aligned}
\frac{\partial}{\partial t}P(a_1(0)\cdots a_N(0)|a_1\cdots a_N t) &= -\sum_{\alpha=1}^{N}\frac{\partial}{\partial a_\alpha}\Big[\sum_{\alpha'=1}^{N}\Big(A_{\alpha\alpha'} + \sum_{\theta=1}^{N}Q_{\alpha\theta\theta\alpha'}\Big) \times a_{\alpha'}P(a_1(0)\cdots a_N(0)|a_1\cdots a_N t)\Big]\\
&+ \sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}\frac{\partial^2}{\partial a_\alpha\partial a_\beta}\Big(\sum_{\alpha'=1}^{N}\sum_{\beta'=1}^{N} \times Q_{\alpha\alpha'\beta\beta'}a_{\alpha'}a_{\beta'}P(a_1(0)\cdots a_N(0)|a_1\cdots a_N t)\Big),
\end{aligned} \quad (97)$$

where $P(a_1(0)\cdots a_N(0)|a_1\cdots a_N t)$ is the probability that $a_1(t) = a_1$, $a_2(t) = a_2, \ldots,$ and $a_N(t) = a_N$ at time $t > 0$ if it was the case that $a_1(t) = a_1(0)$, $a_2(t) = a_2(0), \ldots,$ and $a_N(t) = a_N(0)$ at $t = 0$.

Define $R_{\alpha\alpha'}$ by

$$R_{\alpha\alpha'} \equiv \sum_\theta Q_{\alpha\theta\theta\alpha'}. \quad (98)$$

Equation (40) shows that $R_{\alpha\alpha'}$ has nonpositive eigenvalues.

By using (98), the summation over repeated indices convention, and leaving out the explicit $a_\alpha$ dependence of $P$ leads to

$$\frac{\partial}{\partial t}P = -\frac{\partial}{\partial a_\alpha}[(A_{\alpha\alpha'} + R_{\alpha\alpha'})a_{\alpha'}P] + \frac{\partial^2}{\partial a_\alpha\partial a_\beta}[Q_{\alpha\alpha'\beta\beta}a_{\alpha'}a_{\beta'}P]. \quad (99)$$

Equation (37) implies that $\sum_\alpha \langle a_\alpha^2(t)\rangle$ is a time invariant. This property may also be seen directly from (99). Averages are given in terms of $P$ by

$$\begin{aligned}
\langle a_\alpha(t)\rangle &\equiv \int a_\alpha P(a_1(0)\cdots a_N(0)|a_1\cdots a_N t)da_1\cdots da_N,\\
\langle a_\alpha(t)a_\beta(t)\rangle &\equiv \int a_\alpha a_\beta P(a_1(0)\cdots a_N(0)|a_1\cdots a_N t)da_1\cdots da_N.
\end{aligned} \quad (100)$$

Therefore, using (99) leads to

$$\begin{aligned}
\frac{d}{dt}\sum_\alpha\langle a_\alpha^2(t)\rangle &= \int\sum_\alpha a_\alpha^2\frac{\partial}{\partial t}P\,da_1\cdots da_N\\
&= -\int\sum_{\alpha''}a_{\alpha''}^2\frac{\partial}{\partial a_\alpha}[(A_{\alpha\alpha'} + R_{\alpha\alpha'})a_{\alpha'}P]da_1\cdots da_N\\
&\quad + \int\sum_{\alpha''}a_{\alpha''}^2\frac{\partial^2}{\partial a_\alpha\partial a_\beta}[Q_{\alpha\alpha'\beta\beta}a_{\alpha'}a_{\beta'}P]da_1\cdots da_N
\end{aligned}$$

$$= 2\int a_\alpha(A_{\alpha\alpha'} + R_{\alpha\alpha'})a_{\alpha'}P\,da_1\cdots da_N$$
$$+ 2\int \delta_{\alpha\beta}Q_{\alpha\alpha'\beta\beta'}a_{\alpha'}a_{\beta'}P\,da_1\cdots da_N$$
$$= 2R_{\alpha\alpha'}\langle a_\alpha(t)a_{\alpha'}(t)\rangle + 2Q_{\alpha\alpha'\alpha\beta'}\langle a_{\alpha'}(t)a_{\beta'}(t)\rangle$$
$$= 2R_{\alpha\alpha'}\langle a_\alpha(t)a_{\alpha'}(t)\rangle - 2R_{\alpha'\beta'}\langle a_{\alpha'}(t)a_{\beta'}(t)\rangle = 0. \tag{101}$$

The first equality follows from (100), the second equality follows from (99), the third equality follows from integration by parts, the fourth equality follows from (100), and the last two equalities follow from (98) and a renaming of indices. Therefore, it is seen that the time invariance of $\sum_\alpha \langle a_\alpha^2(t)\rangle$ is guaranteed by (97) or (99). Similarly, in the bilinear complex case, the time invariance of $\sum_\alpha \langle \rho_{\alpha\alpha}(t)\rangle$ will be guaranteed by the corresponding Fokker–Planck equation.

A discussion of the solutions to (99) for general $N$ will be reserved for a sequel to this paper. Here it will suffice to present the complete solution to (99) for the Kubo oscillator which is a one complex component case, and as was proved in Sec. 6 corresponds with a two real components case.

The Kubo oscillator is described by Eq. (12). Write $a(t)$ as $a(t) = a_x(t) + ia_y(t)$ where both $a_x(t)$ and $a_y(t)$ are real. In this way (12) becomes a special $N = 2$ case of (22), where

$$\mathbf{A} = \begin{pmatrix} 0 & -\omega \\ \omega & 0 \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{A}}(t) = \begin{pmatrix} 0 & -\tilde{\varphi}(t) \\ \tilde{\varphi}(t) & 0 \end{pmatrix}, \tag{102}$$

$$Q_{\alpha\alpha'\beta\beta'} = \lambda(\delta_{\alpha 1}\delta_{\alpha' 2}\delta_{\beta 1}\delta_{\beta' 2} + \delta_{\alpha 2}\delta_{\alpha' 1}\delta_{\beta 2}\delta_{\beta' 1} - \delta_{\alpha 1}\delta_{\alpha' 2}\delta_{\beta 2}\delta_{\beta' 1} - \delta_{\alpha 2}\delta_{\alpha' 1}\delta_{\beta 1}\delta_{\beta' 2}). \tag{103}$$

From (103) it is easy to compute $R_{\alpha\alpha'}$ as defined by (98) and this gives

$$\mathbf{R} = \begin{pmatrix} -\lambda & 0 \\ 0 & -\lambda \end{pmatrix}. \tag{104}$$

Using (102)–(104) in (99) for $N = 2$ gives

$$\frac{\partial}{\partial t}P = \omega\left(\frac{\partial}{\partial a_x}a_y - \frac{\partial}{\partial a_y}a_x\right)P + \lambda\left(\frac{\partial}{\partial a_x}a_x + \frac{\partial}{\partial a_y}a_y\right)P$$
$$+ \lambda\left(\frac{\partial^2}{\partial a_x^2}a_y^2 + \frac{\partial^2}{\partial a_y^2}a_x^2 - 2\frac{\partial^2}{\partial a_x \partial a_y}a_x a_y\right)P. \tag{105}$$

At this point introduce polar coordinates: $a_x = r\cos\theta$ and $a_y = r\sin\theta$. This implies

$$\frac{\partial}{\partial a_x} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}$$
$$\text{and} \quad \frac{\partial}{\partial a_y} = \sin\theta\frac{\partial}{\partial r} + \frac{\cos\theta}{r}\frac{\partial}{\partial\theta}. \tag{106}$$

Using (106) in (105) leads, after a modicum of algebra, to

$$\frac{\partial}{\partial t}P = -\omega\frac{\partial}{\partial\theta}P + \lambda\frac{\partial^2}{\partial\theta^2}P, \tag{107}$$

where $P \equiv P(r(0)\theta(0)|r\theta t)$ and $P(r(0)\theta(0)|r\theta 0) = \delta(r - r(0))\delta(\theta - \theta(0))$. From (107) it is seen that $P$ may be factored,

$$P(r\theta t) = R(rt)\,W(\theta t), \tag{108}$$

and (107) becomes two equations:

$$\frac{\partial}{\partial t}R(rt) = 0 \quad \text{and}$$
$$\frac{\partial}{\partial t}W(\theta,t) = -\omega\frac{\partial}{\partial\theta}W(\theta,t) + \lambda\frac{\partial^2}{\partial\theta^2}W(\theta,t). \tag{109}$$

With the initial condition for $P$ given beneath (107) the solution to (109) for $R$ is $R(rt) = \delta[r - r(0)]$. The solution for $W(\theta,t)$ with periodic boundary conditions is given by

$$W(\theta,t) = \frac{1}{\sqrt{4\pi\lambda t}}\sum_{K=-\infty}^{\infty}\exp\left(-\frac{(\theta - \theta(0) + 2K\pi - \omega t)^2}{4\lambda t}\right). \tag{110}$$

This describes a diffusion process on a circle coupled with a streaming term given by $\omega t$. The complete solution to (105) is then given by

$$P(r(0)\theta(0)|r\theta t) = \delta[r - r(0)]\frac{1}{\sqrt{4\pi\lambda t}}$$
$$\times\sum_{K=-\infty}^{\infty}\exp\left(-\frac{[\theta - \theta(0) + 2K\pi - \omega t]^2}{4\lambda t}\right). \tag{111}$$

It is possible to use (111) to reconfirm (15).

## 10. CONCLUDING REMARKS

The physical implications of the equations presented in this paper are relevant in the areas of nonequilibrium thermodynamics and nonequilibrium statistical mechanics. A fuller treatment of the appropriate physical interpretations for these equations will be presented in a sequel to this work. For the present it will suffice to indicate several immediately obvious points.

Additive stochastic processes have been used to explain Brownian motion by Langevin's equation, to explain nonequilibrium thermodynamics close to full equilibrium by the Onsager and Machlup equations, and to explain these first two cases, as well as the fluctuating hydrodynamic theory of Landau of Lifshitz, and the fluctuating Boltzmann equation, by the general theory of stationary, Gaussian, Markov processes presented by Fox and Uhlenbeck. All of these cases are limited to dynamical behavior near full equilibrium, and all of these cases are classical.

Multiplicative stochastic processes, as presented in this paper, suggest physical applications in the following cases. The most simple case is the case of frequency fluctuation for the harmonic oscillator, as was originally proposed by Kubo. The generalization to the real $N$-component case as given by (22) and (27) corresponds with the Liouville equation with a Hamiltonian that contains a fluctuating contribution to the overall energy.[9] Equation (22) is the matrix representation of the partial differential equation which provides the classical Liouville description. The complex $N$-component case corresponds with the Heisenberg matrix representation of the Schrödinger equation. Equation (42) is the relevant equation and contains a Hamiltonian which has a fluctuating contribution. Averaging (42) leads to (48) which depicts the decay of total probability as may be seen using (63). In order to avoid this physically unreasonable consequence, the density matrix formulation is presented by Eq. (65), and (74) corresponds with the

averaged density matrix equation. Equation (79), in contrast with (48) and (63), implies conservation of total probability, even though (75) guarantees that (74) describes irreversible behavior for the whole averaged density matrix. In the literature (74) is referred to as the Redfield equation.[6] Here, the potential physical applicability of (74) is greater than the nuclear magnetic resonance context usually associated with Redfield's equation. In the special case in which (85) is realized, the Redfield equation (74) is seen to reduce to (89) and (92) which comprise the Pauli master equation for the diagonal elements of the average density matrix.[15]

All these cases show that multiplicative stochastic processes pertain to both classical and quantum mechanical considerations. The restriction of additive stochastic processes to physical applicability corresponding with dynamical behavior close to full equilibrium does not apply to multiplicative stochastic processes. This follows from the difference in the levels of description each case involves. In the additive stochastic process case the description is relatively macroscopic such as in fluctuating hydrodynamics, in the fluctuating Boltzmann equation, and in nonequilibrium thermodynamics. These levels of descriptions are usually nonlinear; but their linear approximations are required in order to obtain their stochastic description. The linearization step requires the restriction of applicability to near full equilibrium. In contrast, in the multiplicative stochastic process case the description is relatively microscopic such as in the fluctuating Liouville equation and in the fluctuating density matrix equation. The levels of description are intrinsically already linear, so that no linearization step is required, and, consequently, there is no corresponding attendant limitation to physical applicability.

The possible limitations to physical applicability of multiplicative stochastic processes arise with respect to the validity of introducing a part of the total Hamiltonian which is a purely random, stationary, Gaussian process. This consideration will be made in detail in a sequel to this work which stresses the physical context. For the present, simply note the existence of the rigorous theorem, the proof of which is found in the Appendix and the consequences of which are found in the text, for multiplicative stochastic processes "driven" by purely random, stationary, Gaussian "forces."

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## APPENDIX: PROOF OF EQ. (27)

Define $R_\alpha(t)$ by

$$R_\alpha(t) \equiv \sum_{\alpha'} [e^{-\mathbf{A}t}]_{\alpha\alpha'} a_{\alpha'}(t), \tag{A1}$$

where $\mathbf{A}$ denotes the matrix with components $A_{\alpha\alpha'}$, and

$$[e^{-\mathbf{A}t}]_{\alpha\alpha'} \equiv \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} (\mathbf{A}^n)_{\alpha\alpha'} t^n.$$

Also define $\tilde{L}_{\alpha\alpha'}(t)$ by

$$\tilde{L}_{\alpha\alpha'}(t) \equiv \sum_{\beta} \sum_{\beta'} [e^{-\mathbf{A}t}]_{\alpha\beta} \tilde{A}_{\beta\beta'}(t) [e^{\mathbf{A}t}]_{\beta'\alpha'}. \tag{A2}$$

Via (A1) and (A2), (22) may be written as

$$\frac{d}{dt} R_\alpha(t) = \sum_{\alpha'} \tilde{L}_{\alpha\alpha'}(t) R_{\alpha'}(t). \tag{A3}$$

Because $\tilde{\mathbf{L}}(t)$ and $\tilde{\mathbf{L}}(s)$ do not necessarily commute for $t \neq s$, (A3) must be solved using time-ordered integrals:

$$\begin{aligned} R_\alpha(t) = \sum_{\alpha'} \sum_{k=0}^{\infty} \int_0^t \int_0^{s_k} \int_0^{s_{k-1}} \cdots \int_0^{s_3} \int_0^{s_2} \\ \times \sum_{\mu_{k-1}} \sum_{\mu_{k-2}} \cdots \sum_{\mu_2} \sum_{\mu_1} \\ \times \tilde{L}_{\alpha\mu_{k-1}}(s_k) \tilde{L}_{\mu_{k-1}\mu_{k-2}}(s_{k-1}) \cdots \tilde{L}_{\mu_2\mu_1}(s_2) \\ \times \tilde{L}_{\mu_1\alpha'}(s_1) ds_1 \cdots ds_k R_{\alpha'}(0), \end{aligned} \tag{A4}$$

where $t \geq s_k \geq s_{k-1} \geq \cdots \geq s_2 \geq s_1 \geq 0$. Define $W^k_{\alpha\alpha'}(t)$ by

$$\begin{aligned} W^k_{\alpha\alpha'}(t) \equiv \int_0^t \int_0^{s_k} \cdots \int_0^{s_2} \sum_{\mu_{k-1}} \cdots \\ \times \sum_{\mu_1} \langle \tilde{L}_{\alpha\mu_{k-1}}(s_k) \cdots \tilde{L}_{\mu_1\alpha'}(s_1) \rangle ds_1 \cdots ds_k. \end{aligned} \tag{A5}$$

Equations (25) and (A2) imply that

$$W^k_{\alpha\alpha'}(t) = 0 \quad \text{for all odd } k. \tag{A6}$$

Consider all even $k$, such that $k = 2m$ for $m = 1, 2, \cdots$. Notice that Eqs. (26) and (A2) imply that

$$\begin{aligned} \langle \tilde{L}_{\mu_{2m}\nu_{2m}}(s_{2m}) \cdots \tilde{L}_{\mu_1\nu_1}(s_1) \rangle \\ = \frac{1}{2^m m!} \sum_{p \in S_{2m}} \prod_{j=1}^{m} \langle \tilde{L}_{\mu_{p(2j)}\nu_{p(2j)}}(s_{p(2j)}) \\ \times \tilde{L}_{\mu_{p(2j-1)}\nu_{p(2j-1)}}(s_{p(2j-1)}) \rangle, \end{aligned} \tag{A7}$$

where

$$\begin{aligned} \langle \tilde{L}_{\mu\nu}(s) \tilde{L}_{\mu'\nu'}(s') \rangle \\ = \sum_{\alpha} \sum_{\alpha'} \sum_{\beta} \sum_{\beta'} \langle [e^{-\mathbf{A}s}]_{\mu\alpha} \tilde{A}_{\alpha\alpha'}(s) [e^{\mathbf{A}s}]_{\alpha'\nu} \\ \times [e^{-\mathbf{A}s'}]_{\mu'\beta} \tilde{A}_{\beta\beta'}(s') [e^{\mathbf{A}s'}]_{\beta'\nu'} \rangle \\ = 2 \sum_{\alpha} \sum_{\alpha'} \sum_{\beta} \sum_{\beta'} [e^{-\mathbf{A}s}]_{\mu\alpha} [e^{\mathbf{A}s}]_{\alpha'\nu} Q_{\alpha\alpha'\beta\beta'} \\ \times [e^{-\mathbf{A}s}]_{\mu'\beta} [e^{\mathbf{A}s}]_{\beta'\nu'} \delta(s - s'). \end{aligned} \tag{A8}$$

In particular, (A8) leads to

$$\begin{aligned} \sum_{\theta} \langle \tilde{L}_{\mu\theta}(s) \tilde{L}_{\theta\nu}(s') \rangle \\ = 2 \sum_{\alpha} \sum_{\beta'} [e^{-\mathbf{A}s}]_{\mu\alpha} \sum_{\theta} Q_{\alpha\theta\theta\beta'} [e^{\mathbf{A}s}]_{\beta'\nu} \delta(s - s'). \end{aligned} \tag{A9}$$

Using (A7) in (A5) for $k = 2m$ gives

$$W^k_{\alpha\alpha'}(t) = \int_0^t \int_0^{s_k} \cdots \int_0^{s_2} \sum_{\mu_k} \cdots \sum_{\mu_1} \sum_{\nu_k} \cdots \sum_{\nu_1} \times \delta_{\alpha\mu_k}\delta_{\alpha'\nu_1} \prod_{l=1}^{k-1} \delta_{\mu_l\nu_{l+1}} \frac{1}{2^m m!} \sum_{p\in S_{2m}} \prod_{j=1}^{m} \times \langle \tilde{L}_{\mu_{p(2j)}\nu_{p(2j)}}(s_{p(2j)})\tilde{L}_{\mu_{p(2j-1)}\nu_{p(2j-1)}} \times (s_{p(2j-1)})\rangle ds_1 \cdots ds_k. \quad \text{(A10)}$$

Using (A8) in (A10) gives

$$W^k_{\alpha\alpha'}(t) = \int_0^t \int_0^{s_k} \cdots \int_0^{s_2} \sum_{\mu_k} \cdots \sum_{\mu_1} \sum_{\nu_k} \cdots \sum_{\nu_1} \times \delta_{\alpha\mu_k}\delta_{\alpha'\nu_1} \prod_{l=1}^{k-1} \delta_{\nu_{l+1}\mu_l} \frac{1}{2^m m!} \sum_{p\in S_{2m}} 2^m \times \prod_{j=1}^{m} \sum_{\alpha_j}\sum_{\alpha_j'}\sum_{\beta_j}\sum_{\beta_j'} [e^{-\mathbf{A}s_{p(2j)}}]_{\mu_{p(2j)}\alpha_j} \times [e^{\mathbf{A}s_{p(2j)}}]_{\alpha_j'\nu_{p(2j)}} Q_{\alpha_j\alpha_j'\beta_j\beta_j'} [e^{-\mathbf{A}s_{p(2j)}}]_{\mu_{p(2j-1)}\beta_j} \times [e^{\mathbf{A}s_{p(2j)}}]_{\beta_j'\nu_{p(2j-1)}} \delta(s_{p(2j)} - s_{p(2j-1)}) ds_1 \cdots ds_k. \quad \text{(A11)}$$

This complex expression for $W^k_{\alpha\alpha'}(t)$ reveals its inner structure and leads to major simplifications. Define $f^{kp}_{\alpha\alpha'}(s_k \cdots s_1)$ by

$$f^{kp}_{\alpha\alpha'}(s_k \cdots s_1) \equiv \sum_{\mu_k} \cdots \sum_{\mu_1} \sum_{\nu_k} \cdots \times \sum_{\nu_1} \delta_{\alpha\mu_k}\delta_{\alpha'\nu_1} \prod_{l=1}^{k-1} \delta_{\nu_{l+1}\mu_l} \prod_{j=1}^{m} \sum_{\alpha_j}\sum_{\alpha_j'}\sum_{\beta_j} \times \sum_{\beta_j'} [e^{-\mathbf{A}s_{p(2j)}}]_{\mu_{p(2j)}\alpha_j} [e^{\mathbf{A}s_{p(2j)}}]_{\alpha'\nu_{p(2j)}} \times Q_{\alpha_j\alpha_j'\beta_j\beta_j'} [e^{-\mathbf{A}s_{p(2j)}}]_{\mu_{p(2j-1)}\beta_j} [e^{\mathbf{A}s_{p(2j)}}]_{\beta_j'\nu_{p(2j-1)}} \quad \text{(A12)}$$

for each $p \in S_{2m}$. Therefore, putting (A12) into (A11) gives

$$W^k_{\alpha\alpha'}(t) = \frac{1}{2^m m!} \sum_{p\in S_{2m}} 2^m \int_0^t \int_0^{s_k} \cdots \int_0^{s_2} f^{kp}_{\alpha\alpha'}(s_k \cdots s_1) \prod_{j=1}^{m} \delta(s_{p(2j)} - s_{p(2j-1)}) \times ds_1 \cdots ds_k. \quad \text{(A13)}$$

Now, define $I^{kq}_{\alpha\alpha'}(t)$ by

$$I^{kq}_{\alpha\alpha'}(t) \equiv \int_0^t \int_0^{s_k} \cdots \int_0^{s_2} f^{kq}_{\alpha\alpha'}(s_k \cdots s_1) \times \prod_{j=1}^{m} \delta(s_{q(2j-1)} - s_{q(2j-1)}) ds_1 \cdots ds_k \quad \text{(A14)}$$

for each $q \in S_{2m}$. Let the set $N$ be given by

$$N \equiv \{q \in S_{2m} | \prod_{j=1}^{m} \delta(s_{q(2j)} - s_{q(2j-1)}) \text{ contains the factor } \delta(s_k - s_{k-1})\},$$

and let the set $Z$ be defined by

$$Z \equiv \{q \in S_{2m} | \prod_{j=1}^{m} \delta(s_{q(2j)} - s_{q(2j-1)}) \text{ does not contain the factor } \delta(s_k - s_{k-1})\}.$$

Clearly, $Z$ contains $q$'s such that $\prod_{j=1}^{m} \delta(s_{q(2j)} - s_{q(2j-1)})$ contains the factor $\delta(s_k - s_l)$ for $l \neq k-1$. Since the order of the two time arguments in a delta function does not alter its value, and since the order of the delta functions in a product does not alter its value, then there are $2^m m!$ permutations in $S_{2m}$ which yield identical $\prod_{j=1}^{m} \delta(s_{q(2j)} - s_{q(2j-1)})$. The number of permutations in $N$ is $2m[(2m-2)!]$; because there are two ways of ordering $s_k$ and $s_{k-1}$ in $\delta(s_k - s_{k-1})$, there are $m$ ways of ordering the product with respect to the factor $\delta(s_k - s_{k-1})$ and $m-1$ other factors, and there are $(2m-2)!$ ways of permuting the remaining $2m-2$ time variables. The number of permutations in $Z$ is $2m(2m-2)[(2m-2)!]$; because there are two ways of ordering $s_k$ and $s_l$ in $\delta(s_k - s_l)$, there are $m$ ways of ordering the product with respect to the factor $\delta(s_k - s_l)$ and $m-1$ other factors, there are $(2m-2)$ choices for $l \neq k-1$, and there are $(2m-2)!$ ways of permuting the remaining $2m-2$ time variables. In summary, it follows that $S_{2m} = N \cup Z$, $N \cap Z = \emptyset$, and $(2m)! = 2m[(2m-2)!] + 2m(2m-2)[(2m-2)!]$. If $g(s, s')$ is an arbitrary function of two time variables, then the preceding counting scheme leads to

$$\left\{\prod_{j=1}^{m} g(s_{q(2j)}, s_{q(2j-1)}) | q \in N\right\} = \left\{g(s_k, s_{k-1}) \prod_{j=1}^{m-1} g(s_{r(2j)} - s_{r(2j-1)}) | r \in S_{2m-2}\right\}. \quad \text{(A15)}$$

Each term on the left-hand side of (A15) is redundant $2m$ times if $g(s, s')$ is symmetric in $s$ and $s'$. A special instance of (A15) is: $\{\prod_{j=1}^{m} \delta(s_{q(2j)} - s_{q(2j-1)}) | q \in N\} = \{\delta(s_k - s_{k-1}) \prod_{j=1}^{m-1} \delta(s_{r(2j)} - s_{r(2j-1)} | r \in S_{2m-2}\}$. Equation (A15) will be useful later, and the redundancy factor $2m$ should be noted.

Using (A14) in (A13) gives

$$W^k_{\alpha\alpha'}(t) = \frac{1}{2^m m!} \sum_{p\in S_{2m}} 2^m I^{kp}_{\alpha\alpha'}(t) = \frac{1}{m!} \sum_{q\in N} I^{kq}_{\alpha\alpha'}(t) + \frac{1}{m!} \sum_{q\in Z} I^{kq}_{\alpha\alpha'}(t). \quad \text{(A16)}$$

It will now be shown that

$$I^{kq}_{\alpha\alpha'}(t) = 0 \quad \text{for each } q \in Z. \quad \text{(A17)}$$

Because $q \in Z$,

$$I^{kq}_{\alpha\alpha'}(t) = \int_0^t \int_0^{s_k} \cdots \int_0^{s_2} f^{kq}_{\alpha\alpha'}(s_k \cdots s_1) \times \delta(s_k - s_l)\delta(s_{k-1} - s_i) \times \prod_{j=1}^{m'} \delta(s_{q(2j)} - s_{q(2j-1)}) ds_1 \cdots ds_k, \quad \text{(A18)}$$

where $\prod_{j=1}^{m'} \delta(s_{q(2j)} - s_{q(2j-1)})$ is defined by

$$\prod_{j=1}^{m} \delta(s_{q(2j)} - s_{q(2j-1)}) \equiv \delta(s_k - s_l)\delta(s_{k-1} - s_i) \prod_{j=1}^{m'} \delta(s_{q(2j)} - s_{q(2j-1)}). \quad \text{(A19)}$$

Recall that $q \in Z$ implies that $l \neq k-1$. Therefore, there is some $i$ such that $i \neq k$ and $i \neq l$ and $\delta(s_{k-1} - s_i)$ appears as a factor in the product

$\Pi_{j=1}^{m} \delta(s_{q(2j)} - s_{q(2j-1)})$. Note that $I_{\alpha\alpha'}^{kq}(0) = 0$ and

$$\frac{d}{dt} I_{\alpha\alpha'}^{kq}(t) = \int_0^t \int_0^{s_{k-1}} \cdots \int_0^{s_2} f_{\alpha\alpha'}^{kq}(t, s_{k-1}, \ldots, s_1) \times \delta(t - s_l)\delta(s_{k-1} - s_i) \prod_{j=1}^{m'} \delta(s_{q(2j)} - s_{q(2j-1)}) \times ds_1 \cdots ds_{k-1}. \quad \text{(A20)}$$

The time ordering of the integrals requires that

$$t \geq s_{k-1} \geq \cdots \geq s_l \geq \cdots \geq s_2 \geq s_1 \geq 0. \quad \text{(A21)}$$

The only singular contributions to the integrand of (A20) are in the product of delta functions since $f_{\alpha\alpha'}^{kq}(t, s_{k-1}, \ldots, s_1)$ is a bounded integrable function as is seen from (A12). The integrations in (A20) are performed in the order $ds_1, ds_2, \ldots, ds_{k-1}$. After the $ds_i$ integration, the $\delta(s_{k-1} - s_i)$ term will no longer be present, and the functional dependence of the remaining integrand will no longer be singular in $s_{k-1}$ because no other delta function besides $\delta(s_{k-1} - s_i)$ contains $s_{k-1}$ or $s_i$. For all $s_{k-1} < t$, the $\delta(t - s_l)$ term and (A21) imply that the integrand is zero. Therefore, only $s_{k-1} = t$ can contribute to the over-all integration with respect to $s_{k-1}$. Thus, when the $ds_{k-1}$ integration is finally performed, the remaining integrand is zero for $s_{k-1} < t$ and is not singular in $s_{k-1}$ anywhere in the interval $[0, t]$. Therefore, the Riemann integral over $ds_{k-1}$ from 0 to $t$ gives zero. This proves that for $q \in Z$, $(d/dt) I_{\alpha\alpha'}^{kq}(t) = 0$. Coupling this result with $I_{\alpha\alpha'}^{kq}(0) = 0$ implies that for each $q \in Z$ $I_{\alpha\alpha'}^{kq}(t) = 0$ for all $t$. Consequently, (A17) is proved.

Returning to (A16), (A17) implies that

$$W_{\alpha\alpha'}^{k}(t) = \frac{1}{m!} \sum_{q \in N} I_{\alpha\alpha'}^{kq}(t). \quad \text{(A22)}$$

Using (A12) and (A14) yields

$$\begin{aligned}
\sum_{q\in N} I_{\alpha\alpha'}^{kq}(t) &= \sum_{q\in N} \int_0^t \int_0^{s_k} \cdots \int_0^{s_2} f_{\alpha\alpha'}^{kq}(s_k \cdots s_1) \times \prod_{j=1}^{m} \delta(s_{q(2j)} - s_{q(2j-1)}) ds_1 \cdots ds_k \\
&= \sum_{q\in N} \int_0^t \int_0^{s_k} \cdots \int_0^{s_2} \sum_{\mu_k} \sum_{\mu_{k-1}} \sum_{\nu_k} \sum_{\nu_{k-1}} \\
&\times \sum_{\mu_{k-2}} \cdots \sum_{\mu_1} \sum_{\nu_{k-2}} \cdots \sum_{\nu_1} \delta_{\alpha\mu_k} \delta_{\nu_k \mu_{k-1}} \delta_{\alpha'\nu_1} \\
&\times \prod_{l=1}^{k-2} \delta_{\nu_{l+1}\mu_l} \sum_{\alpha_m} \sum_{\alpha'_m} \sum_{\beta_m} \sum_{\beta'_m} [e^{-\mathbf{A}s_k}]_{\mu_k \alpha_m} \\
&\times [e^{\mathbf{A}s_k}]_{\alpha'_m \nu_k} Q_{\alpha_m \alpha'_m \beta_m \beta'_m} [e^{-\mathbf{A}s_k}]_{\mu_{k-1}\beta_m} \\
&\times [e^{\mathbf{A}s_k}]_{\beta'_m \nu_{k-1}} \prod_{j=1}^{m-1} \sum_{\alpha_j} \sum_{\alpha'_j} \sum_{\beta_j} \sum_{\beta'_j} \\
&\times [e^{-\mathbf{A}s_{q(2j)}}]_{\mu_{q(2j)}\alpha_j} [e^{\mathbf{A}s_{q(2j)}}]_{\alpha'_j \nu_{q(2j)}} Q_{\alpha_j \alpha'_j \beta_j \beta'_j} \\
&\times [e^{-\mathbf{A}s_{q(2j)}}]_{\mu_{q(2j-1)}\beta_j} [e^{\mathbf{A}s_{q(2j)}}]_{\beta'_j \nu_{q(2j-1)}} \\
&\times \delta(s_k - s_{k-1}) \prod_{i=1}^{m''} \delta(s_{q(2i)} - s_{q(2i-1)}) \\
&\times ds_1 \cdots ds_k, \quad \text{(A23)}
\end{aligned}$$

wherein $\Pi''_{i=1}^{m} \delta(s_{q(2i)} - s_{q(2i-1)})$ is defined by

$$\prod_{i=1}^{m} \delta(s_{q(2i)} - s_{q(2i-1)}) \equiv \delta(s_k - s_{k-1}) \prod_{i=1}^{m''} \delta(s_{q(2i)} - s_{q(2i-1)}).$$

If

$$\prod_{l=1}^{k-2} \delta_{\nu_{l+1}\mu_l} = \delta_{\nu_{k-1}\mu_{k-2}} \prod_{l=1}^{k-3} \delta_{\nu_{l+1}\mu_l}$$

and (A15) are used, then the expression in (A23) becomes

$$\begin{aligned}
\sum_{q\in N} I_{\alpha\alpha'}^{kq}(t) &= 2m \sum_{r \in S_{2m-2}} \int_0^t \int_0^{s_k} \int_0^{s_{k-1}} \cdots \int_0^{s_2} \\
&\times \sum_{\nu_{k-1}} \sum_{\alpha_m} \sum_{\beta'_m} [e^{-\mathbf{A}s_k}]_{\alpha\alpha_m} \sum_{\theta_m} Q_{\alpha_m \theta_m \theta_m \beta'_m} \\
&\times [e^{\mathbf{A}s_k}]_{\beta'_m \nu_{k-1}} \delta(s_k - s_{k-1}) \\
&\times \sum_{\mu_{k-2}} \cdots \sum_{\mu_1} \sum_{\nu_{k-2}} \cdots \\
&\times \sum_{\nu_1} \delta_{\nu_{k-1}\mu_{k-2}} \delta_{\alpha'\nu_1} \prod_{l=1}^{k-3} \delta_{\nu_{l+1}\mu_l} \prod_{j=1}^{m-1} \\
&\times \sum_{\alpha_j} \sum_{\alpha'_j} \sum_{\beta_j} \sum_{\beta'_j} [e^{-\mathbf{A}s_{r(2j)}}]_{\mu_{r(2j)}\alpha_j} \\
&\times [e^{\mathbf{A}s_{r(2j)}}]_{\alpha'_j \nu_{r(2j)}} Q_{\alpha_j \alpha'_j \beta_j \beta'_j} \\
&\times [e^{-\mathbf{A}s_{r(2j)}}]_{\mu_{r(2j-1)}\beta_j} [e^{\mathbf{A}s_{r(2j)}}]_{\beta'_j \nu_{r(2j-1)}} \\
&\times \prod_{i=1}^{m-1} \delta(s_{r(2i)} - s_{r(2i-1)}) ds_1 \cdots \\
&\times ds_{k-2} ds_{k-1} ds_k. \quad \text{(A24)}
\end{aligned}$$

The factor $2m$ comes from the redundancy requirement discussed following relation (A15). Because $r \in S_{2m-2}$, it also follows that

$$\prod_{i=1}^{m''} (s_{q(2i)} - s_{q(2i-1)}) = \prod_{i=1}^{m-1} \delta(s_{r(2j)} - s_{r(2i-1)}) \text{ for } q \in N,$$

and this has been used to get (A24) from (A23). Using (A12) for $k - 2$ shows that (A24) is equivalent to

$$\begin{aligned}
\sum_{q\in N} I_{\alpha\alpha'}^{kq}(t) &= 2m \sum_{r \in S_{2m-2}} \int_0^t \int_0^{s_k} \sum_{\nu_{k-1}} \sum_{\alpha_m} \sum_{\beta'_m} \\
&\times [e^{-\mathbf{A}s_k}]_{\alpha\alpha_m} \sum_{\theta_m} Q_{\alpha_m \theta_m \theta_m \beta'_m} [e^{\mathbf{A}s_k}]_{\beta'_m \nu_{k-1}} \\
&\times \delta(s_k - s_{k-1}) \int_0^{s_{k-1}} \cdots \int_0^{s_2} f_{\nu_{k-1}\alpha'}^{k-2\, r} \\
&\times (s_{k-2} \cdots s_1) \prod_{i=1}^{m-1} \delta(s_{r(2i)} - s_{r(2i-1)}) \\
&\times ds_1 \cdots ds_{k-2} ds_{k-1} ds_k \\
&= 2m \sum_{r \in S_{2m-2}} \int_0^t \int_0^{s_k} \sum_{\nu_{k-1}} \sum_{\alpha_m} \sum_{\beta'_m} [e^{-\mathbf{A}s_k}]_{\alpha\alpha_m} \\
&\times \sum_{\theta_m} Q_{\alpha_m \theta_m \theta_m \beta'_m} [e^{\mathbf{A}s_k}]_{\beta'_m \nu_{k-1}} \\
&\times \delta(s_k - s_{k-1}) I_{\nu_{k-1}\alpha'}^{k-2\, r}(s_{k-1}) ds_{k-1} ds_k. \quad \text{(A25)}
\end{aligned}$$

The second equality in (A25) follows from (A14) for $k - 2$.

By using (A13) and (A14) it also follows that

$$W^{k-2}_{\nu_{k-1}\alpha'}(s_{k-1}) = \frac{1}{(m-1)!} \sum_{r \in S_{2m-2}} I^{k-2\,r}_{\nu_{k-1}\alpha'}(s_{k-1}) \tag{A26}$$

because $k - 2 = 2(m-1)$. Now, if one last quantity $N_{\alpha\nu_{k-1}}(s_k)$ is defined by

$$N_{\alpha\nu_{k-1}}(s_k) \equiv \sum_{\alpha_m} \sum_{\beta'_m} [e^{-\mathbf{A}s_k}]_{\alpha\alpha_m} \sum_{\theta_m} Q_{\alpha_m\theta_m\theta_m\beta'_m} [e^{\mathbf{A}s_k}]_{\beta'_m\nu_{k-1}}, \tag{A27}$$

then together with (A13), (A14), (A25), and (A26) this leads to

$$\begin{aligned} W^k_{\alpha\alpha'}(t) &= 2 \sum_{\nu_{k-1}} \int_0^t \int_0^{s_k} N_{\alpha\nu_{k-1}}(s_k)\delta(s_k - s_{k-1}) \\ &\quad \times W^{k-2}_{\nu_{k-1}\alpha'}(s_{k-1})\, ds_{k-1} ds_k \\ &= \sum_{\nu_{k-1}} \int_0^t N_{\alpha\nu_{k-1}}(s_k) W^{k-2}_{\nu_{k-1}\alpha'}(s_k)\, ds_k, \end{aligned} \tag{A28}$$

wherein the $ds_{k-1}$ integration with $\delta(s_k - s_{k-1})$ in the integrand and $s_k$ as an integration limit introduced a factor of $\frac{1}{2}$ which cancelled the 2. By differentiation, (A28) gives

$$\frac{d}{dt} W^k_{\alpha\alpha}(t) = \sum_{\nu_{k-1}} N_{\alpha\nu_{k-1}}(t) W^{k-2}_{\nu_{k-1}\alpha'}(t). \tag{A29}$$

By returning to (A4) and (A5), (A29) permits the writing of

$$\begin{aligned} \frac{d}{dt}\langle R_\alpha(t)\rangle &= \sum_{\alpha'} \sum_{k=0}^{\infty} \frac{d}{dt} W^k_{\alpha\alpha'}(t) R_{\alpha'}(0) \\ &= \sum_{\alpha'} \sum_{m=0}^{\infty} \frac{d}{dt} W^{2m}_{\alpha\alpha'}(t) R_{\alpha'}(0) \\ &= \sum_{\alpha'} \sum_{m=1}^{\infty} \sum_{\nu} N_{\alpha\nu}(t) W^{2m-2}_{\nu\alpha'}(t) R_{\alpha'}(0) \\ &= \sum_{\nu} N_{\alpha\nu}(t) \sum_{\alpha'} \sum_{m=0}^{\infty} W^{2m}_{\alpha\alpha'}(t) R_{\alpha'}(0) \\ &= \sum_{\nu} N_{\alpha\nu}(t) \langle R_\nu(t)\rangle. \end{aligned} \tag{A30}$$

Using (A1) and (A27) finishes the proof of (27) with

$$\frac{d}{dt}\langle a_\alpha(t)\rangle = \sum_{\alpha'} A_{\alpha\alpha'}\langle a_{\alpha'}(t)\rangle + \sum_{\alpha'} \sum_{\theta} Q_{\alpha\theta\theta\alpha'}\langle a_{\alpha'}(t)\rangle.$$

It should be noted that this result is equivalent with the statement that the time-ordered integrals which arise in the formal solution to (22) yield nonzero quantities upon averaging, only if the product of delta functions which occurs is "properly ordered." By "properly ordered" is meant that

$$\prod_{j=1}^{m} \delta(s_{p(2j)} - s_{p(2j-1)}) = \prod_{j=1}^{m} \delta(s_{(2j)} - s_{(2j-1)}), \tag{A31}$$

since $\prod_{j=1}^{m} \delta(s_{(2j)} - s_{(2j-1)})$ in the integrand of the time-ordered integral leads to a nonzero quantity, whereas any other pairing of time variables leads to zero. Therefore, only permutations which satisfy (A31) give "properly ordered" delta function products. In the proof presented here this property has been arrived at by "peeling off" two time variables at a time, and noting that to get a nonzero result that the two time variables "peeled off" were "properly ordered" relative to all possible time variables.

Reference to these properties of "properly ordered" products are made in Sec. 9 with respect to rigorously justifying the Fokker–Planck equations given in that section.


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## Long-Wavelength Normal Modes of Crystals with Coulomb Interactions


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An investigation is made of the behavior of the normal modes of vibration in the long-wavelength limit for infinite crystal lattices in which Coulomb interactions are present. The work is applicable to point ion models with any crystal structure. Rules are derived which are helpful in determining the long-wavelength behavior of the normal modes from symmetry considerations. A study is made of the conditions under which the branches of the phonon dispersion relations will approach definite frequencies in the long-wavelength limit. Finally, a number of examples are presented which illustrate the preceding analysis.

### I. INTRODUCTION

The presence of Coulomb interactions in an infinite lattice has a marked effect on its lattice dynamics at long wavelengths. Neither the dynamical matrix nor the phonon dispersion relations have well-defined values at infinite wavelength for such lattices. In fact, in some cases, a branch of the dispersion relations will not even approach a definite frequency (independent of the direction of the propagation vector) as the propagation vector approaches zero.[1] The standard methods of group theory used to analyze the behavior of the dispersion relations at long wavelengths must

By using (A13) and (A14) it also follows that

$$W^{k-2}_{\nu_{k-1}\alpha'}(s_{k-1}) = \frac{1}{(m-1)!} \sum_{r \in S_{2m-2}} I^{k-2\,r}_{\nu_{k-1}\alpha'}(s_{k-1}) \tag{A26}$$

because $k - 2 = 2(m-1)$. Now, if one last quantity $N_{\alpha\nu_{k-1}}(s_k)$ is defined by

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### I. INTRODUCTION

The presence of Coulomb interactions in an infinite lattice has a marked effect on its lattice dynamics at long wavelengths. Neither the dynamical matrix nor the phonon dispersion relations have well-defined values at infinite wavelength for such lattices. In fact, in some cases, a branch of the dispersion relations will not even approach a definite frequency (independent of the direction of the propagation vector) as the propagation vector approaches zero.[1] The standard methods of group theory used to analyze the behavior of the dispersion relations at long wavelengths must

be modified when Coulomb interactions are present.[2] In this paper we give a mathematical analysis of the long-wavelength behavior of the phonon dispersion relations for such lattices. The analysis applies to point ion models[3] in the harmonic approximation. This work is a generalization of earlier work on simple cubic lattices[4] and lattices of the NaCl and CaCl structures.[5]

We begin our analysis in Sec. II by forming the dynamical matrix[6] for a lattice whose particles interact harmonically through a potential varying with distance $r$ as $r^{-p}$, where temporarily it is assumed that $p > 1$. In Sec. III we review some symmetry properties of dynamical matrices for crystals in which long-range forces are absent. Then in Sec. IV we show how these symmetry properties must be modified at long wavelengths in the limit of $p = 1$. In spite of these modifications, a great deal of information about the long-wavelength behavior of the dispersion relations for crystals with Coulomb interactions can still be obtained from symmetry considerations. These methods are developed in Secs. V–VII. In Secs. VIII and IX we derive conditions under which the branches of the dispersion relations will approach definite frequencies (independent of direction) as the propagation vector approaches zero. Finally, in Secs. X–XII several examples are presented which illustrate the mathematical results developed in Secs. IV–IX.

## II. THE SYSTEMS TO BE ANALYZED

Although the primary purpose of this paper is to study the behavior of the dispersion relations at long wavelengths for a large variety of infinite crystal lattices in which Coulomb interactions exist between particles, we begin by assuming that, in addition to short-range forces, the particles interact through potentials varying with distance $r$ as $r^{-p}$, where $p > 1$. Then we assume that lattices in which Coulomb interactions are present are to be treated by letting $p \to 1$ in our initial results. The reasons for proceeding in this manner will be made clear in Sec. IV.

Consider a lattice with $f$ particles per unit cell with equilibrium positions $\mathbf{x}(l\kappa) = \mathbf{x}(l) + \mathbf{x}(\kappa)$, where $\kappa = 1, 2, \ldots, f$. We choose $a$ to be some typical dimension for a unit cell and define the dimensionless equilibrium position $\boldsymbol{\eta}(l\kappa)$ by $\boldsymbol{\eta}(l\kappa) = \mathbf{x}(l\kappa)/a$. The corresponding dimensionless displacement of a particle from equilibrium is denoted by $\mathbf{u}(l\kappa)$. Suitable Cartesian coordinates are imbedded in the lattice along which vectors are resolved into components.

The particles interact harmonically through short-range forces and through forces derived from long-range potentials. The long-range potentials are such that the potential energy (due to long-range interactions) of the $\kappa_0$th particle in the zeroth cell is

$$V^L = a^{-p} G \sum_{l,\kappa}{}' Z_\kappa Z_{\kappa_0} \times \left[\sum_i (\eta_i(l\kappa) + u_i(l\kappa) - \eta_i(0\kappa_0) - u_i(0\kappa_0))^2\right]^{-p/2}. \quad (1)$$

The prime on the summation sign indicates that $l, \kappa = 0, \kappa_0$ is to be omitted from the sum. In the limit of $p = 1$, we identify $G$ with the electronic charge squared and $Z_\kappa$ with the fraction of an electronic charge on the $\kappa$th particle. Since the net charge per cell is zero, we set

$$\sum_\kappa Z_\kappa = 0. \quad (2)$$

We choose the normal mode solutions to the equations of motion for the lattice in the harmonic approximation to be of the form

$$u_i(l\kappa) = (\mu_\kappa)^{-1/2} \Psi_i(\kappa, \boldsymbol{\phi}) \exp[2\pi i \boldsymbol{\phi} \cdot \boldsymbol{\eta}(l\kappa) - i\omega(\boldsymbol{\phi})t], \quad (3)$$

where $\boldsymbol{\phi}$ is a dimensionless propagation vector, $\omega(\boldsymbol{\phi})$ is the frequency, and $\mu_\kappa = m_\kappa/m$, where $m_\kappa$ is the mass of the $\kappa$th particle and $m$ is some typical particle mass. Substituting Eq. (3) into the equations of motion, we obtain the following eigenvector equation giving the dispersion relations and normal mode eigenvectors for the lattice:

$$\sum_{j,\kappa} C_{ij}(\kappa_0\kappa|\boldsymbol{\phi})\Psi_j(\kappa;\boldsymbol{\phi}) = \lambda(\boldsymbol{\phi})\Psi_i(\kappa_0;\boldsymbol{\phi}). \quad (4)$$

In the above equation $\lambda(\boldsymbol{\phi}) = a^{p+2} m\omega^2(\boldsymbol{\phi})/G$, the elements $C_{ij}(\kappa_0\kappa|\boldsymbol{\phi})$ form a $3f$-dimensional, Hermitian, dynamical matrix[7] $\mathbf{C}(\boldsymbol{\phi})$, and the elements $\Psi_j(\kappa;\boldsymbol{\phi})$ form a $3f$-component vector $\boldsymbol{\Psi}(\boldsymbol{\phi})$.

We shall order the elements of $\mathbf{C}(\boldsymbol{\phi})$ according to the rule $(i\kappa_0) < (j\kappa)$ if $\kappa_0 < \kappa$ or if $\kappa_0 = \kappa$ and $i < j$. Such an ordering automatically breaks $\mathbf{C}(\boldsymbol{\phi})$ into $f^2$ $3 \times 3$ submatrices $\mathbf{C}_{\kappa_0\kappa}(\boldsymbol{\phi})$ consisting of elements with the same ordered pair $\kappa_0\kappa$; and, at the same time, it breaks the column matrix for $\boldsymbol{\Psi}(\boldsymbol{\phi})$ into three-component column matrices (vectors) $\boldsymbol{\Psi}_\kappa(\boldsymbol{\phi})$. Throughout this and the following paper, we shall use Greek subscripts to denote such submatrices and use Roman subscripts to denote particular elements of such submatrices.

We may express $\mathbf{C}(\boldsymbol{\phi})$ in the form

$$\mathbf{C}(\boldsymbol{\phi}) = \mathbf{C}^S(\boldsymbol{\phi}) + \mathbf{C}^L(\boldsymbol{\phi}), \quad (5)$$

where $\mathbf{C}^L(\boldsymbol{\phi})$ gives the contribution of the long-range interactions and $\mathbf{C}^S(\boldsymbol{\phi})$ gives the contribution of the short-range forces. The eigenvectors of $\mathbf{C}(\boldsymbol{\phi})$ span a $3f$-dimensional linear vector space. We shall denote this space by the symbol $S_{3f}$ (total).

## III. SOME SYMMETRY PROPERTIES OF LATTICES

Before beginning our analysis, we briefly mention some symmetry properties which are known to hold for infinite lattices in the absence of long-range interactions. Here we draw mainly from a review article by Maradudin and Vosko.[8] [We have made some minor changes in their equations because the dynamical matrix $\mathbf{C}(\boldsymbol{\phi})$ which follows from Eq. (3) differs slightly from that used in Ref. 8.] The space group for a crystal consists of elements $\{\mathbf{R}|\boldsymbol{\nu}(\mathbf{R}) + \boldsymbol{\eta}(l)\}$. The $3 \times 3$ orthogonal matrices $\mathbf{R}$ form the point group of the space group of the lattice (henceforth referred to as the point group for the lattice). The symbol $\boldsymbol{\eta}(l) = \mathbf{x}(l)/a$ represents a translation vector for the crystal and $\boldsymbol{\nu}(\mathbf{R})$ represents a vector smaller than any primitive translation.

Construct the $3f \times 3f$ matrices $\boldsymbol{\Lambda}(\boldsymbol{\phi};\{\mathbf{R}|\boldsymbol{\nu}(\mathbf{R})\})$ defined by

$$\Lambda_{ij}(\kappa\kappa'|\boldsymbol{\phi};\{\mathbf{R}|\boldsymbol{\nu}(\mathbf{R})\}) = R_{ij}\delta(\kappa, F_0(\kappa', \mathbf{R})) \exp[-2\pi i \mathbf{R}\boldsymbol{\phi} \cdot \boldsymbol{\nu}(\mathbf{R})], \quad (6)$$

where $F_0(\kappa', \mathbf{R})$ is the index denoting the type of posi-

tion into which a particle originally in a position of type $\kappa'$ is brought by the space group operation. It can then be shown that

$$\mathbf{\Lambda}(\boldsymbol{\phi};\{\mathbf{R}|\boldsymbol{\nu}(\mathbf{R})\})\mathbf{C}(\boldsymbol{\phi})\mathbf{\Lambda}^{\dagger}(\boldsymbol{\phi};\{\mathbf{R}|\boldsymbol{\nu}(\mathbf{R})\}) = \mathbf{C}(\mathbf{R}\boldsymbol{\phi}). \quad (7)$$

In order to gain information concerning the eigenvalues and eigenvectors of $\mathbf{C}(0)$ (the dynamical matrix at $\boldsymbol{\phi} = 0$), construct the $3f \times 3f$ matrices $T(0;\mathbf{R})$ defined by

$$T_{ij}(\kappa\kappa'|0;\mathbf{R}) = R_{ij}\,\delta(\kappa, F_0(\kappa',\mathbf{R})). \quad (8)$$

These matrices form a representation of the point group for the lattice, and it follows from Eqs. (6) and (7) that each $\mathbf{T}(0;\mathbf{R})$ commutes with $\mathbf{C}(0)$. Thus, by resolving the representation $\{\mathbf{T}(0;\mathbf{R})\}$ into irreducible representations of the point group for the lattice, we may determine the degeneracies of the various branches of the phonon dispersion relations at $\boldsymbol{\phi} = 0$. If the eigenvectors of $\mathbf{C}(0)$ are transformed by the $\mathbf{T}(0;\mathbf{R})$, sets of eigenvectors transform among themselves according to these irreducible representations. The projection operator to the subspace of $S_{3f}$ (total) spanned by eigenvectors transforming according to the $s$th irreducible representation is given by

$$\mathbf{P}^{(s)}(0) = (n_s/g)\sum_{\mathbf{R}} \chi^{(s)*}(0;\mathbf{R})\mathbf{T}(0;\mathbf{R}), \quad (9)$$

where $\chi^{(s)}(0;\mathbf{R})$ is the character of $\mathbf{R}$ in the $s$th irreducible representation, $g$ is the order of the point group for the lattice, and $n_s$ is the dimension of the $s$th irreducible representation.

Let $\mathbf{C}_{\kappa\nu}(0)$ be a $3 \times 3$ submatrix of $\mathbf{C}(0)$. Because of the invariance of the total force on any atom under a rigid translation of the crystal, these submatrices must obey the relation

$$\sum_{\kappa} \mu_{\kappa}^{1/2}\mathbf{C}_{\kappa\nu}(0) = \sum_{\nu} \mu_{\nu}^{1/2}\,\mathbf{C}_{\kappa\nu}(0) = 0. \quad (10)$$

The existence of three independent acoustic modes follows from this property. Finally, we point out that $\mathbf{C}(0)$ is a real, symmetric matrix.

## IV. BEHAVIOR OF THE DYNAMICAL MATRIX AT LONG WAVELENGTHS AS $p \to 1$

The elements of $\mathbf{C}^S(\boldsymbol{\phi})$ are analytic functions of $\boldsymbol{\phi}$, since they are given by finite sums [of the same form as in Eq. (A1)]. In Appendix A we list expressions for the elements of $\mathbf{C}^L(\boldsymbol{\phi})$, which are obtained from Eq. (1). The elements are not analytic functions of $\boldsymbol{\phi}$ at $\boldsymbol{\phi} = 0$; however, expansions for them about $\boldsymbol{\phi} = 0$ may be obtained by using Ewald's method.[1] These expansions are in the form of a nonanalytic term plus a power series in the components of $\boldsymbol{\phi}$ and are discussed in Appendix B. From Appendix B it is easily seen that if $1 < p < 2$ [or $1 < p < 3$ for $\mathbf{C}(\boldsymbol{\phi})$ real], then the behavior of $\mathbf{C}(\boldsymbol{\phi})$ near $\boldsymbol{\phi} = 0$ is given by

$$\mathbf{C}(\boldsymbol{\phi}) = \mathbf{A} + k\boldsymbol{\phi}^{p-1}\mathbf{N}(\hat{\boldsymbol{\phi}}) + \text{remainder}, \quad (11)$$

where the remainder can be neglected for sufficiently small $\boldsymbol{\phi}$. The matrices $\mathbf{A}$ and $\mathbf{N}(\hat{\boldsymbol{\phi}})$ are real and symmetric. The matrix $\mathbf{N}(\hat{\boldsymbol{\phi}})$ is composed of $3 \times 3$ submatrices $\mathbf{N}_{\kappa\nu}(\hat{\boldsymbol{\phi}})$ defined by

$$\mathbf{N}_{\kappa\nu}(\hat{\boldsymbol{\phi}}) = (\mu_\kappa\mu_\nu)^{-1/2}Z_\kappa Z_\nu\mathbf{L}(\hat{\boldsymbol{\phi}}), \quad (12)$$

where

$$\mathbf{L}(\hat{\boldsymbol{\phi}}) = \phi^{-2}\begin{bmatrix}\phi_1^2 & \phi_1\phi_2 & \phi_1\phi_3\\ \phi_1\phi_2 & \phi_2^2 & \phi_2\phi_3\\ \phi_1\phi_3 & \phi_2\phi_3 & \phi_3^2\end{bmatrix}. \quad (13)$$

The constant $k$ is defined by

$$k = 2p\pi^{p+1/2}\,\frac{\Gamma(-\frac{1}{2}p + \frac{3}{2})}{\Gamma(\frac{1}{2}p + 1)}\,\frac{a^3}{v_a}, \quad (14)$$

where $v_a$ is the volume of a unit cell and $a$ is the typical cell dimension introduced in Sec. II.

If $p > 1$, then the term $k\boldsymbol{\phi}^{p-1}\mathbf{N}(\hat{\boldsymbol{\phi}})$ in Eq. (11) goes to zero as $\boldsymbol{\phi}$ approaches zero. Thus, $\mathbf{C}(0)$ is well defined by $\mathbf{C}(0) = \mathbf{A}$, and $\mathbf{A}$ has all of the symmetry properties of a dynamical matrix at $\boldsymbol{\phi} = 0$ discussed in Sec. III.

In the limiting case of $p = 1$, the term $k\boldsymbol{\phi}^{p-1}\mathbf{N}(\hat{\boldsymbol{\phi}})$ is not defined at $\boldsymbol{\phi} = 0$. The value approached depends upon the relative rates at which $\boldsymbol{\phi}$ and $p$ approach zero and one respectively, and upon the direction from which $\boldsymbol{\phi}$ approaches zero. Thus, the dynamical matrix is not defined at $\boldsymbol{\phi} = 0$ for infinite lattices in which Coulomb interactions are present, and we exclude this single point from our analysis. For any other $\boldsymbol{\phi}$, $k\boldsymbol{\phi}^{p-1}\mathbf{N}(\hat{\boldsymbol{\phi}})$ approaches the well-defined value $(4\pi a^3/v_a)\mathbf{N}(\hat{\boldsymbol{\phi}})$ as $p$ approaches one. However, the latter matrix cannot be neglected in comparison to $\mathbf{A}$ no matter how small we make the value of $\boldsymbol{\phi} > 0$. Thus, the long-wavelength behavior of the normal modes of crystals with Coulomb interactions is not governed by $\mathbf{A}$ alone but by a matrix $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ defined by

$$\mathbf{C}^0(\hat{\boldsymbol{\phi}}) = \mathbf{A} + (4\pi a^3/v_a)\mathbf{N}(\hat{\boldsymbol{\phi}}). \quad (15)$$

The term $(4\pi a^3/v_a)\mathbf{N}(\hat{\boldsymbol{\phi}})$ is equivalent to the macroscopic electric dipole field contribution to the dynamical matrix first derived by Born.[1]

We saw above that when $p > 1$, the matrix $\mathbf{A}$ has all of the symmetry properties of a dynamical matrix at $\boldsymbol{\phi} = 0$ discussed in Sec. III. Referring to Appendix B, we see that the elements of $A$ vary continuously as we let $p \to 1$. It follows that $\mathbf{A}$ must still possess these symmetry properties in the limit of $p = 1$. In particular, the matrix $\mathbf{A}$ in Eq. (15) obeys Eq. (7) with $\boldsymbol{\phi} = 0$ in the form

$$\mathbf{\Lambda}(0;\{\mathbf{R}|\boldsymbol{\nu}(\mathbf{R})\})\mathbf{A}\,\mathbf{\Lambda}^{\dagger}(0;\{\mathbf{R}|\boldsymbol{\nu}(\mathbf{R})\}) = \mathbf{A}, \quad (16)$$

and obeys Eq. (10) in the form

$$\sum_{\kappa} \mu_{\kappa}^{1/2}\mathbf{A}_{\kappa\nu} = \sum_{\nu} \mu_{\nu}^{1/2}\,\mathbf{A}_{\kappa\nu} = 0. \quad (17)$$

Further, the eigenvalues and eigenvectors of $\mathbf{A}$ may still be studied using the group theoretical analysis of Sec. III. However, we again emphasize that the long-wavelength behavior of the normal modes is now governed by $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ and not by $\mathbf{A}$.

We could now proceed with our analysis of lattices with Coulomb interactions by either of two routes. We might attempt to study the long-wavelength behavior of their normal modes by directly considering symmetry properties of $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$. However, we shall take the alternative route of studying how conclusions based upon the properties of $\mathbf{A}$ are to be modified because of the presence of the macroscopic field term $(4\pi a^3/v_a)\mathbf{N}(\hat{\boldsymbol{\phi}})$.

## V. PROPERTIES OF THE LONG-WAVELENGTH DYNAMICAL MATRIX FOR THE COULOMB CASE

If Coulomb interactions are present in a lattice, then the long-wavelength eigenvalues $\lambda^0(\hat{\phi})$ and eigenvectors $\Psi^0(\hat{\phi})$ are solutions of the eigenvector equation

$$\mathbf{C}^0(\hat{\phi})\Psi^0(\hat{\phi}) = (\mathbf{A} + (4\pi a^3/v_a)\mathbf{N}(\hat{\phi}))\Psi^0(\hat{\phi}) = \lambda^0(\hat{\phi})\Psi^0(\hat{\phi}). \quad (18)$$

The matrix $\mathbf{C}^0(\hat{\phi})$ is real and symmetric; and, thus, its eigenvectors span $S_{3f}$(total). If two or more branches of the dispersion relations become degenerate in the long-wavelength limit, Eq. (18) will not give their long-wavelength eigenvectors but only a subspace of $S_{3f}$ (total) in which they lie. However, many qualitative properties of these eigenvectors can be deduced from knowledge of this subspace.

Since both of the matrices $\mathbf{A}$ and $\mathbf{N}(\hat{\phi})$ are real and symmetric, their eigenvectors also span $S_{3f}$ (total). The eigenvalues and eigenvectors of $\mathbf{A}$ are given by

$$\mathbf{A}\Psi^a = \lambda^a\Psi^a. \quad (19)$$

Because $\mathbf{A}$ obeys Eq. (17), it has a threefold degenerate eigenvalue of zero. The corresponding eigenvectors (the acoustic modes of $\mathbf{A}$) are represented by $3f$-component column matrices consisting of three-component submatrices $\Psi_\kappa$ which are of the form

$$\Psi_\kappa = \mu_\kappa^{1/2}\psi, \quad (20)$$

where $\psi$ is an arbitrary three-component vector. The acoustic modes of $\mathbf{A}$ occupy a three-dimensional subspace $S_3$(acoustic) of $S_{3f}$(total). This subspace is the first of several subspaces of $S_{3f}$(total) which will be defined in this paper. To aid the reader, we list each such subspace together with its qualitative description in Table I.

Next we consider some properties of $\mathbf{N}(\hat{\phi})$. Using Eqs. (2) and (12), we see that

$$\sum_\kappa \mu_\kappa^{1/2}\mathbf{N}_{\kappa\nu} = \sum_\nu \mu_\nu^{1/2}\mathbf{N}_{\kappa\nu} = 0. \quad (21)$$

It follows from Eq. (15) that the acoustic modes of $\mathbf{A}$ are also acoustic modes for $\mathbf{C}^0(\hat{\phi})$. In order to determine the eigenvectors of $\mathbf{N}(\hat{\phi})$, we first determine those of the matrix $\mathbf{L}(\hat{\phi})$ which appears in Eq. (12). Using Eq. (13), we see that

$$\mathbf{L}(\hat{\phi})\hat{\phi} = \hat{\phi}. \quad (22)$$

Let $\hat{\eta}(\hat{\phi})$ be a three-component transverse vector. Again using Eq. (13), we find

$$\mathbf{L}(\hat{\phi})\hat{\eta}(\hat{\phi}) = 0. \quad (23)$$

Thus, any three-component transverse (longitudinal) vector is an eigenvector of $\mathbf{L}(\hat{\phi})$ corresponding to the eigenvalue zero (one).

It follows from Eqs. (12) and (23) that any transverse, $3f$-component vector $\Psi^t(\hat{\phi})$ will be an eigenvector of $\mathbf{N}(\hat{\phi})$ corresponding to the eigenvalue zero. There are $2f$ independent vectors of this type in $S_{3f}$ (total). Next consider the longitudinal vectors. In the long-wavelength limit any $3f$-component, longitudinal vector $\Psi^l(\hat{\phi})$ will consist of three-component submatrices of the form

$$\Psi_\kappa^l(\hat{\phi}) = \psi_\kappa^l(\hat{\phi})\hat{\phi}, \quad (24)$$

where $\psi_\kappa^l(\hat{\phi})$ is an arbitrary scalar function. With the aid of Eqs. (12) and (22), we find that

$$(\mathbf{N}(\hat{\phi})\Psi^l(\hat{\phi}))_\kappa = \sum_\nu (\mu_\kappa\mu_\nu)^{-1/2}Z_\kappa Z_\nu\Psi_\nu^l(\hat{\phi}). \quad (25)$$

From the above equation, it is clear that any $\Psi^l(\hat{\phi})$ obeying the equation

$$\sum_\kappa \mu_\kappa^{-1/2}Z_\kappa\Psi_\kappa^l(\hat{\phi}) = 0 \quad (26)$$

will be an eigenvector of $\mathbf{L}(\hat{\phi})$ corresponding to the eigenvalue zero. There are $f-1$ linearly independent longitudinal vectors in $S_{3f}$ (total) satisfying Eq. (26), and physically they represent vibrational modes which are longitudinal and produce no change in the electric dipole moment per cell in the long-wavelength limit. Thus, the eigenvalue zero of $\mathbf{N}(\hat{\phi})$ is $(3f-1)$-fold degenerate and the corresponding eigenvectors occupy a $(3f-1)$-dimensional subspace of $S_{3f}$ (total). We shall denote this subspace by the symbol $S_{3f-1}(\lambda_N = 0; \hat{\phi})$.

We must determine one more independent eigenvector of $\mathbf{N}(\hat{\phi})$. Define the normalized longitudinal vector $\Psi^{ln}(\hat{\phi})$ by

$$\Psi_\kappa^{ln}(\hat{\phi}) = \left(\sum_\nu \mu_\nu^{-1}Z_\nu^2\right)^{-1/2}\mu_\kappa^{-1/2}Z_\kappa\hat{\phi}. \quad (27)$$

Using Eq. (25), we see that $\Psi^{ln}(\hat{\phi})$ is an eigenvector of $\mathbf{N}(\hat{\phi})$ corresponding to the eigenvalue $\sum_\nu Z_\nu^2/\mu_\nu$ and is thus the additional vector required. Clearly $\Psi^{ln}(\hat{\phi})$ is a unit vector normal to the subspace $S_{3f-1}(\lambda_N = 0; \hat{\phi})$. The projection operator of $S_{3f}$ (total) onto $\Psi^{ln}(\hat{\phi})$ is $(\sum_\nu Z_\nu^2/\mu_\nu)^{-1}\mathbf{N}(\hat{\phi})$. It follows that the projection operator to the subspace $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ is given by

$$\mathbf{P}(S_{3f-1}(\lambda_N = 0; \hat{\phi})) = \mathbf{I} - \left(\sum_\nu Z_\nu^2/\mu_\nu\right)^{-1}\mathbf{N}(\hat{\phi}), \quad (28)$$

TABLE I. Summary of subspaces and vectors.

| Space or vector | Description(s) |
|---|---|
| $S_{3f}$ (total) | The space of normal mode eigenvectors |
| $S_3$ (acoustic) | The subspace spanned by long-wavelength acoustic mode vectors |
| $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ | The subspace spanned by the eigenvectors of $\mathbf{N}(\hat{\phi})$ corresponding to the eigenvalue zero; the subspace of long-wavelength eigenvectors (for the given $\hat{\phi}$) whose longitudinal components produce no change in the electric dipole moment per cell |
| $S_{3f-2}(\lambda_M = 0; \hat{\phi})$ | The subspace spanned by the eigenvectors of $\mathbf{M}(\hat{\phi})$ corresponding to the eigenvalue zero; the subspace of long-wavelength eigenvectors (for the given $\hat{\phi}$) whose transverse components produce no change in the electric dipole moment per cell |
| $S_{3f-3}$ (zero) | The subspace of vectors contained in $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ for all $\hat{\phi}$ |
| | The intersection of $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ and $S_{3f-2}(\lambda_M = 0; \hat{\phi})$; the subspace of long-wavelength eigenvectors which produce no change in the electric dipole moment per cell |
| $\Psi^{ln}(\phi)$ | The unit normal to $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ |
| $S_3$ (normal) | The subspace of vectors normal to $S_{3f-3}$ (zero); the subspace of all vectors parallel to $\Psi^{ln}(\phi)$ for some $\hat{\phi}$ |

where **I** is the $3f \times 3f$ unit matrix

## VI. CRITERIA FOR DETERMINING EIGENVALUES AND EIGENVECTORS OF $\mathbf{C}^0(\hat{\phi})$ FROM THOSE OF THE MATRIX A

In Sec. IV we saw that the matrix **A** possesses all of the symmetry properties of a dynamical matrix at $\phi = 0$ for a lattice in which Coulomb interactions are absent. It is, thus, of interest to compare the eigenvectors $\Psi^a$ and eigenvalues $\lambda^a$ of **A** with those of $\mathbf{C}^0(\hat{\phi})$.

We first consider under what circumstances an eigenvector $\Psi^a$ of **A** will be an eigenvector of $\mathbf{C}^0(\hat{\phi})$ for a particular $\hat{\phi}$. From the treatment in Sec. V, it is clear that we have the following cases;

(1) If $\Psi^a \in S_{3f-1}(\lambda_N = 0; \hat{\phi})$, then $\Psi^a$ is also an eigenvector of $\mathbf{C}^0(\hat{\phi})$ with the same eigenvalue $\lambda^a$.

(2) If $\Psi^a = \text{const} \times \Psi^{ln}(\hat{\phi})$, then $\Psi^a$ is also an eigenvector of $\mathbf{C}^0(\hat{\phi})$. However, it follows from Eq. (18) and the discussion following Eq. (27) that the corresponding eigenvalue of $\mathbf{C}^0(\hat{\phi})$ is not $\lambda^a$ but instead is $\lambda^a + (4\pi a^3/v_a)\sum_\kappa (Z_\kappa^2/\mu_\kappa)$.

(3) If neither case (1) nor case (2) holds true, then $\Psi^a$ is not an eigenvector of $\mathbf{C}^0(\hat{\phi})$.

In the preceding paragraph we regard $\hat{\phi}$ as having some fixed value. We now discuss conditions under which eigenvectors of **A** will be eigenvectors of $\mathbf{C}^0(\hat{\phi})$ for all $\hat{\phi}$. Notice that as $\hat{\phi}$ varies, the subspace $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ and its normal $\Psi^{ln}(\hat{\phi})$ vary. As $\hat{\phi}$ takes on all possible values, the vectors parallel to $\Psi^{ln}(\hat{\phi})$ fill out a three-dimensional subspace of $S_{3f}$ (total) consisting of all vectors $\Psi$ of the form

$$\Psi_\kappa = \mu_\kappa^{-1/2} Z_\kappa \psi, \tag{29}$$

where $\psi$ is an arbitrary three-component vector. We denote this subspace by $S_3$ (normal). It follows that there is a $(3f-3)$-dimensional subspace of $S_{3f}$ (total) which is contained in $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ for all $\hat{\phi}$. This subspace is the subspace of all vectors orthogonal to every vector in $S_3$ (normal). We denote it by the symbol $S_{3f-3}$ (zero), and it follows from Eq. (29) that $\Psi \in S_{3f-3}$ (zero) if and only if its three-component submatrices $\Psi_\kappa$ obey the relation

$$\sum_\kappa \mu_\kappa^{-1/2} Z_\kappa \Psi_\kappa = 0. \tag{30}$$

Physically, a $\Psi$ obeying Eq. (30) is a long-wavelength mode which produces no change in the electric dipole moment per cell.

We can now state some important cases under which eigenvectors of **A** will be eigenvectors of $\mathbf{C}^0(\hat{\phi})$ for all $\hat{\phi}$.

### Case (a)

If $\Psi^a$ is an eigenvector of **A** with the eigenvalue $\lambda^a$ and if $\Psi^a \in S_{3f-3}$ (zero), then $\Psi^a$ is an eigenvector of $\mathbf{C}^0(\hat{\phi})$ corresponding to the same eigenvalue $\lambda^a$ for all $\hat{\phi}$.

### Case (b)

Assume **A** has a $q$-fold degenerate eigenvalue $\lambda^a$. The eigenvectors corresponding to this degenerate eigenvalue span a $q$-dimensional subspace $S_q$ of $S_{3f}$ (total). If this subspace is contained in $S_{3f-3}$ (zero), these eigenvectors of **A** are also eigenvectors of $\mathbf{C}^0(\hat{\phi})$ for all $\hat{\phi}$. Even if the above is not true, the intersection of $S_q$ with $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ must be at least $(q-1)$-dimensional for each $\hat{\phi}$.[9] Thus, for each $\hat{\phi}$ we can construct $q-1$ mutually orthogonal eigenvectors of **A** which lie in $S_{3f-1}(\lambda_N = 0; \hat{\phi})$, and these vectors will be eigenvectors of $\mathbf{C}^0(\hat{\phi})$ corresponding to the eigenvalue $\lambda^a$. (Of course, perturbation theory must be used to determine the proper vectors if $q - 1 > 1$.) As $\hat{\phi}$ varies, these vectors vary and trace out the long-wavelength behavior of the normal modes for $q-1$ branches of the dispersion relations. Each of these branches approaches the frequency $\lambda^a$ in the long-wavelength limit.

### Case (c)

Assume that, as in Case (b), **A** has a $q$-fold degenerate eigenvalue $\lambda^a$, where now $q \geq 3$, and $S_q$ contains $S_3$ (normal). Then for each $\hat{\phi}$ there is an eigenvector of **A** which is parallel to $\Psi^{ln}(\hat{\phi})$ and is, therefore, an eigenvector of $\mathbf{C}^0(\hat{\phi})$ corresponding to the eigenvalue $\lambda^a + (4\pi a^3/v_a)\sum_\kappa Z_\kappa^2/\mu_\kappa$. In addition we can construct $q-1$ independent eigenvectors of **A** which are orthogonal to $\Psi^{ln}(\hat{\phi})$ and, therefore, lie in $S_{3f-1}(\lambda_N = 0; \hat{\phi})$ for each $\hat{\phi}$. These vectors will be eigenvectors of $\mathbf{C}^0(\hat{\phi})$ corresponding to the eigenvalue $\lambda^a$. In the long-wavelength limit the dispersion relations for the lattice will contain one branch approaching a frequency corresponding to the former eigenvalue and $q-1$ branches approaching a frequency corresponding to the latter eigenvalue. The branch approaching the higher eigenvalue will become purely longitudinal in this limit.

The standard methods of group theory discussed in Secs. III and IV can be applied to determine the degeneracies of the eigenvalues of **A** and to gain information concerning the subspaces of $S_{3f}$ (total) in which the corresponding eigenvectors lie. The results in Cases (a)–(c) can then be applied in order to gain information about the eigenvalues and eigenvectors of $\mathbf{C}^0(\hat{\phi})$.

## VII. SOME CONSEQUENCES OF CASE (a)

In this section we give some useful results which follow immediately from the discussion under Case (a) of Sec. VI.

Consider the acoustic mode vectors of **A**. Using Eqs. (2), (20), and (30), we see that these eigenvectors lie in $S_{3f-3}$ (zero). It follows from Case (a) that the acoustic mode vectors of **A** are also acoustic mode vectors of $\mathbf{C}^0(\hat{\phi})$. (The same result was obtained more directly in Sec. V.)

Next assume that **A** is invariant under the transposition $(\kappa_0 \nu_0)$ of two particular indices of its submatrices. (That is, $\mathbf{A}_{\nu_0\nu_0} = \mathbf{A}_{\kappa_0\kappa_0}$, $\mathbf{A}_{\kappa_0\nu_0} = \mathbf{A}_{\nu_0\kappa_0}$, and $\mathbf{A}_{\kappa_0\lambda} = \mathbf{A}_{\nu_0\lambda}$ if $\lambda \neq \nu_0$ or $\kappa_0$.) Further, assume that $Z_{\kappa_0} = Z_{\nu_0}$ and $\mu_{\kappa_0} = \mu_{\nu_0}$. Then, using Eq. (19) and the fact that **A** is real and symmetric, one can easily show that **A** has three linearly independent eigenvectors, each of the general form

$$\Psi_\lambda = 0 \quad \text{if } \lambda \neq \kappa_0 \text{ or } \nu_0, \qquad \text{and} \qquad \Psi_{\nu_0} = -\Psi_{\kappa_0}. \tag{31}$$

Clearly these eigenvectors obey Eq. (30) and lie in $S_{3f-3}$ (zero), so that the discussion under Case (a) is applicable. These eigenvectors of $\mathbf{A}$ are also eigenvectors of $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ with the same eigenvalues.

More generally, if $\mathbf{A}$ is invariant under the product of $n$ independent transpositions of indices of its submatrices, $(\kappa_1\nu_1)(\kappa_2\nu_2)\cdots(\kappa_n\nu_n)$ with $Z_{\kappa_j} = Z_{\nu_j}$ and $\mu_{\kappa_j} = \mu_{\nu_j}$, then $\mathbf{A}$ has $3n$ independent eigenvectors of the general form

$$\Psi_\lambda = 0 \quad \text{if } \lambda \neq \kappa_j \text{ or } \nu_j, \qquad \text{and} \qquad \Psi_{\kappa_j} = -\Psi_{\nu_j}. \tag{32}$$

Again Eq. (30) is satisfied and Case (a) is applicable. All $3n$ eigenvectors of $\mathbf{A}$ are eigenvectors of $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ with the same eigenvalues.

## VIII. DIRECTIONAL DEPENDENCE OF THE FREQUENCY AT LONG WAVELENGTHS

Suppose we start with a solution $\Psi^0(\hat{\boldsymbol{\phi}})$ of Eq. (18) for a particular $\hat{\boldsymbol{\phi}}$. If we now vary $\hat{\boldsymbol{\phi}}$ continuously, then $\Psi^0(\hat{\boldsymbol{\phi}})$ varies continuously and traces out the long-wavelength behavior of the normal modes for a particular branch of the frequency spectrum. In general, it is possible that $\lambda^0(\hat{\boldsymbol{\phi}})$ will also vary as we trace out the branch. In such a case, the branch will not approach a definite frequency as $\phi$ approaches zero, but instead the value approached will depend upon the direction from which $\phi$ approaches zero.

In order to study the directional dependence of $\lambda^0(\hat{\boldsymbol{\phi}})$, we must first determine how $\mathbf{N}(\hat{\boldsymbol{\phi}})$ and $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ vary as $\hat{\boldsymbol{\phi}}$ varies. If $\hat{\boldsymbol{\phi}}$ is rotated to $\hat{\boldsymbol{\phi}}'$, then $\hat{\boldsymbol{\phi}}' = \mathbf{R}\hat{\boldsymbol{\phi}}$, where $\mathbf{R}$ is a three-dimensional orthogonal matrix. The set of all $\mathbf{R}$ forms an irreducible representation $O(3)$ of the rotation group. Using Eq. (13), we find that

$$\mathbf{L}(\mathbf{R}\hat{\boldsymbol{\phi}}) = \mathbf{R}\mathbf{L}(\hat{\boldsymbol{\phi}})\mathbf{R}^{-1}. \tag{33}$$

It then follows from Eq. (12) that

$$\mathbf{N}(\mathbf{R}\hat{\boldsymbol{\phi}}) = \boldsymbol{\Theta}\mathbf{N}(\hat{\boldsymbol{\phi}})\boldsymbol{\Theta}^{-1}, \tag{34}$$

where $\boldsymbol{\Theta}$ is a $3f \times 3f$ matrix consisting of $3 \times 3$ submatrices given by

$$\boldsymbol{\Theta}_{\kappa\nu} = \delta_{\kappa\nu}\mathbf{R}. \tag{35}$$

Since $\mathbf{A}$ is independent of $\hat{\boldsymbol{\phi}}$, we find that

$$\mathbf{C}^0(\mathbf{R}\hat{\boldsymbol{\phi}}) = \mathbf{A} + (4\pi a^3/v_a)\boldsymbol{\Theta}\mathbf{N}(\hat{\boldsymbol{\phi}})\boldsymbol{\Theta}^{-1}. \tag{36}$$

An immediate result of Eq. (36) is that $\mathrm{Tr}[\mathbf{C}^0(\mathbf{R}\hat{\boldsymbol{\phi}})] = \mathrm{Tr}[\mathbf{C}^0(\hat{\boldsymbol{\phi}})]$ for all $\mathbf{R}$. Thus, even if $\lambda^0(\hat{\boldsymbol{\phi}})$ depends upon the direction for some branches, the sum over all branches $\sum_{j=1}^{3f}\lambda_j^0(\hat{\boldsymbol{\phi}})$ is independent of $\hat{\boldsymbol{\phi}}$. This is the long-wavelength limit of a sum rule first discussed by Blackman[10] and later by other authors.[11,12]

A necessary and sufficient condition that $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ and $\mathbf{C}^0(\mathbf{R}\hat{\boldsymbol{\phi}})$ have the same spectrum of eigenvalues is that there exist a matrix $\mathbf{Q}(\mathbf{R}, \hat{\boldsymbol{\phi}})$ such that

$$\mathbf{C}^0(\mathbf{R}\hat{\boldsymbol{\phi}}) = \mathbf{Q}(\mathbf{R}, \hat{\boldsymbol{\phi}})\mathbf{C}^0(\hat{\boldsymbol{\phi}})\mathbf{Q}^{-1}(\mathbf{R}, \hat{\boldsymbol{\phi}}). \tag{37}$$

Suppose that $\mathbf{R}$ is an element of the point group for the lattice. The matrix $\mathbf{N}(\hat{\boldsymbol{\phi}})$ is invariant under any permutation of indices of its submatrices if these indices correspond to particles having the same charge and mass. It then follows from Eqs. (37), (36), (16), and (8) that we can choose $\mathbf{Q}(\mathbf{R}, \hat{\boldsymbol{\phi}}) = \mathbf{T}(0, \mathbf{R})$ for any $\hat{\boldsymbol{\phi}}$. Thus, even if $\lambda^0(\hat{\boldsymbol{\phi}})$ depends upon $\hat{\boldsymbol{\phi}}$, $\lambda^0(\hat{\boldsymbol{\phi}})$ is invariant under a transformation of $\hat{\boldsymbol{\phi}}$ which is an element of the point group for the lattice.

A necessary and sufficient condition that all branches of the dispersion relations for a lattice approach definite values in the long-wavelength limit is that for some $\hat{\boldsymbol{\phi}}$ the matrix $\mathbf{Q}(\mathbf{R}, \hat{\boldsymbol{\phi}})$ exists for all $\mathbf{R} \in O(3)$. Thus, a sufficient (but not necessary) condition is that $\boldsymbol{\Theta}$ commute with $\mathbf{A}$ for all $\mathbf{R} \in O(3)$, for then we can choose $\mathbf{Q}(\mathbf{R}, \phi) = \mathbf{Q}(\mathbf{R}) = \boldsymbol{\Theta}$. The condition $\boldsymbol{\Theta}\mathbf{A} = \mathbf{A}\boldsymbol{\Theta}$ for all $\mathbf{R}$ is equivalent to the condition $\mathbf{R}\mathbf{A}_{\kappa\nu} = \mathbf{A}_{\kappa\nu}\mathbf{R}$ for all $\kappa$, $\nu$, and $\mathbf{R}$. It follows from one of Schur's lemmas[13] that the latter condition holds if and only if

$$\mathbf{A}_{\kappa\nu} = a_{\kappa\nu}\mathbf{I}, \tag{38}$$

where $a_{\kappa\nu}$ is a number and $\mathbf{I}$ is the $3 \times 3$ identity matrix. The point group for any lattice contains a subgroup for which the quantity $\delta(\kappa, F_0(\kappa', \mathbf{R}))$ in Eq. (6) equals $\delta_{\kappa\kappa'}$. Using Eq. (16), we see that if this subgroup contains the tetrahedral group $T$, then all submatrices $\mathbf{A}_{\kappa\nu}$ of $\mathbf{A}$ will obey Eq. (38). Thus, all branches of such lattices will approach definite frequencies in the long-wavelength limit. Examples are such structures as NaCl, CsCl, $CaF_2$, and ZnS.

The above sufficiency condition is too restrictive to be a necessary condition. For example, the following generalization can be made immediately. Suppose that $\mathbf{A}$ is not required by Eq. (16) to have the form of Eq. (38), but that a matrix $\mathbf{U}$ exists having the properties that $\mathbf{U}\mathbf{N}(\hat{\boldsymbol{\phi}})\mathbf{U}^{-1} = \mathbf{N}(\hat{\boldsymbol{\phi}})$ for all $\hat{\boldsymbol{\phi}}$ and that $\mathbf{U}\mathbf{A}\mathbf{U}^{-1}$ has the form given in Eq. (38). Then we can choose $\mathbf{Q}(\mathbf{R}, \hat{\boldsymbol{\phi}}) = \mathbf{Q}(\mathbf{R}) = \mathbf{U}^{-1}\boldsymbol{\Theta}\mathbf{U}$. It follows that all branches of the dispersion relations approach definite frequencies in the long-wavelength limit. An illustration of this case is given in Sec. XII.

## IX. DIRECTIONAL DEPENDENCE OF THE FREQUENCY FOR PARTICULAR BRANCHES AT LONG WAVELENGTHS

In Sec. VIII we considered the question of whether or not all branches of the dispersion relations for a given lattice approach definite frequencies in the long-wavelength limit. In this section we will derive a necessary and sufficient condition that a given single branch approach a definite frequency in this limit. A sufficient (but not necessary) condition follows immediately from the work in Secs. VI and VIII: A branch will approach a definite frequency in the long-wavelength limit if, in this limit, either its eigenvectors lie in $S_{3f-1}(\lambda_N = 0; \hat{\boldsymbol{\phi}})$ for all $\hat{\boldsymbol{\phi}}$ or are parallel to $\Psi^{ln}(\hat{\boldsymbol{\phi}})$ for all $\hat{\boldsymbol{\phi}}$.

We now derive a necessary and sufficient condition that the term $\lambda^0(\hat{\boldsymbol{\phi}})$ in Eq. (18) be independent of $\hat{\boldsymbol{\phi}}$ for a given branch of the dispersion relations. The $\Psi^0(\hat{\boldsymbol{\phi}})$ which give the long-wavelength behavior of the normal modes for a particular branch of the dispersion relations are solutions of Eq. (18) and vary continuously as $\hat{\boldsymbol{\phi}}$ varies continuously. Suppose that we make an infinitesimal rotation of $\hat{\boldsymbol{\phi}}$. According to Eq. (34), the matrix $\mathbf{N}(\hat{\boldsymbol{\phi}})$ in Eq. (18) is then transformed into $\boldsymbol{\Theta}\mathbf{N}(\hat{\boldsymbol{\phi}})\boldsymbol{\Theta}^{-1}$. Referring to Eq. (35) and remembering that the transformation is infinitesimal, we see

that $\Theta$ may be written in the form $\Theta = \mathbf{I} + \mathbf{E}$, where $\mathbf{I}$ is the $3f \times 3f$ identity matrix and $\mathbf{E}$ consists of $3 \times 3$ submatrices of the form

$$\mathbf{E}_{\kappa\nu} = \delta_{\kappa\nu}\epsilon, \tag{39}$$

where $\epsilon$ is an antisymmetric, infinitesimal matrix of the form

$$\epsilon = \begin{bmatrix} 0 & \gamma & -\beta \\ -\gamma & 0 & \alpha \\ \beta & -\alpha & 0 \end{bmatrix}. \tag{40}$$

Referring to Eq. (15) and neglecting second-order infinitesimal terms, we find that the change produced in $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ by an infinitesimal rotation of $\hat{\boldsymbol{\phi}}$ is given by

$$\delta\mathbf{C}^0(\hat{\boldsymbol{\phi}}) = (4\pi a^3/v_a)[\mathbf{E}\mathbf{N}(\hat{\boldsymbol{\phi}}) - \mathbf{N}(\hat{\boldsymbol{\phi}})\mathbf{E}]. \tag{41}$$

The resulting change $\delta\lambda^0(\hat{\boldsymbol{\phi}})$ in $\lambda^0(\hat{\boldsymbol{\phi}})$ is determined from first-order perturbation theory. It is given by

$$\delta\lambda^0(\hat{\boldsymbol{\phi}}) = \Psi^{0\dagger}(\hat{\boldsymbol{\phi}})[\delta\mathbf{C}^0(\hat{\boldsymbol{\phi}})]\Psi^0(\hat{\boldsymbol{\phi}}), \tag{42}$$

where we assume that $\Psi^0(\hat{\boldsymbol{\phi}})$ is normalized. A necessary and sufficient condition that $\lambda^0(\hat{\boldsymbol{\phi}})$ be independent of $\hat{\boldsymbol{\phi}}$ for the entire branch of the dispersion relations is that $\delta\lambda^0(\hat{\boldsymbol{\phi}}) = 0$ for all $\hat{\boldsymbol{\phi}}$ and for arbitrary values of the parameters $\alpha, \beta$, and $\gamma$ in Eq. (40). Using Eqs. (12), (39), and (42), we see that this condition reduces to the condition that

$$\sum_{\kappa,\nu} Z_\kappa Z_\nu \, (\mu_\kappa\mu_\nu)^{-1/2}\Psi_\kappa^{0\dagger}(\hat{\boldsymbol{\phi}})(\epsilon\mathbf{L}(\hat{\boldsymbol{\phi}}) - \mathbf{L}(\hat{\boldsymbol{\phi}})\epsilon)\Psi_\nu^0(\hat{\boldsymbol{\phi}}) = 0 \tag{43}$$

for all $\boldsymbol{\phi}, \alpha, \beta$, and $\gamma$.

Express $\Psi^0(\hat{\boldsymbol{\phi}})$ in the form of the sum of its longitudinal and transverse parts. That is, write

$$\Psi_\kappa^0(\hat{\boldsymbol{\phi}}) = \psi_\kappa^l(\hat{\boldsymbol{\phi}})\hat{\boldsymbol{\phi}} + \psi_\kappa^t(\hat{\boldsymbol{\phi}})\hat{\boldsymbol{\eta}}_\kappa(\hat{\boldsymbol{\phi}}), \tag{44}$$

where the functions $\psi_\kappa^l(\hat{\boldsymbol{\phi}})$ and $\psi_\kappa^t(\hat{\boldsymbol{\phi}})$ are scalars, and $\hat{\boldsymbol{\eta}}_\kappa(\hat{\boldsymbol{\phi}})$ is a unit, three-component, transverse vector. Using Eqs. (22), (23), (40), and (44), we find that Eq. (43) will hold for arbitrary $\alpha, \beta$, and $\gamma$ if and only if

$$\left[\sum_\kappa \mu_\kappa^{-1/2}Z_\kappa \psi_\kappa^l(\hat{\boldsymbol{\phi}})\hat{\boldsymbol{\phi}}\right] \times \left[\sum_\nu \mu_\nu^{-1/2}Z_\nu \psi_\nu^t(\hat{\boldsymbol{\phi}})\hat{\boldsymbol{\eta}}_\kappa(\hat{\boldsymbol{\phi}})\right] = 0, \tag{45}$$

where the symbol $\times$ is the usual cross product from vector analysis.

Equation (45) holds true if and only if either one or the other of the two factors vanishes. Thus, a branch of the dispersion relations will approach a definite frequency in the long-wavelength limit if and only if, for all $\hat{\boldsymbol{\phi}}$, either

$$\sum_\kappa \mu_\kappa^{-1/2}Z_\kappa \psi_\kappa^l(\hat{\boldsymbol{\phi}})\hat{\boldsymbol{\phi}} = 0, \tag{46}$$

or

$$\sum_\kappa \mu_\kappa^{-1/2}Z_\kappa \psi_\kappa^t(\hat{\boldsymbol{\phi}})\hat{\boldsymbol{\eta}}_\kappa(\hat{\boldsymbol{\phi}}) = 0. \tag{47}$$

Physically Eq. (46) states that, in the long-wavelength limit, the longitudinal part of the mode produces no net change in the electric dipole moment per cell, and Eq. (47) states the same thing for the transverse part of the mode. We emphasize that either the condition of Eq. (46) or the condition of Eq. (47), for all $\hat{\boldsymbol{\phi}}$, is sufficient.

Both of the situations mentioned in the first paragraph of this section are included in the above result. The condition that Eq. (46) hold true for all $\hat{\boldsymbol{\phi}}$ is equivalent to the condition that $\Psi^0(\hat{\boldsymbol{\phi}}) \in S_{3f-1}(\lambda_N = 0, \hat{\boldsymbol{\phi}})$ for all $\hat{\boldsymbol{\phi}}$. Any branch of the dispersion relations which is purely longitudinal in the long-wavelength limit satisfies Eq. (47) for all $\hat{\boldsymbol{\phi}}$. Thus, any vector parallel to $\Psi^{ln}(\hat{\boldsymbol{\phi}})$ for all $\hat{\boldsymbol{\phi}}$ satisfies this condition.

We conclude this section by deriving some properties of the subspace of $S_{3f}$ (total) consisting of vectors satisfying Eq. (47) for a particular $\hat{\boldsymbol{\phi}}$. Define the $3f \times 3f$ matrix $\mathbf{M}(\hat{\boldsymbol{\phi}})$ by

$$\mathbf{M}_{\kappa\nu}(\hat{\boldsymbol{\phi}}) = (\mu_\kappa\mu_\nu)^{-1/2}Z_\kappa Z_\nu \mathbf{T}(\hat{\boldsymbol{\phi}}), \tag{48}$$

where the matrix $\mathbf{T}(\hat{\boldsymbol{\phi}})$ is given by

$$\mathbf{T}(\hat{\boldsymbol{\phi}}) = \phi^{-2}\begin{bmatrix} \phi_2^2 + \phi_3^2 & -\phi_1\phi_2 & -\phi_1\phi_3 \\ -\phi_1\phi_2 & \phi_3^2 + \phi_1^2 & -\phi_2\phi_3 \\ -\phi_1\phi_3 & -\phi_2\phi_3 & \phi_1^2 + \phi_2^2 \end{bmatrix}. \tag{49}$$

The matrix $\mathbf{M}(\hat{\boldsymbol{\phi}})$ has properties analogous to those of $\mathbf{N}(\hat{\boldsymbol{\phi}})$ with the roles of transverse and longitudinal vectors reversed. The submatrix $\mathbf{T}(\hat{\boldsymbol{\phi}})$ obeys the equations

$$\mathbf{T}(\hat{\boldsymbol{\phi}})\hat{\boldsymbol{\phi}} = 0 \tag{50}$$

and

$$\mathbf{T}(\hat{\boldsymbol{\phi}})\hat{\boldsymbol{\eta}}(\hat{\boldsymbol{\phi}}) = \hat{\boldsymbol{\eta}}(\hat{\boldsymbol{\phi}}), \tag{51}$$

where $\hat{\boldsymbol{\eta}}(\hat{\boldsymbol{\phi}})$ is a unit, three-component, transverse vector. A vector satisfies Eq. (47) if and only if it is an eigenvector of $\mathbf{M}(\hat{\boldsymbol{\phi}})$ corresponding to the eigenvalue zero. Carrying out an analysis similar to that given in the last part of Sec. V, we find that there are $3f - 2$ independent vectors of this type. Thus, we denote the subspace of vectors obeying Eq. (47) by $S_{3f-2}(\lambda_M = 0; \hat{\boldsymbol{\phi}})$. [The matrix $\mathbf{M}(\hat{\boldsymbol{\phi}})$ also has the twofold degenerate eigenvalue $\sum_\kappa (Z_\kappa^2/\mu_\kappa)$ with corresponding eigenvectors of the form $\Psi_\kappa(\hat{\boldsymbol{\phi}}) \propto (Z_\kappa/\mu_\kappa^{1/2})\hat{\boldsymbol{\eta}}(\hat{\boldsymbol{\phi}})$.]

From the above discussion, we can easily construct a projection operator $\mathbf{P}(S_{3f-2}(\lambda_M = 0; \hat{\boldsymbol{\phi}}))$ to $S_{3f-2}(\lambda_M = 0; \hat{\boldsymbol{\phi}})$. It is given by

$$\mathbf{P}(S_{3f-2}(\lambda_M = 0; \hat{\boldsymbol{\phi}})) = \mathbf{I} - (\sum_\nu Z_\nu^2/\mu_\nu)^{-1}\mathbf{M}(\hat{\boldsymbol{\phi}}), \tag{52}$$

where $\mathbf{I}$ is the $3f \times 3f$ identity matrix. Finally, we note that the intersection of $S_{3f-1}(\lambda_N = 0; \hat{\boldsymbol{\phi}})$ and $S_{3f-2}(\lambda_M = 0; \hat{\boldsymbol{\phi}})$ is the subspace $S_{3f-3}$ (zero).

With this section we conclude our general mathematical development for this paper. In the following sections we apply some of the above results to specific examples.

## X. CRYSTALS WITH TWO PARTICLES PER CELL

For our first example we consider crystals having two particles per cell, where the point ion model is used. The space $S_{3f}$ (total) $= S_6$ (total) is six dimensional. There are three independent acoustic mode vectors which are of the general form given by Eq. (20) with $\kappa = 1$ and 2. There remain three independent optical mode vectors which must be orthogonal to the acoustic mode vectors and thus have the general form

$$\Psi = \begin{bmatrix} \mu_1^{-1/2}\psi \\ -\mu_2^{-1/2}\psi \end{bmatrix}, \tag{53}$$

where $\psi$ is a three-component vector.

We now consider the conditions under which an optical branch will approach a definite frequency as $\phi \to 0$. According to the discussion in Sec. IX, a necessary and sufficient condition that the above be true is that either $\Psi^0(\hat{\phi}) \in S_5(\lambda_N = 0; \hat{\phi})$ or $\Psi^0(\hat{\phi}) \in S_4(\lambda_M = 0; \hat{\phi})$ for all $\hat{\phi}$, where $\Psi^0(\hat{\phi})$ gives the long-wavelength behavior of the eigenvectors for the branch. The above condition is equivalent to stating that either $\mathbf{P}(S_5(\lambda_N = 0; \hat{\phi}))\Psi^0(\hat{\phi}) = \Psi^0(\hat{\phi})$ or $\mathbf{P}(S_4(\lambda_M = 0; \hat{\phi}))\Psi^0(\hat{\phi}) = \Psi^0(\hat{\phi})$ for all $\hat{\phi}$. Using Eqs. (28) and (52), we impose each of these conditions on a vector $\Psi^0(\hat{\phi})$ of the form given by Eq. (53) and obtain the following result: An optical branch for a crystal with two particles per cell (and Coulomb interactions) will approach a definite frequency in the long-wavelength limit if and only if, in that limit, the branch becomes either purely transverse or purely longitudinal.

Next we obtain eigenvalue equations for $\mathbf{A}$ and $\mathbf{C}^0(\hat{\phi})$ with vectors of the form given in Eq. (53). Attach the superscript $a$ to $\psi$ in Eq. (53) and substitute the result into Eq. (19). Using Eq. (17), we obtain the following result:

$$(1 + \mu_1/\mu_2)\mathbf{A}_{11}\psi^a = \lambda^a\psi^a. \tag{54}$$

Attach the superscript 0 to $\psi$ and substitute the result into Eq. (18). With the aid of Eqs. (2), (12), and (17), we find that

$$(1 + \mu_1/\mu_2)[\mathbf{A}_{11} + (4\pi a^3/v_a)(Z_1^2/\mu_1)\mathbf{L}]\psi^0(\hat{\phi}) = \lambda^0(\hat{\phi})\psi^0(\hat{\phi}). \tag{55}$$

From Eqs. (22) and (23), it follows that $\psi^0(\hat{\phi})$ will be a purely transverse or purely longitudinal solution of Eq. (55) if and only if it is also a solution of Eq. (54) for all $\hat{\phi}$. Thus, eigenvectors of $\mathbf{C}^0(\hat{\phi})$ which are transverse (longitudinal) for all $\hat{\phi}$ can be found by determining eigenvectors of $\mathbf{A}_{11}$ which are transverse (longitudinal) for all $\hat{\phi}$ and by substituting the results into Eq. (53).

In the remainder of this section we analyze the long-wavelength behavior of the optical branches for the various crystal symmetries. The two particles in each cell cannot be identical since $Z_1 = -Z_2$. Thus, the factor $\delta(\kappa, F_0(\kappa', \mathbf{R}))$ in Eq. (6) must equal $\delta_{\kappa\kappa'}$. Equation (16) then reduces to

$$\mathbf{R}\mathbf{A}_{11}\mathbf{R}^{\dagger} = \mathbf{A}_{11}, \tag{56}$$

where $\mathbf{R}$ is any element of the point group for the lattice. Equation (56) and the fact that $\mathbf{A}_{11}$ is real and symmetric can be used to determine the form imposed on $\mathbf{A}_{11}$ by the crystal symmetry.

If the point group for the lattice belongs to either the triclinic or monoclinic system, we find that $\mathbf{A}_{11}$ has three distinct eigenvalues (barring accidental degeneracy). But in this case the directions of the eigenvectors of Eq. (54) are fixed, and a vector which is transverse or longitudinal for all $\hat{\phi}$ cannot be a solution. Therefore, in the long-wavelength limit none of the optical modes approaches a definite frequency.

For crystals whose point groups fall into the trigonal, tetragonal, or hexagonal systems, we find that $\mathbf{A}_{11}$ may be reduced to the form

$$\mathbf{A}_{11} = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \gamma \end{bmatrix}, \tag{57}$$

where in all cases we chose the $z$ axis to be the principle rotational axis of the point group. Since $\mathbf{A}_{11}$ (and thus $\mathbf{A}$) has a twofold degenerate eigenvalue, the discussion under Case (b) of Sec. VI is applicable, and $\mathbf{C}^0(\hat{\phi})$ has at least one eigenvector lying in $S_5(\lambda_N = 0; \hat{\phi})$ for all $\hat{\phi}$. Clearly, one such vector is obtained by setting $\psi^0(\hat{\phi}) = \psi^a = \hat{\eta}^1(\hat{\phi})$ in Eq. (54), where

$$\hat{\eta}^1(\hat{\phi}) = (\phi_1^2 + \phi_2^2)^{-1/2}\begin{bmatrix} \phi_2 \\ -\phi_1 \\ 0 \end{bmatrix}. \tag{58}$$

The corresponding eigenvalue is $\lambda^0 = (1 + \mu_1/\mu_2)\alpha$. In the long-wavelength limit one optical branch is purely transverse and approaches a definite frequency given by the above value of $\lambda^0$. The two remaining solutions of Eq. (55) must be of the form $\psi^0(\hat{\phi}) = c_1\hat{\phi} + c_2\hat{\eta}^2(\hat{\phi})$, where $c_1$ and $c_2$ are constants and $\hat{\eta}^2(\hat{\phi})$ is a unit transverse vector orthogonal to $\hat{\eta}^1(\hat{\phi})$. Substituting this vector into Eq. (55), we obtain the eigenvalues

$$\lambda_{\pm}^0 = \tfrac{1}{2}(1 + \mu_1/\mu_2)\{(\alpha + \gamma + \Omega) \pm [(\alpha - \gamma - \Omega)^2 + 4(\alpha - \gamma)\Omega \sin^2\theta]^{1/2}\}, \tag{59}$$

where $\Omega = (4\pi a^3/v_a)(Z_1^2/\mu_1)$, and $\theta$ is the angle between $\hat{\phi}$ and the $z$ axis. Barring accidental degeneracy ($\alpha = \gamma$), the frequencies approached by these optical branches in the long-wavelength limit depend upon $\theta$. Neither branch is purely transverse or purely longitudinal in this limit.

Finally consider lattices whose point groups belong to the regular system. For such lattices, it follows from Eq. (56) that $\mathbf{A}_{11} = \alpha\mathbf{I}$. We can easily solve Eq. (55) for this case; however, in order to illustrate some of the material in the preceding sections, we instead give the following arguments. The matrix $\mathbf{A}$ has the threefold degenerate eigenvalue $(1 + \mu_1/\mu_2)\alpha$, and the corresponding eigenvectors span a three-dimensional subspace $S_3'$ of $S_6$ (total), where $S_3'$ is orthogonal to the subspace $S_3$ (acoustic). But in $S_6$ (total) the subspace $S_3$ (acoustic) coincides with $S_3$ (zero). Thus, $S_3'$ coincides with $S_3$ (normal), and the discussion under Case (c) of Sec. VI is applicable. One of the eigenvectors coincides with $\Psi^{ln}(\hat{\phi})$, defined by Eq. (27) with $\kappa = 1$ and 2, for all $\hat{\phi}$. The corresponding eigenvalue is $(1 + \mu_1/\mu_2)[\alpha + (4\pi a^3/v_a)(Z_1^2/\mu_1)]$. The remaining two eigenvectors lie in $S_5(\lambda_N = 0; \hat{\phi})$ and correspond to the eigenvalue $(1 + \mu_1/\mu_2)\alpha$. The latter two vectors are transverse, because $S_5(\lambda_N = 0; \hat{\phi})$ can contain only one longitudinal vector and this vector lies in $S_3$ (acoustic). Thus, in the long-wavelength limit all three optical branches

approach definite frequencies. Two branches become purely transverse and degenerate in this limit and the remaining branch becomes purely longitudinal.

## XI. THE WURTZITE STRUCTURE

For a second example consider point ion models for lattices having the Wurtzite structure. Such lattices consist of two geometrically identical, interpenetrating, hexagonal close-packed structures. The first consists of identical cations ($\kappa = 1$ and 2), and the second consists of identical anions ($\kappa = 3$ and 4). The two close-packed structures are displaced from each other in the direction perpendicular to the bases of the unit hexagonal prisms. There are four particles per unit cell, and thus $S_{3f}$ (total) $= S_{12}$ (total). The point group for the lattice is $C_{6v}$.

We imbed a Cartesian coordinate system in the lattice with the origin at the position of one of the cations (with $\kappa = 1$). The $z$ axis is chosen perpendicular to the base of a hexagonal prism. The $x$ axis intersects a vertex of the hexagon of particles with $\kappa = 1$ centered about the origin, and the $y$ axis bisects a side of the same hexagon. Then, using Eqs. (6) and (16) and the fact that $\mathbf{A}$ is real and symmetric, we find that the form for $\mathbf{A}$ required by symmetry is

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{A}_{13} & \mathbf{A}_{23} \\ \mathbf{A}_{12} & \mathbf{A}_{11} & \mathbf{A}_{23} & \mathbf{A}_{13} \\ \mathbf{A}_{13} & \mathbf{A}_{23} & \mathbf{A}_{33} & \mathbf{A}_{34} \\ \mathbf{A}_{23} & \mathbf{A}_{13} & \mathbf{A}_{34} & \mathbf{A}_{33} \end{bmatrix}, \tag{60}$$

where

$$\mathbf{A}_{\nu\kappa} = \mathbf{A}_{\kappa\nu} = \begin{bmatrix} \alpha_{\kappa\nu} & 0 & 0 \\ 0 & \alpha_{\kappa\nu} & 0 \\ 0 & 0 & \beta_{\kappa\nu} \end{bmatrix}. \tag{61}$$

In addition the $\mathbf{A}_{\kappa\nu}$ obey Eq. (17).

We must determine the long-wavelength behavior of the twelve branches of the dispersion relations. Three of these are acoustic mode branches, which lie in $S_9$ (zero). Equation (60) shows that $\mathbf{A}$ is invariant under a product of transpositions of its indices of the form (12)(34). It follows from the analysis in Sec. VII, that $\mathbf{A}$ and $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ have six additional linearly independent eigenvectors lying in $S_9$ (zero). According to Eq. (32), the general form of these vectors is given by

$$\Psi = \begin{bmatrix} \psi_1 \\ -\psi_1 \\ \psi_2 \\ -\psi_2 \end{bmatrix}, \tag{62}$$

where $\psi_1$ and $\psi_2$ are three component vectors. The corresponding eigenvectors and eigenvalues of $\mathbf{A}$ and $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ are easily found by substituting Eqs. (60), (61), and (62) into Eq. (19). We will not list the results here but point out that there are two twofold degenerate eigenvalues and two nondegenerate eigenvalues.

So far we have established that at least nine of the twelve branches of the dispersion relations approach definite frequencies in the long-wavelength limit. To study the three remaining branches, construct a general vector which is orthogonal to $S_3$ (acoustic) and to any vector of the form given in Eq. (62). The form of such a vector is

$$\Psi = \begin{bmatrix} \mu_3^{1/2}\psi \\ \mu_3^{1/2}\psi \\ -\mu_1^{1/2}\psi \\ -\mu_1^{1/2}\psi \end{bmatrix}, \tag{63}$$

where $\psi$ is a three-component vector.

Eigenvectors of $\mathbf{A}$ or of $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ of this form can be determined by substituting Eqs. (60), (61), and (63) into Eq. (19) or Eq. (18), respectively. Mathematically, the remainder of the problem is identical to the problem of determining the optical modes for a hexagonal (etc.) crystal with two particles per cell discussed in Sec. X. We find that for one eigenvector of $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$, $\psi$ in Eq. (63) is proportional to $\hat{\boldsymbol{\eta}}^1(\hat{\boldsymbol{\phi}})$ as defined in Eq. (58). The corresponding branch of the dispersion relations is purely transverse in the long-wavelength limit and approaches a definite frequency corresponding to $\lambda^0 = (1 + \mu_3/\mu_1)(\alpha_{33} + \alpha_{34})$. The remaining two branches of the dispersion relations are neither purely transverse nor longitudinal in this limit and do not approach definite frequencies. The eigenvalues of $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$ for these branches are given by

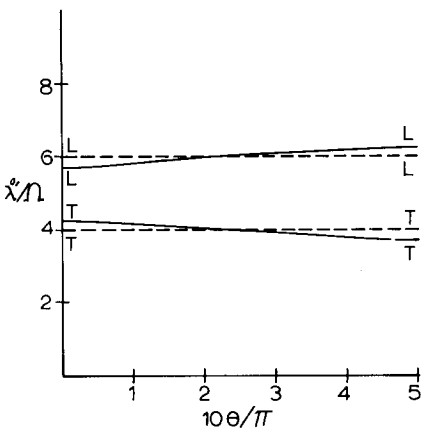


FIG. 1. $\lambda^0/\Omega$ as a function of $\theta$ for lattices of the wurtzite structure with $\lambda'_L + \lambda'_T = 10\Omega$. The solid line results from $\lambda'_L - \lambda'_T = (3/2)\Omega$ and the broken line from $\lambda'_L - \lambda'_T = 2\Omega$.

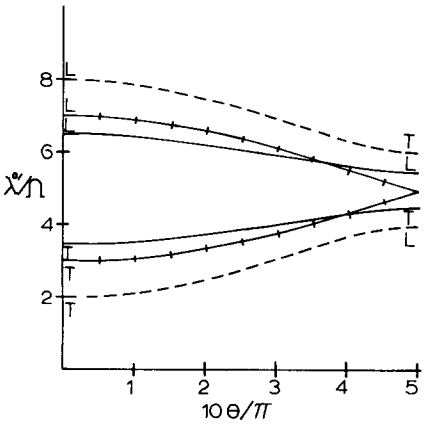


FIG. 2. $\lambda^0/\Omega$ as a function of $\theta$ for lattices of the wurtzite structure with $\lambda'_L + \lambda'_T = 10\Omega$. The solid line results from $\lambda'_L - \lambda'_T = 3\Omega$, the hatched line from $\lambda'_L - \lambda'_T = 4\Omega$, and the broken line from $\lambda'_L - \lambda'_T = 6\Omega$.

$$\lambda_{\pm}^{0\prime}(\hat{\phi}) = \tfrac{1}{2}(\lambda_L' + \lambda_T') \pm \tfrac{1}{2}[(\lambda_L' - \lambda_T')^2 + 8\Omega(\lambda_T' - \lambda_L' + 2\Omega)\sin^2\theta]^{1/2}, \quad (64)$$

where $\lambda^{0\prime} = \lambda^0/(1 + \mu_3/\mu_1)$, $\Omega = (4\pi a^3/v_a)(Z_1^2/\mu_3)$, $\lambda_T' = (\alpha_{33} + \alpha_{34})$, and $\lambda_L' = (\beta_{33} + \beta_{34}) + 2\Omega$. The quantity $\theta$ is the angle between $\hat{\phi}$ and the $z$ axis.

In Figs. 1 and 2 we illustrate the $\theta$-dependence of the two branches for some hypothetical models with $\lambda_L' + \lambda_T' = 10\Omega$ and with values of $\lambda_L' - \lambda_T'$ ranging between $(3/2)\Omega$ and $6\Omega$. The branches are either longitudinal or transverse at $\theta = 0$ and $\theta = \pi/2$, and this property is shown by an $L$ or $T$ on the graph. The model with $\lambda_L' - \lambda_T' = (3/2)\Omega$ is qualitatively similar to a model for Cadmium Sulfide studied by Nusimovici and Birman.[14] Finally notice that if $\lambda_L' - \lambda_T' = 2\Omega$, then both branches approach definite frequencies in the long-wavelength limit. In this case $(\alpha_{33} + \alpha_{34}) = (\beta_{33} + \beta_{34})$, and all three of the modes just analyzed become accidentally degenerate. The matrix **A** then has a threefold degenerate eigenvalue whose eigenvectors span $S_3$ (normal) and the discussion under Case (c) of Sec. VI becomes applicable.

## XII. THE CUBIC PEROVSKITE STRUCTURE

For a final example, we consider a lattice of the cubic perovskite structure. Such a lattice consists of three types of ions, $A$, $B$, and $C$. There is an ion of type $A$ ($\kappa = 1$) at the corner of each cube, an ion of type $B$ ($\kappa = 2$) at the center of each cube, and an ion of type $C$ ($\kappa = 3, 4$ and 5) at the center of each cube edge. Thus, there are five particles per unit cell and the space $S_{3f}$ (total) $= S_{15}$ (total) is fifteen dimensional. The point group for the lattice is $O_h$. We choose Cartesian coordinates along cube edges and, using Eq. (16), find that the form of **A** required by symmetry is

$$\mathbf{A} = \begin{bmatrix} \alpha\mathbf{I} & \beta\mathbf{I} & \mathbf{F}(\delta,\epsilon,\epsilon) & \mathbf{F}(\epsilon,\delta,\epsilon) & \mathbf{F}(\epsilon,\epsilon,\delta) \\ \beta\mathbf{I} & \gamma\mathbf{I} & \mathbf{F}(\zeta,\nu,\nu) & \mathbf{F}(\nu,\zeta,\nu) & \mathbf{F}(\nu,\nu,\zeta) \\ \mathbf{F}(\delta,\epsilon,\epsilon) & \mathbf{F}(\zeta,\nu,\nu) & \mathbf{F}(\sigma,\tau,\tau) & \mathbf{F}(\rho,\rho,\omega) & \mathbf{F}(\rho,\omega,\rho) \\ \mathbf{F}(\epsilon,\delta,\epsilon) & \mathbf{F}(\nu,\zeta,\nu) & \mathbf{F}(\rho,\rho,\omega) & \mathbf{F}(\tau,\sigma,\tau) & \mathbf{F}(\omega,\rho,\rho) \\ \mathbf{F}(\epsilon,\epsilon,\delta) & \mathbf{F}(\nu,\nu,\zeta) & \mathbf{F}(\rho,\omega,\rho) & \mathbf{F}(\omega,\rho,\rho) & \mathbf{F}(\tau,\tau,\sigma) \end{bmatrix}, \quad (65)$$

where

$$\mathbf{F}(x,y,z) = \begin{bmatrix} x & 0 & 0 \\ 0 & y & 0 \\ 0 & 0 & z \end{bmatrix}. \quad (66)$$

We now show that all branches of the dispersion relations approach definite frequencies as $\phi$ approaches zero. Define the matrix **U** by

$$\mathbf{U} = \begin{bmatrix} \mathbf{I} & 0 & 0 & 0 & 0 \\ 0 & \mathbf{I} & 0 & 0 & 0 \\ 0 & 0 & \mathbf{F}(1,0,0) & \mathbf{F}(0,1,0) & \mathbf{F}(0,0,1) \\ 0 & 0 & \mathbf{F}(0,1,0) & \mathbf{F}(0,0,1) & \mathbf{F}(1,0,0) \\ 0 & 0 & \mathbf{F}(0,0,1) & \mathbf{F}(1,0,0) & \mathbf{F}(0,1,0) \end{bmatrix}. \quad (67)$$

Using Eqs. (65), (66), and (67), we see that $\mathbf{UAU}^{-1}$ has the form given in Eq. (38). Further, using Eq. (12) and the fact that particles with $\kappa = 3$, 4, and 5 have equal charges and masses, one finds that $\mathbf{UN}(\hat{\phi})\mathbf{U}^{-1} = \mathbf{N}(\hat{\phi})$ for all $\hat{\phi}$. Referring to the last paragraph of Sec. VIII, we conclude that all branches of the dispersion relations approach definite frequencies in the long-wavelength limit.

We conclude this section by giving a qualitative discussion of the behavior of the fifteen branches of the dispersion relations as $\phi$ approaches zero. Using Eq. (8), we construct the matrices $\mathbf{T}(0;\mathbf{R})$ for the lattice. The resulting representation of the point group $O_h$ reduces to $4\Gamma_{15} \oplus \Gamma_{25}$. Since both of the irreducible representations $\Gamma_{15}$ and $\Gamma_{25}$ are three dimensional, the matrix **A** has five threefold degenerate eigenvalues. With the aid of Eq. (9), we construct a projection operator to the three-dimensional subspace of vectors in $S_{15}$ (total) transforming according to $\Gamma_{25}$. Then, operating upon a general vector with this projection operator, we find [with the aid of Eq. (30)] that any vector transforming according to $\Gamma_{25}$ lies in the subspace $S_{12}$ (zero); and, thus, the discussion under Case (a) of Sec. VI is applicable. Three branches of the dispersion relations for the lattice become degenerate as $\phi$ approaches zero. Using Eq. (19), we easily find that the frequency approached corresponds to $\lambda = \tau - \omega$.

The subspace of vectors transforming according to $\Gamma_{15}$ is the subspace of vectors orthogonal to all vectors transforming according to $\Gamma_{25}$. There are four sets of such vectors, each set corresponding to a threefold degenerate eigenvalue of **A**. One set provides three independent acoustic mode vectors for **A** which are also acoustic mode vectors for $\mathbf{C}^0(\hat{\phi})$. Consider any one of the remaining three sets of vectors. Since the corresponding eigenvalue $\lambda^a$ of **A** is threefold degenerate, the discussion under Case (b) of Sec. VI is applicable. For every $\hat{\phi}$ at least two linearly independent vectors from this set lie in $S_{14}(\lambda_N = 0;\hat{\phi})$ and are, therefore, eigenvectors of $\mathbf{C}^0(\hat{\phi})$ corresponding to the eigenvalue $\lambda^a$. We do not expect the entire set of vectors to lie in $S_{14}(\lambda_N = 0;\hat{\phi})$ for any $\hat{\phi}$ except accidentally, for if it did, a vector from the set could be found which lies both in $S_{14}(\lambda_N = 0;\hat{\phi})$ and $S_{13}(\lambda_M = 0;\hat{\phi})$.[9] But the intersection of $S_{14}(\lambda_N = 0;\hat{\phi})$ and $S_{13}(\lambda_M = 0;\hat{\phi})$ is $S_{12}$ (zero), and only the acoustic mode vectors and those transforming according to $\Gamma_{25}$ are required to lie in $S_{12}$ (zero) by symmetry. Thus, each of the remaining three sets of vectors (each set corresponding to a threefold degenerate eigenvalue of **A**) provides us with two linearly independent vectors corresponding to a twofold degenerate eigenvalue of $\mathbf{C}^0(\hat{\phi})$. [The eigenvalues are the same for **A** and $\mathbf{C}^0(\hat{\phi})$.] In the long-wavelength limit there are three sets of twofold degenerate branches of the dispersion relations.

There remain to be considered three eigenvectors of

$\mathbf{C}^0(\hat{\boldsymbol{\phi}})$. These are not required by symmetry to lie in $S_{14}(\lambda_N = 0; \hat{\boldsymbol{\phi}})$. Since in the long-wavelength limit the corresponding branches of the dispersion relations must approach definite frequencies, it follows from the work in Sec. IX that these vectors must lie in $S_{13}(\lambda_M = 0; \hat{\boldsymbol{\phi}})$. The branches will not be degenerate in the long-wavelength limit except by accident.

## XIII. CONCLUDING REMARKS

In this paper we considered the behavior of the dispersion relations only in the limit of infinite wavelengths. In order to obtain information about such properties as the contributions of the various branches to the phonon frequency spectrum in the long-wavelength limit, it is necessary to determine the behavior of the dispersion relations at somewhat shorter wavelengths. A general procedure for such an analysis is the following. Using methods outlined in Appendix B, we expand the dynamical matrix to second order in the form

$$\mathbf{C}(\boldsymbol{\phi}) = \mathbf{C}^0(\hat{\boldsymbol{\phi}}) + \mathbf{C}^1(\boldsymbol{\phi}) + \mathbf{C}^2(\boldsymbol{\phi}) + \text{remainder}, \quad (68)$$

where $\mathbf{C}^1(\boldsymbol{\phi})$ is purely imaginary and of first order in the components of $\boldsymbol{\phi}$ and $\mathbf{C}^2(\boldsymbol{\phi})$ is real and of second order. The forms of $\mathbf{C}^1(\boldsymbol{\phi})$ and $\mathbf{C}^2(\boldsymbol{\phi})$ for a given crystal symmetry can be determined by using Eq. (7). We regard $\mathbf{C}^1(\boldsymbol{\phi}) + \mathbf{C}^2(\boldsymbol{\phi})$ to be a perturbation of $\mathbf{C}^0(\hat{\boldsymbol{\phi}})$. The corrections to $\lambda^0(\hat{\boldsymbol{\phi}})$ given by perturbation theory determine the analytic behavior of $\lambda(\boldsymbol{\phi})$ in the neighborhood of $\boldsymbol{\phi} = 0$. So far, we have used this procedure to successfully analyze a limited number of cubic structures, including point ion and shell models. However, we do not consider our present results to be of sufficient generality to include them in this paper.

## APPENDIX A

The contribution of the long-range interactions to the dynamical matrix is given by

$$\mathbf{C}^L_{js}(\kappa_0\kappa\,|\,\boldsymbol{\phi}) = a^{p+2}G^{-1}\sum_l (\mu_{\kappa_0}\mu_\kappa)^{-1/2}\boldsymbol{\Phi}^L_{js}\begin{pmatrix}0 & l\\ \kappa_0 & \kappa\end{pmatrix} \times \exp[2\pi i\boldsymbol{\phi}\cdot\boldsymbol{\eta}(l\kappa\kappa_0)], \quad (A1)$$

where if $0, \kappa_0 \neq l, \kappa$, then

$$\Phi^L_{js}\begin{pmatrix}0 & l\\ \kappa_0 & \kappa\end{pmatrix} = pGZ_\kappa Z_{\kappa_0} a^{-(p+2)} \times \left[-(p+2)\eta_j(l\kappa\kappa_0)\eta_s(l\kappa\kappa_0)\left(\sum_i \eta_i^2(l\kappa\kappa_0)\right)^{-(p/2)-2} + \delta_{js}\left(\sum_i \eta^2(l\kappa\kappa_0)\right)^{-(p/2)-1}\right], \quad (A2)$$

and

$$\Phi^L_{js}\begin{pmatrix}0 & 0\\ \kappa_0 & \kappa_0\end{pmatrix} = -\sum_{l,\kappa\neq 0,\kappa_0}\Phi^L_{js}\begin{pmatrix}0 & l\\ \kappa_0 & \kappa\end{pmatrix}. \quad (A3)$$

After applying the Ewald transformation to Eq. (A1), we obtain the following results:

(1) If $\kappa \neq \kappa_0$, then

$$C^L_{js}(\kappa_0\kappa\,|\,\phi) = [p\pi^{(p/2)+1}/\Gamma(\tfrac{1}{2}p+1)][Z_{\kappa_0}Z_\kappa/(\mu_{\kappa_0}\mu_\kappa)^{1/2}] \times \Big[(2\pi a^3/v_a)\sum_h [\phi_j + \xi_j(h)][\phi_s + \xi_s(h)] \times \exp\{-2\pi i\boldsymbol{\xi}(h)\cdot[\boldsymbol{\eta}(\kappa) - \boldsymbol{\eta}(\kappa_0)]\} \times \Phi_{-1/2p+1/2}(\pi[\boldsymbol{\phi} + \boldsymbol{\xi}(h)]^2) - 2\pi\sum_l \eta_j(l\kappa\kappa_0) \times \eta_s(l\kappa\kappa_0)\exp[2\pi i\boldsymbol{\phi}\cdot\boldsymbol{\eta}(l\kappa\kappa_0)] \times \Phi_{(p/2)+1}(\pi\eta^2(l\kappa\kappa_0)) + \delta_{js}\sum_l \exp[2\pi i\boldsymbol{\phi}\cdot\boldsymbol{\eta}(l\kappa\kappa_0)] \times \Phi_{p/2}(\pi\eta^2(l\kappa\kappa_0))\Big]. \quad (A4)$$

(2) If $\kappa_0 = \kappa$, then

$$C^L_{js}(\kappa\kappa\,|\,\boldsymbol{\phi}) = B^L_{js}(\kappa\kappa\,|\,\boldsymbol{\phi}) - B^L_{js}(\kappa\kappa\,|\,0) - \sum_{\kappa'\neq\kappa}(\mu_{\kappa'}/\mu_\kappa)^{1/2}C^L_{js}(\kappa\kappa'\,|\,0). \quad (A5)$$

The quantity $B^L_{js}(\kappa\kappa\,|\,0)$ is given by

$$B^L_{js}(\kappa\kappa\,|\,0) = [p\pi^{(p/2)+1}/\Gamma(\tfrac{1}{2}p+1)](Z_\kappa^2/\mu_\kappa) \times \Big((2\pi a^3/v_a)\sum_h [\phi_j + \xi_j(h)][\phi_s + \xi_s(h)] \times \Phi_{-1/2p+1/2}(\pi[\boldsymbol{\phi} + \boldsymbol{\xi}(h)]^2) - 2\pi\sum_{l\neq 0}\eta_j(l) \times \eta_s(l)\exp[2\pi i\boldsymbol{\phi}\cdot\boldsymbol{\eta}(l)]\Phi_{(p/2)+1}(\pi\eta^2(l)) - (\tfrac{1}{2}p+1)^{-1}\delta_{js} + \delta_{js}\sum_{l\neq 0}\Phi_{p/2}(\pi\eta^2(l)) \times \exp[2\pi i\boldsymbol{\phi}\cdot\boldsymbol{\eta}(l)]\Big). \quad (A6)$$

The subscript $h$ indicates a summation over the reciprocal lattice, and $\boldsymbol{\xi}(h) = a\mathbf{y}(h)$, where $\mathbf{y}(h)$ is a reciprocal lattice vector. The function $\Phi_m(x)$ is an incomplete gamma function defined by

$$\Phi_m(x) = \int_1^\infty t^m e^{-xt}dt. \quad (A7)$$

## APPENDIX B

The elements of $C^S(\boldsymbol{\phi})$ are known to be analytic functions of $\boldsymbol{\phi}$ at $\boldsymbol{\phi} = 0$. Expressions for the expansion of $\Phi_m(x)$ from $x = 0$ into regions of positive $x$ are given in Appendix B of Ref. 4. Using these expansions and the relation $\Phi'_m(x) = -\Phi_{m+1}(x)$, we can obtain expansions of the elements of $\mathbf{C}^L(\boldsymbol{\phi})$ about $\boldsymbol{\phi} = 0$ from Eqs. (A4)–(A6). These expansions consist of a single nonanalytic term plus a power series in the components of $\boldsymbol{\phi}$. The constant and nonanalytic terms in the expansion for $1 < p < 3$ are given by the following equations:

(1) If $\kappa_0 \neq \kappa$, then

$$C^L_{js}(\kappa_0\kappa\,|\,\boldsymbol{\phi}) = C_{\kappa_0\kappa}(p)F_{js}(\boldsymbol{\eta}(\kappa_0) - \boldsymbol{\eta}(\kappa)) + Z_{\kappa_0}Z_\kappa(\mu_{\kappa_0}\mu_\kappa)^{-1/2}k_p\phi^{p-3}\phi_j\phi_s + \text{remaining power series terms.} \quad (B1)$$

(2) If $\kappa_0 = \kappa$, then

$$C^L_{js}(\kappa\kappa\,|\,\boldsymbol{\phi}) = -\sum_{\kappa'\neq\kappa}(\mu_{\kappa'}/\mu_\kappa)^{1/2}C^L_{js}(\kappa\kappa'\,|\,0) + Z_\kappa^2\mu_\kappa^{-1}k_p\phi^{p-3}\phi_j\phi_s + \text{remaining power series terms.} \quad (B2)$$

In the above equations,

$$k_p = 2p\pi^{p+1/2}\frac{\Gamma(-\frac{1}{2}p+\frac{3}{2})}{\Gamma(\frac{1}{2}p+1)}\frac{a^3}{v_a}, \tag{B3}$$

$$C_{\kappa_0\kappa}(p) = \frac{p\pi^{(p/2)+1}}{\Gamma(\frac{1}{2}p+1)}\frac{Z_{\kappa_0}Z_\kappa}{(\mu_{\kappa_0}\mu_\kappa)^{1/2}}, \tag{B4}$$

and

$$F_{js}(\boldsymbol{\eta}(\kappa_0)-\boldsymbol{\eta}(\kappa)) = (2\pi a^3/v_a)\sum_{h\neq 0}\xi_j(h)\xi_s(h) \times \exp\{-2\pi i\boldsymbol{\xi}(h)\cdot[\boldsymbol{\eta}(\kappa)-\boldsymbol{\eta}(\kappa_0)]\}\Phi_{-1/2p+1/2}(\pi\xi^2(h)) - 2\pi\sum_l \eta_j(l\kappa\kappa_0)\eta_s(l\kappa\kappa_0)\Phi_{(p/2)+1}(\pi\eta^2(l\kappa\kappa_0)) + \delta_{js}\sum_l \Phi_{p/2}(\pi\eta^2(l\kappa\kappa_0)). \tag{B5}$$


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# On the Finite Transformations of $SU(3)$


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The finite transformations in an arbitrary irreducible representation of the $SU(3)$ group are obtained by considering the reduced matrix elements of the operator $e^{-i\nu\lambda_4}$. The special case of $\nu = \frac{1}{2}\pi$ is also worked out and shown to be in agreement with earlier derivations. Symmetry properties and addition theorems for the resulting matrix elements are explicitly stated. As a useful application of the method, the finite transformations of the Weyl subgroup on the basis vectors of an arbitrary irreducible representation of $SU(3)$ are also given.


## 1. INTRODUCTION

Although the infinitesimal transformations of the $SU(3)$ have received considerable attention,[1] it is only in the past few years that the matrices of the finite transformations in an arbitrary irreducible representation of the group have begun to attract the attention of some authors.[2–4] A general element $U$ of the group was first parametrized in the form

$$U = D(\delta_1,\delta_2)U_{23}(\phi_2,\sigma_3)U_{12}(\theta_1,\sigma_2)U_{13}(\phi_1,\sigma_1) \tag{1.1}$$

by Murnaghan.[5] Here $D$ is a diagonal matrix with elements $\exp i\delta_1$, $\exp i\delta_2$, $\exp(-i\delta_1-i\delta_2)$, and $U_{pq}(\phi,\sigma)$ is a $3\times 3$ unitary unimodular matrix which, for instance for $p=1$, $q=2$ has the form

$$U_{12}(\phi,\sigma) = \begin{pmatrix} \cos\phi & -\sin\phi\,\exp(-i\sigma) & 0 \\ \sin\phi\,\exp(i\sigma) & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{1.2}$$

An alternative which is analogous to the $SU(2)$ Euler angle parametrization and which is more convenient for finding the finite transformations of $SU(3)$ has also been obtained recently by Nelson.[6] His result is

$$U = e^{-i\beta T_8}e^{-i\alpha_3 T_3}e^{-i\alpha_2 T_2}e^{-i\gamma T_3}e^{-i\nu\lambda_4}e^{i\gamma' T_3}e^{i\alpha'_2 T_2} \times e^{i\alpha'_3 T_3}, \tag{1.3}$$

where $T_8 = (1/\sqrt{3})\lambda_8$, $T_i = \frac{1}{2}\lambda_i$ $(i=1,2,3)$, and $\lambda_j$ are the Gell-Mann $SU(3)$ matrices.[1] Since $\lambda_3$ and $\lambda_8$ are diagonal it follows immediately that

$$\langle IMY|e^{-i\alpha_3 T_3}e^{-i\alpha_2 T_2}e^{-i\gamma T_3}|I'M'Y'\rangle = D^I_{MM'}(\alpha_3,\alpha_2,\gamma)\delta_{YY'}\delta_{II'}, \tag{1.4}$$

and

$$\langle IMY|e^{-i\beta T_8}|I'M'Y'\rangle = e^{-i\beta Y}\delta_{YY'}\delta_{II'}\delta_{MM'}. \tag{1.5}$$

$I$ is the isotopic spin, $M$ the third component of $I$, and $Y$ the hypercharge. Instead of $Y$ we shall, in the following, use the more convenient notation $\delta$, which is related to $Y$ by

$$\delta = \tfrac{1}{2}Y + \tfrac{1}{3}(p-q), \tag{1.6}$$

$p$ and $q$ being nonnegative integers characterizing an irreducible representation of the group.

Using Eqs. (1.4) and (1.5), the matrix elements of Equation (1.3) can be written as

$$k_p = 2p\pi^{p+1/2}\frac{\Gamma(-\frac{1}{2}p+\frac{3}{2})}{\Gamma(\frac{1}{2}p+1)}\frac{a^3}{v_a}, \tag{B3}$$

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$p$ and $q$ being nonnegative integers characterizing an irreducible representation of the group.

Using Eqs. (1.4) and (1.5), the matrix elements of Equation (1.3) can be written as

$$\langle IMY|U|I'M'Y'\rangle = e^{-i\beta Y}\sum_{M'',M'''} D^{I}_{MM''}(\alpha_3,\alpha_2,\gamma)\langle IM''Y|e^{-i\nu\lambda_4}|I'M'''Y'\rangle \times D^{I'}_{M'''M'}(-\gamma',-\alpha'_2,-\alpha'_3). \quad (1.7)$$

The problem then reduces to finding the matrix elements

$$D^{p,q}_{IMY,I'M'Y'}(\nu) = \langle IMY|e^{-i\nu\lambda_4}|I'M'Y'\rangle. \quad (1.8)$$

A number of authors[2-4] have carried out this calculation by observing that $e^{-i\nu\lambda_4}$ can be expressed as a product of three terms:

$$e^{-i\nu\lambda_4} = e^{-i(\pi/2)\lambda_6}e^{-i\nu\lambda_2}e^{i(\pi/2)\lambda_6} \quad (1.9)$$

and therefore evaluating the simpler matrix

$$E^{p,q}_{IMY,I'M'Y'} = \langle IMY|e^{i(\pi/2)\lambda_6}|I'M'Y'\rangle. \quad (1.10)$$

Because Chacón and Moshinsky[2] published their result as a letter, they had to be brief and could give hardly any details. Holland's result[3] was presented in a form which makes practical applications very difficult; we found Majumdar's and Basu's[4] approach not easy to follow. Taking these considerations into account and because our method seems more straightforward, we rederive in Sec. 2 the matrix elements $E^{p,q}_{IMY,I'M'Y'}$.

However, we believe that, the direct evaluation of $D^{p,q}_{IMY,I'M'Y'}(\nu)$ is no more difficult than that of the $E$-matrices. The details of this are presented in Sec. 3 where it is shown that the matrix elements can be expressed in an alternative way as a product of two Jacobi polynomials and a Clebsch–Gordan coefficient. The main results of the paper are Eqs. (2.11) and (3.11). In Sec. 4 we study the properties of $D^{p,q}_{IMY,I'M'Y'}(\nu)$ for special values of $\nu$. This enables us to write down the orthogonality property and various sum rules and addition theorems of the $E$-matrices. In Sec. 5, we consider the finite transformations of the Weyl subgroup of $SU(3)$ and use our method to obtain the effect of the Weyl reflections on the basis vectors of an arbitrary irreducible representations of $SU(3)$. Finally, in the Appendix, we derive a relationship between the Racah coefficient (which is essentially what the $E$ matrices are) and the generalized hypergeometric function ${}_4F_3(1)$. This relation may prove useful in applications to many-body problems.

## 2. THE $E^{p,q}_{IMY,I'M'Y'}$ MATRIX ELEMENTS

The orthonormal basis state of $SU(3)$ in the unitary irreducible representation $(p,q)$ is[7,8]

$$|p,q;jmY\rangle = |jm\delta\rangle = [(p+q+1)!p!q!]^{1/2}N_{jm\delta}\sum_r \frac{x^{j+\delta-r}(-\bar{x})^{j-m-r}y^r(\bar{y})^{m-\delta+r}z^{p-j-\delta}(\bar{z})^{q-j+\delta}}{(j+\delta-r)!(j-m-r)!r!(m-\delta+r)!(p-j-\delta)!(q-j+\delta)!} \quad (2.1)$$

where

$$N_{jm\delta} = \left(\frac{(2j+1)(j+m)!(j-m)!(j+\delta)!(j-\delta)!(p-j-\delta)!(q-j+\delta)!}{(p+j-\delta+1)!(q+j+\delta+1)!}\right)^{1/2} \quad (2.2)$$

and $\delta$ is as defined in Eq. (1.6).

From Eq. (2.1) one obtains the inverse relation

$$x^{j+\delta-r}(-\bar{x})^{j-m-r}y^r(\bar{y})^{m-\delta+r}z^{p-j-\delta}(\bar{z})^{q-j+\delta} = M_{j\delta mr}\sum_I \left(\frac{(p-I-\delta)!(q-I+\delta)!(q+I+\delta+1)!(p+I-\delta+1)!}{(j-I)!(j+I+1)!}\right)^{1/2} \times C\{\tfrac{1}{2}(j+\delta),\tfrac{1}{2}(j-\delta),I;\tfrac{1}{2}(j+\delta-2r),\tfrac{1}{2}(2m+2r-j-\delta),m\}|Im\delta\rangle, \quad (2.3)$$

where

$$M_{j\delta mr} = \left(\frac{(j+\delta-r)!(j-m-r)!r!(m-\delta+r)!}{p!q!(p+q+1)!}\right)^{1/2} \quad (2.4)$$

and $C(j_1j_2j;m_1m_2m)$ is the $SU(2)$ Clebsch–Gordan coefficient.[9]

From Eqs. (2.1) and (2.3) we obtain in a straightforward manner the matrix elements $E^{p,q}_{jm\delta,j'm'\delta'}$ as

$$E^{p,q}_{j'm'\delta',jm\delta} = \langle j'm'\delta|e^{i(\pi/2)\lambda_6}|jm\delta\rangle = N_{jm\delta}\left(\frac{(p-j'-\delta')!(q-j'+\delta')!(q+j'+\delta'+1)!(p+j'-\delta'+1)!}{(p-j-\delta)!(q-j+\delta)!}\right)^{1/2} \times \sum_r \frac{C\{\frac{1}{2}(p-r),\frac{1}{2}(q-m+\delta-r),j';\frac{1}{2}(2j+2\delta-p-r),\frac{1}{2}(m+\delta+q-2j+r),m'\}}{r!(m-\delta+r)![(j+\delta-r)!(j-m-r)!(p-j'-\delta'-r)!(p+j'-\delta'+1-r)!]^{1/2}} \quad (2.5)$$

with

$$2\delta' = p-q+m-\delta, \qquad m+\delta = m'+\delta'. \quad (2.6)$$

Substituting in Eq. (2.5) Racah's expression for the Clebsch–Gordan coefficients, viz.,

$$C(j_1j_2j_3;m_1m_2m_3)=\delta_{m_3,m_1+m_2}\left((2j_3+1)\frac{(j_1+j_2-j_3)!(j_3+j_1-j_2)!(j_3+j_2-j_1)!}{(j_1+j_2+j_3+1)!}\right)^{1/2}$$
$$\times[(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j_3+m_3)!(j_3-m_3)!]^{1/2}$$
$$\times\sum_s\frac{(-1)^s}{s!}[(j_1+j_2-j_3-s)!(j_1-m_1-s)!(j_2+m_2-s)!(j_3-j_2+m_1+s)!$$
$$\times(j_3-j_1-m_2+s)!]^{-1} \tag{2.7}$$

and using in Eq. (2.5), Eq. (2.6) and the relation

$$\sum_r\frac{1}{r!(m-\delta+r)!(p+j'+1-\delta'-r)!(p-\delta'-j'-s-r)!}$$
$$=\frac{(p+q+1-s)!}{(p+j'+1-\delta')!(q+\delta'-j'-s)!(p-\delta'-j'-s)!(q+j'+\delta'+1)!}, \tag{2.8}$$

we obtain the result

$$E^{p,q}_{j'm'\delta',jm\delta}=(-1)^{\delta'-m'}N_{jm\delta}N_{j'm'\delta'}$$
$$\times\sum_\nu\frac{(-1)^{p+q+\nu}(\nu+1)!}{(p+q-\nu)!(j+j'+p+m'-\delta-\nu)!(j+j'+q+\delta-m'-\nu)!}$$
$$\times\frac{1}{(\nu+\delta'-j'-p)!(\nu-j'-q-\delta')!(\nu-\delta-j-q)!(\nu+\delta-j-p)!}, \tag{2.9}$$

where we have replaced $s$ by

$$\nu=p+q-s=2p+m-\delta-2\delta'-s. \tag{2.10}$$

From (A1) we see that Eq. (2.9) can be written as a Racah coefficient. Thus

$$E^{p,q}_{j'm'\delta',jm\delta}=(-1)^{\delta'-m'}[(2j+1)(2j'+1)]^{1/2}$$
$$\times W(\tfrac{1}{2}(2\delta+q),\tfrac{1}{2}(p-\delta-m),\tfrac{1}{2}q;\tfrac{1}{2}(2\delta'+q);j',j)). \tag{2.11}$$

By virtue of Eq. (2.6) the above result can be written in various forms. This result is in agreement with those of Chacón and Moshinsky[2] and Majumdar and Basu.[4] Holland's result[3] is equivalent to our Eq. (2.5).

From Eq. (2.9), the following symmetry properties of the $E$ matrices are easily derived. Thus

$$E^{pq}_{j'm'\delta',jm\delta}=E^{qp}_{j'-m'-\delta',j-m-\delta}=(-1)^{2\delta-2\delta'}E^{pq}_{jm\delta,j'm'\delta'}. \tag{2.12}$$

Thus from Eqs. (1.9) and (2.11), it is a straightforward matter to write down the matrix elements $D^{p,q}_{IMY,I'M'Y'}$.

## 3. THE $D^{p,q}_{IMY,I'M'Y'}$ MATRIX ELEMENTS

The purpose of this section is to carry out the evaluation of the matrix elements (1.8) directly. Applying the operator $e^{-i\nu\lambda_4}$ to Eq. (2.1) is equivalent to the replacements

$$x\to x\cos\nu-iz\sin\nu,\qquad \bar{x}\to\bar{x}\cos\nu+i\bar{z}\sin\nu,$$
$$y\to y,\qquad \bar{y}\to\bar{y}, \tag{3.1}$$
$$z\to -ix\sin\nu+z\cos\nu,\qquad \bar{z}\to i\bar{x}\sin\nu+\bar{z}\cos\nu.$$

Thus

$$|jm\delta\rangle'=e^{-i\nu\lambda_4}|jm\delta\rangle=[p!q!(p+q+1)!]^{1/2}N_{jm\delta}$$
$$\times\sum_{r,a,b,c,d}\frac{(-1)^{2j+\delta-m-2r-a+c+b+d}(\cos\nu)^{a+b+p+q-2j-c-d}(i\sin\nu)^{2j+\delta-m+c+a-2r-a-b}}{r!a!b!c!d!(j+\delta-r-a)!(j-m-r-b)!(p-j-\delta-c)!}$$
$$\times\frac{x^{a+c}(-\bar{x})^{b+d}y^r(\bar{y})^{m-\delta+r}z^{p-r-a-c}(\bar{z})^{q+\delta-m-r-b-d}}{(q-j+\delta-d)!(m-\delta+r)!}. \tag{3.2}$$

With the choice

$$\delta'=\tfrac{1}{2}(a+c-b-d-m+\delta),\quad m'=\tfrac{1}{2}(a+c-b-d+m-\delta),$$
$$I'=\tfrac{1}{2}(a+c+b+d+m-\delta+2r),\quad m'-\delta'=m-\delta, \tag{3.3}$$

$x^{a+c}(-\bar{x})^{b+d}y^r(\bar{y})^{m-\delta+r}z^{p-r-a-c}(\bar{z})^{q-m+\delta-r-b-d}$ becomes $x^{I'+\delta'-r}(-\bar{x})^{I'-m'-r}y^r(\bar{y})^{m'-\delta'+r}z^{p-I'-\delta'}(\bar{z})^{q-I'+\delta'}$.

Observing that

$$\sum_a\sum_c=\sum_{a+c}\sum_{a-c=-(a+c)}^{a+c}=\sum_\alpha\sum_{t=-\alpha}^{\alpha}, \tag{3.4}$$

Equation (3.2) can now be written as

$$e^{-i\nu\lambda_4}|jm\delta\rangle = [p!q!(p+q+1)!]^{1/2}N_{jm\delta}$$
$$\times \sum_r \sum_{s,\alpha} \sum_{t=-\alpha}^{\alpha} \sum_{\beta=-s}^{s} \frac{(-1)^{2j-2r+\delta-m-t-s}(-i\cot\nu)^{t+\beta}(\cos\nu)^{p+q-2j}(i\sin\nu)^{2j+\delta-m-2r}}{r![\tfrac{1}{2}(\alpha+t)]![\tfrac{1}{2}(s+\beta)]![\tfrac{1}{2}(\alpha-t)]![\tfrac{1}{2}(s-\beta)]!(m-\delta+r)!}$$
$$\times \frac{x^{I'+\delta'-r}(-\bar{x})^{I'-m'-r}y^r(\bar{y})^{m'-\delta'+r}z^{p-I'-\delta'}(\bar{z})^{q-I'+\delta'}}{[j+\delta-r-\tfrac{1}{2}(\alpha+t)]![j-m-r-\tfrac{1}{2}(s+\beta)]![p-j-\delta-\tfrac{1}{2}(\alpha-t)]![q-j+\delta-\tfrac{1}{2}(s-\beta)]!}, \tag{3.5}$$

where $\alpha = s + m' + \delta'$, $m' - \delta' = m - \delta$, and $I' = s + m' + r$. (3.6)

From Eqs. (2.3) and (3.5), it follows immediately that

$$\langle j'm'\delta'|e^{-i\nu\lambda_4}|jm\delta\rangle = N_{jm\delta}[(p-j'-\delta')!(q-j'+\delta')!(j'+\delta'+q+1)!(j'-\delta'+p+1)!]^{1/2} \sum_{r,s,\alpha} \sum_{t=-\alpha}^{\alpha} \sum_{\beta=-s}^{s}$$
$$\times \frac{(-1)^{2j+\delta-m-2r+s+\beta}s!\alpha!(\cos\nu)^{p+q-2j}(i\sin\nu)^{2j-m+\delta-2r}(i\cot\nu)^{t+\beta}}{[\tfrac{1}{2}(\alpha+t)]![\tfrac{1}{2}(\alpha-t)]![\tfrac{1}{2}(s+\beta)]![\tfrac{1}{2}(s-\beta)]![r!s!\alpha!(r+\alpha-j'-\delta')!(r+\alpha+j'-\delta'+1)!(m'-\delta'+r)!]^{1/2}}$$
$$\times \frac{C\{\tfrac{1}{2}(r+\alpha), \tfrac{1}{2}(r+\alpha-2\delta'), j'; \tfrac{1}{2}(\alpha-r), \tfrac{1}{2}(m'-\delta'+r-s), m'\}}{[j+\delta-r-\tfrac{1}{2}(\alpha+t)]![p-j-\delta-\tfrac{1}{2}(\alpha-t)]![j-m-r-\tfrac{1}{2}(s+\beta)]![q-j+\delta-\tfrac{1}{2}(s-\beta)]}. \tag{3.7}$$

The $t$ and $\beta$ summations can be easily carried out. Since

$$y = \sum_n \frac{x^n}{n!(\alpha-n)!(\beta+n)!(\gamma-n)!} = \frac{1}{\alpha!\beta!\gamma!}\,{}_2F_1(-\alpha,-\gamma;\beta+1;x) \tag{3.8}$$

and $\alpha = s + m' + \delta'$, Eq. (3.7) becomes

$$\langle j'm'\delta'|e^{-i\nu\lambda_4}|jm\delta\rangle = N_{jm\delta}[(p-j'-\delta')!(q-j'+\delta')!(j'+\delta'+q+1)!(j'-\delta'+p+1)!]^{1/2}$$
$$\times \sum_{r,s} \frac{(\cos\nu)^{p+q-2j-m'-\delta'-2s}(-i\sin\nu)^{2j+2\delta'-2r+2s}}{[s!r!(s+m'+\delta')!(s+j'+m'+r+1)!(-j'+m'+r+s)!(m'-\delta'+r)!]^{1/2}}$$
$$\times \frac{C\{\tfrac{1}{2}(m'+\delta'+r+s), \tfrac{1}{2}(m'-\delta'+r+s), j'; \tfrac{1}{2}(m'+\delta'+s-r), \tfrac{1}{2}(m'-\delta'+r-s), m'\}}{(p-j-\delta-m'-\delta'-s)!(j+\delta-r)!(-j+\delta+q-s)!(j-m-r)!}$$
$$\times {}_2F_1(-m'-\delta'-s,-j-\delta+r;1+p-j-\delta-m'-\delta'-s;-\cot^2\nu)$$
$$\times {}_2F_1(-s,-j+m+r;1+q-j+\delta-s;-\cot^2\nu). \tag{3.9}$$

Equation (3.9) is the desired result. It can, however, be written in a more convenient form as follows. Since the Jacobi polynomial is related to ${}_2F_1$ by[10]

$$P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(n+\beta+1)}{n!\Gamma(\beta+1)}\,{}_2F_1\left(-n,-n-\alpha;\beta+1;\frac{x+1}{x-1}\right), \tag{3.10}$$

Eq. (3.9) can be expressed in the alternative form

$$D^{p,q}_{j'm'\delta',jm\delta}(\nu) = \frac{N_{jm\delta}[(p-j'-\delta')!(q-j'+\delta')!(j'+\delta'+q+1)!(j'-\delta'+p+1)!]^{1/2}}{(p-j-\delta)!(q-j+\delta)!}$$
$$\times \sum_{r,s}\left(\frac{s!(s+m'+\delta')!}{r!(m'-\delta'+r)!(j'+m'+1+s+r)!(-j'+m'+s+r)!}\right)^{1/2}$$
$$\times \frac{(\cos\nu)^{p+q-2j-m'-\delta'-2s}(-i\sin\nu)^{2j-2m'-2r-2s}}{(j-m-r)!(j+\delta-r)!}\, C\{\tfrac{1}{2}(m'+\delta'+s+r), \tfrac{1}{2}(m'-\delta'+s+r), j';$$
$$\tfrac{1}{2}(m'+\delta'+s-r), \tfrac{1}{2}(m'-\delta'+r-s), m'\}\, P_s^{(j-m-r-s,q-j+\delta-s)}(\cos 2\nu)P_{s+m'+\delta'}^{(j+\delta-m'-\delta'-r-s,p-j-\delta-m'-\delta'-s)}(\cos 2\nu). \tag{3.11}$$

This form will prove useful for the consideration of special values of the parameter $\nu$. It is, in fact, the one we shall adopt. However, since the Clebsch–Gordan coefficient is a ${}_3F_2(1)$ function, Eq. (3.11) can also be expressed in an equally convenient form as

$$D^{p,q}_{j'm'\delta',jm\delta}(\nu) = N_{jm\delta}N_{j'm'\delta'}\frac{(j'-\delta'+p+1)!(j'+\delta'+q+1)!}{(p-j-\delta)!(q-j+\delta)!}$$
$$\times \sum_{r,s} \frac{(\cos\nu)^{p+q-2j-m'-\delta'-2s}(-i\sin\nu)^{2j-2m'-2r-2s}s!(s+m'+\delta')!}{r!(j+\delta-r)!(j-m-r)!(j'+\delta'-r)!(j'-m'-r)!(-j'+m'+s+r)!}$$

$$\times \frac{{}_3F_2(-r, j'-m'-s-r, -m'+\delta'-r; j'+\delta'-r+1, j'-m'-r+1; 1)}{(s+r+j'+m'+1)!(m'-\delta'+r)!}$$
$$\times P_s^{(j-m-r-s,q-j+\delta+s)}(\cos 2\nu)\, P_{s+m'+\delta'}^{(j-m'+\delta-\delta'-r-s,p-j-\delta-m'-\delta'-s)}(\cos 2\nu). \quad (3.12)$$

*Note added in proof:* Equation (3.11) and its equivalent can be written in a more symmetrical form by means of the replacements $s \to s + \frac{1}{2}m' + \frac{1}{2}\delta'$ and $r \to j - \frac{1}{2}m + \frac{1}{2}\delta - r = j - \frac{1}{2}m' + \frac{1}{2}\delta' - r$.

## 4. SPECIAL CASES AND ADDITION THEOREM

An important check on our work is the evaluation of the special value of $\nu = -\pi/2$ in any of the three equations (3.9), (3.11), and (3.12). Using Eq. (3.11), we easily obtain the result

$$D^{p,q}_{j'm'\delta',jm\delta}(-\pi/2) = (-1)^{j+m+\delta-j'} E^{p,q}_{j'-m'\delta',jm\delta}, \quad (4.1)$$

which, as expected, is of the same form as Eq. (2.11). Also

$$D^{p,q}_{j'm'\delta',jm\delta}(\pi) = (-1)^{p+q+m-\delta} D^{p,q}_{j'm'\delta',jm\delta}(0)$$
$$= (-1)^{p+q+m-\delta}\, \delta_{j'j}\delta_{m'm}\delta_{\delta'\delta}. \quad (4.2)$$

Thus since $p + q + m - \delta$ is an integer, the $D$-matrix is periodic in $\nu$ with period $2\pi$.

The orthonormality condition of the $E$-matrices follows from Eq. (1.9). Using that equation, we have

$$\delta_{jj'}\delta_{mm'}\delta_{\delta\delta'} = \sum_{j''m''\delta''} (E^{p,q}_{jm\delta,j''m''\delta''})^{\dagger} E^{p,q}_{j''m''\delta'',j'm'\delta'}, \quad (4.3)$$

where the dagger denotes Hermitian conjugation. We then obtain the generalized form of the orthonormality property of the Racah coefficients,[11]

$$\delta_{jj'}\delta_{mm'}\delta_{\delta\delta'} = \sum_{j''} (2j''+1)[(2j+1)(2j'+1)]^{1/2}$$
$$\times W(\tfrac{1}{2}(2\delta+q), \tfrac{1}{2}(p-\delta-m), \tfrac{1}{2}q,$$
$$\tfrac{1}{2}(p+m'-\delta'); j'', j) W(\tfrac{1}{2}(2\delta'+q),$$
$$\tfrac{1}{2}(p-\delta'-m'), \tfrac{1}{2}q, \tfrac{1}{2}(p+m-\delta); j'', j'). \quad (4.4)$$

Again by putting $\nu = -\pi/2$ in Eq. (1.9) and using Eq. (4.1), we obtain the sum rule

$$(-1)^{j+m+\delta-j'} E^{p,q}_{j'-m'\delta',j-m,\delta} = \sum_{j''m''\delta''m''} (E^{p,q}_{j'm'\delta',j''m''\delta''})^{\dagger}$$
$$\times d^{j''}_{m''m''}(-\pi) \times E^{p,q}_{j''m'''\delta'',jm\delta}, \quad (4.5)$$

which in terms of the Racah coefficients reads

$$(-1)^{j-j'+m+\delta} W(\tfrac{1}{2}(2\delta+j), \tfrac{1}{2}(p-\delta+m),$$
$$\tfrac{1}{2}q, \tfrac{1}{2}(p-m-\delta); j', j)$$
$$= \sum_{j''} (-1)^{p-q-2\delta-j''}(2j''+1)$$
$$\times W(\tfrac{1}{2}(2\delta'+q), \tfrac{1}{2}(p-\delta'-m'), \tfrac{1}{2}q, \tfrac{1}{2}(p+m'-\delta');$$
$$j'', j') W(\tfrac{1}{2}(2\delta+q), \tfrac{1}{2}(p-\delta-m), \tfrac{1}{2}q, \tfrac{1}{2}(p+m-\delta);$$
$$j'', j). \quad (4.6)$$

Equations (4.4) and (4.6) are the usual sum rules of the Racah coefficients which have now appeared quite naturally in our analysis.

## 5. THE FINITE TRANSFORMATIONS OF THE WEYL SUBGROUP

As an application of the above method, we wish to consider the finite transformations of the Weyl subgroup on the basis states of an arbitrary irreducible representation of $SU(3)$, since this is probably the most immediately useful set of finite transformations of $SU(3)$.[12] As is well known, invariance under $SU(3)$ implies invariance under Weyl reflections.

The matrix representations of the Weyl reflections are denoted by $W_1$, $W_2$, $W_3$ and these are defined as

$$W_1 = -\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad W_2 = -\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad W_3 = -\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad (5.1)$$

where

$$W_1^2 = W_2^2 = W_3^2 = 1 \quad (5.2)$$

and

$$W_3 = W_1 W_2 W_1. \quad (5.3)$$

Thus the Weyl reflections and their distinct products form a discrete group of order 6, isomorphic to the symmetric group $S_3$ on three objects and called the Weyl group of $SU(3)$.

Having described the method of approach in detail in Secs. 3 and 4, it will suffice at this stage to state only the relevant results.

Thus using (5.1), we see that

$$W_1\colon (x, y, z, \bar{x}, \bar{y}, \bar{z}) \to (-y, -x, -z; -\bar{y}, -\bar{x}, -\bar{z}),$$
$$W_2\colon (x, y, z, \bar{x}, \bar{y}, \bar{z}) \to (-x, -z, -y; -\bar{x}, -\bar{z}, -\bar{y}),$$
$$W_3\colon (x, y, z, \bar{x}, \bar{y}, \bar{z}) \to (-z, -y, -x; -\bar{z}, -\bar{y}, -\bar{x}). \quad (5.4)$$

and therefore the matrix elements of $W_1$, $W_2$, and $W_3$ are easily obtained as

$$\langle j'm'\delta'|W_1|jm\delta\rangle = (-1)^{p+q+j'-\delta'}\delta_{j'j}\delta_{m'-m}\delta_{\delta'\delta}, \quad (5.5)$$

$$\langle j'm'\delta'|W_2|jm\delta\rangle = (-1)^{p+q} E^{p,q}_{j'm'\delta',jm\delta}, \quad (5.6)$$

and

$$\langle j'm'\delta'|W_3|jm\delta\rangle = (-1)^{j'+j+\delta'+m} E^{pq}_{j'-m'\delta',j-m\delta} \quad (5.7)$$

The three matrix elements clearly satisfy the operator equation (5.3). That Eq. (5.5) is indeed correct follows since $W_1$ is just a reflection in the isospin space and as such only introduces a phase. Notice also the similarity between Eq. (4.2) and Eq. (5.5), the former being just a reflection on the $x - z$ space.

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## APPENDIX: THE RACAH COEFFICIENT AS A ${}_4F_3(1)$ FUNCTION

Since there are algebraic and numerical tables[13] available for the Racah coefficient, it may be useful to show directly a relationship between these coefficients and the ${}_4F_3(1)$ generalized hypergeometric functions for which no such tables are readily available. The advantage in expressing the Racah coefficient as a ${}_4F_3(1)$ function is the ease with which one can prove the properties satisfied by the former.

The Racah coefficient is defined as[14]

$$W(abcd,ef) = \Delta(abe)\Delta(cde)\Delta(acf)\Delta(bdf) \times \sum_n \frac{(-1)^{a+b+c+d+n}(n+1)!}{(n-a-b-e)!(n-c-d-e)!(n-a-c-f)!(n-b-d-f)!(a+b+c+d-n)!} \times \frac{1}{(a+d+e+f-n)!(b+c+e+f-n)!} \tag{A1}$$

$$\text{where } \Delta(abc) = \left(\frac{(a+b-c)!(a-b+c)!(-a+b+c)!}{(a+b+c+1)!}\right)^{1/2}. \tag{A2}$$

Let $\nu = a+b+c+d-n$. Then we can write (A1) as

$$W(abcd,ef) = \Delta(abe)\Delta(cde)\Delta(acf)\Delta(bdf)\sum_\nu \times \frac{(-1)^\nu(a+b+c+d+1-\nu)!}{\nu!(e+f-c-b+\nu)!(e+f-a-d+\nu)!(c+d-e-\nu)!(a+b-e-\nu)!(b+d-f-\nu)!(a+c-f-\nu)!}. \tag{A3}$$

Using the formula

$$\frac{\Gamma(z-\nu)}{\Gamma(z)} = (-1)^\nu \frac{\Gamma(-z+1)}{\Gamma(-z+\nu+1)} \tag{A4}$$

and introducing the notation

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}, \tag{A5}$$

Eq. (A3) becomes

$$\begin{aligned} W(abcd,ef) &= \frac{(a+b+c+d+1)!\Delta(abe)\Delta(cde)\Delta(acf)\Delta(bdf)}{(a+b-e)!(c+d-e)!(a+c-f)!(b+d-f)!(e+f-a-d)!(e+f-b-c)!} \\ &\quad \times \sum_\nu \frac{(e-c-d)_\nu(e-a-b)_\nu(f-b-d)_\nu(f-a-c)_\nu}{\nu!(-a-b-c-d-1)_\nu(e+f+1-b-c)_\nu(e+f+1-a-d)_\nu} \\ &= \frac{(a+b+c+d+1)!\Delta(abe)\Delta(cde)\Delta(acf)\Delta(bdf)}{(a+b-e)!(c+d-e)!(a+c-f)!(b+d-f)!(e+f-a-d)!(e+f-b-c)!} \\ &\quad \times {}_4F_3\left[\begin{matrix} e-c-d, e-a-b, f-b-d, f-a-c; 1 \\ -a-b-c-d-1, e+f+1-b-c, e+f+1-a-d \end{matrix}\right] \end{aligned} \tag{A6}$$

which is a terminating Saalschützian series.[15] Properties of such series are well known.

*Note added in manuscript:* After completion of this work, the authors came across a paper by Minton[16] in which he also derives Eq. (A6) and then uses it to obtain a new (unphysical) symmetry of the Racah coefficients.

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# Applications of Function Space Integrals to Problems in Wave Propagation in Random Media*

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Two problems in wave propagation governed by the reduced wave equation with a random refractive index are studied. Problem (a) is concerned with radiation from a source in an infinite medium, and problem (b) pertains to the scattering by a random half-space at high frequencies. By transforming the reduced wave equation into a generalized heat equation, it becomes possible to express the moments of solutions in terms of Wiener integrals. Concrete results are obtained for certain special cases. By systematically approximating the functional integral representation for the moments, various perturbation equations come forth. Among them is Kraichnan's direct interaction approximation. By examining the errors involved, the accuracy in each approximation is ascertained and the nature of the approximation becomes transparent.

## 1. INTRODUCTION

The problems of wave propagation in random media have been subject to intensive study in the past decade. Mathematically, most works have been confined to the problems of time-harmonic wave propagation governed by the wave equation with a random field of refractive index which is independent of time. Due to the well-known difficulty in obtaining exact solutions, nearly all problems have been analyzed under the assumption that the random fluctuation of the medium is small. Then the perturbation methods are applicable. For a comprehensive account of these methods and their applications, one is referred to two important papers by Keller[1,2] and a recent paper by Papanicolaou and Keller.[3] Concerning other methods and various physical applications, they can be found in an up-to-date review article by Barabanekov, Rytov, and Tatarski.[4]

The present work was motivated by an interesting article by Frisch[5] who showed that the radiation problem for the random reduced wave equation can be transformed into a complex heat equation with a random potential. The random solution can therefore be written in terms of a Wiener integral. However, no concrete results were obtained from that integral representation. On the other hand, the method of parabolic approximation has become prominent in random scattering problems due to Chernov[6] and Tatarski.[7] In view of similarity in equations, these two problems are amenable to the same treatment. By means of the Feynman–Kac[8,9] formula, the exact random solution can be expressed in terms of a Wiener integral from which various moments of the solution can be derived. In the process, it is expedient to interchange the order of functional integration and mathematical expectation. However the Wiener integral involved is not an integral in the measure-theoretic sense as pointed out by Cameron[10] who termed it a sequential Wiener integral. It is for this reason that Fubini's theorem for justifying the interchange of the order of integrations ceases to apply and the computation has to be carried out in a formal manner. Nevertheless, judged by the fact that our results agree with certain known results obtained previously by other procedures, this interchange does not seem to lead to any error.

The principal aim of the present paper is to extract some concrete results from the functional integral representation of the solutions related to the two physical problems indicated above. Concerning the problem of scattering by a half-space, one generalizes the results for the correlation functions on one plane to that on different planes. At high frequency the asymptotic results of the first two moments are obtained for this problem as well as for the radiation problem for the general correlation function of the random refractive index. The most interesting results in this paper are the revelation of the true nature of Kraichnan's direct interaction approximation and the clarification of interconnections between various known approximations as applied to a random parabolic equation. As it stands, Kraichran's derivation of his nonlinear moment equations based on physical argument is very difficult to justify mathematically. The present approach yields a convincing evidence of the validity of Kraichnan's approximation. This may provide a firm basis for the rigorous proof of his method in the future.

Formulation of the problems and transformation into a complex heat equation are given in Sec. 2. Then, in Sec. 3, the exact solution to this random heat equation is obtained by using the Feynman–Kac formula, and the statistical moments of the solution are expressed as Wiener integrals involving the characteristic functional of the given random field as their integrands. For computational convenience, the results are specialized to the case of a Gaussian random field in Sec. 4. The results for the stationary, homogeneous Gaussian field are also obtained there. When the Gaussian correlation function is assumed to be delta-correlated in time, the exact evaluation of certain functional integrals become possible. In particular the first two moments agree with those obtained by Chernov[6] and Tatarski[7] by different methods. These results are contained in Sec. 5. In the following section the differential equations satisfied by the moments of the solution are derived. In the process, the relation of the two-time, two-point correlation function to the simultaneous two-point correlation function is found. The possibility of reducing the evaluation of multiple-time moments to that of simultaneous moments is pointed out. At high frequency, the asymptotic evaluation of the functional integrals for arbitrary correlation functions is performed in Sec. 7. Results are obtained when the scale of random fluctuation and the wave-

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length are of the same order of magnitude. In other cases, one finds that the stationary path can be complex. The asymptotic evaluation is not feasible. When the previous results are specialized to the radiation problem, the results for high frequency radiation follow. This is shown in Sec. 8. An attempt is made in Sec. 9 to approximate the integrands of functional integrals in order to derive differential equations for moments. One of such approximations leads to Kraichnan's direct interaction equation for moments. In Sec. 10 it is shown that certain approximate integrands yield the results obtained by perturbation methods, such as the Born approximation, the method of smooth perturbation[5] and the two-time method.[3] The connection between various perturbation methods is thus established. Finally remarks are made concerning the use of the functional integral approach to stochastic wave propagation problems in general. Possible extensions are also discussed. In the appendices, some details in the main body of the paper are illustrated.

## 2. FORMULATION OF PROBLEMS

Let us consider two problems in stochastic wave propagation mentioned in the introduction. These problems will be formulated briefly here. The original versions can be found in Refs 5, and 6 and 7, respectively.

*Problem a: the radiation problem in a random medium:* Let $v$ be the solution of the radiation problem

$$\Delta v + k^2 n^2(\mathbf{r}) v = \delta(\mathbf{r}), \tag{2.1}$$

$$\lim_{|\mathbf{r}|\to\infty} |\mathbf{r}| \left( \frac{\partial v}{\partial |\mathbf{r}|} - ikn v \right) = 0. \tag{2.2}$$

This describes the radiation from a source of unit strength located at the origin $\mathbf{r} = 0$. The refractive index $n(\mathbf{r})$ is a given random field. The wavenumber $k$ is taken to be complex with $\mathrm{Im}\{k\} > 0$. At the same time, we introduce the following initial-value problem

$$\frac{\partial u}{\partial t} = \frac{i}{k} [\Delta + \mu(\mathbf{r})] u, \quad t > 0, \tag{2.3}$$

$$u(0, \mathbf{r}) = \delta(\mathbf{r}), \tag{2.4}$$

where $\mu$ is a random field to be specified. If one denotes the Laplace transform of $u$ by $\hat{u}$ defined by

$$\hat{u}(s, \mathbf{r}) = \int_0^\infty u(t, \mathbf{r}) e^{-st} dt, \quad \mathrm{Re}\{s\} > 0, \tag{2.5}$$

a Laplace transform of Eq. (2.3), noting (2.4), yields

$$\Delta \hat{u} + (iks + \mu) \hat{u} = \delta(\mathbf{r}). \tag{2.6}$$

The above equation reduces to Eq. (2.1) if one sets

$$n^2(\mathbf{r}) = 1 + k^{-2} \mu(\mathbf{r}), \tag{2.7}$$

$$v(\mathbf{r}) = (ik)^{-1} \hat{u}(\mathbf{r}, -ik) = (ik)^{-1} \int_0^\infty u(t, \mathbf{r}) e^{ikt} dt, \quad \mathrm{Im}\{k\} > 0. \tag{2.8}$$

In this way the original radiation problem can be embedded in the initial-value problem (2.3) and (2.4).

*Problem b: scattering by a random half-space:* It is supposed that a time-harmonic wave propagates in a medium which is homogeneous for $x < 0$ and randomly inhomogeneous for $x \geq 0$. The variable $x$ denotes the first component of the space variable $\mathbf{x}$ so that $\mathbf{x} = (x, \mathbf{r})$, where $\mathbf{r}$ is the transverse variable. The wavefunction $v(\mathbf{x})$ satisfies the reduced wave equation

$$\Delta v + k^2 n^2(\mathbf{x}) v = 0, \quad x > 0, \tag{2.9}$$

$$\Delta v + k^2 v = 0, \quad x < 0 \tag{2.10}$$

in which $v$ and $v_x$ are continuous at $x = 0$ and $v$ is outgoing at infinity. In this case the random refractive index is assumed to be expressible as

$$n^2(\mathbf{x}) = 1 + \eta(x, \mathbf{r}). \tag{2.11}$$

For a wave $f(\mathbf{r}) e^{ikx}$ incident from the left half-plane, one may seek a solution, for $x > 0$, in the form

$$v(\mathbf{x}) = u(\mathbf{x}) e^{ikx}, \quad x > 0. \tag{2.12}$$

Upon substituting (2.12) into (2.9) and neglecting the term $u_{xx}$ in the resulting equation, one obtains

$$\frac{\partial u}{\partial x} = \frac{i}{2k} (\Delta_T + \mu) u, \quad x > 0, \tag{2.13}$$

where $\Delta_T$ stands for the transverse Laplacian and

$$\mu = k^2 \eta(x, \mathbf{r}). \tag{2.14}$$

The correct condition at $x = 0$ is the "initial" condition

$$u(0, \mathbf{r}) = f(\mathbf{r}). \tag{2.15}$$

The reduction of the full problem to the initial-value problem (2.13) and (2.15) is known as the parabolic equation approximation, which is valid for large $k$.[6,7] It is worth noting that the approximation is a singular perturbation. A more systematic expansion in the inverse power of $k$, which takes into account back scattering, was given by Keller, Papanicolaou and the author.[11]

It is seen that the solutions to the above physical problems, to be abbreviated as problem (a) and problem (b) in the sequel, are derivable from the corresponding solutions to an initial-value problem for a generalized, random heat equation. In problem (b), $x$ is the timelike variable and the random field $\mu$ is therefore "time" dependent, while $\mu$ in problem (a) is not. The other noticeable difference is in the spatial dimensions of these two problems—three dimensions in problem (a) and two dimensions in problem (b).

## 3. SOLUTIONS BY WIENER INTEGRALS

To treat problem (a) and problem (b) concurrently, let us consider the fundamental solution $u$ of the generalized heat equation in $n$ dimensions:

$$\frac{\partial u}{\partial t} = \frac{\alpha}{2} [\Delta + \mu(t, \mathbf{r}, \omega)] u, \quad t > 0, \tag{3.1}$$

$$u(0, \mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}') \tag{3.2}$$

where $\alpha$ is a complex number with $\mathrm{Re}\{\alpha\} > 0$, $\mathbf{r}$ and $\mathbf{r}'$ are two points in $R_n$ ($n$-dimensional Euclidean space) and $\Delta$ is the Laplacian in $\mathbf{r}$. The random field

$\mu(t,\mathbf{r},\omega)$, for each fixed $\omega$, is an element of certain set of functions $S$ defined over $R_n \times [0,\infty]$, and $\omega$ designates an elementary event in a sample space $\Omega$. It is supposed that a probability measure $P$ is defined over the $\sigma$-field of events in $\Omega$. For any functional $\phi[\mu]$ which is defined in $S$ and measurable with respect to $P$, the expected value of $\phi$ is denoted by $\langle\phi[\mu]\rangle$. By taking $\Omega = S$, this is an integration of $\phi$ over $S$ given by

$$\langle\phi[\mu]\rangle = \int_S \phi[\mu]P(d\mu). \tag{3.3}$$

Assuming that $\mu$ is stochastically continuous, a constructive method of specifying the random process $\mu$ is to exhibit its characteristic functional $F[\lambda]$ defined as

$$F[\lambda] = \left\langle \exp\left( i \int_0^\infty \int_{R_n} \lambda(t,\mathbf{r})\mu(t,\mathbf{r},\omega)dt\, d\mathbf{r}\right)\right\rangle. \tag{3.4}$$

The integral in the above exponent is usually taken to be a Stieltjes integral. Therefore, the parametric function $\lambda(t,\mathbf{r})$ is allowed to be a generalized function. From $F[\lambda]$, various moments of $\mu$ can be obtained by taking functional derivatives.[12]

For $0 \le \tau \le t$, let $\mathbf{z}(\tau)$ be elements in the space $c(0,t)$ of continuous, $n$-vector-valued functions with $\mathbf{z}(0) = 0$. For a suitable functional $G[\mathbf{z}]$, e.g., an analytic functional, the sequential Wiener integral (or simply, the Wiener integral) of $G$ generated by the heat equation

$$\frac{\partial\psi}{\partial t} = \frac{\alpha}{2}\Delta\psi, \quad t > 0, \tag{3.5}$$

$$\psi(0,\mathbf{r}) = \delta(\mathbf{r}) \tag{3.6}$$

is known to exist.[10] Let $\{\tau_1,\tau_2,\ldots,\tau_n\}$ be a partition of $[0,t]$ so that $0 = \tau_0 < \tau_1 < \tau_2 < \cdots < \tau_n = t$, and let $\mathbf{z}(\tau_i) = \xi_i$. To approximate $\mathbf{z}$, one introduces a polygonal function $\mathbf{z}_{\tau,\xi}(t)$ such that

$$\mathbf{z}_{\tau,\xi}(\tau_i) = \xi_i, \quad i = 0,1,2,\ldots,m, \tag{3.7}$$

and $\mathbf{z}_{\tau,\xi}$ is linear on $[\tau_{i-1},\tau_i]$. Then the sequential Wiener integral is defined as the limit, if it exists:

$$E_z\{G[\mathbf{z}]\} = \lim_{\substack{\max|\tau_j-\tau_{j-1}|\to 0 \\ 1\le j\le m}} \int_{R_n} d\xi_1 \overset{(m)}{\cdots} \int_{R_n} d\xi_m\, G[\mathbf{z}_{\tau,\xi}] \times \prod_{j=1}^{m} \left( \frac{\exp\left(-\dfrac{(\xi_j-\xi_{j-1})^2}{2\alpha(\tau_j-\tau_{j-1})}\right)}{[2\pi\alpha(\tau_j-\tau_{j-1})]^{n/2}} \right) \tag{3.8}$$

Let $E_z\{G[\mathbf{z}]\,|\,\mathbf{z}\in c_0\}$ denote the Wiener integral over a subset $c_0$ of $c$. For computational purposes, it is found convenient to write this integral symbolically as

$$E_z\{G[\mathbf{z}]\,|\,\mathbf{z}\in c_0\} = \frac{\int_{c_0} G[\mathbf{z}]\exp\left(-(1/2\alpha)\int_0^t[\dot{\mathbf{z}}(\tau)]^2 d\tau\right)d_w\mathbf{z}}{\int_{c_0}\exp\left(-(1/2\alpha)\int_0^t[\dot{\mathbf{z}}(\tau)]^2 d\tau\right)d_w\mathbf{z}}. \tag{3.9}$$

According the Feynman–Kac formula, the solution of (3.1) and (3.2) for a rather general class of $\mu$, can be represented as a functional integral

$$u(t,\mathbf{r},\mathbf{r}',\omega) = E_z\left[\exp\left(\frac{\alpha}{2}\int_0^t \mu(\tau,\mathbf{z}(\tau),w)d\tau\right)\,\middle|\,\mathbf{z}\in c(0,t),\ \mathbf{z}(t) = \frac{\exp[-(\mathbf{r}-\mathbf{r}')^2/2\alpha(t-\tau)]}{[2\pi\alpha(t-\tau)]^{n/2}}\right], \tag{3.10}$$

which is an integration over all continuous paths starting from the origin at $\tau = 0$ and reaching $\mathbf{r}-\mathbf{r}'$ at $\tau = t$. To remove the terminal condition on each path, Eq. (3.10) can be rewritten as

$$u(t,\mathbf{r},\mathbf{r}',\omega) = E_z\left[\exp\left(\frac{\alpha}{2}\int_0^t \times \mu(\tau,\mathbf{z}(\tau)+\mathbf{r}',\omega)d\tau\right)\delta[\mathbf{z}(t)-\mathbf{r}+\mathbf{r}']\right], \tag{3.11}$$

where $\delta$ is the Dirac delta function.

If one sets $\mu \equiv 0$, $\mathbf{r}' = 0$ in (3.11), it yields the solution of (3.5) and (3.6) in the form

$$\psi(t,\mathbf{r}) = E_z\{\delta[\mathbf{z}(t)-\mathbf{r}]\} = (2\pi\alpha t)^{-n/2}\exp(-\mathbf{r}^2/2\alpha t) \tag{3.12}$$

This simple formula will be found useful later. Next, the statistical moments of the solution will be determined. To this end, one defines the $n$th moment $\Gamma_n$ of the fundamental solution to be

$$\Gamma_n(t_1,t_2,\ldots,t_n;\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n) = \langle u_1(t_1,\mathbf{r}_1)u_2(t_2,\mathbf{r}_2)\ldots u_n(t_n,\mathbf{r}_n)\rangle. \tag{3.13}$$

Here the following convention has been adopted:

$$u_j \equiv \begin{cases} u, & \text{for odd } j \\ \bar{u}, & \text{for even } j \end{cases}, \tag{3.14}$$

where $\bar{u}$ means the complex conjugate of $u$.

In general the arguments in $\Gamma_n$ need not be distinct. For example, $\Gamma_2(t,t;\mathbf{r}_1,\mathbf{r}_2) \equiv \Gamma_2(t;\mathbf{r}_1,\mathbf{r}_2)$ will be called the simultaneous (or one-time), two-point second moment of $u$ and so on. Let us first compute the first moment (or the mean) of $u$:

$$\Gamma_1(t,\mathbf{r}) = \langle u(t,\mathbf{r},\omega)\rangle = \left\langle E_z\left[\exp\left(\frac{\alpha}{2}\int_0^t \mu(\tau,\mathbf{z}(\tau),\omega)d\tau\right)\right]\delta[\mathbf{z}(t)-\mathbf{r}]\right\rangle, \tag{3.15}$$

where, without loss of generality, $\mathbf{r}'$ in (3.11) has been set to zero and $u(t,\mathbf{r},0,\omega) \equiv u(t,\mathbf{r},\omega)$. To simplify (3.15), one formally interchanges the order of the $\langle\rangle$ and $E_z$; for the reason given in Sec. 1, it is not easily justifiable. Nevertheless, it is assumed here and hereafter that this kind of interchange is always permissible. Then (3.15) can be rewritten as

$$\Gamma_1(t,\mathbf{r}) = E_z\left\{\left\langle\exp\left[\tfrac{1}{2}\int\mu(\tau,\mathbf{z}(\tau),w)d\tau\right]\right\rangle\delta[\mathbf{z}(t)-\mathbf{r}]\right\}. \tag{3.16}$$

If one lets

$$\lambda_1(t-\tau,\mathbf{r}-\mathbf{z}) = (\alpha/2i)\delta[\mathbf{r}-\mathbf{z}(\tau)]H(t-\tau), \tag{3.17}$$

where $H$ is the Heaviside function, then, in view of (3.4), the following relation holds:

$$F[\lambda_1] = \left\langle\exp\left(\frac{\alpha}{2}\int_0^t \mu(\tau,\mathbf{z}(\tau),\omega)d\tau\right)\right\rangle. \tag{3.18}$$

Upon using (3.18) in (3.16), it becomes

$$\Gamma_1(t,\mathbf{r}) = E_z\{F[\lambda_1]\delta[\mathbf{z}(t)-\mathbf{r}]\}. \tag{3.19}$$

Introducing $\lambda_2$, defined by

$$\begin{aligned}\lambda_2[t_1-\tau,t_2-\tau;\mathbf{r}-\mathbf{z}_1,\mathbf{r}-\mathbf{z}_2] &= (\alpha/2i)\delta[\mathbf{r}-\mathbf{z}_1(\tau)]H(t_1-\tau)\\ &\quad+(\bar\alpha/2i)\delta[\mathbf{r}-\mathbf{z}_2(\tau)]H(t_2-\tau),\end{aligned} \tag{3.20}$$

the two-time, two-point second moment (or the correlation function) of $u$ can also be expressed in terms of the characteristic functional as follows:

$$\begin{aligned}\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) &= \Big\langle E_{z_1}\Big[\exp\Big(\frac{\alpha}{2}\int_0^{t_1}\mu(\tau_1,\mathbf{z}_1(\tau_1),\omega)d\tau_1\Big)\\ &\quad\times\delta[\mathbf{z}_1(t_1)-\mathbf{r}_1]\Big]\,E_{z_2}\Big[\exp\Big(\frac{\bar\alpha}{2}\int_0^{t_2}\\ &\quad\times\mu(\tau_2,\mathbf{z}_2(\tau_2),\omega)d\tau_2\Big)\delta[\mathbf{z}_2(t_2)-\mathbf{r}_2]\Big]\Big\rangle\\ &= E_{z_1z_2}\{F[\lambda_2]\delta[\mathbf{z}_1(t_1)-\mathbf{r}_1]\delta[\mathbf{z}_2(t_2)-\mathbf{r}_2]\}.\end{aligned} \tag{3.21}$$

Here $E_{z_1z_2}=E_{z_1}\cdot E_{z_2}$ means a double Wiener integration, where $E_{z_1}$ is the Wiener integration defined in (3.8), and $E_{z_2}$ is the same integration with a parameter $\bar\alpha$. In general the $m$th moment can be written down in a compact form

$$\begin{aligned}\Gamma_m(t_1,t_2,\ldots,t_m;\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m) &= E_{z_1z_2,\ldots,z_m}\{F[\lambda_m]\delta_1[\mathbf{z}_1(\tau_1)-\mathbf{r}_1]\\ &\quad\times\delta[\mathbf{z}_2(\tau_2)-\mathbf{r}_2]\cdots\delta[\mathbf{z}_m(\tau_m)-\mathbf{r}_m]\},\end{aligned} \tag{3.22}$$

which is an $m$-fold Wiener integral. The parameter function $\lambda_m$ in this case is defined to be

$$\begin{aligned}&\lambda_m(t_1-\tau,t_2-\tau,\ldots,t_m-\tau;\\ &\quad\mathbf{r}-\mathbf{z}_1,\mathbf{r}-\mathbf{z}_2,\ldots,\mathbf{r}-\mathbf{z}_m)\\ &\quad=\frac{1}{2i}\sum_{j=1}^{m}\alpha_j\delta[\mathbf{r}-\mathbf{z}_j(\tau)]H(t_j-\tau).\end{aligned} \tag{3.23}$$

To $E_{z_j}$ and $\alpha_j$, the convention (3.14) applies.

## 4. GAUSSIAN RANDOM FIELD

Let $\mu$ be a Gaussian random field with the mean function $a(t,\mathbf{r})$ and the covariance function $R(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2)$. Then the characteristic functional assumes the form

$$\begin{aligned}F[\lambda] &= \exp\Big(i\int_0^\infty\int_{R_n}\lambda(\tau,\mathbf{r})a(\tau,\mathbf{r})d\tau d\mathbf{r}\\ &\quad-\tfrac12\int_0^\infty\int_0^\infty\int_{R_n}\int_{R_n}\lambda(\tau_1,\mathbf{r}_1)\lambda(\tau_2\mathbf{r}_2)R(\tau_1,\tau_2;\\ &\quad\mathbf{r}_1,\mathbf{r}_2)d\tau_1d\tau_2d\mathbf{r}_1d\mathbf{r}_2\Big).\end{aligned} \tag{4.1}$$

In this case, the moments of the solution given by (3.19), (3.21), and (3.22) yield

$$\begin{aligned}\Gamma_1(t,r) &= E_z\Big[\exp\Big(\frac{\alpha}{2}\int_0^t a(\tau,\mathbf{z}(\tau))d\tau\\ &\quad+\frac{\alpha^2}{8}\int_0^t\int_0^t R(\tau_1,\tau_2;\mathbf{z}_1(\tau_1),\\ &\quad\mathbf{z}_2(\tau_2))d\tau_1d\tau_2\Big)\delta[\mathbf{z}(t)-\mathbf{r}]\Big],\end{aligned} \tag{4.2}$$

$$\begin{aligned}\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) &= E_{z_1z_2}\Big[\exp\Big(\frac{\alpha}{2}\int_0^{t_1}a(\tau,\mathbf{z}_1(\tau))d\tau\\ &\quad+\frac{\bar\alpha}{2}\int_0^{t_2}a(\tau,\mathbf{z}_2(\tau))d\tau\\ &\quad+\frac{\alpha^2}{2}\int_0^{t_1}\int_0^{t_1}R(\tau_1,\tau_2;\mathbf{z}_1(\tau_1),\mathbf{z}_1(\tau_2))d\tau_1d\tau_2\\ &\quad+\frac{\bar\alpha^2}{2}\int_0^{t_2}\int_0^{t_2}R(\tau_1,\tau_2;\mathbf{z}_2(\tau_1),\mathbf{z}_2(\tau_2))d\tau_1d\tau_2\\ &\quad+\frac{\alpha\bar\alpha}{4}\int_0^{t_1}\int_0^{t_2}R(\tau_1,\tau_2;\mathbf{z}_1(\tau_1),\mathbf{z}_2(\tau_2))d\tau_1d\tau_2\Big)\\ &\quad\times\delta[\mathbf{z}_1(t_1)-\mathbf{r}_1]\delta[\mathbf{z}_2(t_2)-\mathbf{r}_2]\Big],\end{aligned} \tag{4.3}$$

and

$$\begin{aligned}\Gamma_m(t_1,t_2,\ldots,t_m;\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m) &= E_{z_1z_2\cdots z_m}\Big[\exp\Big(\tfrac12\sum_{j=1}^m\alpha_j\int_0^{t_1}a(\tau,\mathbf{z}_j(\tau))d\tau\\ &\quad+\tfrac18\sum_{j=1}^m\alpha_j^2\int_0^{t_j}\int_0^{t_j}R(\tau_1,\tau_2;\mathbf{z}_j(\tau_1),\\ &\quad\mathbf{z}_j(\tau_2))d\tau_1d\tau_2\,\tfrac14\sum_{j<k}\alpha_j\alpha_k\\ &\quad\times\int_0^{t_j}\int_0^{t_k}R(\tau_1,\tau_2;\mathbf{z}_1(\tau_1),\mathbf{z}_2(\tau_2))d\tau_1d\tau_2\Big)\\ &\quad\times\delta[\mathbf{z}_1(\tau_1)-\mathbf{r}_1]\delta[\mathbf{z}_2(\tau_2)-\mathbf{r}_2]\cdots\\ &\quad\times\delta[\mathbf{z}_m(\tau_m)-\mathbf{r}_m]\Big].\end{aligned} \tag{4.4}$$

The symbol $\sum_{j<k}$ means summation over all possible pairs of distinct indices without repetition. For other random processes with known characteristic functionals, one can, of course, write down the moments of $u$ in terms of Wiener integrals in a similar manner. When the process $\mu$ is homogeneous and stationary, the mean function $a$ reduces to a constant. The covariance function depends only on the difference in space and time variables, respectively,

$$R(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2)=R(t_1-t_2;\mathbf{r}_1-\mathbf{r}_2). \tag{4.5}$$

In this case, the results (4.2)–(4.4) simplify to

$$\begin{aligned}\Gamma_1(t,\mathbf{r}) &= e^{(\alpha/2)at}E_z\Big[\exp\Big(\frac{\alpha^2}{8}\int_0^t\int_0^t R(\tau_1-\tau_2,\mathbf{z}(\tau_1)\\ &\quad-\mathbf{z}(\tau_2))d\tau_1d\tau_2\Big)\delta[\mathbf{z}(t)-\mathbf{r}]\Big],\end{aligned} \tag{4.6}$$

$$\begin{aligned}\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) &= e^{(a/2)(\alpha+\bar\alpha)t}E_{z_1z_2}\Big[\exp\Big(\tfrac18\alpha^2\int_0^{t_1}\int_0^{t_1}\\ &\quad\times R(\tau_1-\tau_2,\mathbf{z}_1(\tau_1)-\mathbf{z}_1(\tau_2))d\tau_1d\tau_2\\ &\quad+\tfrac18\bar\alpha^2\int_0^{t_2}\int_0^{t_2}R(\tau_1-\tau_2,\mathbf{z}_2(\tau_1)-\mathbf{z}_2(\tau_2))d\tau_1d\tau_2\\ &\quad+\tfrac14\alpha\bar\alpha\int_0^{t_1}\int_0^{t_2}R(\tau_1-\tau_2,\mathbf{z}_1(\tau_1)-\mathbf{z}_2(\tau_2))d\tau_1d\tau_2\Big)\\ &\quad\times\delta[\mathbf{z}_1(t_1)-\mathbf{r}_1]\delta[\mathbf{z}_2(t_2)-\mathbf{r}_2]\Big]\end{aligned} \tag{4.7}$$

and

$$\begin{aligned}\Gamma_m(t_1,t_2,\ldots,t_m;\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m) &= e^{(a/2)\sum_{j=1}^m\alpha_jt}E_{z_1z_2\cdots z_m}\Big[\exp\Big(\tfrac18\sum_{j=1}^m\alpha_j^2\int_0^{t_j}\int_0^{t_j}\\ &\quad\times R(\tau_1-\tau_2,\mathbf{z}_j(\tau_1)-\mathbf{z}_j(\tau_2))d\tau_1d\tau_2\end{aligned}$$

$$+\tfrac{1}{4}\sum_{j<k}\alpha_j\alpha_k\int_0^{t_j}\int_0^{t_k} R(\tau_1-\tau_2,\mathbf{z}_j(\tau_1)-\mathbf{z}_k(\tau_2))d\tau_1 d\tau_2\Big)\delta[\mathbf{z}_1(\tau_1)-\mathbf{r}_1]\times\delta[\mathbf{z}_2(\tau_2)-\mathbf{r}_2]\cdots\delta[\mathbf{z}_m(\tau_m)-\mathbf{r}_m]\Big]. \quad (4.8)$$

It is seen that the mean value of $\mu$ only introduces an exponential factor in each moment of $u$. The remaining part of the paper is devoted exclusively to the case where $\mu$ is a stationary, homogeneous, centered Gaussian process, although some results may be extended to other Gaussian processes.

## 5. THE CASE OF DELTA CORRELATION IN TIME

It is supposed that the mean value $a = 0$ and the correlation function $R$ is delta correlated in $t$ so that

$$R(t_1-t_2,\mathbf{r}_1-\mathbf{r}_2)=\delta(t_1-t_2)g(\mathbf{r}_1-\mathbf{r}_2). \quad (5.1)$$

In the context of problem (b), this means that, with $t = x$, the $\mu$ process has the characteristics of a white noise in the $x$ direction. Using (5.1) in (4.6) with $a = 0$ and noting (3.12), there results

$$\Gamma_1(t,\mathbf{r})=E_z\{\exp[\tfrac{1}{8}\alpha^2 g(0)t]\delta[\mathbf{z}(t)-\mathbf{r}]\}=\psi(t,\mathbf{r})e^{(\alpha^2/8)g(0)t}, \quad (5.2)$$

where $\psi$ is defined by (3.12).

For an arbitrary initial condition $u(0,\mathbf{r}) = f(\mathbf{r})$, the mean solution, denoted by $\Gamma_{f,1}$, can be constructed from (5.2) as follows:

$$\Gamma_{f,1}(t,\mathbf{r})=e^{(\alpha^2/2)g(0)t}\int_{R_n}\psi(t,\mathbf{r}-\mathbf{r}')f(\mathbf{r}')d\mathbf{r}'. \quad (5.3)$$

Similarly, the second moment (4.7) becomes

$$\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2)=e^{(1/8)g(0)(\alpha^2 t_1+\alpha^2 t_2)}\times E_{z_1z_2}\Big[\exp\Big(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^{t_{12}} g(\mathbf{z}_1(\tau)-\mathbf{z}_2(\tau))d\tau\Big)\delta[\mathbf{z}_1(t_1)-\mathbf{r}_1]\delta[\mathbf{z}_2(t_2)-\mathbf{r}_2]\Big], \quad (5.4)$$

where $t_{12} = \min\{t_1, t_2\}$.

For arbitrary initial data $f$, it is found that

$$\Gamma_{f,2}(t_1,t_2;\mathbf{r}_1\mathbf{r}_2)=e^{(1/8)g(0)(\alpha^2 t_1+\alpha^2 t_2)}\times E_{z_1z_2}\Big[\exp\Big(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^{t_{12}} g(\mathbf{z}_1(\tau)-\mathbf{z}_1(t_1)-\mathbf{z}_2(\tau)+z_2(t_2)+\mathbf{r}_1-\mathbf{r}_2)d\tau\Big)\times f[\mathbf{r}_1-\mathbf{z}_1(t_1)]\bar{f}[\mathbf{r}_2-\mathbf{z}_2(t_2)]\Big]. \quad (5.5)$$

In general it is difficult to evaluate the above double integral in a closed form. This is, however possible if $t_1 = t_2 = t$ and $f$ has the property of a plane wave in $R_n$ so that

$$f(\mathbf{r}_1)\bar{f}(\mathbf{r}_2)=h(\mathbf{r}_1-\mathbf{r}_2). \quad (5.6)$$

To see this, one has to effect a change of the variables of integration in (5.5). Let two new variables $\mathbf{p}_1$ and $\mathbf{p}_2$ be defined so that, for $\tau \le t$,

$$\mathbf{p}_1(\tau)=\mathbf{z}_1(\tau)-\mathbf{z}_2(\tau), \quad (5.7)$$

$$\mathbf{p}_2(\tau)=\mathbf{z}_1(\tau)+\mathbf{z}_2(\tau). \quad (5.8)$$

Then it is a simple matter to check that $\mathbf{p}_1$ and $\mathbf{p}_2$ are real, dependent Wiener processes with a common variance parameter $2\mathrm{Re}\{\alpha\}$. In what follows, the terms, such as mathematical expectation and conditional expectation in probability theory will be used analogously to their counterparts for a real Wiener process. Let $I_1$ denote the integral appearing in the right-hand side of (5.5) for $t_{12} = t$. That is

$$I_1=E_{z_1z_2}\Big[\exp\Big(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^t g(\mathbf{z}_1(\tau)-\mathbf{z}_1(t)-\mathbf{z}_2(\tau)+\mathbf{z}_2(t)+\mathbf{r}_1-\mathbf{r}_2)d\tau\Big)f[\mathbf{r}_1-\mathbf{z}_1(t)]\bar{f}[\mathbf{r}_2-\mathbf{z}_2(t)]\Big] \quad (5.9)$$

which becomes, after a change of variables according to (5.7), (5.8) and invoking (5.6)

$$I_1=E_{p_1p_2}\Big[\exp\Big(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^t g(\mathbf{p}_1(\tau)-\mathbf{p}_1(t)+\mathbf{r}_1-\mathbf{r}_2)d\tau\Big)h[\mathbf{r}_1-\mathbf{r}_2-\mathbf{p}_1(t)]\Big] \quad (5.10)$$
$$=E_{p_1}\Big[\exp\Big(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^t g(\mathbf{p}_1(\tau)-\mathbf{p}_1(t)+\mathbf{r}_1-\mathbf{r}_2)d\tau\Big)h[\mathbf{r}_1-\mathbf{r}_2-\mathbf{p}_1(t)]E_{p_1p_2|p_1}(1)\Big].$$

In obtaining the last expression, one made use of an identity in mathematical expectation $E_{p_1p_2}=E_{p_1}\cdot E_{p_1p_2|p_1}$, where $E_{\cdot|p_1}$ means the conditional expectation with respect to $\mathbf{p}_1$. Since $E_{\cdot|p_1}(1)=1$, Eq. (5.10) reduces to

$$I_1=E_{p_1}\Big[\exp\Big(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^t g(\mathbf{p}_1(\tau)-\mathbf{p}_1(t)+\mathbf{r}_2-\mathbf{r}_1)d\tau\Big)\times h[\mathbf{r}_1-\mathbf{r}_2-\mathbf{p}_1(t)]\Big]. \quad (5.11)$$

In terms of the symbolic integral as shown in (3.9), $I_1$ takes the form

$$I_1(t,\mathbf{r}_1,\mathbf{r}_2;\alpha)=\int_{c(0,t)}\exp\Big(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^t g[\mathbf{p}_1(\tau)-\mathbf{p}_1(t)+\mathbf{r}_1-\mathbf{r}_2]d\tau-\frac{1}{\alpha_1}\int_0^t[\dot{\mathbf{p}}_1(\tau)]^2d\tau\Big)\times h[\mathbf{r}_1-\mathbf{r}_2-\mathbf{p}_1(t)]d_w\mathbf{p}_1, \quad (5.12)$$

where $\alpha_1 = \mathrm{Re}\{\alpha\}$.

For problem (b), one has $\alpha = 1/ik$. When $k$ approaches real axis from above, $a$ tends to the imaginary axis from the right, i.e., $\alpha_1 \to 0^+$. The limit of $I_1$ as $\alpha_1 \to 0^+$ or $1/\alpha_1 \to \infty$ can be computed as follows

$$\lim_{\alpha_1\to 0} I_1(t,\mathbf{r}_1,\mathbf{r}_2;\alpha)=\lim_{(1/\alpha_1)\to\infty}\int_{c(0,t)}\exp\Big(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^t g[\mathbf{p}_1(\tau)-\mathbf{p}_1(t)+\mathbf{r}_1-\mathbf{r}_2]d\tau-\frac{1}{\alpha_1}\int_0^t[\dot{\mathbf{p}}_1(\tau)]^2d\tau\Big)\times h[\mathbf{r}_1-\mathbf{r}_2-\mathbf{p}_1(t)]d_w\mathbf{p}_1$$
$$=h(\mathbf{r}_1-\mathbf{r}_2)e^{(\alpha_2^2/4)g(\mathbf{r}_1-\mathbf{r}_2)t}, \quad (5.13)$$

where $\alpha_2 = \mathrm{Im}\{\alpha\}$. The justification of the above result is shown in Appendix A. Formally this result can be easily obtained by using the method of stationary phase to be discussed in Sec. 7. Inserting (5.13) in (5.5) and setting $\alpha_2 = ik^{-1}$, one obtains

$$\Gamma_{h,2}(t,\mathbf{r}_1,\mathbf{r}_2) = h(\mathbf{r}_1-\mathbf{r}_2)e^{-(1/4k^2)[g(0)-g(\mathbf{r}_1-\mathbf{r}_2)]t}. \tag{5.14}$$

For $f \equiv 1$, hence $h \equiv 1$, the results (5.3) and (5.14) reduce to that obtained by Chernov[6] and Tatarski.[7]

The exact evaluation of the higher moments is more difficult. The corresponding expression for the $m$th moment is given by

$$\begin{aligned}\Gamma_m(t_1,t_2,\ldots,t_m;\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m) &= E_{z_1z_2\cdots z_m}\Big[\exp\Big(\tfrac{1}{8}\sum_{j=1}^{m}\alpha_j^2 g(0)t_j \\ &+ \tfrac{1}{4}\sum_{j<k}\alpha_j\alpha_k\int_0^{t_j} g(\mathbf{z}_j(\tau)-\mathbf{z}_k(\tau))d\tau\Big)\delta[\mathbf{z}_1(t_1) \\ &- \mathbf{r}_1]\delta[\mathbf{z}_2(t_2)-\mathbf{r}_2]\cdots\delta[\mathbf{z}_m(t_m)-\mathbf{r}_m]\Big].\end{aligned} \tag{5.15}$$

Here, for convenience, the sequence $t_j$, $j = 1,2,\ldots,m$, has been taken to be nondecreasing so that $t_1 \le t_2 \le \cdots \le t_m$. In particular, when $t_1 = t_2 = \cdots = t_m$, (5.15) becomes

$$\begin{aligned}\Gamma_m(t,\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m) &= E_{z_1z_2\cdots z_m} \\ &\times\Big[\exp\Big(\tfrac{1}{8}\sum_{j=1}^{m}\alpha_j^2 g(0)t + \tfrac{1}{4}\sum_{j<k}\alpha_j\alpha_k\int_0^t g(\mathbf{z}_j(\tau) \\ &- \mathbf{z}_k(\tau))d\tau\Big)\delta[\mathbf{z}_1(t)-\mathbf{r}_1]\delta[\mathbf{z}_2(t) \\ &- \mathbf{r}_2]\cdots\delta[\mathbf{z}_m(t)-\mathbf{r}_m]\Big].\end{aligned} \tag{5.16}$$

To evaluate the above integral, one borrows an idea of Kac's[13] which suggests the use of the method of differential equations.

## 6. EVALUATION OF $\Gamma_m$ AND DIFFERENTIAL EQUATIONS

To derive a differential equation for $\Gamma_m$, one will use an operational method which seems to yield the desired results more readily. This approach was first used by Donsker[14] to verify the Feynman–Kac formula for the nonrandom heat equation. For the purpose of illustration, the equation for $\Gamma_2$ will be derived in detail. The equation for higher moments can be obtained in a similar fashion. One starts with the following identity

$$\begin{aligned}\exp\Big(\beta\int_0^t g[\mathbf{z}(\tau)]d\tau\Big) &= 1 \\ &+ \beta\int_0^t g[\mathbf{z}(\sigma)]\exp\Big(\beta\int_0^\sigma g[\mathbf{z}(\tau)]d\tau\Big)d\sigma.\end{aligned} \tag{6.1}$$

Multiplying Eq. (5.4) by $e^{-(1/8)g(0)(\alpha^2t_1+\bar{\alpha}^2t_2)}$ with $t_1 \le t_2$ and invoking (6.1), it yields

$$\begin{aligned}e^{-(1/8)g(0)(\alpha^2t_1+\bar{\alpha}^2t_2)}&\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) \\ &= E_{z_1z_2}\{\delta[\mathbf{z}_1(t_1)-\mathbf{r}_1]\delta[\mathbf{z}_2(t_2)-\mathbf{r}_2]\} \\ &+ E_{z_1z_2}\Big[\frac{\alpha\bar{\alpha}}{4}\int_0^{t_1} g[\mathbf{z}_1(\sigma) \\ &- \mathbf{z}_2(\sigma)]\exp\Big(\frac{\alpha\bar{\alpha}}{4}\int_0^\sigma g(\mathbf{z}_1(\tau) \\ &- \mathbf{z}_2(\tau))d\tau\Big)\delta[\mathbf{z}_1(t_1)-\mathbf{r}_1]\delta[\mathbf{z}_2(t_2)-\mathbf{r}_2]\Big]d\sigma.\end{aligned} \tag{6.2}$$

In view of (3.12), it is found that

$$\begin{aligned}T(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) &\equiv \Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) \\ &- \psi(t_1,\mathbf{r}_1)\bar{\psi}(t_2,\mathbf{r}_2)\,e^{(1/8)g(0)(\alpha^2t_1+\bar{\alpha}^2t_2)} \\ &= \frac{\alpha\bar{\alpha}}{4(2\pi)^n}e^{(1/8)g(0)(\bar{\alpha}^2t_1+\alpha^2t_2)}\int_0^{t_1}\int\!\!\int_{R_n} \\ &\times e^{-i(\mu_1\cdot\mathbf{r}_1+\mu_2\cdot\mathbf{r}_2)}d\mu_1\,d\mu_2\int\!\!\int_{R_n} g(\rho_1 \\ &- \rho_2)e^{i(\mu_1\cdot\rho_1+\mu_2\cdot\rho_2)}E_{z_1z_2}\Big[\exp\Big(\frac{\alpha\bar{\alpha}}{4}\int_0^\sigma g(\mathbf{z}_1(\tau) \\ &- \mathbf{z}_2(\tau))d\tau\Big)\delta[\mathbf{z}_1(\sigma)-\rho_1]\delta[\mathbf{z}_2(\sigma) \\ &- \rho_2]\exp[i\mu_1\cdot(\mathbf{z}_1(t_1)-\mathbf{z}_1(\sigma)) \\ &+ i\mu_2\cdot(\mathbf{z}_2(t_2)-\mathbf{z}_2(\sigma))\Big]d\rho_1d\rho_2d\sigma.\end{aligned} \tag{6.3}$$

In obtaining the above expression, use has been made of the formal representation of the delta function

$$\delta(\mathbf{r}) = \frac{1}{(2\pi)^n}\int_{R_n} e^{i\mu\cdot\mathbf{r}}d\mu. \tag{6.4}$$

By the property of independent increments for a Wiener process and the definition of $\Gamma_2$ given by (5.4), (6.3) can be simplified to give

$$\begin{aligned}T(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) &= \frac{\alpha\bar{\alpha}}{4}\int_0^{t_1}\int\!\!\int_{R_n}\psi(t_2-\sigma,\rho_1-\mathbf{r}_1)\bar{\psi}(t_2 \\ &- \sigma,\rho_2-\mathbf{r}_2)e^{(1/8)g(0)[\alpha^2(t_1-\sigma)+\bar{\alpha}^2(t_2-\sigma)]}g(\rho_1 \\ &- \rho_2)\Gamma_2(\sigma,\rho_2,\rho_2)d\rho_1d\rho_2d\sigma.\end{aligned} \tag{6.5}$$

In view of (5.2) and (6.3), one has

$$\begin{aligned}\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) &= \Gamma_1(t_1,\mathbf{r}_1)\bar{\Gamma}_1(t_2,\mathbf{r}_2) \\ &+ \frac{\alpha\bar{\alpha}}{4}\int_0^{t_1}\int\!\!\int_{R_n}\Gamma_1(t_1-\sigma,\rho_1-\mathbf{r}_1)\bar{\Gamma}_1(t_2 \\ &- \sigma,\rho_2-\mathbf{r}_2)g(\rho_1-\rho_2) \\ &\times\Gamma_2(\sigma,\rho_1,\rho_2)d\rho_1d\rho_2d\sigma, \quad t_1 \le t_2.\end{aligned} \tag{6.6}$$

This relates the two-time correlation function to the simultaneous correlation function through the mean solution $\Gamma_1$.[15] To obtain an equation for $\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2)$, let $t_1 = t_2 = t$ in (6.6). In this way, it yields an integral equation for $\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2)$:

$$\begin{aligned}\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2) &= \Gamma_1(t_1,\mathbf{r}_1)\bar{\Gamma}_1(t_2,\mathbf{r}_2) + \frac{\alpha\bar{\alpha}}{4}\int_0^t\int\!\!\int_{R_n}\Gamma_1(t \\ &- \sigma,\rho_1-\mathbf{r}_1)\bar{\Gamma}_1(t-\sigma,\rho_2-\mathbf{r}_2)g(\rho_1 \\ &- \rho_2)\Gamma_2(\sigma,\rho_1,\rho_2)d\rho_1d\rho_2d\sigma.\end{aligned} \tag{6.7}$$

From (3.13) and (5.2), one observes that the product $(\Gamma_1\bar{\Gamma}_1)$, as the kernel in the above integral equation, is the fundamental solution of the diffusion equation in $2$-$n$ dimensions:

$$\left(\frac{\partial}{\partial t} - \tfrac{1}{2}(\alpha\Delta_1 + \bar{\alpha}\Delta_2) - \tfrac{1}{8}(\alpha^2 + \bar{\alpha}^2)g(0)\right)[\Gamma_1(t,\mathbf{r}_1) \times \bar{\Gamma}_1(t,\mathbf{r}_2)] = 0, \quad t > 0, \quad (6.8)$$

where $\Delta_1, \Delta_2$ are the Laplacians in $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. Consequently, the integral equation (6.7) is equivalent to the initial-value problem

$$\frac{\partial}{\partial t}\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2) = \tfrac{1}{2}(\alpha\Delta_1 + \bar{\alpha}\Delta_2)\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2) + [\tfrac{1}{8}(\alpha^2 + \bar{\alpha}^2)g(0) + \tfrac{1}{4}\alpha\bar{\alpha}g(\mathbf{r}_1 - \mathbf{r}_2)]\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2), \quad t > 0, \quad (6.9)$$

$$\Gamma_2(0,\mathbf{r}_1,\mathbf{r}_2) = \delta(\mathbf{r}_1)\delta(\mathbf{r}_2). \quad (6.10)$$

When $\alpha = ik^{-1}$ the result (6.9) and (6.10) agrees with that of Chernov[6] and Tatarski[7] obtained by entirely different methods. Furthermore, with $t = x$, (6.6) generalizes their results for the correlation function to two different planes. As an example, let the initial condition be $\Gamma_{f,2}(0,\mathbf{r}_1,\mathbf{r}_2) = h(\mathbf{r}_1 - \mathbf{r}_2)$. Then, after simplification, (6.6) yields

$$\Gamma_{h,2}(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) = e^{(1/8)g(0)(\alpha^2 t_1 + \bar{\alpha}^2 t_2)}\int_{R_n} h(\boldsymbol{\rho})e^{(1/4)\alpha\bar{\alpha}g(\boldsymbol{\rho})t_1} \times \bar{\Gamma}_1(t_2 - t_1, \boldsymbol{\rho} + \mathbf{r}_1 - \mathbf{r}_2)d\boldsymbol{\rho}, \quad t_1 \le t_2. \quad (6.11)$$

Since $\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) = \bar{\Gamma}_2(t_2,t_1;\mathbf{r}_2,\mathbf{r}_1)$, it follows that

$$\Gamma_{h,2}(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) = e^{(1/8)g(0)(\alpha^2 t_1 + \bar{\alpha}^2 t_2)}\int_{R_n} h(\boldsymbol{\rho})e^{(1/4)\alpha\bar{\alpha}g(\boldsymbol{\rho})t_2} \times \Gamma_1(t_1 - t_2, \boldsymbol{\rho} + \mathbf{r}_2 - \mathbf{r}_1)d\boldsymbol{\rho}, \quad t_1 \ge t_2 \quad (6.12)$$

The results (6.11) and (6.12) are new. For $t_1 = t_2 = t$, either one of them reduces to (5.14) as to be expected.

For higher moments, the multitime correlation function can be related to the corresponding lower-order time correlations, and eventually the simultaneous correlation function. This reduction is achieved by a repeated use of formula (6.1) and by breaking up the range of integration into nonoverlapping time intervals so that the property of independent increments is applicable. This observation is important in the context of the parabolic equation approximation because, in general, one has to deal with one-plane correlation only. Hence the problem is greatly simplified. The details will not be shown here. Instead the equation for $\Gamma_m(t,\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_m)$ will be derived. By almost the same steps that lead one from (6.2) to (6.7), the following integral equation results:

$$\Gamma_m(t,\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m) = \prod_{j=1}^{m}\Gamma_{1,j}(t,\mathbf{r}_j) + \tfrac{1}{4}\int_0^t\int_{R_n}\cdots^{(m)}\int_{R_n}\sum_{j<k}\alpha_j\alpha_k g(\boldsymbol{\rho}_j - \boldsymbol{\rho}_k) \times\left(\prod_{l=1}^{m}\Gamma_{1,l}(t-\sigma,\boldsymbol{\rho}_1 - \mathbf{r}_l)\right)\Gamma_m(\sigma,\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_m) \times d\boldsymbol{\rho}_1\cdots d\boldsymbol{\rho}_m d\sigma, \quad (6.13)$$

where the following convention is in effect:

$$\Gamma_{1,j} = \begin{cases}\Gamma_1, & \text{for odd } j\\ \bar{\Gamma}_1, & \text{for even } j\end{cases}. \quad (6.14)$$

It is not difficult to see that the integral equation (6.13) is equivalent to the initial-value problem

$$\frac{\partial}{\partial t}\Gamma_m(t,\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m) = \left(\tfrac{1}{2}\sum_{j=1}^{m}\alpha_j\Delta_j + \tfrac{1}{8}g(0)\sum_{j=1}^{m}\alpha_j^2 + \tfrac{1}{4} \times\sum_{j<k}\alpha_j\alpha_k g(\mathbf{r}_j - \mathbf{r}_k)\right)\Gamma_m(t,\mathbf{r}_1,\mathbf{r}_2\cdots\mathbf{r}_m), \quad (6.15)$$

$$\Gamma_m(0,\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_m) = \prod_{j=1}^{m}\delta(\mathbf{r}_j). \quad (6.16)$$

This equation has not been solved for $n > 2$.

## 7. ASYMPTOTIC EVALUATION OF FUNCTIONAL INTEGRALS

The method of stationary phase (or the Laplace method, in general) has been applied to many problems in quantum physics (see, e.g., Ref. 16). It is of interest to carry out certain computations of this kind here. Let $c(t,r)$ be the set of all functions $\mathbf{z}(\tau)$ in $c(0,t)$ with $\mathbf{z}(t) = \mathbf{r}$. Suppose that $G[\mathbf{z}]$ and $\int_0^t \phi[\mathbf{z}(\tau)]d\tau$ are two smooth functionals on $c(t,r)$ so that the following integral exists:

$$I(t,\mathbf{r},\beta) = \int_{c(t,r)} G[\mathbf{z}]\exp\left(\beta\int_0^t[\phi(\mathbf{z}(\tau)) - \tfrac{1}{2}(\dot{\mathbf{z}}(\tau))^2]d\tau\right)d_w\mathbf{z}, \quad (7.1)$$

where $\beta$ is a complex parameter and $|\beta| \gg 1$.

The method consists of finding the extremal paths $\mathbf{z}^*(\tau)$ which render the exponent stationary. One then evaluates $I$ by approximating $\phi[\mathbf{z}]$ by a quadratic functional about $\mathbf{z}^*$. The variational problem for determining $\mathbf{z}^*$ gives rise to the Euler equation

$$\frac{d^2\mathbf{z}}{d\tau^2} + \nabla\phi(\mathbf{z}) = 0, \quad (7.2)$$

$$\mathbf{z}(0) = 0, \quad \mathbf{z}(t) = \mathbf{r}. \quad (7.3)$$

If the above boundary-value problem has a unique solution $\mathbf{z}^*$ (multiple solutions are admitted), one has, for large $|\beta|$

$$I(t,\mathbf{r},\beta) \sim \exp\left(\beta\int_0^t[\phi(\mathbf{z}^*(\tau)) - \tfrac{1}{2}(\dot{\mathbf{z}}^*(\tau))^2]d\tau\right) \times\int_{c(t,0)} G[\mathbf{z}^* + \mathbf{y}]\exp\left[\tfrac{1}{2}\beta\int_0^t\int_0^\tau\int_0^\tau \mathbf{y}(\tau_1)\cdot\left(\frac{\delta^2\phi}{\delta\mathbf{z}(\tau_1)\delta\mathbf{z}(\tau_2)}\Big|_{\mathbf{z}=\mathbf{z}^*}\right)\cdot\mathbf{y}(\tau_2)d\tau_1 d\tau_2 d\tau - \beta\int_0^t\dot{\mathbf{z}}^*(\tau)\cdot d\mathbf{y}(\tau)\right]d_w\mathbf{y}, \quad (7.4)$$

where $\mathbf{y} = \mathbf{z} - \mathbf{z}^*$, and $\delta^2\phi/\delta\mathbf{z}(\tau_1)\delta\mathbf{z}(\tau_2)$, a second order tensor, denotes the second variational derivative of $\phi[z]$. Thereby one reduces the integral (7.1) to a Wiener integral involving a quadratic functional. The asymptotic expansion for a double Wiener integral can be carried out in a similar fashion.

To apply formula (7.4) to $\Gamma_1$ given by (4.6) with $a = 0$, one rewrites it as follows:

$$\Gamma_1(t,\mathbf{r}) = \int_{c(t,r)}\exp\left(-\frac{k^2\epsilon^2}{8}\int_0^t\int_0^t S[\tau_1 - \tau_2, \mathbf{z}_1(\tau_1) - \mathbf{z}_2(\tau_2)]d\tau_1 d\tau_2 + \frac{ik}{2}\int_0^t[\dot{\mathbf{z}}(\tau)]^2 d\tau\right)d_w\mathbf{z}. \quad (7.5)$$

Here the result is specialized to problem (b), where $\alpha = ik^{-1}$, and $S$ is related to $R$ by the assumption

$$R(t_1 - t_2, \mathbf{r}_1 - \mathbf{r}_2) = k^4\epsilon^2 S(t_1 - t_2, \mathbf{r}_1 - \mathbf{r}_2), \quad (7.6)$$

in which $\epsilon$ is a small parameter measuring the scale of random fluctuation of $\eta$. Two limiting cases will be considered in the following.

*Case (a):* $|k| \gg 1$ *and* $k\epsilon = O(1)$*:* Physically this means that the wavelength is short and is of the same order of magnitude as that of the scale of random fluctuations in the medium. By comparing (7.5) with (7.4), one sees that $\beta = -ik$, $\phi \equiv 0$, and

$$G[\mathbf{z}] = \exp\left(-\frac{k^2\epsilon^2}{2}\int_0^t\int_0^t S[\tau_1 - \tau_2, \mathbf{z}_1(\tau_1), \mathbf{z}_2(\tau_2)]d\tau_1 d\tau_2\right). \quad (7.7)$$

The stationary path in this case is given by the free particle trajectory

$$\mathbf{z}^*(\tau) = (\tau/t)\mathbf{r} \quad (7.8)$$

using a three-term functional Taylor series expansion of $G[\mathbf{y} + \mathbf{z}^*]$ in $\mathbf{y}$ about $\mathbf{z}^*$ given by (7.7), and noting (7.8) and (7.4), the asymptotic result for $\Gamma_1$ is found after evaluating the resulting integrals in (7.5)

$$\Gamma_1(t,\mathbf{r}) \sim \psi(t,\mathbf{r})\exp\left[-\frac{k^2\epsilon^2}{4}\int_0^t\int_0^\sigma S\left(\sigma - \tau, \frac{1}{t}(\sigma-\tau)\mathbf{r}\right]d\sigma d\tau\right)\Big\{1 + i\frac{k^3\epsilon^4}{16}\int_0^t\cdots\int_0^t \nabla S\left[\tau_1-\tau_2,\frac{1}{t}(\tau_1-\tau_2)\mathbf{r}\right]\cdot\nabla S\left[\tau_3-\tau_4,\frac{1}{t}(\tau_3-\tau_4)\mathbf{r}\right][D(\tau_1,\tau_3) - D(\tau_1,\tau_4) - D(\tau_2,\tau_3) + D(\tau_2,\tau_4)]d\tau_1\cdots d\tau_4 - i\frac{k\epsilon^2}{4}\frac{1}{t}\int_0^t \tau(t^2-\tau^2)\nabla\cdot\nabla S\left(\tau,\frac{\tau}{t}\mathbf{r}\right)d\tau\Big\}, \quad (7.9)$$

where the function $D$ has the following definition:

$$D(\tau_1,\tau_2) = \begin{cases}(\tau_1/t)(t-\tau_2), & \text{if } \tau_1 \le \tau_2\\ (\tau_2/t)(t-\tau_1), & \text{if } \tau_1 > \tau_2\end{cases}. \quad (7.10)$$

Similarly the second moment $\Gamma_2$, referring to (4.7), can be expanded and the result is

$$\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) \sim \psi(t_1,\mathbf{r}_1)\bar{\psi}(t_2,\mathbf{r}_2)\exp\left(-\frac{k^2\epsilon^2}{4}\right)\left(\int_0^{t_1}\int_0^\sigma S\left[\sigma-\tau,\frac{1}{t_1}(\sigma-\tau)\mathbf{r}_1\right]d\sigma d\tau + \int_0^{t_2}\int_0^\sigma S\left[\sigma-\tau_1,\frac{1}{t_2}(\sigma-\tau)\mathbf{r}_2\right]d\sigma d\tau - \int_0^{t_1}\int_0^{t_2} S\left[\sigma-\tau_1\frac{\sigma}{t_1}\mathbf{r}_1 - \frac{\tau}{t_2}\mathbf{r}_2\right]d\sigma d\tau\right)\Big\{1 - i\frac{k\epsilon^2}{4}\sum_{j=1}^{2}\frac{1}{t_j}\int_0^{t_j}\tau(t_j^2-\tau^2)\nabla\cdot\nabla S\left(\tau_1-\tau_2,\frac{\tau_1}{t_1}\mathbf{r}_1 - \frac{\tau_2}{t_2}\mathbf{r}_2\right)[D(\tau_1,\tau_1) + D(\tau_2,\tau_2)]d\tau_1 d\tau_2 + i\frac{k^3\epsilon^4}{16}\sum_{j=1}^{2}\int_0^{t_j}\cdots\int_0^{t_j}\nabla S\left[\tau_1-\tau_2,\frac{1}{t_j}(\tau_1-\tau_2)\mathbf{r}_j\right]\cdot\nabla S\left[\tau_3-\tau_4,\frac{1}{t_j}(\tau_3-\tau_4)\mathbf{r}_j\right][D(\tau_1,\tau_3) - D(\tau_1,\tau_4) - D(\tau_2,\tau_3) + D(\tau_2,\tau_4)]d\tau_1\cdots d\tau_4\Big\} - i\frac{k^3\epsilon^4}{8}\sum_{\substack{j,k=1\\ j\neq k}}^{2}\int_0^{t_j}\int_0^{t_j}\int_0^{t_k}\int_0^{t_k}\nabla S\left[\tau_1-\tau_2,\frac{1}{t_j}(\tau_1-\tau_2)\mathbf{r}_j\right]\cdot\nabla S\left(\tau_j-\tau_k,\frac{\tau_3}{t_j}\mathbf{r}_j - \frac{\tau_4}{t_k}\mathbf{r}_k\right)[D(\tau_1,\tau_3) - D(\tau_2,\tau_3)]d\tau_1\cdots d\tau_4\cdot\nabla S\left[\tau_3-\tau_4,\frac{1}{t_j}(\tau_3-\tau_4)\mathbf{r}_j\right][D(\tau_1,\tau_3) - D(\tau_1,\tau_4) - D(\tau_2,\tau_3) + D(\tau_2,\tau_4)]d\tau_1\cdots d\tau_4\Big\} - i\frac{k^3\epsilon^4}{8}\sum_{\substack{j,k=1\\ j\neq k}}^{2}\int_0^{t_j}\int_0^{t_j}\int_0^{t_k}\int_0^{t_k}\nabla S\left[\tau_1-\tau_2,\frac{1}{t_j}(\tau_1-\tau_2)\mathbf{r}_j\right]\cdot\nabla S\left(\tau_j-\tau_k,\frac{\tau_3}{t_j}\mathbf{r}_j - \frac{\tau_4}{t_k}\mathbf{r}_k\right)[D(\tau_1,\tau_3) - D(\tau_2,\tau_3)]d\tau_1\cdots d\tau_4 + i\frac{k^3\epsilon^4}{8}\int_0^{t_1}\int_0^{t_1}\int_0^{t_2}\int_0^{t_2}\nabla S\left(\tau_1-\tau_2,\frac{\tau_1}{t_1}\mathbf{r}_1 - \frac{\tau_2}{t_2}\mathbf{r}_2\right)\cdot\nabla S\left(\tau_3-\tau_4,\frac{\tau_3}{t_1}\mathbf{r}_1 - \frac{\tau_4}{t_2}\mathbf{r}_2\right)[D(\tau_1,\tau_3) + D(\tau_2,\tau_4)]d\tau_1\cdots d\tau_4. \quad (7.11)$$

The asymptotic expressions for higher moments become too lengthy to be given here.

*Case (b):* $|k| \gg 1$ *and* $k\epsilon^2 = O(1)$*:* This is the case where the scale of random fluctuations is comparable to the square root of the wavelength. Setting $b = \frac{1}{8}k\epsilon^2$, the Euler equation (7.2) corresponding to the mean solution (7.5) is found to be

$$i\frac{d^2\mathbf{z}}{d\tau^2} - b\int_0^t \nabla S[\tau-\sigma, \mathbf{z}(\tau) - \mathbf{z}(\sigma)]d\sigma = 0. \quad (7.12)$$

It is easy to show that, for real $k$, there exists no real solution which satisfies the boundary condition (7.3). This means that there is no stationary path in the class $c(t,r)$. Hence the asymptotic expansion cannot be obtained this way. However it is worth mentioning a recent paper by McLaughlin[17] in which the asymptotic evaluation of Feynman integrals for various limiting values of parameters is studied and slightly complex path is admitted. The results obtained in this section, with $t$ replaced by $x$, pertains to the problem (b), the random scattering by a half-space.

## 8. HIGH FREQUENCY RADIATION

Let us keep only one term in the asymptotic results for $\Gamma_1$ and $\Gamma_2$ obtained in the previous section and specialize them to problem (a) with $n = 3$. In this case $S$ is time independent and $k$ must be replaced by $\frac{1}{2}k$ in (7.9) and (7.11). Then these equations yield, with $r = |\mathbf{r}|$,

$$\Gamma_1(t,\mathbf{r}) \sim \left(\frac{k}{4\pi i t}\right)\frac{3}{2}\exp\left(ik\frac{r^2}{t} - k^2\epsilon^2\int_0^t\int_0^\sigma S\left[\frac{1}{t}(\sigma-\tau)\mathbf{r}\right]d\sigma d\tau\right) \quad (8.1)$$

and

$$\Gamma_2(t_1,t_2;\mathbf{r}_1,\mathbf{r}_2) \sim \left(\frac{|k|^2}{16\pi^2 t_1 t_2}\right)^{3/2}\exp\left\{ik\frac{r_1^2}{t_1} - ik\frac{r_2^2}{t_2}\right.$$

$$- k^2\epsilon^2\left(\int_0^{t_1}\int_0^{\sigma} S\left[\frac{1}{t_1}(\sigma-\tau)\mathbf{r}_1\right]d\sigma d\tau\right) + \int_0^{t_2}\int_0^{\sigma} S\left[\frac{1}{t_2}(\sigma-\tau)\mathbf{r}_2\right]d\sigma d\tau - \int_0^{t_1}\int_0^{t_2} S\left(\frac{\tau_1}{t_1}\mathbf{r}_1 - \frac{\tau_2}{t_2}\mathbf{r}_2\right)d\tau_1 d\tau_2\Big\}. \quad (8.2)$$

To obtain the mean solution $\langle v\rangle$ and the second moment $\langle v(\mathbf{r})\bar{v}(\mathbf{r})\rangle$ of the radiation field governed by (2.1) and (2.2), one has to transform the above result according to (2.8). In this way, it is found that

$$\langle v(\mathbf{r})\rangle \sim (ik)^{-1}\int_0^{\infty}\left(\frac{k}{4\pi i t}\right)^{3/2}\exp\Big\{ik\left(t+\frac{r^2}{t}\right) - k^2\epsilon^2 \times \int_0^t\int_0^{\sigma} S\left[\frac{1}{t}(\sigma-\tau)\mathbf{r}\right]d\sigma d\tau\Big\}d\tau \quad (8.3)$$

and

$$\langle v(\mathbf{r}_1)\bar{v}(\mathbf{r}_2)\rangle \sim |k|^2\int_0^{\infty}\int_0^{\infty}\left(\frac{|k|^2}{16\pi^2 t_1 t_2}\right)^{3/2}\exp\Big(ik(t_1 + t_1^{-1}\mathbf{r}_1^2) - i\bar{k}(t_2 + t_2^{-1}\mathbf{r}_2) - k^2\epsilon^2\int_0^{t_1}\int_0^{t_2} S\left[\frac{1}{t_1}\times(\sigma-\tau)\mathbf{r}_1\right]d\sigma d\tau + \int_0^{t_2}\int_0^{\sigma} S\left[\frac{1}{t_2}(\sigma-\tau)\mathbf{r}_2\right]\times d\sigma d\tau - \int_0^{t_1}\int_0^{t_2} S\left[\frac{\tau_1}{t_1}\mathbf{r}_1 - \frac{\tau_2}{t_2}\mathbf{r}_2\right]d\tau_1 d\tau_2\Big)\,dt_1 dt_2. \quad (8.4)$$

Since $|k|$ is large, the conventional method of stationary phase is again applicable here. In the integral (8.3), the stationary point is $\tau = r$. The leading term in this evaluation yields

$$\langle v(\mathbf{r})\rangle \sim G(r)\exp\Big(-k^2\epsilon^2\int_0^r\int_0^{\sigma} S[(\sigma-\tau)\hat{r}]d\sigma d\tau\Big), \quad (8.5)$$

where $\hat{r}$ is the unit vector along $\mathbf{r}$ direction and $G$ is the free space Green's function

$$G(r) = e^{ikr}/4\pi r. \quad (8.6)$$

Similarly, the correlation field takes the form

$$\langle v(\mathbf{r}_1)\bar{v}(\mathbf{r}_2)\rangle \sim G(r_1)\bar{G}(r_2)\exp\Big[-k^2\epsilon^2\Big(\int_0^{r_1}\int_0^{\sigma} S((\sigma-\tau)\times\hat{r}_1)d\sigma d\tau + \int_0^{r_2}\int_0^{\sigma} S((\sigma-\tau)\hat{r}_2)d\sigma d\tau - \int_0^{r_1}\int_0^{r_2} S(\tau_1\hat{r}_1 - \tau_2\hat{r}_2)d\tau_1 d\tau_2\Big)\Big]. \quad (8.7)$$

In particular, the auto correlation is seen to be

$$\langle v(\mathbf{r})\bar{v}(\mathbf{r})\rangle \sim G(r)\bar{G}(r). \quad (8.8)$$

As far as one can tell, the results (8.6)–(8.8) have not been obtained before. They show clearly how a centered-Gaussian field of refractive indices affect the mean and correlation fields at high frequency.

First one observes that the mean-square intensity (8.8) remains unchanged by the random fluctuation about the zero mean. This is a form of energy conservation at high frequency which is shared by the previous results (5.14) and (7.11) for problem (b). If $S$ is isotropic and monotonically descreasing, the mean field (8.5) attenuates and the correlation field (8.7) falls off to zero as the separation $|\mathbf{r}_1 - \mathbf{r}_2|$ tends to infinity. The higher moments can also be evaluated if it is so desired.

## 9. NONLINEAR MOMENT EQUATIONS

It is well known that, for stochastic equations like (3.1), the derivation of moment equations leads to an hierarchy of coupled moment equations. This fact is reflected in the difficulty of evaluating the functional integrals in general. To get a set of closed equations for moments, known as the closure problem in turbulence,[18] one must make certain statistical hypothesis about the solution. In view of the integral representation of solution, it is natural to replace the statistical hypothesis by an approximation of the integrand involved. One of such approximations to be presented here leads to Kraichnan's[19] direct interaction equation which was derived by quite involved physical arguments.

To fix the idea, one considers the mean solution $\Gamma_1(t,\mathbf{r})$ given by (4.6) with $a = 0$. By virtue of (6.1), it can be rewritten as

$$\Gamma_1(t,\mathbf{r}) = \psi(t,\mathbf{r}) + \frac{\alpha^2}{4}\int_0^t E_z\Big[\int_0^s R[\tau - s, \mathbf{z}(\tau) - \mathbf{z}(s)]d\tau \times \exp\Big(\frac{\alpha^2}{8}\int_0^s\int_0^s R(\tau_1 - \tau_2, \mathbf{z}(\tau_1) - \mathbf{z}(\tau_2))d\tau_1 d\tau_2\Big)\delta[\mathbf{z}(t) - \mathbf{r}]\Big]\,ds. \quad (9.1)$$

For convenience, one introduces a function $Q(t,\mathbf{r})$ defined by

$$Q(t,\mathbf{r}) = \frac{\alpha^2}{4}\int_0^t E_z\Big[\int_0^s R[\tau - s, \mathbf{z}(\tau) - \mathbf{z}(s)]d\tau \times \exp\Big(\frac{\alpha^2}{8}\int_0^s\int_0^s R(\tau_1 - \tau_2, \mathbf{z}(\tau_1) - \mathbf{z}(\tau_2))d\tau_1 d\tau_2\Big)\delta[\mathbf{z}(t) - \mathbf{r}]\Big]ds, \quad (9.2)$$

which is, so to speak, the first order remainder. In terms of $Q$, Eq. (9.1) becomes

$$\Gamma_1(t,\mathbf{r}) = \psi(t,\mathbf{r}) + Q(t,\mathbf{r}). \quad (9.3)$$

By manipulating the integrand of $Q$ similar to steps taken in Sec. 6, there results

$$Q(t,\mathbf{r}) = \frac{\alpha^2}{4}\int_0^t\int_0^s\int_{R_n}\int_{R_n}\psi(t-s, \mathbf{r} - \boldsymbol{\rho}_1 - \boldsymbol{\rho}_2) \times E_z\Big[\exp\Big(\frac{\alpha^2}{4}\int_0^s\int_0^s R(\tau_1 - \tau_2, \mathbf{z}(\tau_1) - \mathbf{z}(\tau_2))d\tau_1 d\tau_2\Big)\delta[\mathbf{z}(s) - \boldsymbol{\rho}_1]\delta[\mathbf{z}(\tau) - \boldsymbol{\rho}_2]\Big] \times ds d\tau d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2. \quad (9.4)$$

Now let the following closure hypothesis be proposed: Approximate the exponent in the right-hand side of (9.4) according to

$$\int_0^s\int_0^s R(\tau_1 - \tau_2, \mathbf{z}(\tau_1) - \mathbf{z}(\tau_2))d\tau_1 d\tau_2 \approx \Big(\int_0^{\tau}\int_0^{\tau} + \int_{\tau}^s\int_{\tau}^s\Big) R(\tau_1 - \tau_2, \mathbf{z}(\tau_1) - \mathbf{z}(\tau_2))d\tau_1 d\tau_2. \quad (9.5)$$

This approximation will be called the direct integral decomposition. Using (9.5) in (9.4), one obtains an approximation $Q_1$ to $Q$ which can be simplified to give

$$Q_1(t,\mathbf{r}) = \frac{\alpha^2}{4}\int_0^t\int_0^s\int_{R_n}\int_{R_n}\psi(t-s, \mathbf{r} - \boldsymbol{\rho}_1) \times R(s-\tau, \boldsymbol{\rho}_1 - \boldsymbol{\rho}_2)\Gamma_1(s-\tau, \boldsymbol{\rho}_1 - \boldsymbol{\rho}_2) \times \Gamma_1(\tau, \boldsymbol{\rho}_2)ds d\tau d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2. \quad (9.6)$$

In obtaining the above expression, one used the Markovian property of the Wiener path in simplifying the expectation of the product of two functionals defined over two nonoverlapping time intervals and Eq. (4.6). When $Q_1$ given by (9.6) is used in place of $Q$ in (9.3), it yields an integral equation for $\Gamma_1$. The integral equation thus obtained is equivalent to the nonlinear integro-differential equation

$$\frac{\partial \Gamma_1(t,\mathbf{r})}{\partial t} - \frac{\alpha}{2}\Delta\Gamma_1(t,\mathbf{r}) = \frac{\alpha^2}{4}\int_0^t \int_{R_n} R(t-s,\mathbf{r}-\rho) \times \Gamma_1(t-s,\mathbf{r}-\rho)\Gamma_1(s,\rho)dsd\rho, \quad (9.7)$$

$$\Gamma_1(0,\mathbf{r}) = \delta(\mathbf{r}). \quad (9.8)$$

For $\alpha = \frac{1}{2}$ in (9.7) and $R$ being independent of $t$, it becomes identical with Kraichnan's[19] equation derived by stochastic model equations and using the diagram method. In this derivation, the assumptions on homogeneity and stationarity can be removed. Let the error involved in this approximation be denoted by $\Delta Q_1$. That is

$$\Delta Q_1 = Q - Q_1. \quad (9.8')$$

Let $\Delta Q_1 f$ be the error involved when the initial function $f$ is smooth. Then one can show, by the definition of a fundamental solution, that

$$\Delta Q_1 f = \frac{\alpha^2}{4}\int_0^t\int_0^s E_z\left\{\int_{R_n}\psi[t-s,\mathbf{r}-\mathbf{z}(s)] \times R[s-\tau,\mathbf{z}(s)-\mathbf{z}(\tau)-\rho]f(\rho)d\rho \times \exp\left[\frac{\alpha^2}{8}\left(\int_0^\tau\int_0^\tau + \int_\tau^s\int_\tau^s\right)R(\tau_1-\tau_2,\mathbf{z}(\tau_1) - \mathbf{z}(\tau_2))d\tau_1 d\tau_2\right]\left[\exp\left(\frac{\alpha^2}{4}\int_0^\tau\int_\tau^s R(\tau_1-\tau_2,\mathbf{z}(\tau_1) - \mathbf{z}(\tau_2))d\tau_1 d\tau_2\right) - 1\right]\right\} dsd\tau, \quad (9.9)$$

when $\alpha$ is complex, a bound on the error would be difficult. This is so because the integral $E_z$ with the parameter $\alpha$ is not of bounded variation. For real $\alpha$, this is, however, possible. Since this case has no direct physical interest, the result will not be given. For complex $\alpha$, one will proceed heuristically. It is observed that when $R(t,\mathbf{r})$ is delta-correlated in $t$, the error (9.9) is zero. Therefore Eq. (9.6) should provide a good approximation when the correlation function $R$ is peaked at $t = 0$ (or the correlation time is small) even if $|\alpha|$ is moderate. For small $|\alpha|$, one can expand the exponential function, contained in the last factor in the right-hand side of (9.9), into a power series in $\alpha^2$. Thus one finds the error $\Delta Q_1 f = 0(\alpha^4)$ for fixed $t$. This can be made more precise by using a mean-value theorem on this last factor as a function of $s$ and $\tau$ over $[0,t]$. From these considerations, one concludes that Eq. (9.6) is valid either when the correlation time is short or when the scale of random fluctuation is small. In the latter case Eq. (9.6) is correct up to $O(\alpha^2)$ inclusive. The corresponding equation for the second moment $\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2)$ can be derived by making the same closure hypothesis. Without going through the derivation, this equation is found to be

$$\frac{\partial}{\partial t}\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2) - (\alpha\Delta_1 + \bar{\alpha}\Delta_2)\Gamma_2(t,\mathbf{r}_1,\mathbf{r}_2) = \tfrac{1}{4}\int_0^t\int_{R_n}\int_{R_n}[\alpha^2 R(t-s,\mathbf{r}_1-\rho_1) + \bar{\alpha}^2 R(t-s,\mathbf{r}_1-\rho_2) + \alpha\bar{\alpha}R(t-s,\mathbf{r}_2-\rho_1) + \alpha\bar{\alpha}R(t-s,\mathbf{r}_1-\rho_2)]\Gamma_2(t-s,\mathbf{r}_1-\rho_2) \times \Gamma_2(t-s,\mathbf{r}_2-\rho_1)dsd\rho_1 d\rho_2, \quad (9.10)$$

$$\Gamma_2(0,\mathbf{r}_1,\mathbf{r}_2) = \delta(\mathbf{r}_1)\delta(\mathbf{r}_2). \quad (9.11)$$

Equation (9.10) was not given in Ref. 19. These nonlinear equations should be useful when the random fluctuations are not small or when the correlation time is long. In these cases, the perturbation methods, to be discussed in the next section, break down. It is worth noting that, for the first time the derivation of the nonlinear moment equations has been made precise and the error involved in this approximation is displayed explicitly.

## 10. CONNECTION WITH SOME PERTURBATION METHODS

In this section, one will systematically review and compare various perturbation methods applicable to Eq. (3.1) with $\mu = \epsilon\eta$;

$$\frac{\partial u}{\partial t} = \frac{\alpha}{2}[\Delta + \epsilon\eta(t,\mathbf{r},w)]u, \quad t > 0, \quad (10.1)$$

$$u(0,\mathbf{r}) = \delta(\mathbf{r}). \quad (10.2)$$

The small parameter in the perturbation expansion is $\epsilon$. As before $\langle\eta\rangle$ is taken to be zero. The perturbation and other methods to be considered here are the method of Born expansion (MBE), the method of smooth perturbation (MSP), the two-time method (MTT), the method of Markov approximation[4] (MMA) given in Sec. 5, and the method of direct integral decomposition (MDID) proposed in the previous section. This program will be carried out from the view point of approximating the functional integral representation of the solution $u$. The scope is limited to the mean solution $\Gamma_1(t,\mathbf{r})$ up to $O(\epsilon^2)$ inclusive.

As was shown in Sec. 9, the closure hypothesis based on the MDID lead to a nonlinear equation (9.7). In this closure hypothesis, if one further discards the integral from $\tau$ to $s$, i.e., setting in (9.2),

$$\int_0^s\int_0^s R[\tau_1-\tau_2,\mathbf{z}(\tau_1)-\mathbf{z}(\tau_2)]d\tau_1 d\tau_2 \approx \int_0^\tau\int_0^\tau R[\tau_1-\tau_2,\mathbf{z}(\tau_1)-\mathbf{z}(\tau_2)]d\tau_1 d\tau_2, \quad (10.3)$$

a second approximation $Q_2$ to $Q$ is obtained:

$$Q_2(t,\mathbf{r}) = \epsilon^2\frac{\alpha^2}{4}\int_0^t\int_0^\tau\int_{R_n}\int_{R_n}\psi(t-\tau,\mathbf{r}-\rho_1) \times S(t-\tau,\rho_1-\rho_2)E_z\left[\exp\left(\epsilon^2\frac{\alpha^2}{8}\int_0^{\tau'}\int_0^{\tau'} S(\tau_1-\tau_2,\mathbf{z}(\tau_1)-\mathbf{z}(\tau_2))d\tau_1 d\tau_2\right) \times \delta[\mathbf{z}(\tau)-\mathbf{z}(\tau')-\rho_1+\rho_2]\delta[\mathbf{z}(\tau')-\rho_2]\right] \times d\tau d\tau' d\rho_1 d\rho_2 = \epsilon^2\frac{\alpha^2}{4}\int_0^t\int_0^{\tau_1}\int_{R_n}\int_{R_n} \psi(t-\tau_1,\mathbf{r}-\rho_1)S(\tau_1-\tau_2,\rho_1-\rho_2) \times \psi(\tau_1-\tau_2,\rho_1-\rho_2)\Gamma_1(\tau_2,\rho_2)d\tau_1 d\tau_2 d\rho_1 d\rho_2, \quad (10.4)$$

where $S$ is defined to be

$$S(t-t',\mathbf{r}-\mathbf{r}') = \langle \eta(t,\mathbf{r})\eta(t',\mathbf{r}')\rangle, \tag{10.5}$$

when $Q_2$, given by (10.4), is used in (9.3), an integral equation for $\Gamma_1$ is obtained

$$\Gamma_1(t,\mathbf{r}) = \psi(t,\mathbf{r}) + \epsilon^2 \frac{\alpha^2}{4}\int_0^t\int_0^{\tau_1}\int_{R_n}\int_{R_n} \psi(t-\tau_1,\mathbf{r}-\boldsymbol{\rho}_1)S(\tau_1-\tau_2,\boldsymbol{\rho}_1-\boldsymbol{\rho}_2) \times \psi(\tau_1-\tau_2,\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)\Gamma_1(\tau_2,\boldsymbol{\rho}_2)\,d\tau_1 d\tau_2 d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2. \tag{10.6}$$

This integral equation is obviously equivalent to the problem

$$\frac{\partial\Gamma_1(t,\mathbf{r})}{\partial t} - \frac{\alpha}{2}\Delta\Gamma_1(t,\mathbf{r}) = \epsilon^2\frac{\alpha^2}{4}\int_0^t\int_{R_n}\psi(t-\tau,\mathbf{r}-\boldsymbol{\rho}) \times S(t-\tau,\mathbf{r}-\boldsymbol{\rho})\Gamma_1(\tau,\boldsymbol{\rho})\,d\tau d\boldsymbol{\rho}, \tag{10.7}$$

$$\Gamma_1(0,\mathbf{r}) = \delta(\mathbf{r}). \tag{10.8}$$

The integro-differential equation (10.7) can be derived by applying the method of smooth perturbation due to Keller[1] and others. In view of closure hypothesis (10.3), this approximation is less accurate than that of MDID. In fact, a comparison of (10.7) and (9.6) reveals that the former is a linearized version of the latter. The expression for the error involved, similar to (9.9) can be written down. It is found that the error is again zero with $S$ is delta-correlated in time. Although Eq. (10.7) is derivable from (10.1) by MSP based on weak fluctuations, it is valid for strong fluctuation when the correlation time is small. For large correlation time and fixed $t$, the error is of $O(\alpha^4\epsilon^4)$.

Let us consider the next level of approximation. In (10.4), it is assumed that $\Gamma_1$ is representable in terms of slowly varying function $w(\epsilon^2 t,\mathbf{r})$ so that

$$\Gamma_1(t,\mathbf{r}) = \int_{R_n}\psi(t,\mathbf{r}-\boldsymbol{\rho})w(\epsilon^2 t,\boldsymbol{\rho})d\boldsymbol{\rho}. \tag{10.9}$$

The above representation is merely a formal approximation based on the intuitive idea that a small perturbation introduces a slow modulation of the solution. On using (10.9) in (10.7) and integrating the resulting equation from 0 to $t$, one finds, after simplification, that

$$\frac{\partial w(\tau,\mathbf{r})}{\partial\tau} = \frac{\alpha^2}{4}\frac{1}{t}\int_0^t\int_0^{\tau_1}\int_{R_n}\int_{R_n}\int_{R_n}\psi(-\tau_1,\mathbf{r}-\boldsymbol{\rho}_1) \times \psi(\tau_1-\tau_2,\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)S(\tau_1-\tau_2,\boldsymbol{\rho}_1-\boldsymbol{\rho}_2) \times \psi(\tau_2,\boldsymbol{\rho}_2-\boldsymbol{\rho}_3)w(\tau,\boldsymbol{\rho}_3)d\tau_1 d\tau_2 d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2 d\boldsymbol{\rho}_3 \tag{10.10}$$

in which $\tau = \epsilon^2 t$. Let

$$\phi(\tau_1,\boldsymbol{\rho},\mathbf{r}) = \int_0^{\tau_1}\int_{R_n}\int_{R_n}\psi(-\tau,\mathbf{r}-\boldsymbol{\rho}_1) \times \psi(\tau_1-\tau_2,\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)\psi(\tau_2,\boldsymbol{\rho}_2-\boldsymbol{\rho}_3) \times w(\tau,\boldsymbol{\rho})d\tau_2 d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2. \tag{10.11}$$

Then, as $t\to\infty$ with $\tau$ fixed, Eq. (10.10) has the following limiting form

$$\frac{\partial w(\tau,\mathbf{r})}{\partial\tau} = \frac{\alpha^2}{4}\lim_{t\to\infty}\frac{1}{t}\int_0^t\int_{R_n}\phi(\tau,\boldsymbol{\rho},\mathbf{r})w(\tau,\boldsymbol{\rho})d\tau d\boldsymbol{\rho}. \tag{10.12}$$

This equation is shown in Appendix 2 to agree with that obtained by a two-time method.[3] However, the approach given there is a variant of what is proposed in Ref. 3. It is seen that the two-time method can be taken to be an approximation to the method of smooth perturbation under the assumption (10.9) and by taking time-average.

If the correlation function $R = \epsilon^2 S$ is taken to be delta-correlated as shown by (5.1), then it is easy to show, invoking (10.10), that $\Gamma_1$ given by (10.9) satisfies the equation

$$\frac{\partial\Gamma_1(t,\mathbf{r})}{\partial t} = \frac{\alpha}{2}\left(\Delta + \frac{\alpha}{2}g(0)\right)\Gamma_1(t,\mathbf{r}). \tag{10.13}$$

This equation was first derived by Chernov[6] by Markov approximation which is known[7] to be equivalent to assuming the correlation $R$ being delta-correlated in $t$.

Finally, replacing $R$ by $\epsilon^2 S$ in (9.1) and expanding the exponential function in powers of $\epsilon^2$, the one-term expansion yields

$$\Gamma_1(t,\mathbf{r}) = \psi(t,\mathbf{r}) + \epsilon^2\frac{\alpha^2}{4}\int_0^t\int_0^{\tau_1}E_z\{S[\tau_1-\tau_2,\mathbf{z}(\tau_1) - \mathbf{z}(\tau_2)]\delta[\mathbf{z}(t)-\mathbf{r}]\}d\tau_1 d\tau_2 + O(\epsilon^4\alpha^4). \tag{10.14}$$

The expectation in the above integral, depending only on three points $\tau_1, \tau_2$, and $t$ can be easily computed. With this result, (10.14) becomes

$$\Gamma_1(t,\mathbf{r}) = \psi(t,\mathbf{r}) + \epsilon^2\frac{\alpha^2}{4}\int_0^t\int_0^{\tau_1}\int_{R_n}\int_{R_n} \psi(t-\tau_1,\mathbf{r}-\boldsymbol{\rho}_1)S(\tau_1-\tau_2,\boldsymbol{\rho}_1-\boldsymbol{\rho}_2) \times \psi(\tau_1-\tau_2,\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)\,\psi(\tau_2,\boldsymbol{\rho}_2)d\tau_1 d\tau_2 d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2 + O(\epsilon^4\alpha^4). \tag{10.15}$$

Alternatively, if one expands $u$ into a power series in $\epsilon$, the successive approximations for $u$ can be determined from (10.1). The mean solution is found by taking average termwise in the perturbation series. The result $\Gamma_1$ thus obtained coincides with (10.15). This procedure, known as Born approximation, suffers a serious defect, namely the secular behavior of the solution (for a good discussion, see Ref. 5). This limits the validity of the approximation to a small time range. Various modified perturbation methods, such as MSP and MTT, have been designed to circumvent this difficulty.

To compare various perturbation methods it seems reasonable to degree to the following convention: Approximation $A$ is said to be more accurate than approximation $B$ if $B$ is obtainable from $A$ by further approximations which lead to a simplification in finding the solution, and the poorest approximation of all is the one which is not uniformly valid. Then clearly one has the following implication:

$$\text{MDID} \to \text{MSP} \to \text{MTT} \to \text{MMA} \to \text{MBE}, \tag{10.16}$$

where the arrow points in the direction of decrease in accuracy. In passing it is cautioned that the two-time method is not applicable if the random field $\mu$ (or $\eta$) is time independent. A formal argument can be found in the Appendix, Sec. 2.

## 11. CONCLUDING REMARKS

By means of Wiener integrals, two problems arising from wave propagation in random media have been investigated. Certain concrete results are obtained by this approach, notably the results contained in Secs. 5–8. The connection between function space integrals and differential equations may serve to facilitate the actual means of evaluating the integrals as well as to clarify the nature of various approximations. The results presented here are far from complete due to the well-known difficulty in the evaluation of functional integrals. This approach will bear more fruits when the functional integral calculus are advanced and better methods of approximate evaluation become available. In Ref. 20 Daletskii gave a representation for the solution of certain hyperbolic system in terms of a continuous integral (or functional integral). Though concrete results may not be obtainable, the part on the derivation of moment equations can presumely be carried over. Finally one remarks that the results given in this paper can be interpreted in the context of a quantum mechanical problem, the motion of a particle in a force field or random potential.

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## APPENDIX

### 1. The Limit of a Functional Integral

Consider the limit, as $\alpha_1 = \mathrm{Re}\{\alpha\} \to 0$, of the integral $I_1$ defined by (5.11). To show this limit is given by (5.13), one rescales $\mathbf{p}_2$ according to

$$\mathbf{p}(\tau) = (2\alpha_1)^{-1/2}\mathbf{p}_2(\tau). \tag{A1}$$

Then $\mathbf{p}(\tau)$ is a Wiener process with the covariance matrix

$$\langle p_j(\tau_1)p_k(\tau_2)\rangle = \min\{\tau_1, \tau_2\}\delta_{ij}; \tag{A2}$$

upon using (A1) in (5.11), it yields

$$I_1(t, \mathbf{r}_1\mathbf{r}_2, \alpha_1) = E_p\left[\exp\left(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^t g(\sqrt{2\alpha_1}\,\mathbf{p}(\tau) - \sqrt{2\alpha_1}\times \mathbf{p}(t) - \mathbf{r}_1 + \mathbf{r}_2)d\tau\right) h(\mathbf{r}_1 - \mathbf{r}_2 - \sqrt{2\alpha_1}\,\mathbf{p}(t))\right]. \tag{A3}$$

Let it be supposed that the functions $g$ and $h$ are bounded and continuous on $R_n$. Then the functional inside the expectation sign in (A3) is bounded and continuous and hence is Wiener $p$ integrable for each $\alpha_1 > 0$. Invoking the dominated convergence theorem in measure theory, one has the desired result as asserted

$$\begin{aligned}\lim_{\alpha_1\to 0} I_1(t, \mathbf{r}_1\mathbf{r}_2, \alpha_1) &= \lim_{\alpha_1\to 0} E_p \\ &\times \left[\exp\left(\tfrac{1}{4}\alpha\bar{\alpha}\int_0^t g(\sqrt{2\alpha_1}\,\mathbf{p}(\tau) - \sqrt{2\alpha_1}\,\mathbf{p}(t) - \mathbf{r}_1 + \mathbf{r}_2)d\tau\right)\right. \\ &\left.\times h(\mathbf{r}_1 - \mathbf{r}_2 - \sqrt{2\alpha_1}\,\mathbf{p}(t))\right] \\ &= E_p\left[\exp\left(\tfrac{1}{4}\alpha_2\bar{\alpha}_2\int_0^t g(\mathbf{r}_2 - \mathbf{r}_1)d\tau\right)h(\mathbf{r}_1 - \mathbf{r}_2)\right] \\ &= h(\mathbf{r}_1 - \mathbf{r}_2)\exp[\tfrac{1}{4}\alpha_2\bar{\alpha}_2 g(\mathbf{r}_2 - \mathbf{r}_1)t].\end{aligned} \tag{A4}$$

### 2. A Derivation of a Mean Equation by the Two-Time Method

To apply the MTT, one deals with Eq. (10.1) directly. Surpressing the dependence of $u$ on $\mathbf{r}$, one seeks a solution of the form (see Ref. 3)

$$u(t, \epsilon) = v(t, \tau, \epsilon), \tag{A5}$$

where $\tau = \epsilon^2 t$ and $v$ is a function depending on two times $t$ and $\tau$. Here $v$ is different from that defined in Sec. 2. Then one has the following differentiation rule

$$\frac{\partial u}{\partial t} = \frac{\partial v}{\partial t} + \epsilon^2\frac{\partial v}{\partial \tau}. \tag{A6}$$

Using (A5) and (A6) in (10.1) and (10.2) and expanding $v$ into a power series in $\epsilon$,

$$v(t, \tau, \epsilon) = v_0(t, \tau) + \epsilon v_1(t, \tau) + \epsilon^2 v_2(t, \tau) + \cdots. \tag{A7}$$

The resulting equation gives rise to the following recursive system

$$\frac{\partial v_0}{\partial t} - \frac{\alpha}{2}\Delta v_0 = 0, \tag{A8}$$

$$v_0(0, 0) = \delta(\mathbf{r}),$$

$$\frac{\partial v_1}{\partial t} - \frac{\alpha}{2}\Delta v_1 = \frac{\alpha}{2}\eta v_1, \tag{A9}$$

$$v_1(0, 0) = 0,$$

and

$$\frac{\partial v_2}{\partial t} - \frac{\alpha}{2}\Delta v_2 = \frac{\alpha}{2}\eta v_1 - \frac{\partial v_0}{\partial \tau}, \tag{A10}$$

$$v_2(0, 0) = 0,$$

$$\cdots.$$

The solution to (A8) is found to be

$$v_0(t, \tau) = \int_{R_n} \psi(t, \mathbf{r} - \boldsymbol{\rho})\hat{w}(\tau, \boldsymbol{\rho})d\boldsymbol{\rho}, \tag{A11}$$

where $\hat{w}$ is a slowly varying random function to be determined, and it satisfies the initial condition

$$\hat{w}(0, \mathbf{r}) = \delta(\mathbf{r}). \tag{A12}$$

By substituting (A11) into (A9), Eqs. (A9) is then solved to give

$$v_1(t, \tau) = \frac{\alpha}{2}\int_0^t\int_{R_n}\int_{R_n} \psi(t - s, \mathbf{r} - \boldsymbol{\rho}_1)\psi(s, \boldsymbol{\rho}_1 - \boldsymbol{\rho}_2) \times \eta(s, \boldsymbol{\rho}_1)\hat{w}(\tau, \boldsymbol{\rho}_2)ds d\boldsymbol{\rho}_1 d\boldsymbol{\rho}_2. \tag{A13}$$

When (A11) and (A13) are used in (A10), its solution reads

$$v_2(t,\tau) = \frac{\alpha^2}{4}\int_0^t\int_0^s\int_{R_n}\int_{R_n}\int_{R_n}\psi(t-t_1,\mathbf{r}-\rho_1)$$
$$\times\psi(t_1-t_2,\rho_1-\rho_2)\psi(t_2,\rho_2-\rho_3)[\eta(t_1,\rho_1)$$
$$\times\eta(t_2,\rho_2)]\hat{w}(\tau,\rho_3)\,dt_1dt_2d\rho_1d\rho_2d\rho_3$$
$$-t\frac{\partial}{\partial\tau}\int_{R_n}\psi(t,\mathbf{r}-\rho)\hat{w}(\tau,\rho)d\rho. \qquad \text{(A14)}$$

It is seen that the second term on the right-hand side of (A14) grows linearly with $t$. For the mean solution to be bounded in $t$, one requires that

$$\lim_{t\to\infty}\frac{1}{t}\langle v_2\rangle = 0. \qquad \text{(A15)}$$

In view of (A14), condition (A15) gives rise to an equation for $w = \langle\hat{w}\rangle$

$$\frac{\partial w(\tau,\mathbf{r})}{\partial\tau} = \frac{\alpha^2}{4}\lim_{t\to\infty}\frac{1}{t}\int_0^t\int_0^{t_1}\int_{R_n}\int_{R_n}\int_{R_n}\psi(-t_1,\mathbf{r}-\rho_1)$$
$$\times\psi(t_1-t_2,\rho_1-\rho_2)S(t_1-t_2,\rho_1-\rho_2)\psi(t_2,\rho_2-\rho_3)$$
$$\times w(\tau,\rho_3)\,dt_1dt_2d\rho_1d\rho_2d\rho_3. \qquad \text{(A16)}$$

The initial condition (A12) yields

$$w(0,\mathbf{r}) = \delta(\mathbf{r}). \qquad \text{(A17)}$$

Here one tacitly made use of the almost sure stability theorem in probability [see Eq. (4.2) in Ref. 3] before the expectation is taken. This permits the replacement of the time-average of a random function by the time-average of its mean function. It is because of this that Eq. (A16) is no longer valid when the random field $\eta$ is time independent. Therefore the two-time method is not applicable to this case.

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# A Model for Dissipative Behavior in Nonlinear Quantum Optics

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The compatibility of mechanistic, microscopic dynamics with dissipative, macroscopic behavior is proved by solving rigorously a model. This model consists of an infinite chain of two-level atoms interacting with an electromagnetic mode via two-photon emission and absorption.

## INTRODUCTION

The finite lifetimes of unstable particles, and the relaxation times of nonequilibrium thermodynamics are usually treated by approximate methods which tacitly assume that these *dissipative* behaviors are somehow compatible with the *conservative* laws of mechanics. To prove that this assumption is correct is still an open problem in both scattering theory and nonequilibrium statistical mechanics. Two projection techniques have been used in attempts to solve this problem in a manner which would be both mathematically rigorous and physically satisfying. In Sec. 1, we sketch these two approaches and indicate their respective pitfalls. The main body of the paper then treats explicitly an example in which the pitfalls of these projection techniques are avoided. Specifically, we present a quantum *mechanistic* model which admits a set $\mathfrak{M}_0$ of macroscopic observables leading to a *dissipative, selfcontained* macroscopic description of the evolution. We first describe in Sec. 2 a simplified version of the microscopic, mechanistic model. The set $\mathfrak{M}_0$ of the observables of interest and the dissipative character of the evolution relative to $\mathfrak{M}_0$ are discussed in Sec. 3. The full model is presented in Sec. 4. Some mathematical proofs are collected in the appendices. The general significance of the results is indicated in Sec. 5.

## 1. PROJECTION TECHNIQUES

The first evidence we have that a "macroscopic" dissipative description of the evolution is in principle compatible with a finer, or "microscopic," mechanistic description is based on the following embedding theorem due to Sz-Nagy.[1] Let $\{S^t | t \in \mathbf{R}^+\}$ be a continuous, contraction semigroup acting in a Hilbert space $\mathfrak{K}_0$, then there exists a unique (up to isomorphisms) triple $\{\mathfrak{K}, U^t, \mathfrak{D}\}$ constituted by a Hilbert space $\mathfrak{K}$, a continuous unitary group $\{U^t | t \in \mathbf{R}\}$ on $\mathfrak{K}$,

$$v_2(t,\tau) = \frac{\alpha^2}{4}\int_0^t\int_0^s\int_{R_n}\int_{R_n}\int_{R_n}\psi(t-t_1,\mathbf{r}-\rho_1)$$
$$\times\psi(t_1-t_2,\rho_1-\rho_2)\psi(t_2,\rho_2-\rho_3)[\eta(t_1,\rho_1)$$
$$\times\eta(t_2,\rho_2)]\hat{w}(\tau,\rho_3)\,dt_1dt_2d\rho_1d\rho_2d\rho_3$$
$$-t\frac{\partial}{\partial\tau}\int_{R_n}\psi(t,\mathbf{r}-\rho)\hat{w}(\tau,\rho)d\rho. \qquad \text{(A14)}$$

It is seen that the second term on the right-hand side of (A14) grows linearly with $t$. For the mean solution to be bounded in $t$, one requires that

$$\lim_{t\to\infty}\frac{1}{t}\langle v_2\rangle = 0. \qquad \text{(A15)}$$

In view of (A14), condition (A15) gives rise to an equation for $w = \langle\hat{w}\rangle$

$$\frac{\partial w(\tau,\mathbf{r})}{\partial\tau} = \frac{\alpha^2}{4}\lim_{t\to\infty}\frac{1}{t}\int_0^t\int_0^{t_1}\int_{R_n}\int_{R_n}\int_{R_n}\psi(-t_1,\mathbf{r}-\rho_1)$$
$$\times\psi(t_1-t_2,\rho_1-\rho_2)S(t_1-t_2,\rho_1-\rho_2)\psi(t_2,\rho_2-\rho_3)$$
$$\times w(\tau,\rho_3)\,dt_1dt_2d\rho_1d\rho_2d\rho_3. \qquad \text{(A16)}$$

The initial condition (A12) yields

$$w(0,\mathbf{r}) = \delta(\mathbf{r}). \qquad \text{(A17)}$$

Here one tacitly made use of the almost sure stability theorem in probability [see Eq. (4.2) in Ref. 3] before the expectation is taken. This permits the replacement of the time-average of a random function by the time-average of its mean function. It is because of this that Eq. (A16) is no longer valid when the random field $\eta$ is time independent. Therefore the two-time method is not applicable to this case.

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# A Model for Dissipative Behavior in Nonlinear Quantum Optics

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The compatibility of mechanistic, microscopic dynamics with dissipative, macroscopic behavior is proved by solving rigorously a model. This model consists of an infinite chain of two-level atoms interacting with an electromagnetic mode via two-photon emission and absorption.

## INTRODUCTION

The finite lifetimes of unstable particles, and the relaxation times of nonequilibrium thermodynamics are usually treated by approximate methods which tacitly assume that these *dissipative* behaviors are somehow compatible with the *conservative* laws of mechanics. To prove that this assumption is correct is still an open problem in both scattering theory and nonequilibrium statistical mechanics. Two projection techniques have been used in attempts to solve this problem in a manner which would be both mathematically rigorous and physically satisfying. In Sec. 1, we sketch these two approaches and indicate their respective pitfalls. The main body of the paper then treats explicitly an example in which the pitfalls of these projection techniques are avoided. Specifically, we present a quantum *mechanistic* model which admits a set $\mathfrak{M}_0$ of macroscopic observables leading to a *dissipative, selfcontained* macroscopic description of the evolution. We first describe in Sec. 2 a simplified version of the microscopic, mechanistic model. The set $\mathfrak{M}_0$ of the observables of interest and the dissipative character of the evolution relative to $\mathfrak{M}_0$ are discussed in Sec. 3. The full model is presented in Sec. 4. Some mathematical proofs are collected in the appendices. The general significance of the results is indicated in Sec. 5.

## 1. PROJECTION TECHNIQUES

The first evidence we have that a "macroscopic" dissipative description of the evolution is in principle compatible with a finer, or "microscopic," mechanistic description is based on the following embedding theorem due to Sz-Nagy.[1] Let $\{S^t | t \in \mathbf{R}^+\}$ be a continuous, contraction semigroup acting in a Hilbert space $\mathfrak{K}_0$, then there exists a unique (up to isomorphisms) triple $\{\mathfrak{K}, U^t, \mathfrak{D}\}$ constituted by a Hilbert space $\mathfrak{K}$, a continuous unitary group $\{U^t | t \in \mathbf{R}\}$ on $\mathfrak{K}$,

and a projector $\mathfrak{D}$ from $\mathfrak{K}$ onto $\mathfrak{K}_0$ such that $\mathfrak{S}^t = \mathfrak{D}U^t\mathfrak{D}$ for all $t$ in $\mathbf{R}^+$, and $\{U^t\Psi \mid t \in \mathbf{R}, \Psi \in \mathfrak{K}_0\}$ is dense in $\mathfrak{K}$. Several papers[2-4] have recently discussed the idea that this theorem could provide a *conservative*, rigorously mechanistic explanation for the *dissipative*, exponential decay of unstable particles. It would seem natural to consider[5] the same idea in nonequilibrium statistical mechanics. The physical interpretation of the mathematical construction involved in Sz-Nagy's theorem presents, however, even more than in the case of unstable particles, some rather serious difficulties, among which is the physical identification of the observables and states of the microscopic description obtained in this manner.

A line of less resistance thus appears to be the study of the inverse problem where one supposes known the microscopic description and asks whether a dissipative macroscopic evolution does exist. This problem can be decomposed in three steps: First, identify the set $\mathfrak{N}$ of the microscopic observables, the microscopic equations of motion and the set $\mathfrak{M}$ of macroscopic observables; second, obtain a reduced macroscopic description, e.g., in the form of a generalized master equation (GME); third, investigate whether this description is dissipative, i.e., determine under which conditions the GME reduces to a Pauli master equation (PME). A model[5,6] has been proposed, showing that steps (1) and (2) can indeed be carried out, thus setting on a rigorous footing a well defined projection technique in Liouville space. In this model, $\mathfrak{N}$ is the von Neumann algebra $\mathfrak{B}(\mathfrak{K})$ of all bounded operators acting in some Hilbert space $\mathfrak{K}$; the time evolution is given, in the Schrödinger picture, by the von Neumann equation

$$\frac{d}{dt}\rho^t = -iL\rho^t \text{ with } L\cdot = [H,\cdot], \tag{1}$$

and H is the microscopic Hamiltonian; the Liouville operator L is shown to act as a self-adjoint operator on the Hilbert space $\mathfrak{L}(\mathfrak{K})$ of all Hilbert–Schmidt operators on $\mathfrak{K}$. This space, called "Liouville space," contains as vectors the density matrices $\rho$. $\mathfrak{M}$ is taken to be the Abelian von Neumann algebra generated by the "macrocells" $E_\Delta$ (i.e., $\{E_\Delta\}$ is a partition of $\mathfrak{K}$ into mutually orthogonal subspaces which are assumed to be of finite dimension $N_\Delta$). For every macroscopic observable $A = \sum_\Delta A(\Delta)E_\Delta$ in $\mathfrak{M}$ we thus have

$$\langle \rho^t; A\rangle = \sum_\Delta p^t(\Delta)A(\Delta) \tag{2}$$

and the GME

$$\frac{d}{dt}p^t(\Delta) = -\sum_{\Delta'}\int_0^t ds K^s(\Delta,\Delta') \times \left\{\frac{1}{N_{\Delta'}}p^{t-s}(\Delta') - \frac{1}{N_\Delta}p^{t-s}(\Delta)\right\} \tag{3}$$

is then derived without further approximation from the von Neumann equation (1) and the initial condition $\rho^0 = \mathfrak{D}\rho^0$, where the coarse-graining operator $\mathfrak{D}$ is defined as a projector on $\mathfrak{L}(\mathfrak{K})$ by

$$\mathfrak{D}\rho = \sum_\Delta p(\Delta)\rho_\Delta \text{ with } p(\Delta) = \mathrm{Tr}\rho E_\Delta \text{ and } \rho_\Delta = E_\Delta/N_\Delta. \tag{4}$$

Step (3) would then consist in showing that Eq. (3) reduces to

$$\frac{d}{dt}p^t(\Delta) = -\sum_{\Delta'}K(\Delta,\Delta')\left\{\frac{1}{N_{\Delta'}}p^t(\Delta') - \frac{1}{N_\Delta}p^t(\Delta)\right\}. \tag{5}$$

It has been proved,[7] however, and this is the pitfall associated with this projection technique, that this last step is *not* possible, i.e., that (5) is incompatible with (1) for the model as presented up to this point. Gudder and Marchand[8] have proved that $\mathfrak{D}$, as defined by (4), could not be generalized and still keep those of its properties which are essential to its interpretation and which have been used in the derivation of (3).

Various procedures have been proposed to bypass the incompatibility of (5) and (1). All involve some kind of argument to the effect that (5) should be understood to hold only after times large compared to some intrinsic microscopic time, e.g., "collision time." It has been suggested[7] in particular that the incompatibility of (5) and (1) can be removed by the introduction of a time-smoothing operation on $\mathfrak{M}$, accompanied by the corresponding smoothing of the initial conditions. This idea of replacing $\mathfrak{M}$ by a "smoother" set $\mathfrak{M}_0$ of observables which would behave in a truly dissipative manner has been strongly advocated by Prigogine and his school, and it plays a central role in their recent publications.[9] Taking this idea seriously into account, we come to suspect the discreteness of the spectrum of $\mathfrak{M}$ to be the stumbling block which barred (5) from receiving a mechanistic interpretation. The purpose of this paper is to show that this is indeed the case. We produce a mechanistic model which admits a set $\mathfrak{M}_0$ of macroscopic observables such that (i) the time evolution with respect to $\mathfrak{M}_0$ can be described in a self contained manner, (ii) it is dissipative, and (iii) $\mathfrak{M}_0$ has continuous spectrum.

## 2. THE SIMPLIFIED MICROSCOPIC EVOLUTION

We take for the algebra of microscopic observables the von Neumann algebra $\mathfrak{B}(\mathfrak{K})$ of all bounded operators on the Hilbert space $\mathfrak{K} = \mathfrak{L}^2(\mathbf{R})$ of all square integrable functions with respect to Lebesgue measure:

$$\mathfrak{N} = \mathfrak{B}(\mathfrak{L}^2(\mathbf{R}, dx)). \tag{6}$$

We define the time evolution by its action on the vectors of $\mathfrak{L}^2(\mathbf{R})$ as follows:

$$(U^t\Psi)(x) = e^{-t/2}\Psi(e^{-t}x). \tag{7}$$

Clearly $\{U^t \mid t \in \mathbf{R}\}$ is a continuous, one-parameter group of unitary operators acting on $\mathfrak{L}^2(\mathbf{R})$. Its generator, our *microscopic Hamiltonian*, is equal to

$$H = \tfrac{1}{2}(PQ + QP) \tag{8}$$

on the dense linear manifold $\mathfrak{S}(\mathbf{R})$ in $\mathfrak{L}^2(\mathbf{R})$, constituted by all infinitely differentiable functions $\Psi$ from R to C for which

$$\lim_{|x|\to\infty} x^m \frac{d^n\Psi}{dx^n}(x) = 0 \text{ for all } n, m = 0, 1, 2, \cdots. \tag{9}$$

P and Q are defined on $\mathfrak{S}(\mathbf{R})$ as usual by

$$(P\Psi)(x) = -i\frac{d\Psi}{dx}(x), (Q\Psi)(x) = x\Psi(x). \tag{10}$$

Since $\mathfrak{S}(\mathbf{R})$ is stable under P and Q, and since P, Q and H (see Appendix A) are essentially self-adjoint

on $\mathcal{S}(\mathbf{R})$, the formulas (8) and (10) suffice to define the self-adjoint operators P, Q and H.

We notice that the Fourier transform $F$ defined by

$$(F\Psi)(x) = (2\Pi)^{-1/2} \int dy \ \exp(ixy)\Psi(y) \tag{11}$$

acts as a *time-reversal* operator, i.e.,

$$FU^tF^* = U^{-t} \text{ for all } t \text{ in } \mathbf{R}. \tag{12}$$

Since $F$ is unitary, we conclude that

$$FHF^* = -\mathrm{H} \tag{13}$$

in agreement with (8) and the well-known equalities

$$FQF^* = \mathrm{P}, FPF^* = -\mathrm{Q}. \tag{14}$$

The effect (13) of the canonical transformation $F$ on H shows that the spectrum of H is symmetric with respect to 0. A more detailed analysis of (7) or (8) would actually show that the spectrum of H extends from $-\infty$ to $+\infty$, and is continuous with respect to Lebesgue measure. The physical meaning of the last but one property will be discussed in Sec. 4.

To every density matrix $\rho$, i.e., to every normal state on $\mathfrak{N} = \mathfrak{B}(\mathcal{L}^2(\mathbf{R}))$, corresponds a positive Hilbert–Schmidt kernel, i.e., an element $\rho$ in $\mathcal{L}^2(\mathbf{R}^2)$ such that

$$\begin{aligned} &(\rho\Psi)(x) = \int dy \rho(x,y)\Psi(y) \text{ for all } \Psi \text{ in } \mathcal{L}^2(\mathbf{R}), \\ &\iint dxdy\, |\rho(x,y)|^2 < \infty, \\ &\int dx \rho(x,x) = 1. \end{aligned} \tag{15}$$

The time evolution, in the Schrödinger picture (see Sec. 1), takes then the form $\rho(x,y) \to \rho^t(x,y)$ with

$$\rho^t(x,y) = e^{-t}\rho(e^{-t}x, e^{-t}y) \tag{16}$$

and $\{\mathfrak{U}^t | t \in \mathbf{R}\}$ defined on $\mathcal{L}^2(\mathbf{R}^2)$ by

$$(\mathfrak{U}^t R)(x,y) = e^{-t}R(e^{-t}x, e^{-t}y) \tag{17}$$

is clearly a continuous, one parameter group of unitary operators. Its generator [see von Neumann Eq. (1) in Sec. 1] is equal to

$$\mathrm{L} = \tfrac{1}{2}\{\mathrm{P}_x\mathrm{Q}_x + \mathrm{Q}_x\mathrm{P}_x) + (\mathrm{P}_y\mathrm{Q}_y + \mathrm{Q}_y\mathrm{P}_y)\}. \tag{18}$$

The precise definition of $\mathrm{P}_x, \mathrm{Q}_x, \mathrm{P}_y, \mathrm{Q}_y$, and L, and the associated domain questions are disposed of as in the beginning of this section [see the remark following (10), with now $\mathcal{S}(\mathbf{R})$ replaced by $\mathcal{S}(\mathbf{R}^2)$].

## 3. REDUCED DESCRIPTION

We now consider the set $\mathcal{L}^\infty(\mathbf{R})$ of all measurable, essentially bounded functions $f$: $\mathbf{R} \to \mathbf{C}$ with respect to the Lebesgue measure. This set is equipped with the structure of a normed*-algebra by the following definitions:

$$\begin{aligned} (\lambda f)(x) &= \lambda f(x), \\ (f+g)(x) &= f(x) + g(x), \\ (fg)(x) &= f(x)g(x), \\ f^*(x) &= f(x)^*, \\ \|f\| &= \operatorname*{ess-sup}_{x \in \mathbf{R}} |f(x)|, \end{aligned} \tag{19}$$

for every $f, g \in \mathcal{L}^\infty(\mathbf{R})$ and every $\lambda \in \mathbf{C}$. For every $f$ in $\mathcal{L}^\infty(\mathbf{R})$ we then define the bounded operator $A_f$ acting on $\mathcal{L}^2(\mathbf{R})$ by

$$(A_f\Psi)(x) = f(x)\Psi(x). \tag{20}$$

We now consider as the set $\mathfrak{M}_0$ of all "observables of interest" (see Sec. 1) the set

$$\mathfrak{M}_0 = \{A_f | f \in \mathcal{L}^\infty(\mathbf{R})\} \tag{21}$$

and notice[10] that $f \to A_f$ is an isometric isomorphism from the normed*-algebra $\mathcal{L}^\infty(\mathbf{R})$ to $\mathfrak{M}_0$ considered as a normed*-subalgebra of $\mathfrak{B}(\mathcal{L}^2(\mathbf{R}))$; further more $\mathfrak{M}_0$ is a maximal abelian von Neumann subalgebra of $\mathfrak{B}(\mathcal{L}^2(\mathbf{R}))$ and has continuous spectrum, namely R. The physical interpretation of $\mathfrak{M}_0$ is provided by the remark that $\mathfrak{M}_0$ is generated, as a von Neumann algebra by the projectors $\mathrm{E}_\Delta$ defined by

$$(\mathrm{E}_\Delta\Psi)(x) = \mathrm{X}_\Delta(x)\Psi(x), \tag{22}$$

where $\Delta$ runs over all Borel subsets of R, and $\mathrm{X}_\Delta$ is the characteristic function of $\Delta$. Hence $\mathfrak{M}_0$ is the maximal Abelian von Neumann algebra to which the position operator Q is affilated. We remark in passing that $\mathfrak{M}_0$ *maximal* abelian means in physical terms that the self adjoint elements of $\mathfrak{M}_0$ form a complete set of commuting observables; this fact is responsible for some simplifications in the forthcoming argument, but is not essential to its completion. Clearly the restrictions to $\mathfrak{M}_0$ of any normal state $\rho$ on $\mathfrak{N}$ is a normal state on $\mathfrak{M}_0$. Consequently[11] for every $\rho$ normal on $\mathfrak{N}$, there exists one positive element $\tilde{\rho}$ in $\mathcal{L}^1(\mathbf{R})$ such that

$$\langle \rho; A\rangle = \int A(x)\tilde{\rho}(x)dx \text{ for all } A \text{ in } \mathcal{L}^\infty(\mathbf{R}) \tag{23}$$

and, in particular,

$$\int \tilde{\rho}(x)dx = 1. \tag{24}$$

We thus have identified the macroscopic states corresponding to the normal states on $\mathfrak{N}$. Moreover, every normal state $\tilde{\rho}$ on $\mathfrak{M}_0$ can be written[12] as

$$\langle \tilde{\rho}; A\rangle = (\Psi, A\Psi) \tag{25}$$

for some $\Psi$ in $\mathcal{L}^2(\mathbf{R})$ with $\int |\Psi(x)|^2 dx = 1$. Conversely every such $\Psi$ generates a normal state $\tilde{\rho}$ on $\mathfrak{M}_0$, and upon extending (25) to every $A$ in $\mathfrak{N}$, $\Psi$ actually generates a normal state $\rho$ on $\mathfrak{N}$, the restriction of which to $\mathfrak{M}_0$ is evidently $\tilde{\rho}$. We notice that for every such $\Psi$ and every unitary operator $U$ in $\mathfrak{M}_0' = \mathfrak{M}_0$, $\Psi' = U\Psi$ also generates a normal state $\rho' \neq \rho$ on $\mathfrak{N}$, with, however, $\rho'$ equivalent[13] to $\rho$ with respect to $\mathfrak{M}_0$. Hence any normal macroscopic state contains infinitely many linearly independent normal microscopic states. We remark also that $\tilde{\rho}$ is the so-called "diagonal part"[9] of $\rho$; indeed the bridge with Prigogine's notation is provided by the remark that

$$\begin{aligned} &\tilde{\rho}(x) = R_0(x) \text{ with} \\ &R_\eta(\xi) \equiv \rho(\xi - \eta, \xi + \eta). \end{aligned} \tag{26}$$

In the perspective of Sec. 1, $\mathfrak{M}_0$ presents its first remarkable feature with respect to the microscopic time-evolution generated by (7). Indeed the automorphisms $\alpha^t$ of $\mathfrak{N}$ defined for every $t \in \mathbf{R}$ by

$$\alpha^t[A] = U^{-t}AU^t \tag{27}$$

map $\mathfrak{M}_0$ into itself, and actually the restriction of each $\alpha^t$ to $\mathfrak{M}_0$ is an automorphism of $\mathfrak{M}_0$ itself: For each $A$ in $\mathfrak{M}_0$ we have

$$(\alpha^t[A])(x) = A(e^t x). \tag{28}$$

This implies immediately the existence of a self-contained macroscopic description of the time evolution with respect to $\mathfrak{M}_0$:

$$\tilde{\rho}^t(x) = e^{-t}\tilde{\rho}(e^{-t}x). \tag{29}$$

The privileged role of $\mathfrak{M}_0$ with respect to the time evolution is emphasized by the change of variables (26). Indeed, for any normal state $\rho$ on $\mathfrak{N}$ we have

$$R^t_\eta(\xi) = e^{-t}R_{e^{-t}\eta}(e^{-t}\xi) \tag{30}$$

so that the nondiagonal part $R^t_{\eta\neq 0}$ depends, in the course of time, on $R^{t=0}_{\eta'}$ for all values $\eta' = e^{-t}\eta$, whereas the diagonal part $R^t_0$ satisfy Eq. (29), which involves $R^{t=0}_0$ only.

The second remarkable feature of $\mathfrak{M}_0$ is that the reduced description (29) of the time evolution satisfies the "master equation":

$$\frac{d}{dt}\tilde{\rho}^t = -i\tilde{\mathrm{L}}\tilde{\rho}^t$$

with $\tilde{\mathrm{L}}$ defined, for instance on $\mathcal{S}(\mathbf{R}) \subset \mathcal{L}^1(\mathbf{R})$

$$\text{by } \tilde{\mathrm{L}} = \Omega - i\Lambda, \text{ where}$$
$$\Omega = \tfrac{1}{2}(\mathrm{PQ} + \mathrm{QP}) \text{ and } \Lambda = \tfrac{1}{2}I. \tag{31}$$

$\Omega$ gives the usual propagation term, whereas the strictly positive operator $\Lambda$ gives the dissipative part usually associated with a master equation of Pauli type.

Equations (29) and (31) show that the time evolution prescribed by (7) and (16), reduced to $\mathfrak{M}_0$, provides a model for the kind of dissipative behavior looked for in Sec. 1. The dissipative character of the evolution, as viewed from $\mathfrak{M}_0$, can be emphasized by the following three side remarks. First, the macroscopic entropy defined naively by

$$\tilde{S}(t) = -\int dx \tilde{\rho}^t(x) \ln \tilde{\rho}^t(x) \tag{32}$$

is a strictly increasing function of time. Second, $\mathcal{S}(\mathbf{R})$ is stable with respect to $\{U^t | t \in \mathbf{R}\}$ as defined by (7), and the equation

$$\alpha^t[\mathrm{Q}] \equiv U^{-t}\mathrm{Q}U^t = e^t\mathrm{Q} \tag{33}$$

thus make sense on this dense linear manifold $\mathcal{S}(\mathbf{R})$ of $\mathcal{L}^2(\mathbf{R})$ on which Q and hence $\alpha^t[\mathrm{Q}]$ are essentially self adjoint. The obviously dissipative behavior of the operator Q (which is affilated to $\mathfrak{M}_0$), as given by (33), can also be seen from the time behavior of the bounded operators $\mathrm{E}_\Delta$ defined by (22):

$$(\mathrm{E}_\Delta)^t = \mathrm{E}_{\Delta^t}, \text{ where}$$
$$\Delta^t = \{e^{-t}x | x \in \Delta\}. \tag{34}$$

In particular, and this is our third remark, the partition

$$\gamma = \{\mathrm{E}_\Delta | \Delta = [n, n+1], n \in \mathbf{Z}\}, \tag{35}$$

of the identity $I$ on $\mathcal{L}^2(\mathbf{R})$ into orthogonal subspaces satisfies (for $\tau = \ln 2$)

$$\hat{0} \subset \cdots \subset \alpha^{-\tau}[\gamma] \subset \gamma \subset \alpha^{\tau}[\gamma] \subset \cdots \subset \hat{1},$$

with

$$\bigwedge_{n\in\mathbf{Z}} \alpha^{n\tau}[\gamma] = \hat{0},$$
$$\bigvee_{n\in\mathbf{Z}} \alpha^{n\tau}[\gamma] = \hat{1}, \tag{36}$$

a property reminiscent of the behavior of $K$-systems.[14]

## 4. PHYSICAL MODEL

The microscopic time evolution (7) of the simplified model considered in the preceding sections is generated by a Hamiltonian (8), the spectrum of which extends from $-\infty$ to $+\infty$, and hence is unbounded *from below*, as well as from above. From a physical point of view, this is so unacceptable a behavior for a system with a finite number of degrees of freedom (here 1) that one sometimes hears[4] such Hamiltonians referred to as "unphysical." Incidentally, this "trouble" has been diagnosed[3] in the approach via Sz-Nagy's theorem. It should however be pointed out that for systems with an infinite number of degrees of freedom this behavior is the rule[15] rather than the exception. We shall now indicate how our simplified model can be interpreted in this context.

We consider an infinite chain $\mathbf{Z}$ of identical spin-half particles (i.e., "two level atoms") interacting with an electromagnetic mode of frequency $\omega$. This problem is formulated in the manner usual in statistical mechanics by first prescribing the Hamiltonian relative to a finite region $\Omega$ in $\mathbf{Z}$, and then taking the limit of the corresponding time evolution as $\Omega$ tends to $\mathbf{Z}$. We thus define:

$$\mathrm{H}(\Omega) = \mathrm{H}_0(\Omega) + \lambda \mathrm{V}(\Omega), \tag{37}$$

with

$$\mathrm{H}_0(\Omega) = \omega(a^*a + \tfrac{1}{2}) + B\sum_{j\in\Omega}\sigma^z_j \tag{38}$$

and

$$\mathrm{V}(\Omega) = -\mathrm{N}(\Omega)^{-1}\sum_{j\in\Omega}(\sigma^+_j a a + \sigma^-_j a^* a^*). \tag{39}$$

This type of interaction is well known in quantum optics.[16]

The heuristic argument of the standard mean free field method used in the theory of phase transitions can be used here, but this should be done with some care. The mathematical problems connected with this aspect of our model are analyzed, and solved in detail in Appendices A, B, and C. The result is the following.

When the initial state of the system is prepared in such a manner that the EM mode is uncoupled to the spin system, and that the latter is in the canonical equilibrium corresponding, for the natural temperature $\beta$, to the Hamiltonian $-B\Sigma_j\sigma^\gamma_j$, the time evolution corresponding to the thermodynamical limit of (37) is given, for any observable $A_{\mathrm{EM}}$ relative to the electromagnetic mode, by

$$\langle \psi; A_{\mathrm{EM}}\rangle^t = \langle \nu^t_{W,\phi}[\rho_{\mathrm{EM}}]; \alpha^t_{\mathrm{EM}}[A_{\mathrm{EM}}]\rangle, \tag{40}$$

where $\rho_{\mathrm{EM}}$ is the initial normal state of the EM mode, and

$$\nu^t_{W,\phi}[\rho_{EM}] = U^t_{W,\phi}\rho_{EM}U^{-t}_{W,\phi},$$
$$\alpha^t_{EM}[A_{EM}] = U^{-t}_{EM}A_{EM}U^t_{EM}, \tag{41}$$

with $\{U^t_{W,\phi} | t \in R\}$ and $\{U^t_{EM} | t \in R\}$ defined explicitly in Appendix C. The physical interpretation of this result can be given as follows.

The generator $H_{EM}$ of $\{U^t_{EM} | t \in R\}$ is the free Hamiltonian of the EM mode, the fundamental frequency of which corresponds to the resonant situation where a transition from $\sigma^z = +1$ to $\sigma^z = -1$ is accompanied by the emission of two photons of frequency $\omega_0 = B$. This part of the evolution is thus trivial: Its contribution is a periodic motion of frequency $\omega_0$.

The generator $W_\phi$ of $\{U^t_{W,\phi} | t \in R\}$ is more complicated as it describes the occurence of a dissipative behavior. We now substantiate this assertion. We can rewrite (C10) in the form

$$W_\phi = [(\omega - \omega_0)/\omega_0]H_{EM} + \lambda\sigma W, \tag{42}$$

with

$$H_{EM} = \tfrac{1}{2}(P^2 + \omega_0^2 Q^2), \tag{43}$$

$$W = \tfrac{1}{2}(PQ + QP). \tag{44}$$

We use the substitution

$$Q = (2\omega_0)^{-\frac{1}{2}}(a^* + a), \qquad P = i(\tfrac{1}{2}\omega_0)^{\frac{1}{2}}(a^* - a). \tag{45}$$

For the resonnant frequency $\omega_0 = B$, $W_\phi$ reduces then, up to the multiplicative constant $\lambda\sigma$, to the Hamiltonian (7) of our simplified model, the dissipative behavior of which we already discussed. We still might add here that for any initial state $\rho_{EM}$ of the form

$$\langle \rho_{EM}; A_{EM}\rangle = \sum_{n=0}^{\infty} \rho_n(\Psi_n, A_{EM}\Psi_n)$$
with
$$a^*a\Psi_n = n\Psi_n, \tag{46}$$

our Eq. (40) leads to

$$\langle \rho_{EM}; H_{EM}\rangle^t = \langle \rho_{EM}; H_{EM}\rangle \cosh 2\lambda\sigma t, \tag{47}$$
$$\langle \rho_{EM}; Q\rangle^t = 0 = \langle \rho_{EM}; P\rangle^t, \tag{48}$$
$$\langle \rho_{EM}; Q^2\rangle^t = \langle \rho_{EM}; Q^2\rangle\{\exp(2\lambda\sigma t)\cos^2\omega_0 t + \exp(-2\lambda\sigma t)\sin^2\omega_0 t\}, \tag{49}$$
$$\langle \rho_{EM}; P^2\rangle^t = \langle \rho_{EM}; P^2\rangle\{\exp(-2\lambda\sigma t)\cos^2\omega_0 t + \exp(2\lambda\sigma t)\sin^2\omega_0 t\}. \tag{50}$$

We conclude from (47) that the spin system releases its energy to the EM mode in such a manner that the expectation value of the (unperturbed) energy $H_{EM}$ stored in this mode increases monotonically with $|t|$, and actually one has for large $|t|$

$$\langle \rho_{EM}; H_{EM}\rangle^t \approx \tfrac{1}{2}\langle \rho_{EM}; H_{EM}\rangle \exp(2\lambda\sigma|t|). \tag{51}$$

Moreover, (48) implies that (49) and (50) give the evolution of the covariances $\langle \Delta Q\rangle$ and $\langle \Delta P\rangle$ and Q and P, the explicit form obtained for these quantities confirms the interpretation of the dissipative effect of the spin system on the EM mode.

From Eq. (45) on, our discussion was restricted to the study of the resonant mode $\omega = \omega_0 = B$. If, however, $\omega \neq \omega_0$, the situation is somewhat more complicated. Three cases can actually occur depending on whether $\epsilon \equiv |\lambda\sigma/\omega - \omega_0|$ is smaller than, equal to, or larger than 1. In particular, the spectrum of the quadratic Hamiltonian (42) is: (A) discrete and semibounded if $\epsilon < 1$, (B) absolutely continuous, doubly degenerate and semibounded if $\epsilon = 1$, and (C) absolutely continuous on the whole of R if $\epsilon > 1$; actually in the later case (42) is unitarily equivalent, up to a real multiplicative constant, to (44). Hence the kind of dissipative behavior observed for the resonant mode occurs also for the nonresonant modes if and only if the absolute value of the coupling constant $\lambda$ exceed a critical value $\lambda = |(\omega - \omega_0)/\sigma|$ depending on $\omega - \omega_0$, and, through $\sigma$, on the temperature of the spin system.

## 5. CONCLUSION

We obtained the exact solution of the dynamics of an electromagnetic mode (see Eqs. 37–39) with an infinite system of two level atoms (or spins) via two-photon emission or absorption. This solution is expressed in an "interaction picture" (see Eqs. 40–41, and Appendix C) which separates the time evolution into two parts. The first is akin to the free dynamics, whereas the second singles out the dissipative part of the evolution. To uncover the dissipative character of the latter we treated (in Secs. 2 and 3) a simplified model in which the microscopic observables are restricted to the observables of the EM mode, the microscopic Hamiltonian is given by Eq. (8), and the macroscopic observables are assumed to be the self-adjoint elements of the maximal Abelian von Neumann algebra $\mathfrak{M}_0$ to which the position operator Q is affiliated; we found the macroscopic equation of the motion relative to $\mathfrak{M}_0$ (see Eqs. 31 and 33). The underlying reversibility of the microscopic evolution shows itself, on the macroscopic level, through the fact that the Fourier transform, which changes Q into P, acts as a time reversal operator for this simplified model; this implies the existence of a set of observables, $\mathfrak{M}_0(P)$, obtained from $\mathfrak{M}_0 = \mathfrak{M}_0(Q)$ by a time-reversal operation $P^t = e^{-t}P$ (compare with 33). Coming back to the full model, we noticed that the effect of the free part of the interaction picture leads to a uniform rotation in the plane (Q, P). As a consequence, the combined evolution leads in particular to the dissipative Eqs. 47–50, valid for all values of the coupling constant $\lambda$ when the frequency of the EM mode is identical to the resonant frequency $\omega_0 = B$ (where $2B$ is equal to the spacing of the energy levels of the individual atoms). For the off-resonant frequencies, we show that there exists a threshold in the value of the coupling constant; below this threshold, the system behaves in a conservative manner; whereas the type of dissipative behavior described at resonance also occurs above the threshold.

In relation with the two projection techniques which we reviewed in Sec. 1, we would like to point out that the passage (see Sec. 3) from the conservative, microscopic description of the evolution to the reduced description relative to Q (or to P) is not, and actually cannot be,[17] achieved by a projection acting from some Hilbert space $\mathfrak{L}$ to some Hilbert space $\mathfrak{DL}$. Indeed, the continuity of the spectrum of $\mathfrak{M}_0$ implies (see in particular Eq. 26) that the diagonal part $\tilde{\rho}$, with respect to $\mathfrak{M}_0$, of a density matrix $\rho$ on $\mathfrak{B}(\mathfrak{L}^2R))$ is in general an element of $\mathfrak{L}^1(R)$ and the later is not a subspace of the Liouville space $\mathfrak{L}^2(R^2)$. This fact illustrates an intrinsic limitation of the usual projec-

tion technique in Liouville space and in particular provides a reason for its failure to lead to a Pauli-type master equation. The main point of the model is to show that this difficulty can indeed be bypassed. In the same breath, this shows also that the Sz-Nagy theorem, however natural it might seem to be in this connection, is actually not the universal answer to the question of the compatibility of the mechanistic and the dissipative descriptions of a physical system. The physical model presented in this paper admits both descriptions and does not conform to the scheme suggested by this mathematical theorem.

The model also raises some interesting questions of principle which we defer to answer here. The first one is to understand to which extent the model is generic. In fact, given $\mathbf{Q}^t = e^{-t}\mathbf{Q}$ we can construct $\mathfrak{L}^2(\mathbf{R}, dx)$, $\mathfrak{M}_0 = \mathfrak{L}^\infty(\mathbf{R}, dx)$ and $\{U^t | t \in \mathbf{R}\}$ in a canonical manner, and the conjugate variable $\mathbf{P}^t = e^{-t}\mathbf{P}$ then occurs naturally. This construction can clearly be extended to the case of several independent dissipative modes with different decay times. The second question raised by this model stems from its structural analogy with $K$- systems; we suggest that the model might help elucidate the connections between the mathematical theories of dissipative systems (see for instance Arnold and Avez[14]) and the physical approaches followed by van Hove[18] and Prigogine[9], for instance.

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## APPENDIX A

The purpose of this appendix is to prove the self-adjointness of some of the operators used in the main body of the paper.

*Lemma:* Let $\{U^t | t \in \mathbf{R}\}$ be a strongly continuous group of unitary operators acting on some Hilbert space $\mathfrak{K}$ and H be its self-adjoint generator. Let further $\mathfrak{M}$ be a dense linear manifold in $\mathfrak{D}(\mathrm{H})$, stable under $\{U^t | t \in \mathbf{R}\}$. Then the restriction of H to $\mathfrak{M}$ is essentially self adjoint.

*Proof:* For any complex $\lambda$ with $\mathrm{Re}\lambda \neq 0$, form $\mathfrak{N} = (\lambda + i\mathrm{H})\mathfrak{M}$, and let $\Phi$ be in $\mathfrak{N}^\perp$. We have then for every $\Psi$ in $\mathfrak{M}$

$$\frac{d}{dt}(\Phi, U^t\Psi) = (\Phi, -i\mathrm{H}U^t\Psi) = \lambda(\Phi, U^t\Psi) \tag{A1}$$

and, hence,

$$(\Phi, U^t\Psi) = e^{\lambda t}(\Phi\Psi), \tag{A2}$$

and, since $\mathfrak{M}$ is dense,

$$U^t\Phi = e^{-\lambda t}\Phi, \tag{A3}$$

which is incompatible with $\mathrm{Re}\lambda \neq 0$ unless $\Phi = 0$. We therefore conclude that $(\lambda + i\mathrm{H})\mathfrak{M}$ is dense in $\mathfrak{K}$, which is to say[19] that H is essentially self adjoint on $\mathfrak{M}$. Q.E.D.

We now remark that the assumptions of the lemma are satisfied for $\mathfrak{K} = \mathfrak{L}^2(\mathbf{R})$, $\{U^t | t \in \mathbf{R}\}$ defined by (7) and $\mathfrak{M} = \mathcal{S}(\mathbf{R})$, thus implying that the Hamiltonian (8) is essentially self adjoint on $\mathcal{S}(\mathbf{R})$.

This conclusion is easily transfered to the Hamiltonian (42) considered as an operator acting either within $\mathfrak{L}^2(\mathbf{R})$ or within $\mathfrak{L}^2(\mathbf{R}) \otimes \mathfrak{K}_s$, where $\mathfrak{K}_s$ can be any Hilbert space; in the latter case $\mathfrak{M}$ is to be taken as the linear span of $\mathcal{S}(\mathbf{R}) \otimes \mathfrak{K}_s$, and $\overline{\mathrm{W}}_\phi(\Psi \otimes \Phi) \equiv \mathrm{W}_\phi\Psi \otimes \Phi$.

Besides establishing that (42) leads unambiguously to the definition of a time evolution, this remark will also allow us to prove the convergence implicit in our use of the mean free field method. This will be done in Appendix C.

## APPENDIX B

The purpose of this appendix is to devise an interaction picture adapted to computing the time evolution of the expectation values of the observables relative to the EM field.

We first rewrite (37) in the form

$$\mathrm{H}(\Omega) = \mathrm{G}_0(\Omega) + \mathrm{W}(\Omega), \tag{B1}$$

with

$$\mathrm{G}_0(\Omega) = B\left\{\sum_{j\in\Omega} \sigma_j^z + (a^*a + \tfrac{1}{2})\right\} \tag{B2}$$

and

$$\mathrm{W}(\Omega) = (\omega - B)(a^*a + \tfrac{1}{2}) + \tfrac{1}{2}\lambda\{\sigma^+(\Omega)aa + \sigma^-(\Omega)a^*a^*\}, \tag{B3}$$

where

$$\sigma^\pm(\Omega) = \mathrm{N}(\Omega)^{-1}\sum_{j\in\Omega}\sigma_j^\pm. \tag{B4}$$

We notice that

$$[\mathrm{G}_0(\Omega), \mathrm{W}(\Omega)] = 0. \tag{B5}$$

Furthermore, we remark upon comparing (B2) with (38) and (B3) with (39) that at resonance (i.e., where $\omega = \omega_0 \equiv B$) $\mathrm{H}_0(\Omega) = \mathrm{G}_0(\Omega)$ and $\mathrm{W}(\Omega) = \lambda\mathrm{V}(\Omega)$. (B5) implies that for any $\Psi \in \mathfrak{L}^2(\mathbf{R}) \otimes \mathfrak{K}_s(\Omega)$ and any $A \in \mathfrak{B}(\mathfrak{L}^2(\mathbf{R})) \otimes \mathfrak{A}(\Omega)$,

$$\begin{aligned}\langle\psi; A\rangle^t &\equiv (U^t(\Omega)\Psi, AU^t(\Omega)\Psi)\\ &= (U_{\mathrm{W}}^t(\Omega)\Psi, U_0^{-t}(\Omega)AU_0^t(\Omega)U_{\mathrm{W}}^t(\Omega)\Psi),\end{aligned} \tag{B6}$$

where $\{U^t(\Omega) | t \in \mathbf{R}\}$, $\{U_0^t(\Omega) | t \in \mathbf{R}\}$ and $\{U_{\mathrm{W}}^t(\Omega) | t \in \mathbf{R}\}$ are the unitary groups respectively generated by $\mathrm{H}(\Omega)$, $\mathrm{G}_0(\Omega)$, and $\mathrm{W}(\Omega)$.

For every $A$ of the form $B \otimes A(\Lambda)$ where $B \in \mathfrak{B}(\mathfrak{L}^2(\mathbf{R}))$ and $A(\Lambda) \in \mathfrak{A}(\Lambda)$, and for every $\Omega \supseteq \Lambda$ finite, (B6) reduces to

$$\langle\psi; A\rangle^t = (U_{\mathrm{W}}^t(\Omega)\Psi, U_0^{-t}(\Lambda)AU_0^t(\Lambda)U_{\mathrm{W}}^t(\Omega)\Psi). \tag{B7}$$

Consequently, the $\Omega$-dependence of the time evolution enters only through $\sigma^\pm(\Omega)$ in (B3), thus making much more simple the convergence proof involved in replacing our original Hamiltonian by its mean free-field approximation.

## APPENDIX C

The aim of this appendix is to analyze in which sense the mean free field method can be used to approxi-

mate, in the limit where $\Omega$ tends to $\mathbf{Z}$, the time evolution determined by the operator $W(\Omega)$ [see (B3)]. A purely algebraic answer to this question is ruled out by the fact that $\sigma^{\pm}(\Omega)$, although uniformly bounded, do not converge in the norm topology as $\Omega$ tends to $\mathbf{Z}$. We therefore will attempt to work in the strong operator topology attached to the particular representation used in the main body of this paper.

As usual, we denote by $\mathfrak{A}$ the $C^*$-algebra of all quasi local observables on the infinite spin system. We recall that $\mathfrak{A}$ is defined as the $C^*$-inductive limit[20] of the algebras $\mathfrak{A}(\Omega)$ describing the spin system in the finite regions $\Omega$:

$$\mathfrak{A} = \overline{\bigcup_{\Omega \subset \mathbf{Z}} \mathfrak{A}(\Omega)},$$

where

$$\mathfrak{A}(\Omega) = \bigotimes_{j \in \Omega} \mathfrak{A}_j \tag{C1}$$

and $\mathfrak{A}_j$ is the algebra of $2 \times 2$ matrices with complex entries, generated by $(I, \sigma_j^x, \sigma_j^y, \sigma_j^z)$ for every $j \in \Omega$.

We now consider the state $\phi_\Omega$ defined on $\mathfrak{A}(\Omega)$ by

$$\langle \phi_\Omega; A_\Omega \rangle = \mathrm{Tr} \rho_\Omega A_\Omega$$

with

$$\rho_\Omega = \exp\{-\beta H'(\Omega)\}/\mathrm{Tr} \exp\{-\beta H'(\Omega)\} \tag{C2}$$

and

$$H'(\Omega) = -B \sum_{j \in \Omega} \sigma_j^y.$$

We notice immediately that for every $A_\Omega$ of the form $A_\Omega = \bigotimes_{j \in \Omega} A_j$,

$$\langle \phi_\Omega; A_\Omega \rangle = \prod_{j \in \Omega} \langle \phi_j; A_j \rangle$$

with

$$\langle \phi_j; \sum_{\mu=0}^{3} a_j^\mu \sigma_j^\mu \rangle = a_j^0 + a_j^y \tanh \beta B, \tag{C3}$$

where

$$a_j^\mu \in \mathbf{C} \text{ and } (\sigma_j^0, \sigma_j^1, \sigma_j^2, \sigma_j^3) = (I_j, \sigma_j^x, \sigma_j^y, \sigma_j^z),$$

and that $\phi_\Omega$, as a state on $\mathfrak{A}(\Omega)$ is uniquely determined by (C3); we therefore use the notation $\phi_\Omega = \bigotimes_{j \in \Omega} \phi_j$.

For every $A \in \cup \mathfrak{A}(\Omega)$ there exists some finite $\Omega_A$ such that $A \in \mathfrak{A}(\Omega)$ for all $\Omega \supset \Omega_A$ and we can therefore define

$$\langle \phi; A \rangle \equiv \lim_{\Omega \to Z} \langle \phi_\Omega; A \rangle = \langle \bigotimes_{j \in \Omega_A} \phi_j; A \rangle. \tag{C4}$$

The linear function $\phi$ defined by (C4) is positive, bounded, and normalized to 1. It can therefore be uniquely extended to a state $\phi$, denoted $\bigotimes_{j \in \mathbf{Z}} \phi_j$, on the whole $C^*$-algebra $\mathfrak{A}$.

We denote by $\Pi_\phi$: $\mathfrak{A} \to \mathfrak{B}\mathcal{H}_\phi$ the cyclic representation of $\mathfrak{A}$, and by $\Phi$ the cyclic vector, associated to $\phi$ by the GNS construction. We want to assert that, in the strong operator topology of $\mathfrak{B}(\mathcal{H}_\phi)$, $\Pi_\phi(\sigma^{\pm}(\Omega))$ converges. We first notice that for all $\Omega \subset \mathbf{Z}$

$$\langle \phi; \sigma^{\pm}(\Omega) \rangle = \pm i\sigma,$$

where

$$\sigma = \tfrac{1}{2} \tanh \beta B. \tag{C5}$$

Taking into account the fact that $0 < \sigma^2 < \frac{1}{4}$, we see that

$$|\{\Pi_\phi(\sigma^{\pm}(\Omega)) - i\sigma\}\Phi|^2 < \tfrac{1}{2} N(\Omega)^{-1}. \tag{C6}$$

It is then easy to check that for every element $A$ in $\cup \mathfrak{A}(\Omega)$ and every $\epsilon > 0$, there exists some finite $\Omega(\epsilon, A) \subset \mathbf{Z}$ such that

$$|\{\Pi_\phi(\sigma^{\pm}(\Omega)) - i\sigma\}A\Phi|^2 < \epsilon, \Omega \supseteq \Omega(\epsilon, A). \tag{C7}$$

Since $\Phi$ is cyclic and $\{\sigma^+(\Omega) - i\sigma\}$ is uniformly bounded, we conclude that $\Pi_\phi(\sigma^{\pm}(\Omega))$ converges to $\pm i\sigma$ in the strong operator topology of $\mathfrak{B}(\mathcal{H}_\phi)$.

We now consider the Hilbert space

$$\mathfrak{H}_\phi = \mathcal{L}^2(\mathbf{R}) \otimes \mathcal{H}_\phi \tag{C8}$$

and the linear manifold $\mathfrak{M}_\phi$ spanned by the elements of the form $\Psi \otimes \Phi'$ with $\Psi \in \mathcal{S}(\mathbf{R})$ and $\Phi' \in \mathcal{H}_\phi$. On $\mathfrak{M}_\phi$ we then define (see B3)

$$W_\phi(\Omega) = (\omega - B)(a^*a + \tfrac{1}{2}) + \tfrac{1}{2}\lambda\{aa\Pi_\phi(\sigma^+(\Omega)) + a^*a^*\Pi_\phi(\sigma^-(\Omega))\}. \tag{C9}$$

From the strong operator convergence of $\pi_\phi(\sigma^{\pm}(\Omega))$ to $\pm i\sigma$ on $\mathcal{H}_\phi$, we conclude that $W_\phi(\Omega)$ converges strongly to $\overline{W}_\phi = W_\phi \otimes I$, where

$$W_\phi = (\omega - B)(a^*a + \tfrac{1}{2}) + \tfrac{1}{2} i\lambda\sigma(aa - a^*a^*) \tag{C10}$$

on the linear manifold $\mathfrak{M}_\phi$ which is dense in $\mathfrak{H}_\phi$. From Appendix A we know that for any $\lambda$ with $\mathrm{Re}\lambda \neq 0$ $(\lambda + iW_\phi)$, $\mathfrak{M}_\phi$ is dense in $\mathfrak{H}_\phi$. We can therefore conclude, upon using Thm. 5.2 in Ref. 21, that for each $t \in \mathbf{R}$, $U^t_{W,\phi}(\Omega)$ converges strongly to $U^t_{W,\phi}$ where $\{U^t_{W,\phi}(\Omega) | t \in \mathbf{R}\}$ and $\{U^t_{W,\phi} | t \in \mathbf{R}\}$ are the strongly continuous unitary group respectively generated by $W_\phi(\Omega)$ and $\overline{W}_\phi$.

The result of the above analysis is therefore that for any $t \in \mathbf{R}$, any vector $\Psi \in \mathfrak{H}_\phi$ and any operator $A$ of the form $B \otimes A(\Lambda)$ with $B \in \mathfrak{B}(\mathcal{L}^2(\mathbf{R}))$ and $A(\Lambda) \in \Pi_\phi(\mathfrak{A}(\Lambda))$, the limit as $\Omega$ tends to $\mathbf{Z}$, of $(U^t(\Omega)\Psi, AU^t(\Omega)\Psi)$ exists and is equal to

$$(U^{-t}_{W,\phi}\Psi, U_0^{-t}(\Lambda) A U_0^t(\Lambda) U^t_{W,\phi}\Psi). \tag{C11}$$

In particular, if $\Psi$ is of the form $\Psi_{EM} \otimes \Psi_s$, we have

$$\langle \psi; B \otimes A(\Lambda) \rangle^t = (U^t_{W,\phi}\Psi_{EM}, U^{-t}_{EM} B U^t_{EM} U^t_{W,\phi}\Psi_{EM}) \times (\Psi_s, U_s^{-t}(\Lambda) A(\Lambda) U_s^t(\Lambda)\Psi_s), \tag{C12}$$

where $\{U^t_{W,\phi} | t \in \mathbf{R}\}$, $\{U^t_{EM} | t \in \mathbf{R}\}$ and $\{U^t_s | t \in \mathbf{R}\}$ are the unitary groups respectively generated by

$$\begin{aligned} &W_\phi \text{ [see (C10)]}, \\ &H_{EM} = \omega_0(a^*a + \tfrac{1}{2}), \\ &H_s(\Lambda) = B \sum_{j \in \Lambda} \sigma_j^z. \end{aligned} \tag{C13}$$

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# Lattice Green's Function for the Diatomic Lattices

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Attention is called to the fact that the lattice Green's function for a diatomic alternating lattice (regular or irregular) can be calculated from the lattice Green's function for the corresponding monatomic lattice. The definition of the lattice Green's function is given in such a fashion that the imaginary part of the trace of the function gives the level density. The values at the origin are shown by graphs for the square, sc, and bcc diatomic lattices; the sc and bcc diatomic lattices are of the sodium-chloride and cesium-chloride type crystal structures, respectively. Discussions are given of the analytic behaviors and symmetry properties. The real part of the lattice Green's function is used to discuss the localized state of the one-impurity problem in the diatomic lattices. Some symmetry properties for the monatomic alternating lattice are given in the Appendix.

## 1. INTRODUCTION

Much effort has been paid for the numerical calculation and the investigations of the analytic properties of the lattice Green's function of the regular monatomic lattices.[1] The discussions of the regular diatomic lattices are given in a few articles.[2,3] Montroll and Potts[2] showed that the equation determining the eigenvalues of a regular diatomic lattice is obtainable from the corresponding equation for the monatomic lattice by a simple transformation. Maradudin *et al.*[3] used the same transformation in their discussion of the asymptotic behavior of the lattice Green's function outside the band. For the monatomic lattices, the imaginary part of the trace of the lattice Green's function gives the level density. This property does not hold for the lattice Green's function defined by these authors for the diatomic lattices. In the present paper we shall introduce the definition of the function in such a way that the property keeps valid. We show that the lattice Green's function for the diatomic lattice as a function of complex energy variable is expressed by the one for the corresponding monatomic lattice with the aid of a similar transformation as the one used by Montroll *et al.* With the aid of this expression, analytic properties and symmetry properties of the former are discussed from those of the latter. Those properties are illustrated by the graphs at the origin for the square, sc, and bcc lattices.

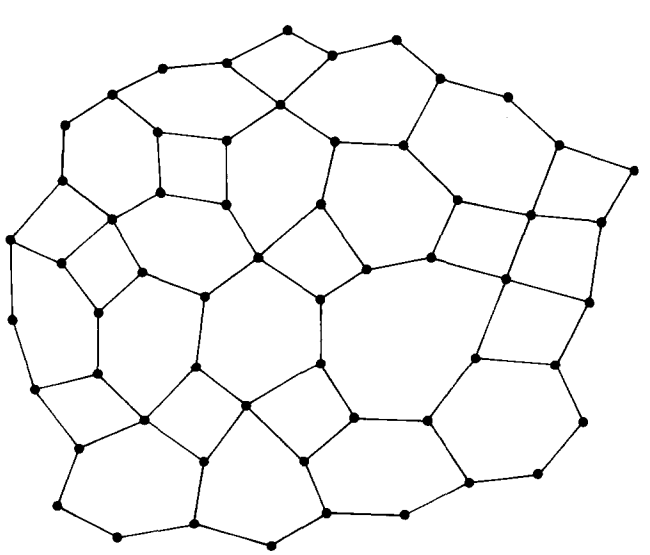

FIG. 1. An example of the "alternating lattice". Note that this lattice consists of polygons with an even number of edges.

General discussions in the present paper are given for the lattices (i) which are composed of two sublattices $A$ and $B$ and (ii) in which the interaction exists only between the lattice sites belonging to different sublattices. We shall name such a lattice an "*alternating lattice.*" Typical examples are the linear, square, honeycomb, sc, bcc, and diamond lattices, if the interaction exists only between nearest neighbor lattice sites. Regularity of the lattice is not required above. Hence even when some sites are missing or a deformation is applied, the above lattices are alternating lattices. A more irregular example is shown in Fig. 1. When all the sites are occupied by the same kind of atoms, the lattice is called a "*monatomic alternating lattice.*" When two sublattices are occupied by different kinds of atoms and each by the same kind of atoms, the lattice is called a "*diatomic alternating lattice*" or simply "*diatomic lattice*" in the present paper.

It is shown in Sec. 2 that the lattice Green's function of the diatomic alternating lattice as a function of the complex energy variable is expressed by that of the monatomic lattice. The analytic properties and symmetry properties of the former are discussed with the aid of those of the latter in Sec. 3. Those properties are illustrated by the curves obtained for the values of the function at the origin for the square, sc, and bcc diatomic lattices, in Secs. 4 and 5. In Sec. 6, the one-impurity problem is discussed.

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Attention is called to the fact that the lattice Green's function for a diatomic alternating lattice (regular or irregular) can be calculated from the lattice Green's function for the corresponding monatomic lattice. The definition of the lattice Green's function is given in such a fashion that the imaginary part of the trace of the function gives the level density. The values at the origin are shown by graphs for the square, sc, and bcc diatomic lattices; the sc and bcc diatomic lattices are of the sodium-chloride and cesium-chloride type crystal structures, respectively. Discussions are given of the analytic behaviors and symmetry properties. The real part of the lattice Green's function is used to discuss the localized state of the one-impurity problem in the diatomic lattices. Some symmetry properties for the monatomic alternating lattice are given in the Appendix.

## 1. INTRODUCTION

Much effort has been paid for the numerical calculation and the investigations of the analytic properties of the lattice Green's function of the regular monatomic lattices.[1] The discussions of the regular diatomic lattices are given in a few articles.[2,3] Montroll and Potts[2] showed that the equation determining the eigenvalues of a regular diatomic lattice is obtainable from the corresponding equation for the monatomic lattice by a simple transformation. Maradudin *et al.*[3] used the same transformation in their discussion of the asymptotic behavior of the lattice Green's function outside the band. For the monatomic lattices, the imaginary part of the trace of the lattice Green's function gives the level density. This property does not hold for the lattice Green's function defined by these authors for the diatomic lattices. In the present paper we shall introduce the definition of the function in such a way that the property keeps valid. We show that the lattice Green's function for the diatomic lattice as a function of complex energy variable is expressed by the one for the corresponding monatomic lattice with the aid of a similar transformation as the one used by Montroll *et al.* With the aid of this expression, analytic properties and symmetry properties of the former are discussed from those of the latter. Those properties are illustrated by the graphs at the origin for the square, sc, and bcc lattices.

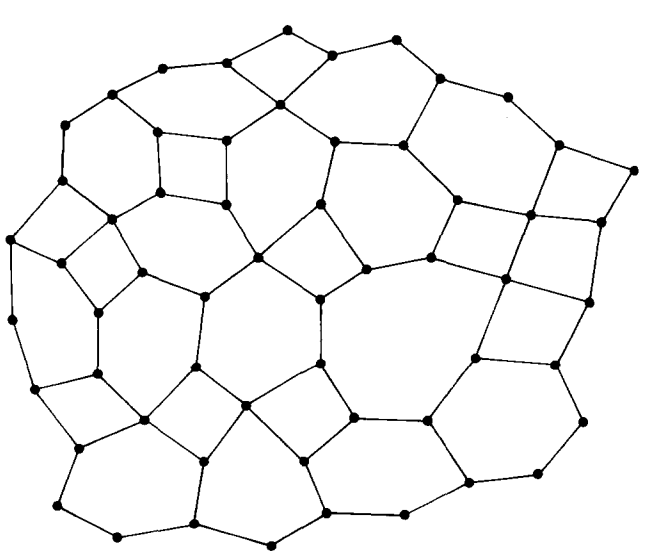

FIG. 1. An example of the "alternating lattice". Note that this lattice consists of polygons with an even number of edges.

General discussions in the present paper are given for the lattices (i) which are composed of two sublattices $A$ and $B$ and (ii) in which the interaction exists only between the lattice sites belonging to different sublattices. We shall name such a lattice an "*alternating lattice.*" Typical examples are the linear, square, honeycomb, sc, bcc, and diamond lattices, if the interaction exists only between nearest neighbor lattice sites. Regularity of the lattice is not required above. Hence even when some sites are missing or a deformation is applied, the above lattices are alternating lattices. A more irregular example is shown in Fig. 1. When all the sites are occupied by the same kind of atoms, the lattice is called a "*monatomic alternating lattice.*" When two sublattices are occupied by different kinds of atoms and each by the same kind of atoms, the lattice is called a "*diatomic alternating lattice*" or simply "*diatomic lattice*" in the present paper.

It is shown in Sec. 2 that the lattice Green's function of the diatomic alternating lattice as a function of the complex energy variable is expressed by that of the monatomic lattice. The analytic properties and symmetry properties of the former are discussed with the aid of those of the latter in Sec. 3. Those properties are illustrated by the curves obtained for the values of the function at the origin for the square, sc, and bcc diatomic lattices, in Secs. 4 and 5. In Sec. 6, the one-impurity problem is discussed.

For the monatomic alternating lattice, some symmetry properties are noticed, which are given in the Appendix.

## 2. BASIC FORMULAS

In this section, we consider a general diatomic alternating lattice. We suppose that an amplitude $\psi(i)$ is associated with $i$th lattice site and that $\psi(i)$ satisfies the following equation:

$$[t + \epsilon(i)]\psi(i) - c(i)\sum_j J(i,j)\psi(j) = 0, \tag{2.1}$$

where $t$ is a complex variable, and $J(i,j)$ is nonzero only when $i$ and $j$ belong to different sublattices. $\epsilon(i)$ and $c(i)$ in Eq. (2.1) take $\epsilon_A$ or $\epsilon_B$ and $c_A$ or $c_B$, respectively, according as $i$ is on the sublattice $A$ or $B$. $c_A$ and $c_B$ are assumed to be positive. $\epsilon_B$ is assumed to be larger than $\epsilon_A$ without loss of generality.

We shall define the lattice Green's function $G(t;i,f)$ as the solution of the inhomogeneous difference equation

$$[t + \epsilon(i)]G(i,f) - c(i)\sum_j J(i,j)G(j,f) = \delta_{if}. \tag{2.2}$$

If the lattice is finite, $G(i,f)$ is defined for $t$ which is not equal to any of the eigenvalues of the set of homogeneous linear equations (2.1). If the lattice is infinite, the boundary condition is

$$G(i,f) \to 0 \quad \text{as} \quad |i-f| \to \infty,$$

and $G(i,f)$ is not defined for real $t$ which is inside of the band.

We introduce factor $g(i)$ which is equal to $g_A$ or $g_B$ according as $i$ is on the sublattice $A$ or $B$, where $g_A$ and $g_B$ are defined such that

$$g_A(t + \epsilon_A)/g_B c_B = g_B(t + \epsilon_B)/g_A c_A = \tilde{t}. \tag{2.3}$$

From this set of equations, one has

$$g_A/g_B = \pm (c_B/c_A)^{1/2}[(t + \epsilon_B)/(t + \epsilon_A)]^{1/2}, \tag{2.4}$$

$$\tilde{t} = \pm [(t + \epsilon_A)(t + \epsilon_B)/c_A c_B]^{1/2}. \tag{2.5}$$

In the following, we shall use the upper signs if otherwise is not stated. The branch cut on the complex $t$ plane is introduced on the real axis from $-\epsilon_B$ to $-\epsilon_A$; cf. Fig. 2(a). The branches of $(t + \epsilon_A)^{1/2}$ and $(t + \epsilon_B)^{1/2}$ are chosen such that they are real and positive when $t + \epsilon_A$ and $t + \epsilon_B$, respectively, are real and positive. Hence if $t = s - i\eta$ and $s < -\epsilon_A$ and $\eta$ is an infinitesimal positive number, $(s - i\eta + \epsilon_A)^{1/2} = -i\sqrt{-s - \epsilon_A}$ where $\sqrt{-s - \epsilon_A}$ is the positive square root of $-s - \epsilon_A$. Equation (2.5) is solved for $t$ as follows:

$$t = -\tfrac{1}{2}(\epsilon_A + \epsilon_B) + t', \tag{2.5'}$$

where

$$t' = \tfrac{1}{2}[(\epsilon_A - \epsilon_B)^2 + 4c_A c_B \tilde{t}^2]^{1/2}.$$

The branch cut from $-\epsilon_B$ to $-\epsilon_A$ on the $t$ plane is mapped to the imaginary axis between $\pm i(\epsilon_B - \epsilon_A)/2(c_A c_B)^{1/2}$ on the $\tilde{t}$ plane as seen from (2.5); cf. Fig. 2(b). The choice of the branch, stated above, corresponds to use the positive real square root on the right-hand side when $\tilde{t}$ is positive. Note that $t'$ changes sign when $\tilde{t}$ changes sign in this choice of the branch cuts.

We define function $\tilde{G}(i,f)$ by

$$\tilde{G}(i,f) = g(i + a)c(i + a)G(i,f)/g(f). \tag{2.6}$$

Here $i + a$ is a lattice site belonging to the sublattice different from the one to which $i$ belongs. We multiply $g(i)/g(f)$ to both sides of (2.2) and use the equality (2.3) and the definition (2.6), and then we obtain the following equation

$$\tilde{t}\tilde{G}(i,f) - \sum_j J(i,j)\tilde{G}(j,f) = \delta_{if}. \tag{2.7}$$

This equation shows that the function $\tilde{G}(i,f)$ is the value of the lattice Green's function for the monatomic lattice at the variable $\tilde{t}$. To show the variable $\tilde{t}$ explicitly, we use the notation $\tilde{G}(\tilde{t};i,f)$ for the solution of Eq. (2.7).

From the knowledge of the lattice Green's function for the monatomic lattice, one can calculate the lattice Green's function for the diatomic lattice via Eq. (2.6) or

$$G(t;i,f) = \frac{g(f)\tilde{G}(\tilde{t};i,f)}{g(i + a)c(i + a)}. \tag{2.8}$$

The ratio $g(f)/[g(i + a)c(i + a)]$ is $g_A/g_B c_B, g_B/g_A c_A$, $1/c_B$, or $1/c_A$. $g_A/g_B$ and $\tilde{t}$ are given by (2.4) and (2.5), respectively. For instance, when $f$ is on the sublattice $A$, this equation is written as follows:

$$G(t;i,f) = (c_A c_B)^{-1/2}[(t + \epsilon_B)/(t + \epsilon_A)]^{1/2}\,\tilde{G}(\tilde{t};i,f) \tag{2.9}$$

if $i$ is also on the sublattice $A$, and

$$G(t;i,f) = (1/c_A)\tilde{G}(\tilde{t};i,f) \tag{2.10}$$

if $i$ is on the other sublattice $B$.

We shall define function $\tilde{\psi}(i)$ by

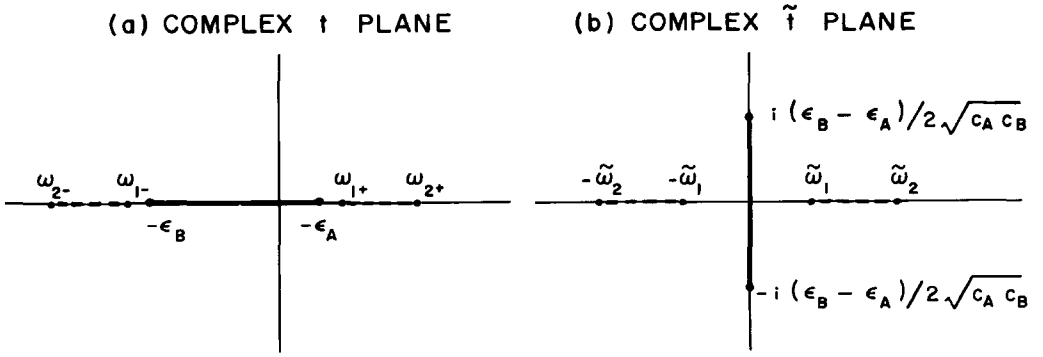


FIG. 2. (a) Complex $t$ plane and (b) complex $\tilde{t}$ plane. Solid lines show the branch cuts which we use for the transformation (2.5) and (2.5'). The dashed lines show the places where the singularities of $G(t;i,f)$ and $\tilde{G}(\tilde{t};i,f)$, respectively, can occur. $\tilde{\omega}_1$, $\tilde{\omega}_2$, $\omega_{1\pm}$, and $\omega_{2\pm}$ are defined in Sec. 3.

$$\tilde{\psi}(i) = g(i + a)c(i + a)\psi(i); \tag{2.11}$$

we multiply $g(i)$ on both sides of (2.1), and then use Eqs. (2.3) and (2.11). As a result, we obtain

$$\tilde{I}\tilde{\psi}(i) - \sum_j J(i,j)\tilde{\psi}(j) = 0. \tag{2.12}$$

Let us assume that the lattice is a finite lattice composed of $N$ lattice sites. We introduce a function $\Delta(i)$ which is + 1 or − 1 according as $i$ belongs to sublattice $A$ or $B$. Then we can easily see that, if $\tilde{w}_k(i)$ is an eigenfunction of (2.12) with eigenvalue $\tilde{\omega}(k)$, then $\Delta(i)\tilde{w}_k(i)$ is another eigenfunction of (2.12) with eigenvalue $-\tilde{\omega}(k)$; a proof is given in the Appendix. In order to cover all the eigenfunctions, we use N/2 labels $k$ and + and − [4]:

$$\tilde{w}_{k+}(i) = \tilde{w}_k(i), \qquad \tilde{w}_{k-}(i) = \Delta(i)\tilde{w}_k(i), \tag{2.13}$$

$$\tilde{\omega}(k\ \pm) = \pm\,\tilde{\omega}(k). \tag{2.14}$$

We assume that $\tilde{w}_{k\pm}(i)$ is normalized unity:

$$\sum_i |\tilde{w}_{k\pm}(i)|^2 = 1. \tag{2.15}$$

Without loss of generality, we assume that

$$\tilde{\omega}(k) \geq 0.$$

Substituting these sets of the eigenfunction and eigenvalues into (2.3) or (2.5) and (2.11), we see that (2.1) is satisfied for

$$t = \omega(k\ \pm), \qquad \psi(i) = w_{k\pm}(i). \tag{2.16}$$

Here

$$\omega(k\ \pm) = -\tfrac{1}{2}(\epsilon_A + \epsilon_B) \pm \tfrac{1}{2}[(\epsilon_A - \epsilon_B)^2 + 4c_A c_B \tilde{\omega}(k)^2]^{1/2}, \tag{2.17}$$

$$w_{k\pm}(i) = C\phi_+(k\ \pm)\tilde{w}_{k+}(i) + C\phi_-(k\ \pm)\tilde{w}_{k-}(i), \tag{2.18}$$

where

$$\phi_+(k\ \pm) = c_A^{1/2}/|\omega(k\ \pm) + \epsilon_A|^{1/2} \pm c_B^{1/2}/|\omega(k\ \pm) + \epsilon_B|^{1/2},$$

$$\phi_-(k\ \pm) = c_A^{1/2}/|\omega(k\ \pm) + \epsilon_A|^{1/2} \mp c_B^{1/2}/|\omega(k\ \pm) + \epsilon_B|^{1/2},$$

$$C = [\phi_+(k\ \pm)^2 + \phi_-(k\ \pm)^2]^{-1/2}. \tag{2.19}$$

When (2.18) is derived, the upper signs of (2.4) and (2.5) are used for $\tilde{I} = \tilde{\omega}(k_+)$ and the lower signs for $\tilde{I} = \tilde{\omega}(k_-)$.

In terms of the eigenvalues $\omega(k\ \pm)$ and the eigenfunctions $w_{k\pm}(i)$ of Eq. (2.1), the lattice Green's function satisfying (2.2) is expressed as follows:

$$G(t; i, f) = \sum_k{}' \sum_{j=\pm} \{w_{kj}(i)w^*_{kj}(f)/[t - \omega(kj)]\}, \tag{2.20}$$

where the prime over the summation sign means that the summation with respect to $k$ is taken over $N/2$ labels. When $t = s - i\eta$ with a real $s$ and an infinitesimal positive number $\eta$, the imaginary part of this expression gives

$$\mathrm{Im}G(s - i\eta; i, f) = \pi \sum_k{}' \sum_{j=\pm} \delta(s - \omega(kj))\, w_{kj}(i)w^*_{kj}(f). \tag{2.21}$$

By putting $i = f$ and summing over $i$, we confirm that the level density per atom $\rho(s)$ is evaluated by

$$\rho(s) = (1/\pi)\ \mathrm{Im}(1/N)\sum_i G(s - i\eta; i, i). \tag{2.22}$$

By using (2.8) or (2.9), one writes this as follows:

$$\rho(s) = (1/\pi)\ \mathrm{Im}[(1/N)(1/c_A c_B \tilde{I})\sum_i [s + \epsilon(i + a)]\,\tilde{G}(\tilde{I}; i, i)], \tag{2.23}$$

where

$$\tilde{I} = [(s - i\eta + \epsilon_A)(s - i\eta + \epsilon_B)/c_A c_B]^{1/2}.$$

If the lattice is a regular lattice composed of two equivalent sublattices, $\tilde{G}(\tilde{I}; i, i)$ are the same for all lattice sites $i$, and (2.23) reduces to

$$\rho(s) = (1/2\pi)\ \mathrm{Im}[\{[(s + \epsilon_A) + (s + \epsilon_B)]/c_A c_B t\}\,\tilde{G}(\tilde{I}; i, i)]. \tag{2.24}$$

For the regular lattices, the numerical calculation of $\tilde{G}(\tilde{I}; i, f)$ has been intensively discussed in a number of recent papers of the present authors' group. Those methods are useful for complex values of $\tilde{I}$. In particular, if the level density is of interest, an extensive table[5] is available for the values at the origin of the lattice Green's function $\tilde{G}(\tilde{I}; i, i)$. The Chebyshev interpolation formulas provided in the table will be useful for the s.c. lattice. For the square and bcc lattices, the expression in terms of the complete elliptic integral of the first kind[6] is very convenient for the calculation of $\tilde{G}(\tilde{I}; i, i)$ for the complex values as well as for the real values of $\tilde{I}$.

In Secs. 4 and 5 curves for the lattice Green's function $G(s - i\eta; i, i)$ for those lattices are given. For that calculation, $\tilde{G}(\tilde{I}; i, i)$ for pure imaginary $\tilde{I}$ is required. That calculation for the b.c.c. lattice is performed with the aid of the formula in terms of the complete elliptic integral of the first kind.[6] For the case of the sc lattice, the formula which expresses $\tilde{G}(\tilde{I}; i, i)$ as a definite integral of a complete elliptic integral of the first kind[7] is used. It has been pointed out that the applicability of the formula to complex $\tilde{I}$ is warranted by the analyticity of the function.[7]

## 3. ANALYTIC PROPERTIES

We assume here that all the positive eigenvalues $\tilde{\omega}(k)$ of the monatomic lattice are between $\tilde{\omega}_1$ and $\tilde{\omega}_2$:

$$\tilde{\omega}_1 \leq \tilde{\omega}(k) \leq \tilde{\omega}_2. \tag{3.1}$$

Then $\omega(k\ \pm)$ given by (2.17) takes values from $\omega_{2-}$ to $\omega_{1-}$ and from $\omega_{1+}$ to $\omega_{2+}$:

$$\begin{aligned} &\omega_{1+} \leq \omega(k_+) \leq \omega_{2+}, \\ &\omega_{2-} \leq \omega(k_-) \leq \omega_{1-}, \end{aligned} \tag{3.2}$$

where

$$\omega_{l\pm} = -\tfrac{1}{2}(\epsilon_A + \epsilon_B) \pm \tfrac{1}{2}[(\epsilon_A - \epsilon_B)^2 + 4c_A c_B \tilde{\omega}_l^2]^{1/2} \tag{3.3}$$

Note that $-\epsilon_A \leq \omega_{1+}$ and $\omega_{1-} \leq -\epsilon_B$; *cf.* Fig. 2. For the regular linear, square, honeycomb, s.c., b.c.c., and diamond lattices, $\tilde{\omega}_1 = 0$ and hence

$$\omega_{1+} = -\epsilon_A, \qquad \omega_{1-} = -\epsilon_B. \tag{3.4}$$

By (2.21), $G(s - i\eta; i, f)$ is real except for these two ranges:

$$\mathrm{Im}G(s - i\eta; i,f) = 0$$

if $s < \omega_{2-}$, or $\omega_{1-} < s < \omega_{1+}$, or $\omega_{2+} < s$.

This fact can be confirmed by (2.8) or (2.9) and (2.10), considering that $\tilde{G}(\tilde{t}; i,f)$ is real for $\tilde{t} > \tilde{\omega}_2$ and $\tilde{t} < -\tilde{\omega}_2$ and $-\tilde{\omega}_1 < \tilde{t} < \tilde{\omega}_1$ and that $\tilde{G}(\tilde{t}; i,f)$ for pure imaginary values of $\tilde{t}$ is pure imaginary if $i$ and $f$ belong to the same sublattice and real if $i$ and $f$ are on different sublattices. These properties of $\tilde{G}(\tilde{t}; i,f)$ are easily confirmed with the aid of formula (A11) given in the Appendix. As a result, we have an energy gap from $\omega_{1-}$ to $\omega_{1+}$, which include the range from $-\epsilon_B$ to $-\epsilon_A$. Thus we conclude that there always occurs an energy gap for the alternating lattice if $\epsilon_A \neq \epsilon_B$.

When $i$ and $f$ are on different sublattices, we have the following symmetry relation:

$$\begin{aligned} G(-\tfrac{1}{2}(\epsilon_A + \epsilon_B) + t'; i,f) &= G(-\tfrac{1}{2}(\epsilon_A + \epsilon_B) - t'; i,f) \\ &= G(-\tfrac{1}{2}(\epsilon_A + \epsilon_B) - t'^*; i,f)^*, \end{aligned} \tag{3.5}$$

which is obtained by substituting (A11) into (2.10). follows from this relation that the real and imaginary parts of the function $G(s - i\eta; i,f)$ are symmetric and antisymmetric, respectively, around $s = -\frac{1}{2}(\epsilon_A + \epsilon_B)$ for an arbitrary value of $\eta$; cf. the argument in the last paragraph of the Appendix for the monatomic lattice. If $i$ and $f$ are on the same sublattice, we have a factor which is not symmetric around $s = -(\epsilon_A + \epsilon_B)/2$; cf. (2.9). What we have for this case is a relation of the function for $i$ and $f$ both on the sublattice $A$ and that for $i$ and $f$ both on the sublattice $B$:

$$\begin{aligned} &G(-\tfrac{1}{2}(\epsilon_A + \epsilon_B) + t'; i,f) \\ &\quad = -G(-\tfrac{1}{2}(\epsilon_A + \epsilon_B) - t'; i + a, f + a) \\ &\quad = -G(-\tfrac{1}{2}(\epsilon_A + \epsilon_B) - t'^*; i + a, f + a)^*. \end{aligned} \tag{3.6}$$

This relation is obtained by substituting (A11) into (2.9). It follows from this relation that the imaginary part of $G(-\frac{1}{2}(\epsilon_A + \epsilon_B) + t'; i,f)$ for $i$ and $f$ both on the sublattice $A$ is equal to the imaginary part of $G(-\frac{1}{2}(\epsilon_A + \epsilon_B) - t'; i,f)$ for $i$ and $f$ both on the sublattice $B$. Their real parts are of different sign. This property is observed in Figs. 3 ~ 4 when (a) and (b) in each figure are compared.

The singularities of $G(t; i,f)$ occur due to the critical points of the spectrum (2.17) of the diatomic lattice. The critical points of the spectrum $\omega(k \pm)$ are determined by the $k$ which make the first derivative of (2.17) with respect to $k$ to zero

$$\frac{\partial \omega(k \pm)}{\partial k_\alpha} = 0,$$

for all components $k_\alpha$ of wave vector $k$. The critical points are called "degenerate" or "nondegenerate," according as the determinant of the Hessian of the spectrum is zero or not.

The first derivative of $\omega(k\pm)$ is given by

$$\frac{\partial \omega(k\pm)}{\partial k_\alpha} = \pm \frac{2c_A c_B \tilde{\omega}(k) \partial \tilde{\omega}(k)/\partial k_\alpha}{[(\epsilon_A - \epsilon_B)^2 + 4c_A c_B \tilde{\omega}(k)^2]^{1/2}}. \tag{3.7}$$

This expression is zero either when

$$\frac{\partial \tilde{\omega}(k)}{\partial k_\alpha} = 0 \tag{3.8}$$

or when

$$\tilde{\omega}(k) = 0. \tag{3.9}$$

The critical points determined by (3.8) have their counterpart for the monatomic lattice. The critical points due to (3.9) are new.

If (3.9) is not satisfied at a critical point determined by (3.8), the corresponding singular behavior is similar to the behavior of the monatomic lattice due to the same critical point. This fact can be easily seen by writing the expression for the determinant of the Hessian. If those critical points are nondegenerate, the singular behaviors due to these are easily obtained with the aid of the general formulas which were recently given by the present authors.[8] Such is the case for the linear, square, and sc regular lattice.

If $\tilde{\omega}_1$, which is the minimum value of $\tilde{\omega}(k)$, is zero, we have the critical points satisfying (3.9). The singular points due to them occur at $t = -\epsilon_A$ and $-\epsilon_B$ as seen from (2.17). When $\tilde{\omega}(k) = 0$, determinant of the Hessian is given by

$$\left|\left(\frac{\partial^2 \omega(k\pm)}{\partial k_\alpha \partial k_\beta}\right)\right| = \pm \frac{2c_A c_B}{\epsilon_B - \epsilon_A} \left|\left(\frac{\partial \tilde{\omega}(k)}{\partial k_\alpha} \frac{\partial \tilde{\omega}(k)}{\partial k_\beta}\right)\right|, \tag{3.10}$$

which is zero except for the one-dimensional lattice, and we have degenerate critical points for two- and three-dimensional lattices. In general, we expect the higher singular behaviors for degenerate critical points than for nondegenerate critical points, in so far as any cancellation does not occur.[8] When (2.18) is substituted in (2.20), we expect such a behavior for each of four terms. When $i$ and $f$ are on different sublattices, the coefficients cancel at the critical points. Thus the leading term of the singular behavior will cancel out. In fact, if we use (2.10) and calculate the singularity of $G(t; i,f)$ from the behavior of $\tilde{G}(\tilde{t}; i,f)$ around $\tilde{t} = 0$, we find that $G(t; i,f)$ is analytic both at $\tilde{t} = -\epsilon_A$ and $-\epsilon_B$ except when $\tilde{G}(\tilde{t}; i,f)$ itself is singular at $\tilde{t} = 0$; in fact, this occurs for the square and bcc lattices. When both $i$ and $f$ are on the same sublattice, say $A$, a cancellation occurs at $t = -\epsilon_B$. These cancellations correspond to the fact that all the atoms on the sublattice $A$ are at rest at $t = -\epsilon_B$ and those on the sublattice $B$ are at rest at $t = -\epsilon_A$. From (2.9), we find that the singular behavior is given by $(t + \epsilon_B)^{1/2}$ at $t \simeq -\epsilon_B$ beside the singular behaviors of the corresponding monatomic lattice; cf. Figs. 3 and 4(a), (b). In Fig. 3, $-\omega^2 = -3.0$ and $-1.5$ correspond to $t = -\epsilon_B$ and $-\epsilon_A$, respectively, etc.

When both $i$ and $f$ are on the same sublattice $A$, any cancellation does not occur at $t = -\epsilon_A$. The singular behavior obtained by (2.9) is

$$G(t; i,f) \simeq [(\epsilon_B - \epsilon_A)/c_A c_B]^{1/2} \tilde{G}(\tilde{t}; i,f)(t + \epsilon_A)^{-1/2} \tag{3.11}$$

where

$$\tilde{t} \simeq [(\epsilon_B - \epsilon_A)/c_A c_B]^{1/2} (t + \epsilon_A)^{1/2}. \tag{3.12}$$

Here $(s - i\eta + \epsilon_A)^{1/2} = -i\sqrt{-s - \epsilon_A}$ if $t = s - i\eta$ and $s < -\epsilon_A$ and $\eta$ is an infinitesimal positive number. As $\tilde{t}$ tends to zero, the monatomic lattice Green's function $\tilde{G}(\tilde{t}; i,f)$ is regular and finite for the linear, rectangular (but not square), orthorhombic (including sc) lattices. For the square and bcc lattices, $\tilde{t} = 0$

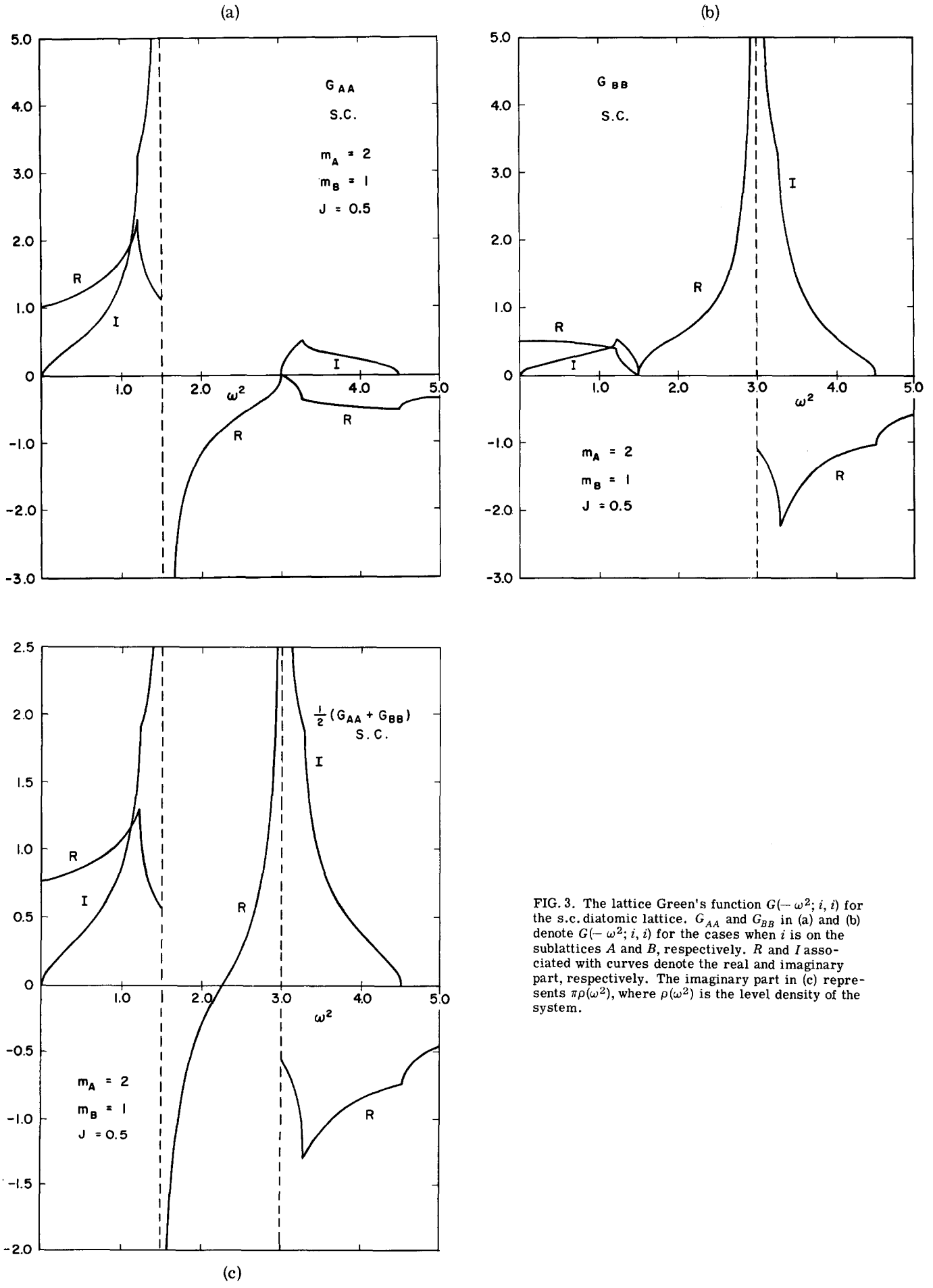


FIG. 3. The lattice Green's function $G(-\omega^2; i, i)$ for the s.c. diatomic lattice. $G_{AA}$ and $G_{BB}$ in (a) and (b) denote $G(-\omega^2; i, i)$ for the cases when $i$ is on the sublattices $A$ and $B$, respectively. $R$ and $I$ associated with curves denote the real and imaginary part, respectively. The imaginary part in (c) represents $\pi\rho(\omega^2)$, where $\rho(\omega^2)$ is the level density of the system.

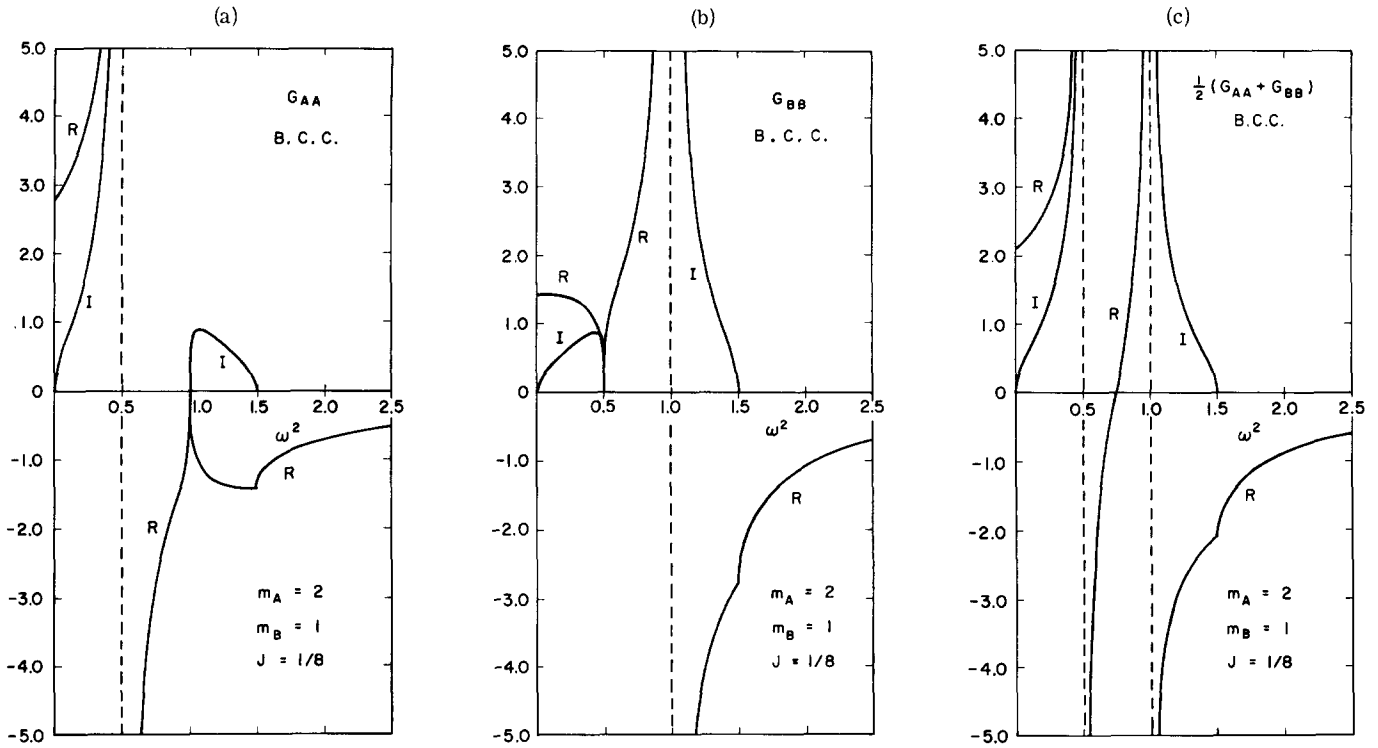


FIG. 4. The lattice Green's function $G(-\omega^2; i, i)$ for the bcc diatomic lattice.

is a singular point of $\tilde{G}(\tilde{t}; i,f)$, and $G(t; i,f)$ involves that singular behavior. The singular behaviors of $\tilde{G}(s - i\eta; i, i)$ are as follows:

Square lattice:

$\tilde{t} = s - i\eta$ and $s$ is real. As $s$ tends to zero,

$$\tilde{G}(s - i\eta; i, i) = 2 + (i/\pi)\ \ln\tfrac{1}{8}s + O(s^2). \tag{3.13}$$

$\tilde{t} = is$ and $s$ is real. As $s$ tends to zero,

$$\tilde{G}(is; i, i) = (i/\pi)\ \ln\tfrac{1}{8}s + O(s^2). \tag{3.14}$$

bcc lattice:

$\tilde{t} = s - i\eta$ and $s$ is real. As $s$ tends to zero,[6,9,10]

$$\tilde{G}(s - i\eta; i, i) = -(2/\pi)\ \ln\tfrac{1}{8}s + i[(2/\pi^2)(\ln\tfrac{1}{8}s)^2 - \tfrac{1}{2}] + O(s^2). \tag{3.15}$$

$\tilde{t} = is$ and $s$ is real. As $s$ tends to zero,

$$\tilde{G}(is; i, i) = -i(2/\pi^2)(\ln\tfrac{1}{8}s)^2 + O(s). \tag{3.16}$$

The singular behaviors for the case when both $i$ and $f$ are on the sublattice $B$ are obtained from the above results with the aid of the symmetry properties of the Green's function discussed generally in the paragraph involving Eq. (3. 6).

As mentioned above, the critical point corresponding to $\tilde{\omega}(k) = 0$ is nondegenerate for the one-dimensional lattice. In a similar way to the cancellations discussed above for the two- and three-dimensional lattices, the singular behavior $(t + \epsilon_A)^{-1/2}$ or $(t + \epsilon_B)^{-1/2}$ for the nondegenerate critical point[8] is cancelled both at $t = -\epsilon_A$ and $-\epsilon_B$ for the case when $i$ and $f$ are on different sublattices and at $t = -\epsilon_B$ when $i$ and $f$ are both on the sublattice $A$ and at $t = -\epsilon_A$ when $i$ and $f$ are both on the sublattice $B$.

## 4. LATTICE VIBRATION

In this section we consider the lattice vibration of regular diatomic lattices. The masses at the lattice site on the sublattice $A$ and $B$ are $m_A$ and $m_B$, respectively. Then the equation of the motion is given by

$$(-m(i)\omega^2 + J_0(i))u(i) - \sum_j J(i,j)u(j) = 0, \tag{4.1}$$

where

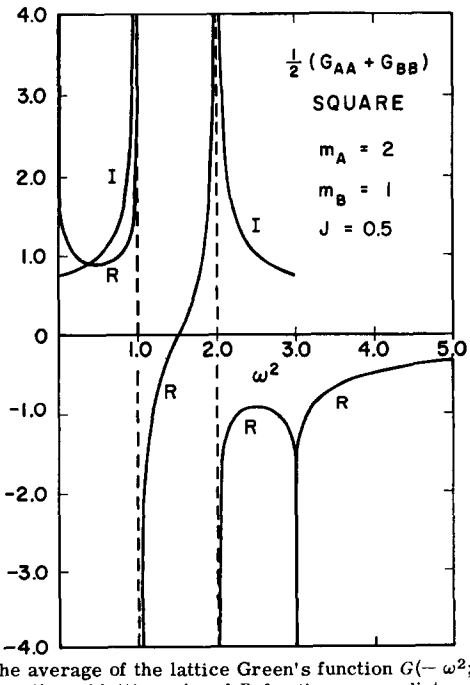


FIG. 5. The average of the lattice Green's function $G(-\omega^2; i, i)$ for the the site $i$ on the sublattices $A$ and $B$, for the square diatomic lattice.

$$J_0(i) = \sum_j J(i,j).$$

We assume that the value of $J_0(i)$ depends only on the sublattice on which $i$ is situated. We denote the value as $J_A$ or $J_B$ according as $i$ is on the sublattice $A$ or $B$. We write this as follows

$$\left(-\omega^2 + \frac{1}{m(i)}J_0(i)\right) u(i) - \frac{1}{m(i)}\sum_j J(i,j)u(j) = 0 \qquad (4.2)$$

and define the lattice Green's function $G(i,f)$ by

$$\left(-\omega^2 + \frac{1}{m(i)}J_0(i)\right) G(i,f) - \frac{1}{m(i)}\sum_j J(i,j) \times G(j,f) = \delta_{if}. \qquad (4.3)$$

Applying the argument in Sec. 2, one has

$$G(-\omega^2; i,f) = \{[g(f)m(i+a)]/g(i+a)\}\,\tilde{G}(\tilde{t}; i,f), \qquad (4.4)$$

where

$$\frac{g_A}{g_B} = \frac{m_A}{m_B}\left(\frac{-m_B\omega^2 + J_B}{-m_A\omega^2 + J_A}\right)^{1/2} \qquad (4.5)$$

and

$$\tilde{t} = [(-m_B\omega^2 + J_B)(-m_A\omega^2 + J_A)]^{1/2}. \qquad (4.6)$$

In the convention we adopted for the branch, we use positive square root when $\omega^2$ is smaller than $J_A/m_A$ and $J_B/m_B$. When $\omega^2$ is larger than both $J_B/m_B$ and

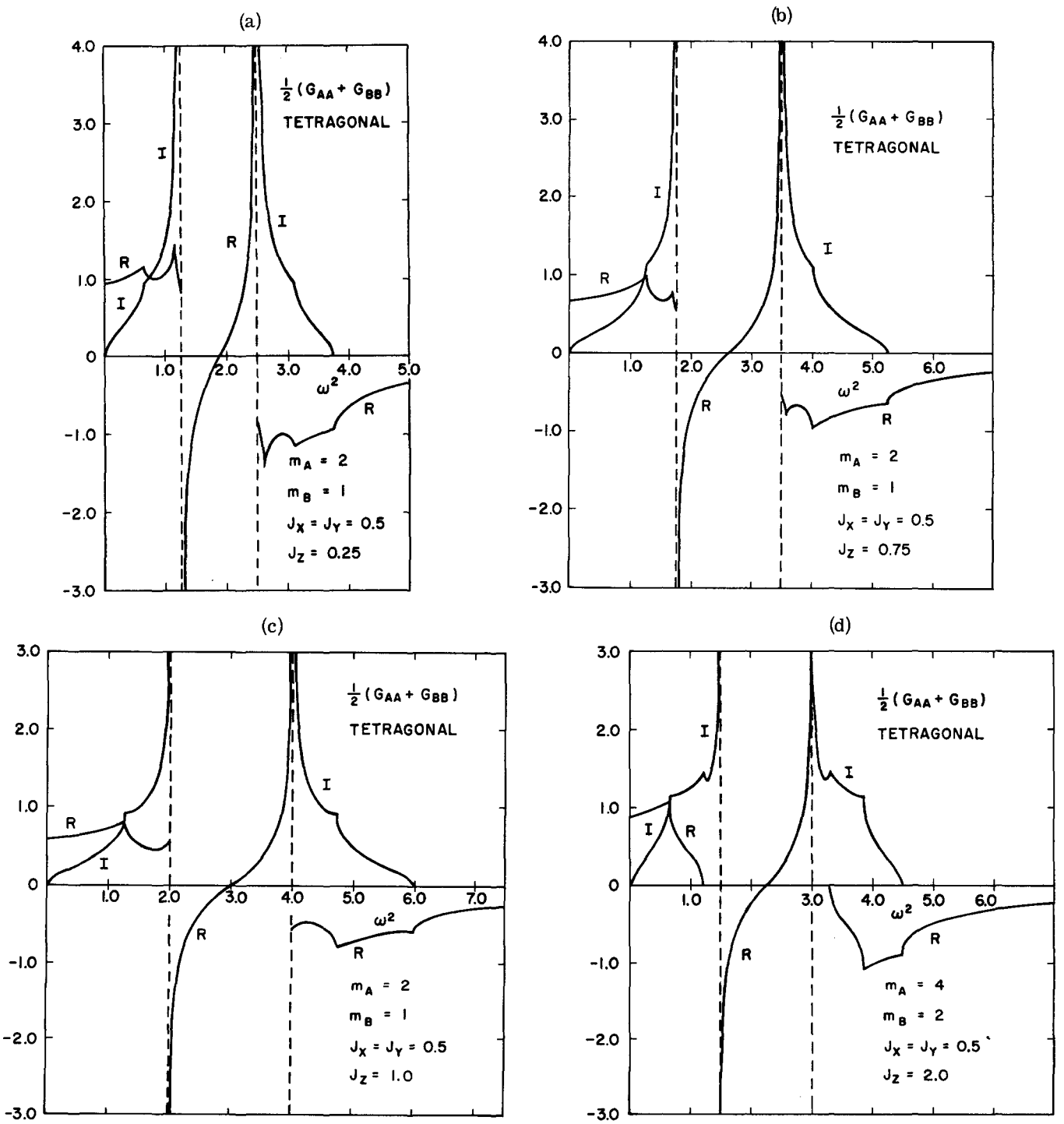


FIG. 6. The average of the lattice Green's function $G(-\omega^2; i, i)$ for the site $i$ on the sublattices $A$ and $B$, for the tetragonal diatomic lattice of various anisotropy constants.

$J_A/m_A$, $\tilde{t}$ is equal to the negative of the square root. Equation (4.4) for the case when $f$ is on the sublattice $A$ is given by

$$G(-\omega^2; i, f) = m_A\left(\frac{-m_B\omega^2 + J_B}{-m_A\omega^2 + J_A}\right)^{1/2} \tilde{G}(\tilde{t}; i, f) \qquad (4.7)$$

if $i$ is also on the sublattice $A$, and by

$$G(-\omega^2; i, f) = m_A\tilde{G}(\tilde{t}; i, f) \qquad (4.8)$$

if $i$ is on the other sublattice $B$.

The expression (2.22) of the level density reads as follows for the present case:

$$\rho(\omega^2) = (1/\pi)\ \mathrm{Im}(1/N)\sum_i G(-\omega^2 - i\eta; i, i). \qquad (4.9)$$

This equation (4.9) is well known for the monatomic lattice. We adopted Eq. (4.3) as the definition of the lattice Green's function so as to keep the property (4.9) for the diatomic lattice. Maradudin *et al.*[3] introduced the delta function on the right-hand side of (4.1) in introducing the lattice Green's function. By their definition, Eq. (4.9) does not hold. With the aid of (4.7), (4.9) is written as follows:

$$\rho(\omega^2) = (m_A m_B/2\pi)\ \mathrm{Im}[\{[-(m_A + m_B)\omega^2 + J_A + J_B]/\tilde{t}\} \times \tilde{G}(\tilde{t}; i, i)]. \qquad (4.10)$$

Figures 3 and 4 show [(a) and (b)] the real and imaginary parts of $G(-\omega^2 - i\eta; i, i)$ for the cases when $i$ is on the sublattice $A$ and $B$, respectively, and (c) their average of which imaginary part is equal to $\pi\rho(\omega^2)$, for the sc and bcc lattices. It is noted that the curves of (b) are obtained from those of (a) by an inversion or a reflection at $\omega^2 = \frac{1}{2}[(1/m_A) + (1/m_B)]\ J_0$, where $J_0 = J_A = J_B$. As a result, the curves of (c) have the same symmetries around the same value of $\omega^2$. The graphs for the square and tetragonal lattices are given in Figs. 5 and 6 only for the average of $G(-\omega^2 - i\eta; i, i)$.

## 5. ELECTRON CONDUCTION

In the simplified treatment of electron conduction, one considers only one Wannier state associated to each lattice site and assume that the transfer integral from site to site is nonzero only between nearest neighbors.[11] In such a system, one meets with the lattice Green's function satisfying the following equation[11]:

$$(-E + \epsilon(i))G(i, f) - \sum_j J(i, j)G(j, f) = \delta_{if}. \qquad (5.1)$$

This equation is identified with Eq. (2.1) by taking

$$t = -E \quad \text{and} \quad c(i) = 1. \qquad (5.2)$$

$G(i, f)$ is now calculated by (2.8) with (2.4) and (2.5).

An example of the curve of $G(-E; i, i)$ obtained for $i$ on the sublattice $B$ is given in Fig. 7. $G(-E; i, i)$ for $i$ on the sublattice $A$ is obtained from the one for the sublattice $B$ by the symmetry property given in Sec. 3. Note a similarity of the graph with a corresponding graph given by Fig. 3(b) for the lattice vibration problem.

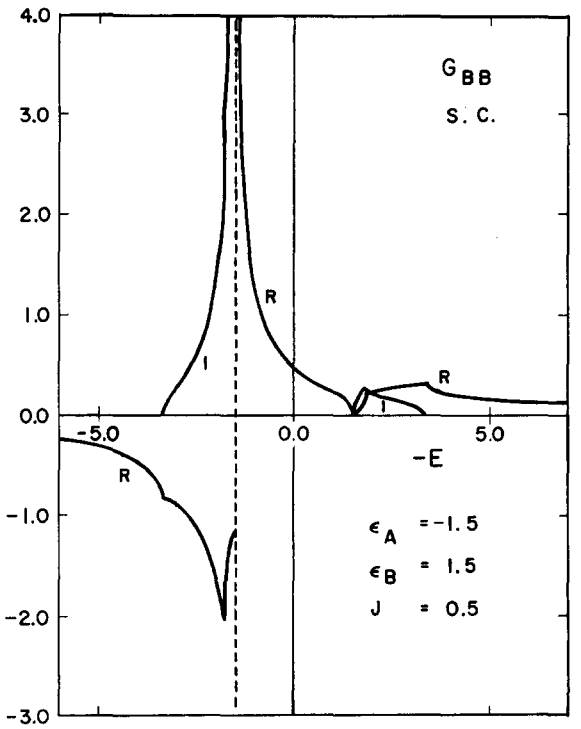


FIG. 7. The lattice Green's function $G(-E; i, i)$ for the site $i$ on the sublattice $B$, for the sc diatomic lattice.

## 6. ONE IMPURITY PROBLEM

In this section, we investigate the eigenvalue problem of the diatomic lattice when one impurity is substituted in place of a site. Let the site occupied by the impurity be $i$th site. We assume that only the value of $\epsilon(i)$ is affected by the impurity. The eigenvalue problem is

$$[t + \epsilon(j)]\psi(j) - c(j)\sum_{j'} J(j, j')\psi(j') = \delta_{j,i}\Delta\epsilon\psi(i). \qquad (6.1)$$

With the aid of the lattice Green's function $G(t; i, f)$ defined by (2.2), this equation is solved as follows:

$$\psi(j) = \Delta\epsilon G(t; j, i)\psi(i). \qquad (6.2)$$

By putting $j = i$, we have the following dispersion relation determining the eigenvalue $t$:

$$G(t; i, i) = (1/\Delta\epsilon). \qquad (6.3)$$

As discussed in Sec. 3, $G(t; i, i)$ is real when $t > \omega_{2+}$, $t < \omega_{2-}$, and $\omega_{1-} < t < \omega_{1+}$. If $t > \omega_{2+}$, we have a localized state as a solution of (6.3) when $\Delta\epsilon$ is positive and greater than a threshold value $G(\omega_{2+}; i, i)^{-1}$. If $t < \omega_{2-}$, a localized state occurs when $\Delta\epsilon$ is negative and smaller than $G(\omega_{2-}; i, i)^{-1}$. We notice in the curves given in the preceding sections that $G(t; i, i)$ takes values from $-\infty$ to 0 and from 0 to $+\infty$ between the two bands ($\omega_{1-} < t < \omega_{1+}$) according as $i$ is on the sublattice $B$ and $A$, respectively. As a result, the localized state always occurs in this range of energy, if $\Delta\epsilon$ is negative and $i$ is on the sublattice $B$ or if $\Delta\epsilon$ is positive and $i$ is on the sublattice $A$.

For the problem of lattice vibration investigated in Sec. 4, the above discussion applies if the impurity is isotopic. $\Delta\epsilon$ is then replaced by $\Delta m\omega^2/m(i) \equiv -\lambda\omega^2$ where $\Delta m$ is equal to the impurity mass $m'$ minus

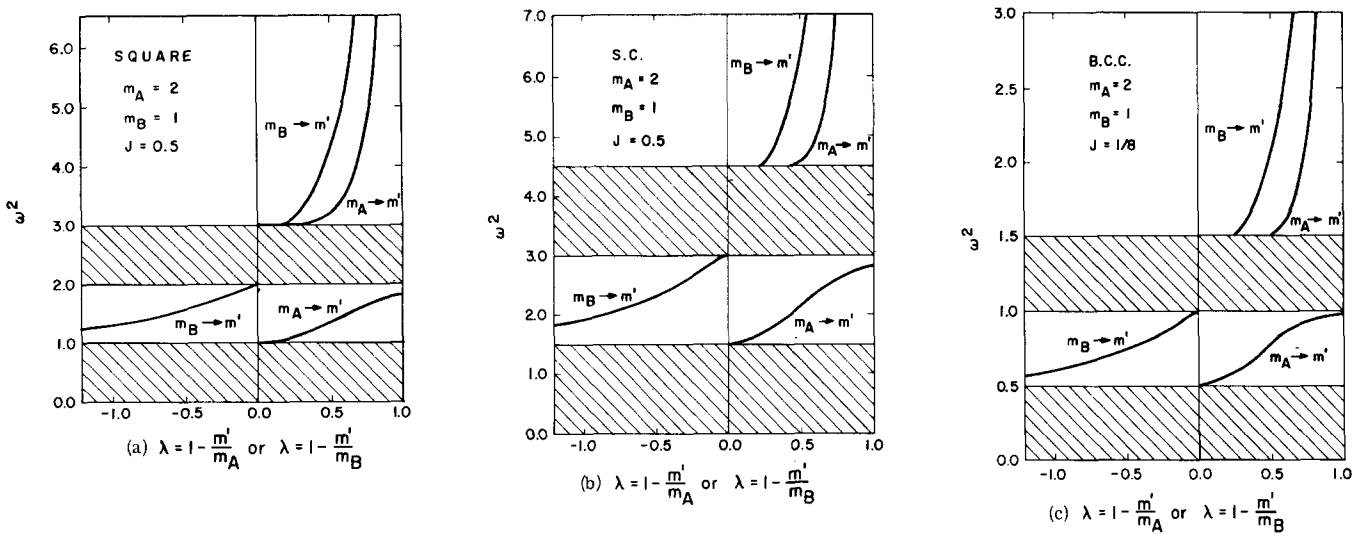


FIG. 8. The frequency of the localized state for the one-impurity problems of the diatomic lattices.

$m(i)$. The top $\omega_L$ of the bands in this problem corresponds to $\omega_{2-}$. The localized state above the top of the band occurs when $\lambda\omega^2$ is positive and greater than $-G(-\omega_L^2; i, i)^{-1}$ or the impurity is lighter than threshold value $m(i)\{1 - [\omega_L^2 G(-\omega_L^2; i, i)]^{-1}\}$. The localized state between the bands always occurs when one of the lighter masses is replaced by a heavier impurity, or one of the heavier masses is replaced by a lighter impurity. The frequency of the localized states is shown in Fig. 8 for the square, s.c., and b.c.c. lattices. For the case of the linear chain, this property has been discussed by Mazur *et al.*[12]

## 7. CONCLUSION

It is shown that the calculation of the lattice Green's function for the diatomic alternating lattice is straightforward from the lattice Green's function for the corresponding monatomic lattice. Some symmetry properties are found to exist for general monatomic and diatomic alternating lattices. For the diatomic lattice, a gap is found to exist if $\epsilon(i)$ in (2.2) are different for two sublattices. As this gap occurs even when the lattice is not regular, this gives another example when a gap occurs for a nonregular lattice.[13]

It has been pointed out that the localized state always occurs between the two bands for the linear chain, when one of the lighter masses is replaced by a heavier impurity or when one of the heavier masses is replaced by a lighter impurity.[12] It is found that this situation is the same also for the square, sc, and bcc lattices. The situation is compared with the one-impurity problem for the linear, square, and fcc monatomic lattices, when the localized state always occurs above the band when the impurity mass is lighter than the host atoms. It is a consequence of the divergence of the real part of the lattice Green's function at the top of the band. This property for the fcc lattice was recently noticed by one of the present authors,[14] after the curves for the lattice Green's function were obtained for the fcc and bcc lattices.[7,9]

## APPENDIX: SYMMETRY OF THE LATTICE GREEN'S FUNCTION FOR THE MONATOMIC ALTERNATING LATTICE

As in the text, we consider an alternating lattice composed of two sublattices $A$ and $B$. In this appendix, we discuss some of the symmetry properties which are valid for the monatomic case, and the notations $\psi(i)$ and $G(t; i, f)$ are used to denote the quantities for the monatomic lattice. The lattice is assumed to be finite.

Amplitude $\psi(i)$ is associated to lattice site $i$ and is assumed to satisfy

$$t\psi(i) - \sum_j J(i, j)\psi(j) = 0. \tag{A1}$$

When the lattice is finite, this equation represents an eigenvalue problem. The lattice Green's function $G(t; i, f)$ is defined by the difference equation

$$tG(t; i, f) - \sum_j J(i, j)G(t; j, f) = \delta_{if}, \tag{A2}$$

where $t$ is not equal to an eigenvalue of (A1). $J(i, j)$ are assumed to be nonzero between pairs of $i$ and $j$ which belong to different sublattices.

It is proved in this appendix (a) that, if $w_k(i)$ is an eigenfunction of (A1) with eigenvalue $\omega(k)$, $\Delta(i)w_k(i)$ is another eigenfunction of (A1) with eigenvalue $-\omega(k)$ and (b) that the Green's function $G(t; i, f)$ satisfies the following symmetry property:

$$G(-t; i, f) = -\Delta(i)\Delta(f)G(t; i, f), \tag{A3}$$

where $\Delta(i)$ is unity or minus unity according as $i$ belongs to the sublattice $A$ or $B$. In the next place it is further assumed that $J(i, j)$ are real: $J(i, j) = J(i, j)^*$. It is then proved (c) that

$$G(t; i, f)^* = G(t^*; i, f). \tag{A4}$$

The symmetry properties derived from properties (A3) and (A4) are discussed. It is further assumed that $J(i, j)$ is symmetric and proved (d) that the level density $\rho(s)$ has the symmetry that

$$\rho(-s) = \rho(s). \tag{A5}$$

(a) $w_k(i)$ is an eigenfunction with the eigenvalue $\omega(k)$

$$\omega(k)w_k(i) - \sum_j J(i, j)w_k(j) = 0. \tag{A6}$$

We multiply $-\Delta(i)$ to this equation and note that

$$\Delta(i)J(i,j) = -\Delta(j)J(i,j), \tag{A7}$$

and then we have

$$-\omega(k)[\Delta(i)w_k(i)] - \sum_j J(i,j)[\Delta(j)w_k(j)] = 0. \tag{A8}$$

This means that $\Delta(i)w_k(i)$ is another eigenfunction with eigenvalue $-\omega(k)$.

(b) We multiply $\Delta(i)\Delta(f)$ to (A2) and write it as follows:

$$(-t)[-\Delta(i)\Delta(f)G(t;i,f)] - \sum_j J(i,j)[-\Delta(j)\Delta(f) \times G(t;j,f)] = \delta_{if}, \tag{A9}$$

where use is made of (A7) and $\Delta(i)\Delta(f)\ \delta_{if} = \delta_{if}$. By comparing this equation with (A2), we identify $-\Delta(i)\Delta(f)G(t;i,f)$ with $G(-t;i,f)$. Thus we confirm (A3).

(c) We take the complex conjugate of Eq. (A2) and have

$$t^*G(t;i,f)^* - \sum_j J(i,j)G(t;j,f)^* = \delta_{if}, \tag{A10}$$

if $J(i,j)$ is real. This equation means (A4); *cf.* (A2) which defines $G(t^*;i,f)$ for variable $t^*$.

By using (A3) and (A4), we have

$$G(-s-i\eta;i,f) = -\Delta(i)\Delta(f)G(s+i\eta;i,f) = -\Delta(i)\Delta(f)G(s-i\eta;i,f)^* \tag{A11}$$

for an arbitrary value of $\eta$ and, hence,

$$\mathrm{Re}G(-s-i\eta;i,f) = -\Delta(i)\Delta(f)\ \mathrm{Re}G(s-i\eta;i,f) \tag{A12}$$

$$\mathrm{Im}G(-s-i\eta;i,f) = \Delta(i)\Delta(f)\ \mathrm{Im}G(s-i\eta;i,f). \tag{A13}$$

(d) By virtue of the above statement (a), the set of eigenfunctions and eigenvalues can be expressed as $w_{k\pm}(i)$ and $\omega(k\pm)$ as follows:

$$w_{k\pm}(i) = \begin{cases} w_k(i) \\ \Delta(i)w_k(i) \end{cases}, \qquad \omega(k\pm) = \pm\omega(k). \tag{A14}$$

We assume that $w_{k\pm}(i)$ is normalized to unity $\sum_i |w_{k\pm}(i)|^2 = 1$. In terms of $w_{k\pm}(i)$ and $\omega(k\pm)$, $G(t;i,f)$ is expressed as follows:

$$G(t;i,f) = \sum_k{}' \sum_{j=\pm} \frac{w_{kj}(i)w_{kj}^*(f)}{t-\omega(kj)}. \tag{A15}$$

When $J(i,j)$ are real and symmetric, all the eigenvalues $\omega(k\pm)$ are real. By putting $i=f$ and summing over $i$, one has

$$\rho(s) = (1/\pi N)\sum_i \mathrm{Im}G(s-i\eta;i,i), \tag{A16}$$

where $\eta$ is an infinitesimal positive number. Using (A13) into this equation, we find that

$$\rho(-s) = \rho(s). \tag{A17}$$

The symmetry properties (A12) and (A13) for different $i$ and $f$ are observed in the curves drawn by Horiguchi[15] for the sc lattice.

In the above derivation, the lattice can be an irregular lattice or $J(i,j) = J(j,i)$ may be random variable. For instance, the above properties must be applicable for the two-dimensional lattice shown in Fig. 1, when the nearest neighbor interaction is assumed.

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4 For a regular alternating lattice composed of two equivalent sublattices, such as the linear, square, honeycomb, s.c., and b.c.c., and diamond diatomic lattices, we naturally use for $k$ all the wave vectors in the first Brillouin zone of the sublattice.

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# The Reproducing Kernel Method. I

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The use of operator-valued reproducing kernels is introduced in order to solve Cauchy problems, $\partial N/\partial t = HN$. A series development of the solution is obtained in terms of the orthogonal functions $\phi_\nu(z)$ in a domain $G$ containing the spectrum of the bounded operator $H$. The optimal character of the approximate solution is stressed.

## 1. INTRODUCTION

Reproducing kernels have been introduced in the mathematical literature by S. Bergman[1] and N. Aronszajn.[2] Their usefulness has been demonstrated in the field of conformal mapping[1,3,4] of partial differential equations[5] and of numerical quadrature.[6] We plan to show in a series of papers, of which this one is the first, that the reproducing kernel method can be applied to new fields of mathematical physics, provided that we extend their definition to operator valued kernels. Among possible applications, we mention the solution of the abstract Cauchy problem $\partial N/\partial t = HN$ with given initial condition $N(0)$ and time-independent operator $H$; perturbation theory with application to the Born series and variational estimates of linear functionals.

The solution of abstract Cauchy problems which is the subject matter of this paper (I) and its companion (II) is usually a formidable numerical undertaking whenever $H$ is an operator in $E^n$ with $n > 2$.

The necessity of taking small time steps is obviated in the reproducing kernel method by a series solution where the time dependence is factored out as in the Neuman series. But although the Neuman series solution is rather inefficient (and incorrect asymptotically), the series obtained by the reproducing kernel method are, in sense, to be defined later (Sec. 3A) optimal from the point of view of convergence.

A knowledge of the spectrum of $H$ is essential for even a qualitative knowledge of the solution. We propose below a method which takes advantage of any knowledge of the spectrum or at least of the regions containing the spectrum. However the search of eigenvalues and eigenfunctions is avoided.

The main characteristics of the method are summarized as follows:

- analytic "time" dependence is combined with numerical "space" dependence;
- the whole time dependence is obtained at once and the solution $N(\vec{r}, t)$ at one time can be computed independently of previous times;
- the large number of time steps in the conventional method is avoided and we have instead only a few (a dozen at most) time-independent problems to solve;
- the accuracy can be indefinitely increased without discarding previous results.

We summarize in Sec. 2 the main properties of reproducing kernels. We show next how operator valued kernels can be defined; the case of compact operators and Hermitian operators is dealt with; the choice of the optimal weight function associated with the reproducing kernel is shown to be closely related with the operator's spectrum.

## 2. REPRODUCING KERNELS

### A. General Properties

Since an extensive use of reproducing kernels will be made in this paper and following, it has been found useful to collect in this paragraph, the main properties of reproducing kernels, which are somewhat scattered in the literature.[1,2]

1. Let $E$ be an abstract set and $F$ a linear class of complex-valued functions defined in $E$. The class $F$ constitutes a Hilbert space with inner product $(f,g) = (f(x), g(x))_x$. Although much of the general theory applies without the assumption that $F$ is separable, we shall for convenience make this assumption.

The function $K(x,y)$ of $x$ and $y$ in $E$ is called a reproducing kernel of $F$ if

(i) for every $y$, $K(x,y)$, as a function of $x$, $\in F$,

(ii) the reproducing property is verified: for every $y \in E$ and every $f \in F$, $f(y) = (f(x), K(x,y))_x$. (2.1)

2. The following theorem has been demonstrated by Aronszajn and Bergman: "$F$ has a reproducing kernel $K$ if and only if there exists, for every $y_0 \in E$, a positive constant $C(y_0)$, depending on $y_0$ such that

$$|f(y_0)| \leq C(y_0)\,\|f\| \quad \text{for all } f \in F. \tag{2.2}$$

3. We can introduce a basis of orthogonal functions $\{f_\nu\}$ for the Hilbert space, with

$$(f_\nu, f_\mu) = \delta_\mu^\nu. \tag{2.3}$$

The kernel function is defined in a formal manner by

$$K(x,y) = \sum_{\nu=1}^{\infty} f_\nu(x)\overline{f_\nu}(y) \quad \text{for } x, y \in E. \tag{2.4}$$

The definition has a meaning only if the series converges. However if $K(x,y)$ belongs to $F$, with property (2.2), the series converges.

The following minimum problem: $\min(f,f)$ with $f(y_0) = 1$, $f$ belonging to the closure of $\{f_\nu\}$ has the solution

$$f(x) = K(x,y_0)/K(y_0,y_0), \tag{2.5}$$

and the value of the minimum is

$$(f,f) = 1/K(y_0,y_0). \tag{2.6}$$

4. If a reproducing kernel exists, it is unique.

5. If the class $F$ possesses a reproducing kernel $K(x,y)$, every sequence $\{f_n\}$ which converges strongly to a function $f$ in $F$, converges also uniformly in every subset in which $K(x,x)$ is bounded. Indeed,

$$|f(y)-f_n(y)| \le \|f-f_n\|(K(y,y))^{1/2}.$$

### B. A Space of Entire Analytic Functions

As a particular class $F$ we have a class of entire functions of one complex variable $z$[7] where $z \in E$, the whole complex plane. They define a Hilbert space with inner product

$$(f,g) = \int f(z)\overline{g}(z)d\mu_z \qquad (2.7)$$

with

$d\mu_z = (1/\pi)\, e^{-|z|^2} d\omega_z$, $d\omega_z$ the elementary area.

Since[7]

$f(z) \le e^{1/2|z|^2}\|f\|$, $F$ admits a reproducing kernel

$$M(z,\zeta) = e^{z\bar{\zeta}}. \qquad (2.8)$$

The class of entire functions is a class for which $(f,f) < \infty$.

We may also use the class $F'$ of functions $\psi(z) = e^{-1/2z^2}f(z)$, where $f \in F$, which define a Hilbert space with inner product

$$(\psi,\varphi) = \int \psi(z)\overline{\varphi}(z)d\mu_z \quad \text{with } d\mu_z = d\omega_z. \qquad (2.9)$$

The reproducing kernel is

$$K(z,\zeta) = e^{-1/2|z-\zeta|^2}. \qquad (2.10)$$

### C. The Space $L_2(G)$

Let $G$ be a bounded and simply connected domain in the complex plane $z$. We define the class $L_2(G)$ as the class of holomorphic functions $f(z)$ defined in $G$, with scalar product $(f,g) = \int_G f(z)\overline{g}(z)d\mu_z$, where $\mu(z)$ is a measure, and such that $(f,f) < \infty$.

We shall from time to time use the special case where $d\mu_z = d\omega_z$ with $d\omega_z = dxdy$. The reproducing kernel associated with $L_2(G)$ and the measure $\mu(z)$ will be written $M(z,\zeta)$. On the other hand the reproducing kernel associated with $L_2(G)$ and the measure $\omega(z)$ will have the distinct notation $K(z,\zeta)$ on behalf of its greater importance.

The importance of $L_2(G)$ is connected with the following minimum problem.

*P1:* Let $\zeta$ be an interior point of $G$ and let $u = h(z)$, $h(\zeta) = 0$, $h'(\zeta) = 1$, be the conformal mapping of the interior of $G$ into the interior of a circle $|u| = R$. Let $d\mu_z = d\omega_z$. Find the function $F(z) \in L_2(G)$, $F(\zeta) = 1$, such that $(F,F)$ is minimum.

The solution is $F_0(z)$ where

$$u = h(z) = \int_\zeta^z F_0(v)dv. \qquad (2.11)$$

The *Bergman kernel* is given by

$$K(z,\zeta) = F_0(z)/(F_0,F_0). \qquad (2.12)$$

Property (2.4) may be rewritten in the following manner[1]: let $\{\phi_\nu(z)\}$ be a closed system of orthogonal functions, which belongs to $L_2(G)$, with $(\phi_\nu,\phi_\mu) = \delta_\mu^\nu$, then the series

$$M(z,\zeta) = \sum_{\nu=1}^{\infty} \phi_\nu(z)\overline{\phi}_\nu(\zeta) \qquad (2.13)$$

converges uniformly and absolutely in any closed domain which is entirely in $G$, to the reproducing kernel $M(z,\zeta)$. The kernel is analytic in $z,\zeta \in G$. We have the reproducing property,

$$f(\zeta) = \int_G \overline{M(z,\zeta)}f(z)d\mu_z \quad \text{for } f \in L_2(G). \qquad (2.14)$$

For the special case where $d\mu_z = d\omega_z$, the reproducing kernel may be written as

$$K(z,\zeta) = (1/\pi)\,[h'(z)\overline{h'(\zeta)}]/[1-h(z)\overline{h(\zeta)}]^2. \qquad (2.15)$$

It is therefore independent of the choice of the $\{\phi_\nu\}$. It is easily seen that since $h'(z) \neq 0$ because $h(z)$ is a one to one mapping, $K(z,\zeta)$ cannot have zeroes for $z,\zeta \in G$.

Let us note, however, that the value of $M(z,\zeta)$ depends not only of the domain $G$, but also of the measure $\mu(z)$, i.e., of the definition of the inner product.

### D. The Space $L_2(C)$

Let $C$ be the boundary of the closed bounded domain $G$ defined in $2C$. We assume that $C$ is an analytic curve. We define the class $L_2(C)$ as the class of holomorphic functions $f(z)$ defined over $C + G$, with inner product $(f,g) = \int_C f(z)\overline{g}(z)d\mu_z$, where $\mu(z)$ is a measure, and such that $(f,f) < \infty$. The reproducing kernel associated with $L_2(C)$ and the measure $\mu(z)$ will be written $\hat{M}(z,\zeta)$. The reproducing kernel associated with $L_2(C)$ and the special case $d\mu_z = ds$ where $ds = |dz|$ is the line element will have the distinct notation $\hat{K}(z,\zeta)$. When $d\mu_z = ds$, the space $L_2(C)$ is connected with the following problem.

*P2:* Let $\zeta$ be an interior point of $G$ and let $u = h(z)$, $h(\zeta) = 0$, $h'(\zeta) = 1$ be the conformal mapping of the interior point of $G$ into the interior of a circle $u = R$. Find the function $F(z) \in L_2(C)$, $F(\zeta) = 1$ such that $(F,F)$ is minimum, $\zeta \in C$. The solution is

$$\hat{F}_0(z) = \left(\frac{dh}{dz}\right)^{1/2}, \quad \text{where} \quad u = h(z) = \int_\zeta^z \hat{F}_0^2(v)dv. \qquad (2.16)$$

The *Szegö kernel* is given by

$$\hat{K}(z,\zeta) = \hat{F}_0(z)/(\hat{F}_0,\hat{F}_0). \qquad (2.17)$$

Property (2.4) may be rewritten in the following manner[1]: Let $\{\hat{\phi}_\nu(z)\}$ be a closed system of orthogonal analytic functions which are regular in $G + C$ and belong to $L_2(C)$, with $(\hat{\phi}_\nu,\hat{\phi}_\mu) = \delta_\mu^\nu$, then the series

$$\hat{M}(z,\zeta) = \sum_{\nu=1}^{\infty} \hat{\phi}_\nu(z)\overline{\hat{\phi}_\nu(\zeta)} \qquad (2.18)$$

converges uniformly and absolutely for $z,\zeta$ in any closed subdomain of $G$ to the reproducing kernel $\hat{M}(z,\zeta)$. We have the reproducing property,

$$f(\zeta) = \int_C \overline{\hat{M}(z,\zeta)}f(z)d\mu_z \quad \text{for} \quad f \in L_2(C). \qquad (2.19)$$

Since $\hat{F}_0^2(z) = F_0(z)$, we have

$$[\hat{K}(z,\zeta)/\hat{K}(\zeta,\zeta)]^2 = K(z,\zeta)/K(\zeta,\zeta), \tag{2.20}$$

which yields a useful relation between the Bergman and the Szegö kernel valid for simply connected domains $G$. Since $\int_G |F_0(z)|^2 d\omega_z = \pi R^2$ and $\int_C |\hat{F}_0(z)|^2 ds = 2\pi R$,

$$4\pi(\hat{K}(z,\zeta))^2 = K(z,\zeta) \tag{2.21}$$

and

$$\hat{K}(z,\zeta) = (1/2\pi)\sqrt{h'(z)\overline{h'(\zeta)}}\,\{1/[1-h(z)\overline{h}(\zeta)]\}. \tag{2.22}$$

### E. Miscellaneous Properties

Let $F_n$ be the class of polynomials of degree at most $n$ and let us assume that $F_n$ is a subclass of the class $L_2(G)$ defined in 3C. This is certainly possible for $d\mu_z = d\omega_z$, although it may not be possible for arbitrary $\mu(z)$. We can restrict therefore the $\{\phi_\nu(z)\}$ to orthogonal polynomials. We define the *partial reproducing kernel*

$$M_n(z,\zeta) = \sum_{\nu=0}^{\infty} \phi_\nu(z)\overline{\phi_\nu(\zeta)} \tag{2.23}$$

associated with the class $F_n$, which projects functions $f \in L_2(G)$ with $F_n \subset L_2(G)$ into the subspace $F_n$.[2] The partial reproducing kernel $M_n(z,\zeta)$ converges uniformly and absolutely to $M(z,\zeta)$ as $n \to \infty$ provided that $F_n \subset L_2(G)$ for all $n$. Completely similar properties are obtained for the partial reproducing kernel $\hat{M}_n(z,\zeta)$ associated with $F_n \subset L_2(C)$. We can extend the definition of the partial reproducing kernel by simply truncating the sum in (2.13) for an arbitrary closed system of orthogonal functions which belong to $L_2(G)$. However we note that if $M(z,\zeta)$ depends only upon $G$ and the metric associated with $G$, i.e., $d\mu_z$, the partial reproducing kernel is not unique and depends also on the choice of $\phi_\nu(z)$.

A simple relation between $M(z,\zeta)$ and $K(z,\zeta)$ may be obtained in case $d\mu_z = |p(z)|^2 d\omega_z$, where $p(z)$ is a regular, single-valued analytic function in $G + C$ which does not vanish in $G + C$. If $f(z) \in L_2(G)$,

$$\int_G \overline{M(z,\zeta)}|p(z)|^2 f(z) d\omega_z = f(\zeta). \tag{2.24}$$

Since $p(z) \neq 0$ in $G + C$, any function of $L_2(G)$ with $d\mu(z) = d\omega_z$ can be brought in the form $p(z)f(z)$ where $f(z) \in L_2(G)$ associated with $d\mu_z = |p(z)|^2 d\omega_z$ and therefore

$$\int_G p(\zeta)\overline{M(z,\zeta)}\,\overline{p(z)}[p(z)f(z)]d\omega_z = p(\zeta)f(\zeta) \tag{2.25}$$

which yields

$$K(z,\zeta) = p(z)\overline{p(\zeta)}M(z,\zeta). \tag{2.26}$$

The same relation is obtained for the class $L_2(C)$,[8] with $d\mu_z = |p(z)|^2 ds$,

$$\hat{K}(z,\zeta) = p(z)\overline{p(\zeta)}\hat{M}(z,\zeta). \tag{2.27}$$

## 3. SOLUTION OF A CAUCHY PROBLEM

### A. Operator-Valued Reproducing Kernels

(a) We have the abstract Cauchy problem: to find $N(t)$, a solution of

$$\frac{\partial N}{\partial t} = HN \tag{3.1}$$

where initial condition $N(0)$ is given.

We assume that $H$ is bounded and defined everywhere (and therefore closed), independent of $t$, with range and domain in a Hilbert space $\mathcal{H}$.

More precisely we assume (i) $H$ is bounded and defined everwhere (ii) $\|R_\lambda(H)\| \leq \text{const}/\lambda - \omega$ for real $\lambda > \omega$, for some real number $\omega$.

Then $H$ is the infinitesimal generator of a strongly continuous semigroup $T(t)$ such that $\|T(t)\| < Ce^{\omega t}$. The solution of (3.1) is unique and given by[9]

$$N(t) = T(t)N(0) \tag{3.2}$$

for any vector $N(0)$. Condition (i) will be satisfied if the halfplane $\mathrm{Re}\lambda > \omega$ lies in the resolvent set of $H$, which is the complementary set of the spectrum $\sigma(H)$.

(b) Let $F(H)$ be the class of complex-valued functions $f$ such that (i) the domain of definition $\Delta(f)$ is an open set of the complex plane which contains $\sigma(H)$. (ii) $f$ is analytic at each point of $\Delta(f)$.

Since $H$ is bounded, it is possible to select a bounded simply connected domain $G$ such that $\Delta(f) \subset G$. Let $G'$ be a simply connected domain such that $\sigma(H) \subset G'$ and $\overline{G'} \subset \Delta(f)$, the boundary $B(G')$ is a closed rectifiable Jordan curve.

We define the function $f(H)$ by the Dunford–Taylor integral

$$f(H) = \frac{1}{2\pi i}\int_{+B(G')} f(\lambda)R_\lambda(H)d\lambda. \tag{3.3}$$

(c) We can define the reproducing kernel $K(z,\zeta)$ associated with the domain $G$ for the class $L_2(G)$.

For fixed $z \in G$, $K(z,\zeta)$ is a bounded regular analytic function of $\zeta \in \overline{G'}$ provided $G'$ is a subdomain entirely in $G$; otherwise $K(z,\zeta)$ may not be defined. Therefore for fixed $z \in G$, $K(z,\zeta)$ is a function of $\zeta(\zeta \in \overline{G'})$, which belongs to $F(H)$, and

$$K(z,H) = \frac{1}{2\pi i}\int_{+B(G')} K(z,\lambda)R_\lambda(H)d\lambda. \tag{3.4}$$

Similarly,

$$K_n(z,H) = \frac{1}{2\pi i}\int_{+B(G')} K_n(z,\lambda)R_\lambda(H)d\lambda, \tag{3.5}$$

$K_n(z,H)$ converges to $K(z,H)$ in the uniform topology of operators.[9] We can define similarly $\phi_\nu(H)$.

(d) Let $f(z) = K(z,H)N(0)$ for $z \in G$, which is a vector-valued function of $z$, defined in the Hilbert space $\mathcal{H}$. Let $\{x_k\}$ be a complete set of elements of $\mathcal{H}$. Then if we write the inner product in $\mathcal{H}$ by $\langle x,y\rangle$ to avoid confusion with the inner product in $L_2(G)$,

$$\langle x_k, f(z)\rangle = \frac{1}{2\pi i}\int_{+B(G')} K(z,\lambda)\langle x_k, R_\lambda(H)N(0)\rangle d\lambda. \tag{3.6}$$

Since $\langle x_k, R_\lambda(H)N(0)\rangle$ is a bounded function of $\lambda$ for $\lambda \in B(G')$, the integral is a regular single-valued function of $z$ for $z \in G$.

In order to prove that $\langle x_k, f(z)\rangle$ belongs to $L_2(G)$ with

measure $d\mu_z = d\omega_z$, we evaluate the norm. Let $f_k(z) = \langle x_k, f(z)\rangle$ and $g_k(\lambda) = \langle x_k, R_\lambda(H)N(0)\rangle$;

$$(f_k(z), f_k(z)) = \frac{1}{(2\pi)^2}\int_G d\omega_z \int_{+B(G')} d\lambda \int_{+B(G')} d\lambda' \times K(z,\lambda)\overline{K(z,\lambda')}g_k(\lambda)\overline{g_k(\lambda')}. \quad (3.7)$$

By Fubini's theorem and using the reproducing property,

$$(f_k(z), f_k(z)) = \frac{1}{(2\pi)^2}\int_{+B(G')} d\lambda \int_{+B(G')} d\lambda' \times K(\lambda',\lambda)g_k(\lambda)g_k(\lambda'). \quad (3.8)$$

Since $g_k(\lambda)$, $g_k(\lambda')$, $K(\lambda,\lambda')$ are bounded for $\lambda, \lambda' \in B(G')$ (which is entirely in $G$) and since $B(G)$ is rectifiable, $\|f_k(z)\| < \infty$ and $f_k(z)$ belongs to $L_2(G)$ associated with $d\mu_z = d\omega_z$. Each component of the vector-valued function $f(z)$ being in $L_2(G)$ we may speak, for short of "functions" $f(z)$ in $L_2(G)$, and apply all properties of Sec. 2.

For $p \notin \overline{G}$, we know that $1/(p-z)$ belongs to $L_2(G)$ for $d\mu_z = d\omega_z$.

Therefore,

$$F(p) = (1/(p-z), f(z)) \quad (3.9)$$

exists and is a vector-valued function of $p$ in Hilbert space $\mathcal{K}$.

Therefore,

$$F(p) = \left(\frac{1}{p-z}, K(z,H)N(0)\right) = \int_G d\omega_z \frac{1}{p-z}\frac{1}{2\pi i} \times \int_{+B(G')} \overline{K(z,\lambda)}R_\lambda(H)N(0)d\lambda. \quad (3.10)$$

By means of Fubini theorem:

$$F(p) = \frac{1}{2\pi i}\int_{+B(G')} R_\lambda(H)N(0)d\lambda \int_G \frac{\overline{K(z,\lambda)}}{p-z} d\omega_z = \frac{1}{2\pi i}\int_{+B(G')} R_\lambda(H)N(0)\frac{d\lambda}{p-\lambda}. \quad (3.11)$$

Since $1/(p-\lambda)$ belongs to the class $F(H)$ for $p \in \overline{G'}$, the last integral is $R_p(H)N(0)$.

(e) As is well known from semigroup theory,

$$T(t)N(0) = \frac{1}{2\pi i}\int_{+B(G')} e^{pt}R_p(H)N(0)dp. \quad (3.12)$$

Substituting (3.10) into (3.12),

$$T(t)N(0) = \frac{1}{2\pi i}\int_{+B(G')} e^{pt}dp \int_G \frac{\overline{K(z,H)}N(0)}{p-z} d\omega_z. \quad (3.13)$$

Again by Fubini's theorem,

$$T(t)N(0) = \int_G \overline{K(z,H)}N(0)d\omega_z \frac{1}{2\pi i}\int_{+B(G')} \frac{e^{pt}}{p-z} dz \quad (3.14)$$

or

$$N(t) = \int_G e^{zt}\,\overline{K(z,H)}N(0)d\omega_z = (e^{zt}, K(z,H)N(0)). \quad (3.15)$$

Equation (3.15) is the main result of this paper.

Although we have used everywhere the space $L_2(G)$ with $d\mu_z = d\omega_z$, all results derived so far in Sec. 3 are valid for the reproducing kernel $M(z,H)$.

Therefore we can write

$$N(t) = \int_G e^{zt}\overline{M(z,H)}N(0)d\mu_z. \quad (3.16)$$

Substituting (2.13) in (3.16),

$$N(t) = \sum_\nu \phi_\nu(H)N(0)\int_G e^{zt}\overline{\phi_\nu}(z)d\mu_z, \quad (3.17)$$

which yields a useful and efficient algorithm, as we shall see later. An interesting feature is the large freedom in the choice of $G$ and $\mu_z$.

It can be easily seen that a similar result is obtained for Szegö kernels, i.e.,

$$N(t) = \int_C e^{zt}\overline{\hat{M}(z,H)}N(0)d\mu_z. \quad (3.18)$$

### B. The Optimum Filtration

We shall solve the problem of the optimal choice of $G$ and $\mu(z)$ for two important cases:

(a) $H$ is a bounded self-adjoint operator,

(b) $H$ is a normal compact operator.

#### 1. *H is a Bounded Self-Adjoint Operator*

Let $\mathcal{E}_\lambda$ be the family of projectors associated with $H$. The resolution of the identity is written[12]

$$Hx = \int_m^M \lambda d\mathcal{E}_\lambda x. \quad (3.19)$$

Let us assume for simplicity that the spectrum is purely continuous. The generalization to a mixed spectrum is obvious.

There exists a finite or infinite system of elements $f_k(\lambda) = \mathcal{E}_\lambda y_k \in \mathcal{K}$ such that, if $\Delta f(\lambda) = f(\beta) - f(\alpha)$,

(a) $\langle \Delta\mathcal{E}_\lambda y_k, \Delta\mathcal{E}_\mu y_k\rangle = 0$ for $k \neq 1$,

(b) $\langle \Delta\mathcal{E}_\lambda y_k, \Delta\mathcal{E}_\mu y_k\rangle = 0$ if intervals $\Delta_\lambda$ and $\Delta_\mu$ do not overlap,

(c) the elements $\Delta f_k(\lambda)$ for $k = 1, 2, \cdots$ and for all intervals $\Delta_\lambda$ form a complete system in $\mathcal{K}$.

Then

$$\rho_k(\lambda) = \|\mathcal{E}_\lambda y_k\|^2$$

is a nondecreasing function of $\lambda$.

We have

$$\mathcal{E}_\mu y = \sum_k \int_m^\mu \frac{d\langle y, \mathcal{E}_\lambda y_k\rangle}{d\rho_k(\lambda)} d\mathcal{E}_\lambda y_k \quad (3.20)$$

Let

$$\sigma_k(\lambda) = \frac{d\langle N(0), \mathcal{E}_\lambda y_k\rangle}{d\rho_k(\lambda)} \quad (3.21)$$

with

$$\mathcal{E}_\mu N(0) = \int_m^\mu \sum_k \sigma_k(\lambda)df_k(\lambda), \quad (3.22)$$

$$M(z,H)N(0) = \sum_k \int_m^M M(z,\lambda)\frac{d\langle N(0), \mathcal{E}_\lambda y_k\rangle}{d\rho_k(\lambda)} d\mathcal{E}_\lambda y_k. \quad (3.23)$$

Therefore

$$N(t) = \int_G e^{zt} d\mu_z \sum_k \int_m^M \overline{M(z,\lambda)}\sigma_k(\lambda) df_k(\lambda). \quad (3.24)$$

Let us consider a family of approximate reproducing kernels $\tilde{M}_n(z,\zeta), n = 1, 2, \ldots$, which is so far arbitrary, except that $M_n(z,\zeta)$ belongs to $L_2(G)$ and converges uniformly in $z, \zeta \in G$ to $M(z,\zeta)$, as $n \to \infty$. We define, correspondingly, approximate solutions of (3.1) by

$$\tilde{N}_n(t) = \int_G e^{zt} d\mu_z \sum_k \int_m^M \overline{\tilde{M}_n(z,\lambda)}\sigma_k(\lambda) df_k(\lambda). \quad (3.25)$$

The uniform convergence of $\tilde{M}_n(z,\lambda)$ to $M(z,\lambda)$ entails the uniform convergence of $N_n(t)$ to $N(t)$. The error is

$$N(t) - \tilde{N}_n(t) = \int_G e^{zt} d\mu_z \sum_k \int_m^M [\overline{M(z,\lambda)} - \overline{\tilde{M}_n(z,\lambda)}]\sigma_k(\lambda) df_k(\lambda). \quad (3.26)$$

Applying Schwarz inequality,

$$\|N(t) - \tilde{N}_n(t)\|^2 \le \int_G e^{2t\,\mathrm{Re}\,\eta} d\mu_\eta \int_G h(z) d\mu_z \quad (3.27)$$

with

$$h(z) = \sum_k \sum_l \int_m^M \int_m^M [M(z,\mu) - \tilde{M}_n(z,\mu)][\overline{M(z,\lambda)} - \overline{\tilde{M}_n[z,\lambda)}]\sigma_k(\lambda)\overline{\sigma_l(\mu)}\langle df_k(\lambda), df_k(\mu)\rangle. \quad (3.28)$$

However,

$$\begin{aligned}\langle df_k(\lambda), df_l(\mu)\rangle &= \langle d\mathcal{E}_\lambda f_k, d\mathcal{E}_\mu f_l\rangle \\ &= \delta_l^k \delta(\lambda - \mu)\langle d\mathcal{E}_\lambda f_k(\lambda), d\mathcal{E}_\lambda f_k(\lambda)\rangle \\ &= \delta_l^k \delta(\lambda - \mu) d\rho_k(\lambda). \end{aligned} \quad (3.29)$$

Therefore

$$h(z) = \sum_k |M(z,\lambda) - \tilde{M}_n(z,\lambda)|^2 |\sigma_k(\lambda)|^2 d\rho_k(\lambda). \quad (3.30)$$

Since

$$\sum_k |\sigma_k(\lambda)|^2 d\rho_k(\lambda) = \sum_k \frac{d\langle N, \mathcal{E}_\lambda y_k\rangle d\langle \overline{N, \mathcal{E}_\lambda y_k}\rangle}{d\rho_k} = \langle N(0), d\mathcal{E}_\lambda N(0)\rangle, \quad (3.31)$$

$$\|N(t) - \tilde{N}_n(t)\|^2 \le \int_G e^{2t\,\mathrm{Re}\,\eta} d\mu_\eta \int_G d\mu_z \int_m^M |M(z,\lambda) - \tilde{M}_n(z,\lambda)|^2 \langle N, d\mathcal{E}_\lambda N\rangle, \quad (3.32)$$

$\tilde{M}_n(z,\lambda)$ being so far arbitrary, we assume that $\tilde{M}_n(z,\lambda) \in L_2(G)$.

The best approximation will be obtained as a two step procedure: First minimize

$$L_n'(z) = \int_m^M |M(z,\lambda) - \tilde{M}_n(z,\lambda)|^2 \langle N, d\mathcal{E}_\lambda N\rangle \quad (3.33)$$

for a given $z$, and then minimize

$$J_n = \int_G L_n'(z) d\mu_z. \quad (3.34)$$

If we had used the Szegö kernel instead of the Bergman kernel, i.e., Eq. (3.18) instead of (3.16), we would have to minimize $J_n = \int_C L_n'(z) d\mu_z$.

**2.** *H is a Compact and Normal Operator*

We shall assume that the eigenvalues are simple. The resolution of the identity is written

$$Hx = \sum_k \lambda_k P_k x, \quad (3.35)$$

where $P_k$ is the eigenprojection associated with $\lambda_k$. Let $N(0)$ be developed in terms of the complete set of eigenvectors $\psi_k$,

$$N(0) = \sum_k \sigma_k \psi_k. \quad (3.36)$$

Since

$$M(z,H)N(0) = \sum_k M(z,\lambda_k)\sigma_k\psi_k, \quad (3.37)$$

the same reasoning as in *b*, leads to the minimization of

$$J_n = \int_G L_n''(z) d\mu_z \quad (3.38)$$

with

$$L_n''(z) = \sum_k |M(z,\lambda_k) - \tilde{M}_n(z,\lambda_k)|^2 |\sigma_k|^2$$

or

$$L_n''(z) = \int_G |M(z,\lambda) - \tilde{M}_n(z,\lambda)|^2 \rho(\lambda)\, d\omega_\lambda \quad (3.39)$$

with

$$\rho(\lambda) = \sum_k |\sigma_k|^2 \delta(\lambda - \lambda_k). \quad (3.40)$$

We introduce now the superscripts $G$ and $R$ to $d\mu_z^G$, $d\mu_\lambda^R$ to emphasize the corresponding measures.

We can summarize both cases by

$$\|N(t) - \tilde{N}_n(t)\|^2 \le J_n \int_G e^{2t\,\mathrm{Re}\,\eta} d\mu_\eta^G \quad (3.41)$$

with the optimal choice obtained from

$$\min J_n = \min \int_G d\mu_z^G \int_R |M(z,\lambda) - \tilde{M}_n(z,\lambda)|^2 d\mu_\lambda^R \equiv \min \int_G d\mu_z^G L_n(z), \quad (3.42)$$

where $R$ is given, as well as $d\mu_\lambda^R$. On the other hand, we have the freedom to choose $G \supset \overline{R}$, the metric $d\mu_z^G$, as well as $\tilde{M}_n(z,\lambda) \subset L^2(G)$, for $z \in G$ and $\lambda \in \overline{R}$. The reproducing kernel $M(z,\lambda)$ is determined as soon as $G$ and $d\mu_z^G$ are fixed. In case of an Hermitian operator, $d\mu_\lambda^R$ degenerates into a one-dimensional measure.

**3.** *Choice of the Optimal Reproducing Kernel*

We shall assume we have a family of bounded domains $G_n$, with

$$G_1 \supset G_2 \supset \cdots G_n \supset \cdots,$$

such that the norm associated with $L_2(G_n)$ is a monotone function of $n$, i.e.,

$$\|f\|_{G_n} \ge \|f\|_{G_{n-1}}. \quad (3.43)$$

Obviously if $f \in L_2(G_n)$, then $f \in L_2(G_{n-1})$. We introduce now the following extremum problem.

*P3:* Let $G$ and $R \subset G_i, i = 1, 2, \cdots$.

Let $\varphi_n(z)$ be a regular single-valued function such that

$$\|\varphi_n\|_R = 1, \quad (\varphi_n, \varphi_{n-\nu})_R = 0, \quad \nu = 1, 2, \ldots, n, \quad (3.44)$$

and

$$\min \|\varphi_n\|_G.$$

Bergman has shown[1] that the set $\{\varphi_n\}, n = 0, 1, \cdots$ is *orthogonal over R, and also over G*. It is closed with respect to $L_2(G)$ but not necessarily so for $L_2(R)$. This will be the case if $R$ is bounded by a finite number of distinct Jordan curves and the inner region of $R$ is such that it separates no point of $G - R$ from the boundary of $G$. We can always choose $G$ and $R$ in this way.

We have $\|\varphi_n\|_G^2 = k_n > 1$, the inequality resulting from the norm monotonicity. The set $\{\varphi_n\}$ is unique. We have also the dual problem,

$$\|\psi_n\|_G = 1, \quad (\psi_n, \psi_{n-\nu})_G = 0, \quad \nu = 1, 2, \cdots, n \tag{3.45}$$

and $\max \|\psi_n\|_R$. We have $\varphi_n = \psi_n k_n^{1/2}$ and $\|\psi_n\|_R^2 = 1/k_n < 1$. We define $\|f\|_G^2$ by $\int_G |f(z)|^2 \, d\mu_z^G$ and $\|f\|_R^2$ by $\int_R |f(z)|^2 d\mu_z^R$. A sufficient condition for the norm monotonicity is $d\mu_z^R < d\mu_z^G$ almost everywhere for $z \in \overline{R}$.

Let $\{\phi_\nu\}$ be a closed system of orthogonal functions over $G$, i.e.,

$$(\phi_\nu, \phi_\mu)_G = \delta_\nu^\mu. \tag{3.46}$$

We have the uniformly convergent development

$$M(z, \lambda) = \sum_\nu \phi_\nu(z)\overline{\phi_\nu(\lambda)}, \quad z, \lambda \in G. \tag{3.47}$$

We choose now $M_n(z, \lambda)$ to be in $L_2(G)$; we can write therefore

$$\tilde{M}_n(z, \lambda) = \sum_{k=0}^{n} a_k(\lambda)\phi_k(z). \tag{3.48}$$

Exchanging the order of integration by means of Fubini theorem, we minimize first

$$\int_G |M(z, \lambda) - \tilde{M}_n(z, \lambda)|^2 d\mu_z^G \tag{3.49}$$

for a given $\lambda \in \overline{R}$. By a classical theorem,[6] the minimum is obtained for the Fourier coefficient:

$$a_k(\lambda) = (M(z, \lambda), \phi_k(z))_G = \overline{\phi}_k(\lambda). \tag{3.50}$$

Therefore

$$J_n = \int_R d\mu_\lambda^R \left(M(\lambda, \lambda) - \sum_{k=0}^{n} |\phi_k(\lambda)|^2\right) = \int_R d\mu_\lambda^R \sum_{k=n+1}^{\infty} |\phi_k(\lambda)|^2. \tag{3.51}$$

We turn now to the problem of finding the best set $\{\phi_\nu\}$. Since

$$J_n = \int_R d\mu_\lambda^R M(\lambda, \lambda) - \sum_{k=0}^{n} \|\phi_k\|_R^2, \tag{3.52}$$

we have to maximize the sum. Indeed $\int_R d\mu_\lambda^R M(\lambda, \lambda)$ is dependent only upon the choice, already made of $G, R, d\mu_z^G, d\mu_\lambda^R$. If we want that for each value of $n$ the approximate solution be optimal, we must minimize $J_n$ sequentially, i.e., find $\phi_n$ such that

$$(\phi_n, \phi_\mu) = \delta_\mu^n, \quad n \geq \mu \tag{3.53}$$

and

$$\max \|\phi_n\|_R^2 = 1/k_n. \tag{3.54}$$

This is precisely problem P3 and therefore the best set $\{\phi_\nu\}$ is the *unique set of functions simultaneously orthogonal over G and R*.

The explicit expressions for the reproducing kernels associated with $L_2(G)$ and $L_2(R)$ can be written down[10]:

$$M_G(z, \lambda) = \sum_\nu \phi_\nu(z)\overline{\phi_\nu(\lambda)}, \tag{3.55}$$

$$M_R(z, \lambda) = \sum_\nu \phi_\nu(z)\phi_\nu(\lambda)k_\nu, \tag{3.56}$$

from which we obtain

$$J_n = \sum_{\nu=n+1}^{\infty} \frac{1}{k_\nu} < \infty. \tag{3.57}$$

We conclude that the best approximate solution $N_n(t)$ is obtained for $M_n(z, \lambda)$ which is the partial reproducing kernel associated with a given domain $G$, a measure $d\mu_z^G$ and the unique set of orthogonal functions over $G$ and $R$, with their respective metric.

Two remarks are in order.

(1) The measure $d\mu_\lambda^R$ is only roughly known, if at all.

(2) It is difficult to evaluate doubly orthogonal functions. Moreover $\phi_\nu(H)$ cannot be easily evaluated for numerical purposes unless $\phi_\nu$ is a polynomial. However, except for special forms of $d\mu_\lambda^R$, the $\phi_\nu$ will not be polynomials.

Obviously a simplification is needed, at the expense of the condition of optimality we have derived. If $G$ is "close" to $R$, as well as $d\mu_z^R$ is "close" to $d\mu_z^G$, a set of orthogonal *polynomials* over $G$, will be "almost" orthogonal over $R$. The departure from optimality is a function, albeit unknown to us, of the closeness of the domains and their associated measure. This departure must be tempered anyway by the fact that $d\mu_z^R$ may be grossly inaccurate. We submit therefore that the best approximation $M_n(z, \zeta)$ be constructed in the following way:

(a) Select a bounded domain $G \supset \overline{R}$;

(b) Select $d\mu_z^G$ close to $d\mu_z^R$ and construct $\{\phi_\nu(z)\}$ as the unique set of orthogonal polynomials associated to $d\mu_z^G$.

The important fact is that, although $\tilde{M}_n(z, \zeta)$ may not be strictly optimal, it is still a partial reproducing kernel and its uniform convergence to $M(z, \zeta)$ ensures that $\tilde{N}_n(t)$ converges to $N(t)$.

It is not allowed to let $G \to R$ with $d\mu_z^G \to d\mu_z^R$, otherwise $k_\nu \to 1$ and $J_n \to \infty$. Although the preceding analysis is limited to Bergman kernels it is easy to see that is also valid for Szegö kernels. Moreover in some particular cases to be examined in the following paper, there are polynomials which are orthogonal not only over a pair $G, R$ but over a family of domains, of which $G, R$ are samples.

We return now to the case of a compact and normal operator, and let us assume that eigenvalues $\lambda_k$ are known. We write therefore

$$d\mu_\lambda^R = \sum_k |\sigma_k|^2 \delta(\lambda - \lambda_k) d\omega_\lambda. \tag{3.58}$$

Let us select $G$ arbitrary as long as $\overline{R} \subset G$ and $d\mu_\lambda^G = \alpha d\mu_\lambda^R$, $\alpha > 1$.

The common set of orthogonal functions for $G$ and $R$ is a set of *finite orthogonal polynomials* $\{p_s(\lambda)\}$. The

orthogonality relation is

$$\sum_{l=1}^{n} |\sigma_l|^2 p_s(\lambda_l) p_k(\lambda_l) = \delta_s^k. \tag{3.59}$$

Obviously

$$p_s(\lambda) = \phi_s(\lambda) = \alpha^{1/2}\psi_s(\lambda), \quad k_s = \alpha > 1.$$

We shall prove that

$$M^*(\lambda_k, \lambda_l) = |\sigma_k|^2 M(\lambda_k, \lambda_l) = \delta_l^k. \tag{3.60}$$

Although this is easily proved for real $\lambda_k$ by means of the Darboux–Christoffel relation for finite orthogonal polynomials, it is not any more possible to use this relation for complex $\lambda_k$. We obtain from (3.59) and (3.60)

$$\sum_{l=1}^{n} |M^*(\lambda_l, \lambda_l)|^2 + \sum_{m \neq l} \sum_{l=1}^{n} |M^*(\lambda_l, \lambda_m)|^2 = n. \tag{3.61}$$

Moreover

$$\sum_{l=1}^{n} M^*(\lambda_l, \lambda_l) = \sum_{l=1}^{n} \sum_{s=1}^{n} |\sigma_l|^2 |p_s(\lambda_l)|^2 = n. \tag{3.62}$$

Therefore the $M^*(\lambda_1, \lambda_1)$ satisfy the relations

$$\sum_{l=1}^{n} |M^*(\lambda_l, \lambda_l)|^2 \leq n,$$

$$\sum_{l=1}^{n} M^*(\lambda_l, \lambda_l) = n. \tag{3.63}$$

The only positive values which satisfy (3.63) are $M^*(\lambda_l, \lambda_l) = 1$ and therefore, by (3.61),

$$M^*(\lambda_l, \lambda_m) = \delta_m^l. \tag{3.64}$$

Therefore

$$N_n(t) = \sum_{k=1}^{n} \sigma_k \psi_k \int_G e^{zt} \overline{M_n(z, \lambda_k)} d\mu_z^R = \sum_{k=1}^{n} \sigma_k \psi_k e^{\lambda_k t}, \tag{3.65}$$

which is of course the expected result. This shows, incidentally, the connection between the reproducing kernel method and the conjugate gradient method[11] which will be examined with more details in the following paper.


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# The Reproducing Kernel Method. II


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The explicit solution of the Cauchy problem $\partial N/\partial t = HN$ by means of reproducing kernels is obtained under various forms: conformal mapping expansions, Sheffer polynomial expansion, polynomials orthogonal on a family of curves; the convergence is studied for both Szegö and Bergman kernels.


We have shown in Paper I[1] how the reproducing kernel in a given Hilbert space of square integrable analytic functions could be used to solve abstract Cauchy problems $\partial N/\partial t = HN$. Many practical problems remain to be solved before using Eq. (I. 3. 16) [Paper I, Eq. (3. 16)] for instance. We show first in Secs. 1A–1C how various scattered results of Szegö and Walsh can be used to generate polynomials orthogonal in the complex plane. Of central importance is the conformal mapping function of a domain $G$ containing the operator's spectrum upon the unit circle. This mapping function allows to use the Sheffer polynomial representation, which gives an explicit solution of the Cauchy problem (Sec. 2A). The use of polynomials orthogonal on a family $C_\gamma$ allows similarly explicit solution for the case where $C_\gamma$ is an ellipse or a parabola. Our principal results are summarized in Eqs. (2. 38), (2. 39) and Eqs. (2. 56), (2. 57). The case of a real interval is examined in Sec. 2C and Sec. 2D. Finally, the convergence is studied briefly in Sec. 3. Although unrelated to the abstract Cauchy problem under examination, we show in the Appendix some connections between the proposed method of reproducing kernels and the conjugate gradient method of Hestenes and Stiefel.[2]

## 1. CONSTRUCTION OF ORTHOGONAL FUNCTIONS

### A. Construction of Orthogonal Functions on $G'$, from a Set Orthogonal on $G$

The method of construction of orthogonal functions on a domain $G$ or a curve $C$ can be found in many textbooks (see, for instance, Refs. 3, 4).

Once orthogonal functions have been built for a given domain $G$, it is easy to build orthogonal functions for a domain $G'$ if the conformal representation of $G'$ upon $G$ is known.

For instance, let $\{\phi_\nu(z)\}$ be a complete orthogonal system on a bounded, simply connected domain $G$, i.e., $(\phi_\nu, \phi_\mu) = \int_G \phi_\nu(z)\overline{\phi}_\mu(z) dw_z = \delta_\mu^\nu$ with $dw_z = dxdy$.

Let $z = g(u)$ be the conformal representation of a bounded simply connected domain $G'$ on $G$. We

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For instance, let $\{\phi_\nu(z)\}$ be a complete orthogonal system on a bounded, simply connected domain $G$, i.e., $(\phi_\nu, \phi_\mu) = \int_G \phi_\nu(z)\overline{\phi}_\mu(z) dw_z = \delta_\mu^\nu$ with $dw_z = dxdy$.

Let $z = g(u)$ be the conformal representation of a bounded simply connected domain $G'$ on $G$. We

assume that $g(u)$ and its inverse function $h(z)$ are univalent. The functions $\phi_\nu(g(u))g'(u)$ form a complete orthogonal system in $G'$.

Indeed

$$\int_{G'}\phi_\nu(g(u))g'(u)\overline{\phi}_\nu(g(u))\overline{g}'(u)dw_u = \int_{G'}\phi_\nu(z)\overline{\phi}_\mu(z)\left|\frac{dg}{du}\right|^2 dw_u = \int_G \phi_\nu(z)\overline{\phi}_\mu(z)dw_z = \delta^\nu_\mu. \tag{1.1}$$

Similarly the functions $\hat{\phi}_\nu(g(u))g'^{1/2}(u)$ form a complete orthonormal system on the boundary $C'$ of $G'$ if $\{\hat{\phi}_\nu(z)\}$ form a complete orthonormal system on the boundary $C$ of $G$.

Indeed

$$\int_{C'}\hat{\phi}_\nu(g(u))g'^{1/2}(u)\overline{\hat{\phi}_\mu(g(u))}\overline{g'^{1/2}}(u)\,|du| = \int_{C'}\hat{\phi}_\nu(z)\overline{\hat{\phi}_\mu(z)}\left|\frac{dg}{du}\right|\cdot|du| = \int_C \hat{\phi}_\nu(z)\overline{\hat{\phi}_\mu(z)}\,|dz| = \delta^\nu_\mu. \tag{1.2}$$

If the original set is orthogonal with respect to a weight function $w(z)$, the new one (in $G'$) is associated with a weight function $w[g(u)]$. For instance let $z = g(u)$ be the conformal representation of $G'$ upon the unit circle, which is the only one which is generally known explicitly, if at all. Since $\{\phi_\nu(z)\} = \{\sqrt{(\nu+1)/\pi}\cdot z^\nu\}$ is an orthogonal set in $G$ the set $\{\sqrt{(\nu+1)/\pi}g^\nu(u)g'(u)\}$ is orthogonal in $G'$ with weight function unity.

Similarly, $(1/\sqrt{2\pi})g^\nu(u)'^{1/2}g'^{1/2}(u)$ is orthogonal on the boundary $C'$ of $G$ with weight function unity.

## B. A Problem of Szegö: Polynomials Orthogonal on a Family of Curves

The following problem has been defined and solved by Szegö.[5]

To determine all Jordan curves $C$ and all analytic functions $D(z)$ regular and nonvanishing outside $C$, $z = \infty$ inclusive, possessing the following property. Let $C_r$ be a level curve in the conformal mapping of the region exterior to $C$ into the region exterior to the circle $|w| = r_0$, the two points at infinity corresponding to each other. The orthogonal polynomials $p_0(z), p_1(z), \ldots$, associated with $C_r$ and with the weight function $|D(z)|^2$ are independent of $r$ for $r > r_0$. In other words it is required that

$$\int_{C_r}|D(z)|^2 p_k(z)\overline{p_l(z)}\,|dz| = 0, \quad k \neq l, \quad r > r_0.$$

There are five categories

1. $C_r$: $|z| = r$, $r > 0$, $D(z) = 1$;

The polynomials are $p_k(z) = z^k$ (unnormalized).

2. $C_r$: $|z| = r$, $r > 1$, $D(z) = 1/(1 - z^{-n})$;

The polynomials are

$$p_k(z) = z^k,\ 0 \le k < n, \qquad p_k(z) = z^{k-n}(z^n - 1),\ k \ge n.$$

3. $C_r$: confocal ellipses with foci $\pm 1$

$$D(z) = [\tfrac{1}{2}(1 - 1/w)]^\alpha[\tfrac{1}{2}(1 + 1/w)]^\beta, \quad \alpha = \beta = \tfrac{1}{2}, \quad 2z = w + 1/w, \ |w| = r \ge 1;$$

the polynomials are

$$p_k(z) = (w^{k+1} - w^{-(k+1)})/(w - w^{-1}).$$

If we let $w = e^{i\theta}$, $z = \cos\theta$, $p_k(z) = (\sin(k+1)\theta/\sin\theta) = U_k(\cos\theta) = U_k(z)$, which are Tchebycheff polynomials of the second kind with

$$|D(z)|^2 = \tfrac{1}{2}\sin\theta = \tfrac{1}{2}\sqrt{1 - z^2}.$$

4. Same as 3 with

$$\alpha = \tfrac{1}{2}, \beta = -\tfrac{1}{2}, \quad |D(z)|^2 = \tan\theta/2, \quad p_k(z) = [\sin(k + \tfrac{1}{2})\theta]/\sin\theta/2 = U_{2k+1}(\cos\theta/2) = U_{2k+1}(\sqrt{(1+z)/2}), \quad r = 1 = (w^{k+1/2} - w^{-(k+1/2)})/(w^{1/2} - w^{-1/2}), \quad r > 1.$$

5. Same as 3 with $\alpha = \beta = -\tfrac{1}{2}$,

$$|D(z)|^2 = \frac{2}{\sin\theta} = \frac{2}{\sqrt{1 - z^2}},$$

$$p_k(z) = \cos k\theta = T_k(\cos\theta) = T_k(z), \quad r = 1 = \tfrac{1}{2}(w^k + w^{-k}), \quad r > 1,$$

i.e., Tchebycheff polynomials of the first kind.

All three polynomials are in fact Jacobi polynomials (See Ref. 5, p. 59).

## C. Polynomials Orthogonal on a Family $C_r$ and in a Domain $G$

Under which conditions polynomials orthogonal on the boundary $C$ of $G$ are also orthogonal in $G$?

Let $u = u(z)$ be the conformal representation of the interior of $G$ upon the interior of the annulus $G'$: $1 \le u \le \rho$. We have the following equalities (Walsh[6])

$$\int_{G'}A(z)p_k\overline{p_l(z)}dS(u) = \int_1^\rho dr\int_{|u|=r}A(z(u))p_k(z(u))\overline{p_l(z(u))}\,|du| = \int_1^\rho dr\int_{z\in C_r}A(z)\left|\frac{du}{dz}\right|p_k(z)\overline{p_l(z)}\,|dz|, \tag{1.3}$$

where $C_r$ is the equipotential curve such that if $z \in C_r$, $|u(z)| = r$, $1 \le r \le \rho$ (see Fig. 1) and $A(z)$ a positive function.

We have also

$$\int_G A(z)p_k(z)\overline{p_l(z)}\left|\frac{du}{dz}\right|^2 d\Sigma(z) = \int_{G'}A(z)p_k(z)\overline{p_l(z)}dS(u). \tag{1.4}$$

Accordingly, polynomials $p_k(z)$ are orthogonal in $G$ relatively to the weight function $A(z)\,|du/dz|^2$ when

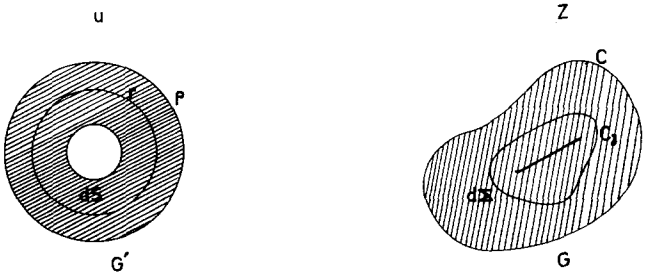


FIG. 1.

they are orthogonal, *on every line* $C_r, 1 \le r \le \rho$, relatively to the weight function $A(z)|du/dz|$.

We state this property in the following way: If $u = u(z)$ is the conformal representation of $G$ on the annulus $G'': 1 \le |u| \le \rho$ and if $\{p_k(z)\}$ is an orthogonal polynomial system on every $C_r: 1 \le r \le \rho$ relatively to the weight function $|D(z)|^2$, then $\{p_k(z)\}$ is orthogonal in $G$ relatively to the weight function $|D(z)|^2\ |du/dz|$.

The reciprocal is true.

We are led back to the problem of finding polynomials orthogonal on a family of curves. If the normalization is such that $\int_{G'} A(z)|p_k(z)|^2 dS = 1$, and if

$$F(r) = \int_{z \in C_r} A(z) \left|\frac{du}{dz}\right| |p_k(z)|^2 |dz|, \tag{1.5}$$

then

$$\int_1^\rho F(r)dr = 1.$$

This method allows (under circumstances described in Sec. 1C) to reduce the integration to one on particular curve of the family (for instance a segment of the real axis) where it is easily performed.

## 2. EXPLICIT SOLUTIONS OF A CAUCHY PROBLEM

### A. Use of the Conformal Representation of a Domain $G'$ upon the Unit Circle

The evaluation of the $m$th order approximation to the Cauchy problem

$$\frac{\partial N}{\partial t} = HN \tag{3.1) of I}$$

is given by Eq. (I. 3. 18),

$$N(t) = \int_{C'} e^{\zeta t}\, \overline{\hat{M}(\zeta, H)} N(0) d\zeta$$

with $d\mu_\zeta = |d\zeta|$, $\hat{M}$ being the Szegö kernel associated with the boundary $C'$ of $G$. Let $z = \psi(\zeta)$ be the mapping function of $G'$ upon the unit circle. Therefore,

$$N(t) = \frac{1}{2\pi} \sum_{\nu=0}^{\infty} \int \overline{\hat{\psi}^\nu(\zeta)\psi'^{1/2}(\zeta)} \times [\psi^\nu(H)\psi'^{1/2}(H)]N(0)e^{\zeta t}\, |d\zeta|. \tag{2.1}$$

In order to evaluate the integral of (2. 1) we may introduce the Sheffer polynomial representation which is a particular case of the generalized Appell polynomial representation introduced by Boas and Buck.[7]

Let

$$A(\psi)e^{tg(\psi)} = \sum_{n=0}^{\infty} \psi^n p_n(t), \tag{2.2}$$

where $\psi$ and $t$ are complex variables. Let $A(\psi)$ and $g(\psi)$ have the following Taylor expansion,

$$A(\psi) = \sum_{n=0}^{\infty} a_n \psi^n, \quad a_0 \neq 0, \tag{2.3}$$

$$g(\psi) = \sum_{n=1}^{\infty} g_n \psi^n, \quad g_1 \neq 0, \tag{2.4}$$

We assume that $A(\psi)$ and $g(\psi)$ are regular for $\psi \in G$ and that $g(\psi)$ is also univalent in the same domain.

Then, as shown by Boas and Buck, (2. 2) is convergent for $\psi$ inside the greatest open disk contained in $G$. In this case $G$ is the unit circle and (2. 2) is convergent in the open disk: $|\psi| < 1$.

The explicit representation of the polynomial $p_n(t)$ is

$$p_n(t) = \sum_{j=0}^{n} \frac{t^j}{j!} B_{j,n} \tag{2.5}$$

with

$$B_{j,n} = \sum a_{k_0} g_{k_1} g_{k_2} \cdots g_{k_j}, \tag{2.6}$$

where the summation extends over all sets of $j + 1$ nonnegative integers $k$ such that $k_0 + k_1 + \cdots + k_j = n$.

Since $g(z)$ is regular, $g'(z)$ is also regular and $g'(z) \neq 0$ since the derivative of an univalent function does not vanish. Therefore if we choose $A(z) = g'^{1/2}(z)$ with the positive branch, $A(z)$ is regular if $|z| < 1$, and $1/A(z)$ is bounded in the same domain. Let $\zeta = g(z) = g(\psi(\zeta))$ be the inverse mapping function of $G'$ upon $G$; we can for simplicity choose $\zeta = 0$ to correspond to $z = 0$. Therefore

$$e^{t\zeta} = e^{tg(\psi)} = \sum_{n=0}^{\infty} \psi^n(\zeta)\psi'^{1/2}(\zeta)p_n(t). \tag{2.7}$$

Substituting (2. 7) into (2. 1), we obtain

$$N(t) = \sum_{\nu=0}^{\infty} \sum_{n=0}^{\infty} p_n(t)[\psi^\nu(H)\psi'^{1/2}(H)N(0)] \frac{1}{2\pi} \times \int_{C'} \overline{\psi}^\nu(\zeta)\overline{\psi}'^{1/2}(\zeta)\psi^n(\zeta)\psi'^{1/2}(\zeta)\, |d\zeta|, \tag{2.8}$$

i.e., because of (2. 2),

$$N(t) = \sum_{n=0}^{\infty} p_n(t)[\psi^n(H)\psi'^{1/2}(H)N(0)]. \tag{2.9}$$

If $g(0) \neq 0$,

$$N(t) = e^{tg(0)} \sum_{n=0}^{\infty} p_n(t)[\psi^n(H)\psi'^{1/2}(H)N(0)]. \tag{2.10}$$

Let us select as an example $z = \psi(\zeta) = (a\zeta + b)/(c\zeta + d)$, the conformal representation of a circle $G'$ upon the unit circle $G$. We have

$$\frac{d\psi}{d\zeta} = \frac{\Delta}{(c\zeta + d)^2} \text{ with } \Delta = ad - bc.$$

Therefore

$$\zeta = g(\psi) = \frac{d\psi - b}{a - c\psi} \text{ and } A(\psi) = \left(\frac{dg}{d\psi}\right)^{1/2} = \frac{\sqrt{\Delta}}{a - c\psi}. \tag{2.11}$$

We have the following identities:

$$a_n = \frac{\sqrt{\Delta}}{a}\left(\frac{c}{a}\right)^n, \quad g_n = \frac{\Delta}{ac}\left(\frac{c}{a}\right)^n \tag{2.12}$$

$$B_{j,n} = \sum a_{k_0} g_{k_1} g_{k_2} \cdots g_{k_j} = \frac{\sqrt{\Delta}}{a}\left(\frac{\Delta}{ac}\right)^j \left(\frac{c}{a}\right)^n P(n, j) \tag{2.13}$$

$$\text{with } P(n, j) = \binom{n}{j}. \tag{2.14}$$

Therefore

$$p_n(t) = \sum_{j=0}^{n} \frac{t^j}{j!}\left(\frac{\Delta}{ac}\right)^j P(n, j)\left(\frac{c}{a}\right)^n \frac{\sqrt{\Delta}}{a}, \tag{2.15}$$

i.e.,

$$N(t) = \frac{\Delta}{ac} e^{-\frac{b}{a}t} \sum_{n=0}^{\infty} \left[\left(H + \frac{b}{a}\right)^n \left(H + \frac{d}{c}\right)^{-(n+1)} N(0)\right] \times L_n\left(-\frac{\Delta}{ac}t\right) \tag{2.16}$$

or

$$N(t) = \frac{\Delta}{ac} e^{-\frac{b}{a}t} \sum_{n=0}^{\infty} A_n L_n\left(-\frac{\Delta}{ac}t\right), \tag{2.17}$$

where $L_n(x)$ is the Laguerre polynomial of order zero and

$$A_n = (H + b/a)^n (H + d/c)^{-(n+1)} N(0) \tag{2.18}$$

i.e.,

$$(H + d/c)A_n = (H + b/a)A_{n-1},$$
$$(H + d/c)A_0 = N(0). \tag{2.19}$$

It would have been easier, of course, to use the generating function for the Laguerre polynomials

$$(1-\psi)^{-(1+\lambda)}\, e^{t(\psi/\psi-1)} = \sum_{n=0}^{\infty} L_n^{(\lambda)}(t)\psi^n, \quad L_n^{(0)}(t) \equiv L_n(t); \tag{2.20}$$

but we have given this example to show all details of calculation by the general method.

If $c \to 0$, we have

$$N(t) = e^{-(b/a)t} \sum_{n=0}^{\infty} \left(H + \frac{b}{a}\right)^n N(0)\, \frac{t^n}{n!}, \tag{2.21}$$

which is the Neuman series solution of the Cauchy problem.

The use of (2.17) and the study of its convergence, as well as the choice of $b/a$ and $d/c$ have been done previously.[8]

### B. Use of Polynomials Orthogonal on a Family $C_r$

Let us use the solution (I. 3. 16) with a Bergman kernel associated with

$$d\mu_z = w(z)d\Sigma(z) \tag{2.22}$$

where $w(z)$ is a positive function

We furnish the domain $G$ with a slit which obviously does not affect (I. 3. 16) because it is of zero measure. However, this is necessary if we wish to use the conformal mapping of $G$ (with a slit) on the annulus $G''$. With the notation of Fig. 1,

$$\begin{aligned} N(t) &= \int_G w(z)\overline{M(z,H)}N(0)e^{zt}\, d\Sigma(z) \\ &= \int_{G''} w(z)\overline{M(z,H)}N(0)e^{zt}\left|\frac{dz}{du}\right|^2 dS(u) \\ &= \int_1^{\rho} dr \int_{|u|=r} w(z)e^{zt}\left|\frac{dz}{du}\right|^2 \overline{M(z,H)}N(0)\,|du|. \end{aligned} \tag{2.23}$$

We expand $M(z, \zeta)$ in terms of complete set of polynomials $P_n(z)$ orthonormal in $G$ relativity to the weight function $w(z)$, i.e.,

$$\int_G P_n(z)\overline{P_m(z)}w(z)d\Sigma(z) = \delta_n^m. \tag{2.24}$$

Let us assume also that the polynomials $P_n(z)$ are also orthogonal on every line $C_r$ defined in Sec. 1C.

Then

$$N(t) = \sum_{n=0}^{\infty} P_n(H)N(0) \int_1^{\rho} dr \int_{z\in C_r} w(z)e^{zt}\left|\frac{dz}{du}\right| \overline{P_n(z)}\,|dz|. \tag{2.25}$$

Since $e^{zt}$ is $L_2(G)$ for a given $t$, $z \in G$, the development

$$e^{zt} = \sum_{n=0}^{\infty} f_n(t)P_n(z) \tag{2.26}$$

is uniformly convergent. The evaluation of $f_n(t)$ may however not be easy.

We define

$$\int_{z\in C_r} e^{zt}\overline{P_n(z)}\left|\frac{dz}{du}\right| w(z)|\,dz| = f_n(r, t) \tag{2.27}$$

and

$$F_n(r) = \int_{|u|=r} w(z)\left|\frac{dz}{du}\right|^2 |P_n(z)|^2\cdot|du|. \tag{2.28}$$

The normalization (2.24) gives $\int_1^{\rho} F_n(r)dr = 1$. Substitution of (2.26) into (2.27) gives $f_n(r, t) = f_n(t)F_n(r)$ and substitution into (2.25) gives

$$\begin{aligned} N(t) &= \sum_{n=0}^{\infty} P_n(H)N(0)f_n(t) \int_1^{\rho} F_n(r)dr \\ &= \sum_{n=0}^{\infty} P_n(H)N(0)f_n(t). \end{aligned} \tag{2.29}$$

Therefore,

$$\begin{aligned} f_n(t) = \int_{z\in C_r} e^{zt}\overline{P_n(z)}\left|\frac{dz}{du}\right| w(z)|\,dz| \Big/ \\ \times \int_{z\in C_r} |P_n(z)|^2\left|\frac{dz}{du}\right| w(z)\cdot|\,dz|. \end{aligned} \tag{2.30}$$

Since $f_n(t)$ is independent of $r$, otherwise the development (2.26) of $e^{zt}$ would not be unique, we can evaluate (2.30) on a particular line $C_{r0}$ where the integrations are easy to perform.

*Example 1:* G is the interior of an ellipse with real foci.

Let us assume that the spectrum of $H$ lies in an ellipse $G$ whose foci are $-\lambda_1$ and $-\lambda_2$ (real numbers, with $H$ either a bounded self-adjoint operator or a normal compact operator (See I, Sec. 3B). As a particular case we have of course the real interval $(-\lambda_1, -\lambda_2)$. Let

$$u = (2z + \lambda_1 + \lambda_2)/(\lambda_2 - \lambda_1), \quad \tau = [(\lambda_2 - \lambda_1)/2]t$$

and therefore $zt = u\tau - [(\lambda_1 + \lambda_2)/(\lambda_2 - \lambda_1)]\tau$ whenever $z \in [-\lambda_1, -\lambda_2]$, $u \in [-1, 1]$.

We shall use an expansion formula given by Erdelyi,[9]

$$\begin{aligned} \phi(a, c, u\tau) = \sum_{n=0}^{\infty} \frac{(g)_n}{(g+n)_n}\, \frac{1}{n!}\, {}_2F_1(-n, g+n, c, u) \\ \times \phi(a+n, g+2n+1, \tau), \end{aligned} \tag{2.31}$$

where $g$ is an arbitrary real number, and $\phi$ the confluent hypergeometric function.

Since $\phi(a, a, u\tau) = e^{u\tau}$, we obtain after some transformations

$$\begin{aligned} e^{u\tau} = \sum_{n=0}^{\infty} \frac{\Gamma(n+\alpha+\beta+1)}{\Gamma(2n+\alpha+\beta+1)}\, P_n^{(\alpha,\beta)}(1-2u)(-\tau)^n \\ \times \phi(n+\alpha+1, 2n+\alpha+\beta+2, \tau), \end{aligned} \tag{2.32}$$

where $\alpha = a - 1$ and $\beta = g - a$ are arbitrary real numbers ($\alpha, \beta > -1$) and $P_n^{(\alpha,\beta)}(1-2u)$ is a Jacobi polynomial. We let $C_r$ be the ellipses confocal with $(-1, 1)$ in the $u$ plane.

We have $e^{u\tau} = e^{\tau}e^{-2\tau(1-u)/2}$ and

$$\begin{aligned} e^{u\tau} = e^{\tau} \sum_{n=0}^{\infty} \frac{\Gamma(n+\alpha+\beta+1)}{\Gamma(2n+\alpha+\beta+1)}\, P_n^{(\alpha,\beta)}(u)(2\tau)^n \\ \times \phi(n+\alpha+1, 2n+\alpha+\beta+2, -2\tau). \end{aligned} \tag{2.33}$$

The normalization is given by

$$\begin{aligned} &\int_{-1}^{1} |P_n^{(\alpha,\beta)}(u)|^2(1-u)^{\alpha}(1+u)^{\beta}\, du = h_n^{(\alpha,\beta)} \\ &= \frac{\Gamma(n+\alpha+1)\,\Gamma(n+\beta+1)}{\Gamma(2n+\alpha+\beta+2)}\, \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1} \end{aligned} \tag{2.34}$$

and

$$P_n(u) = \frac{P_n^{(\alpha,\beta)}(u)}{\sqrt{h_n^{(\alpha,\beta)}}}\ .$$

We can choose as level line $C_{r0}$ the segment $(-1, 1)$ and we have necessarily $\alpha, \beta = \pm\, 1/2$ in order to have

orthogonality on every ellipse $C_r$, with foci $(-1, 1)$, by virtue of Sec. 1C.

Consequently,

$$N(t) = e^{-\lambda_1 t} \sum_{n=0}^{\infty} \frac{\Gamma(n+\alpha+\beta+1)}{\Gamma(2n+\alpha+\beta+1)} \times \phi(n+\alpha+1, 2n+\alpha+\beta+2, (\lambda_1-\lambda_2)t) \times [(\lambda_1-\lambda_2)t]^n P_n^{(\alpha,\beta)}\left(\frac{2H}{\lambda_2-\lambda_1} + \frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}\right) N(0). \quad (2.35)$$

Using Kummer equation $\phi(a, c, x) = e^x \phi(c-a, c, -x)$, we have the alternate representation

$$N(t) = e^{-\lambda_2 t} \sum_{n=0}^{\infty} \frac{\Gamma(n+\alpha+\beta+1)}{\Gamma(2n+\alpha+\beta+1)} \times \phi(n+\beta+1, 2n+\alpha+\beta+2, (\lambda_2-\lambda_1)t) \times [(\lambda_2-\lambda_1)t]^n P_n^{(\alpha,\beta)}\left(\frac{2H}{\lambda_2-\lambda_1} + \frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}\right) N(0). \quad (2.35')$$

It must be recalled that the best choice for $\alpha, \beta$ should be dictated by the best approximation of $|1-u|^\alpha |1+u|^\beta$ to the "eigenvalue distribution", as described in Sec. 3B3 (Paper I). We can now give the explicit forms to the solution for $\alpha, \beta = \pm \frac{1}{2}$.

From

$$I_n(x) = \left(\frac{x}{2}\right)\left(\frac{1}{n!}\right) e^{-x} \phi(n+\tfrac{1}{2}, 2n+1, 2x),$$

the modified Bessel function of the first kind

$$T_n(x) = \frac{n!^2}{(2n)!} 2^{2n} P_n^{(-1/2,-1/2)}(x),$$

the Tchebycheff polynomial of the first kind

$$U_n(x) = \frac{(n+1)!^2}{(2n+1)!} 2^{2n+1} P_n^{(1/2,1/2)}(x),$$

the Tchebycheff polynomial of the second kind,

we obtain

$$N(t) = 2 \sum_{n=0}^{\infty} T_n\left(\frac{2H}{\lambda_2-\lambda_1} + \frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}\right) N(0) \times I_n\left(\frac{\lambda_1-\lambda_2}{2} t\right) e^{-(\lambda_1+\lambda_2)t/2}, \quad \alpha, \beta = -\tfrac{1}{2} \quad (2.36)$$

or

$$N(t) = \sum_{n=0}^{\infty} U_n\left(\frac{2H}{\lambda_2-\lambda_1} + \frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}\right) N(0) \times \frac{I_n[\frac{1}{2}(\lambda_1-\lambda_2)t]}{(n+1)t} e^{-(\lambda_1+\lambda_2)t/2}, \quad \alpha, \beta = +\tfrac{1}{2}. \quad (2.37)$$

The mixed case does not involve particular special functions. Although formulas (2.35) or (2.35′) are valid for $\alpha, \beta = \pm \frac{1}{2}$ when $G$ is an ellipse, they are valid for all values of $\alpha$ and $\beta$ when spectrum is real and contained in the interval $(-1, 1)$ because Jacobi polynomials are orthogonal on this interval. The problem of the validity of (2.35) outside $(-1, 1)$ for arbitrary values of $\alpha$ and $\beta$ will be examined later.

The important point that should be stressed is that (2.35) yields a practical algorithm because of the recurrence relation for the orthogonal polynomials $P_n^{(\alpha,\beta)}(z)$. Although there is no general recurrence relation available for orthogonal polynomials *in the complex plane*, we can use, of course, the recurrence relation for the classical orthogonal polynomials when they happen to be also orthogonal in a complex domain.

In this case,

$$N(t) = e^{-\lambda_1 t} \sum_{n=0}^{\infty} \frac{\Gamma(n+\alpha+\beta+1)}{\Gamma(2n+\alpha+\beta+1)} [(\lambda_2-\lambda_1)t]^n \times \phi(n+\alpha+1, 2n+\alpha+\beta+2, (\lambda_1-\lambda_2)t) A_n \quad (2.38)$$

with

$$A_n = \frac{(2n+\alpha+\beta+1)(2n+\alpha+\beta)}{2n(n+\alpha+\beta)} \times \left(\frac{2}{\lambda_2-\lambda_1} H + \frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}\right) A_{n-1} + \frac{(2n+\alpha+\beta-1)(\alpha^2-\beta^2)}{2n(n+\alpha+\beta)(2n+\alpha+\beta-2)} A_{n-1} - \frac{(n+\alpha-1)(n+\beta+1)(2n+\alpha+\beta)}{n(n+\alpha+\beta)(2n+\alpha+\beta-2)} A_{n-2}, \quad n > 1, \quad (2.39)$$

$$A_0 = N(0), \quad A_1 = \tfrac{1}{2}(\alpha+\beta-2) \times \left(\frac{2}{\lambda_2-\lambda_1} H + \frac{\lambda_1+\lambda_2}{\lambda_2-\lambda_1}\right) N(0) + \tfrac{1}{2}(\alpha-\beta) N(0).$$

The fact that the $A_n$ can be generated recursively is of great importance as well as the fact that $N(t)$ can be evaluated numerically for definite values of $t$ without the usual necessity of taking small time steps to evaluate $N(t)$ for all previous values of $t$.

It should be remarked that the confluent hypergeometric function can itself be computed by means of a recurrence relation although it may not be the best method from the point of view of roundoff.[10]

It might be suggested by (2.31) that Eq. (2.35) has a general validity independently of the value of $\alpha, \beta$.

This can be easily shown by means of the classical expansion formula[11]:

$$\frac{1}{q-u} = \sum_{n=0}^{\infty} \frac{2}{h_n^{(\alpha,\beta)}} (q+1)^\beta (q-1)^\alpha P_n^{(\alpha,\beta)}(u) Q_n^{(\alpha,\beta)}(q) \quad (2.40)$$

valid for $\alpha, \beta > -1$, where $u$ lies inside and $q$ outside an ellipse with foci at $\pm 1$.

From

$$2(q+1)^\beta (q-1)^\alpha Q_n^{(\alpha,\beta)}(q) = \int_{-1}^{1} (1-s)^\alpha (1+s)^\beta \frac{P_n^{(\alpha,\beta)}(s)}{q-s} ds, \quad (2.41)$$

we obtain

$$\frac{1}{q-u} = \sum_{n=0}^{\infty} \frac{1}{h_n^{(\alpha,\beta)}} \times \int_{-1}^{1} \frac{(1-s)^\alpha (1+s)^\beta P_n^{(\alpha,\beta)}(s) P_n^{(\alpha,\beta)}(u) ds}{q-s}. \quad (2.42)$$

We define

$$u = \frac{2z+\lambda_1+\lambda_2}{\lambda_2-\lambda_1}, \quad s = \frac{2v+\lambda_1+\lambda_2}{\lambda_2-\lambda_1}, \quad q = \frac{2p+\lambda_1+\lambda_2}{\lambda_2-\lambda_1}. \quad (2.43)$$

Therefore

$$\frac{1}{p-z}=\sum_{n=0}^{\infty}\frac{1}{h_n}\left[\frac{2}{\lambda_2-\lambda_1}\right]^{\alpha+\beta+1}\int_{-\lambda_2}^{-\lambda_1}\frac{(\lambda_1+v)^{\alpha}(\lambda_2+v)^{\beta}}{p-v}\times P_n^{(\alpha,\beta)}\left(\frac{2z+\lambda_1+\lambda_2}{\lambda_2-\lambda_1}\right)P_n^{(\alpha,\beta)}\left(\frac{2v+\lambda_1+\lambda_2}{\lambda_2-\lambda_1}\right)dv \tag{2.44}$$

is an expansion valid for $p$ outside, and $z$ inside an ellipse of foci $(\lambda_1,\lambda_2)$ which yields after integrating on a Bromwich contour enclosing the ellipse

$$e^{zt}=\frac{2^{\alpha+\beta+1}}{(\lambda_1-\lambda_2)^{\alpha+\beta+1}}\sum_{n=0}^{\infty}\frac{1}{h_n}\int_{\lambda_2}^{\lambda_1}(\lambda_1-v)^{\alpha}(v-\lambda_2)^{\beta}\times e^{-vt}P_n^{(\alpha,\beta)}\left(\frac{2v-\lambda_1-\lambda_2}{\lambda_1-\lambda_2}\right)P_n^{(\alpha,\beta)}\left(\frac{2z-\lambda_1-\lambda_2}{\lambda_1-\lambda_2}\right)dv \tag{2.45}$$

valid for $z$ in an ellipse with foci at $(-\lambda_1,-\lambda_2)$. Using the reproducing property for the analytic function $P_n^{(\alpha,\beta)}\left(\frac{2v-\lambda_1-\lambda_2}{\lambda_1-\lambda_2}\right)\in L_2(G)$, we obtain finally, after substitution of (2.45) into (2.23),

$$N(t)=\int_{\lambda_2}^{\lambda_1}\frac{2^{\alpha+\beta+1}}{(\lambda_1-\lambda_2)^{\alpha+\beta+1}}\sum_{n=0}^{\infty}\frac{e^{-vt}}{h_n}(\lambda_1-v)^{\alpha}(v-\lambda_2)^{\beta}\times P_n^{(\alpha,\beta)}\left(\frac{2v-\lambda_1-\lambda_2}{\lambda_1-\lambda_2}\right)P_n^{(\alpha,\beta)}\left(\frac{2H-\lambda_1-\lambda_2}{\lambda_1-\lambda_2}\right)N(0)dv. \tag{2.46}$$

We have therefore an alternate description of (I. 3. 34) and it can be shown by means of the integral representation of the hypergeometric function that they are fully equivalent. Although (2. 46) is valid for values of $\alpha,\beta>-1$, *we have lost one important property: When the development is truncated, it is no more optimum in the sense of Sec. 3.* Therefore the convergent properties may be affected and the accuracy may be lower.

*Example 2:* The ellipse of Example 1 degenerates into a parabola.

It does not mean, however, that the spectrum of $H$ fills the parabola: Assumptions of example 1 are unchanged. We take the limit of (2. 46) for $\lambda_2\to\infty$: The ellipse degenerates into a parabola.

$$N(t)=\lim_{\lambda_2\to\infty}\int_{\lambda_2}^{\lambda_1}\frac{1}{\lambda_2^{\alpha+1}}\frac{2^{\alpha+\beta+1}}{(\lambda_1/\lambda_2-1)^{\alpha+\beta+1}}\times(\lambda_1-v)^{\alpha}\left(\frac{v}{\lambda_2}-1\right)^{\beta}e^{-vt}\times\sum_n\frac{1}{h_n}P_n^{(\alpha,\beta)}\left(\frac{[(2v-\lambda_1)/\lambda_2]-1}{\lambda_1/(\lambda_2-1)}\right)P_n^{(\alpha,\beta)}\times\left(\frac{[(2H+\lambda_1)\lambda_2]+1}{(1-\lambda_1)\lambda_2}\right)N(0)dv. \tag{2.47}$$

Let us take $\beta/\lambda_2=\gamma$. If $\beta<\infty$, the limit of $N(t)$ is undefined. We shall assume that $\beta\to\infty$ with $\gamma$ a fixed positive number.

Since

$$\lim_{z\to\infty}\left[\frac{\Gamma(z+\alpha)}{\Gamma(z)}-z^{\alpha}\right]=0, \tag{2.48}$$

$$\lim_{\beta\to\infty}\frac{2^{\alpha+\beta+1}}{\lambda_2^{\alpha+1}h_n}=\frac{\Gamma(n+1)}{\Gamma(n+\alpha+1)}\gamma^{\alpha+1}, \tag{2.49}$$

we have also

$$\lim_{\beta\to\infty}P_n^{(\alpha,\beta)}[1-(2x/\beta)]=L_n^{(\alpha)}(x). \tag{2.50}$$

Therefore

$$\lim_{\beta\to\infty}P_n^{(\alpha,\beta)}\left(\frac{1-[(2v-\lambda_1)\gamma/\beta]}{1-(\lambda_1\gamma/\beta)}\right)P_n^{(\alpha,\beta)}\times\left(\frac{1+[(2H+\lambda_1)\gamma/\beta]}{1-(\lambda_1\gamma/\beta)}\right)=L_n^{(\alpha)}((v-\lambda_1)\gamma)\cdot L_n^{(\alpha)}(-(H+\lambda_1)\gamma) \tag{2.51}$$

and

$$\lim_{\beta\to\infty}\frac{[(v/\lambda_2)-1]^{\beta}}{[(\lambda_1/\lambda_2)-1]^{\alpha+\beta+1}}=(-1)^{\alpha+1}e^{\gamma(\lambda_1-v)}. \tag{2.52}$$

Since

$$N(t)=\int_{\infty}^{\lambda_1}\lim_{\beta\to\infty}\sum_{n=0}^{\infty}\left(\frac{\gamma}{\beta}\right)^{\alpha+1}(-1)^{\alpha+1}e^{\gamma(\lambda_1-v)-vt}\times\frac{\Gamma(n+1)(2n+\alpha+\beta+1)}{\Gamma(n+\alpha+1)(n+\beta+1)^{-\alpha}}\times(\lambda_1-v)^{\alpha}L_n^{(\alpha)}(\gamma(v-\lambda_1))\cdot L_n^{(\alpha)}(-(H+\lambda_1)\gamma)Ndv, \tag{2.53}$$

$$\int_0^{\infty}s^{\alpha}L_n^{(\alpha)}(s)e^{-ps}ds=\frac{\Gamma(\alpha+n+1)}{\Gamma(n+1)}\frac{(p-1)^n}{p^{\alpha+n+1}},\qquad \mathrm{Re}\alpha>-1,\ \mathrm{Re}p>0, \tag{2.54}$$

we have

$$N(t)=\gamma^{\alpha+1}e^{-\lambda_1 t}\sum_{n=0}^{\infty}\frac{t^n}{(t+\gamma)^{n+\alpha+1}}L_n^{(\alpha)}(-\gamma(H+\lambda_1))N(0), \tag{2.55}$$

which be obtained also formally from the generating function for Laguerre polynomials. The recurrence relations are given by

$$N(t)=\gamma^{\alpha+1}e^{-\lambda_1 t}\sum_{n=0}^{\infty}\frac{t^n}{(t+\gamma)^{n+\alpha+1}}A_n, \tag{2.56}$$

$$(n+1)A_{n+1}=(2n+\alpha+1)A_n+\gamma(H+\lambda_1)A_n-(n+\alpha)A_{n-1},\qquad n\geq 1,$$
$$A_1=(\alpha+1)A_0+\gamma(H+\lambda_1)A_0,$$
$$A_0=N(0). \tag{2.57}$$

It should be remarked that if the order of truncation is fixed beforehand, the sum (2. 55) may be evaluated "in reverse" by a nested procedure, which is stable for roundoff.[10]

### C. Finite Orthogonal Polynomials on a Real Interval $C$

When the operator is bounded and Hermitian, with its spectrum on a finite segment $R(m,M)$ of the real axis, we can write the resolvent operator, using (I. 2. 18) and (I. 3. 18 )

$$R_p(H)=\sum_{\nu}\phi_{\nu}(H)\int_G\frac{\overline{\phi_{\nu}}(z)}{p-z}\,d\mu_z^G,\quad p\notin G, \tag{2.58}$$

where $G$ is a bounded domain with the real interval $R(m, M)$ in its interior. As shown in Sec. 3B3 (Paper I), if the operator is compact,

$$d\mu_\lambda^R = \sum_k |\sigma_k|^2 \delta(\lambda - \lambda_k)\, d\omega_\lambda, \tag{I. 3. 58}$$

we may select $G \supset \bar{R}$ and choose $d\mu_\lambda^G$ as close as possible to $d\mu_\lambda^R$. We shall therefore write for the *approximate* resolvent operator in this case, Eq. (2. 58) with

$$d\mu_z^G = \sum_{k=1}^N \alpha_k\, \delta(z - a_k)|dz|, \tag{2. 59}$$

where we have substituted the one-dimensional measure, $\delta(z - a_k)$ being the usual Dirac function [and not the two-dimensional definition as in (I. 3. 58)]. The $a_k$ are approximations of the $\lambda_k$ and the $\alpha_k$ of the $|\sigma_k|^2$. However, in general, we shall write

$$\tilde{R}_p(H) = \sum_\nu \hat{\phi}_\nu(H) \int_{\bar{R}} \frac{\overline{\hat{\phi}_\nu(z)}}{p - z}\, d\mu_z, \tag{2. 60}$$

where $d\mu_z$ is a one-dimensional measure approximating $d\mu_\lambda^R = \langle N, d\mathcal{E}_\lambda N\rangle$ (see I. 3. 33) and where the integral is a line integral along the real segment $R$.

If we define the moments $c_n = \int_R z^n\, d\mu_z$ and $p_{kn}$ the $k$th zero of the orthogonal polynomials $\hat{\phi}_n(z)$ associated with $d\mu_z$, i.e., $\int_R \hat{\phi}_n(z)\overline{\hat{\phi}_m}(z) d\mu_z = \delta_n^m$, we have from the general theory of orthogonal polynomials[11]:

$$\int_R \frac{d\mu_z}{p - z} = \lim_{N\to\infty} \frac{C_0^2}{(C_0 C_1 - C_2^2)^{1/2}} \frac{R_N(p)}{S_N(p)} = \lim_{N\to\infty} \sum_{k=1}^N \frac{\beta_{kN}}{p - p_{kN}}.$$

However, for the particular choice $d\mu_z \equiv d\mu_z^G$, the set of orthogonal polynomials is finite and $\alpha_k = \beta_{kN}$, $a_k = p_{kN}$ where $\beta_{kN}$ are the Christoffel numbers.

The orthogonality relation is

$$\sum_{k=1}^N \alpha_k \hat{\phi}_p\ (a_k)\hat{\phi}_q(a_k) = \delta_q^p. \tag{2. 61}$$

A second "orthogonality" relation derived from the Christoffel–Darboux equation

$$\sum_{i=0}^N \hat{\phi}_i(z)\hat{\phi}_i(p) = \frac{k_N}{k_{N+1}} \frac{\hat{\phi}_{N+1}(z)\hat{\phi}_N(p) - \hat{\phi}_{N+1}(p)\hat{\phi}_N(p)}{z - p} \tag{2. 62}$$

gives

$$\sum_{i=0}^N \hat{\phi}_i(a_k)\hat{\phi}_i(a_l) = \frac{\delta_l^k}{\beta_{kN}}, \tag{2. 63}$$

which is a finite closure relation.

Obviously, only the numbers $\phi_i(a_k)$, $i = 0, 1, 2, \ldots, N$, $k = 1, 2, \ldots, N$ are needed to evaluate (2. 58). They are obtained from the three-term recurrence

$$\hat{\phi}_n(a_k) = (A_n a_k + B_n)\hat{\phi}_{n-1}(a_k) - C_n \hat{\phi}_{n-2}(a_k), \tag{2. 64}$$

and the orthogonality relation (2. 61) yields

$$\frac{B_n}{A_n} = -\sum_{k=1}^N \alpha_k a_k \hat{\phi}_{n-1}^2(a_k),$$

$$\frac{C_n}{A_n} = -\sum_{k=1}^N \alpha_k a_k \hat{\phi}_{n-1}(a_k)\hat{\phi}_{n-2}(a_k), \tag{2. 65}$$

$$\frac{1}{A_n^2} = \sum_{k=1}^N \alpha_k a_k \left[\left(a_k + \frac{B_n}{A_n}\right)\hat{\phi}_{n-1}(a_k) - \frac{C_n}{A_n}\hat{\phi}_{n-2}(a_k)\right]\hat{\phi}_{n-1}(a_k).$$

Since $\phi_N(a_k) = 0$, the recurrence stops at $\nu = N$. Consequently, we obtain from (2. 60)

$$\tilde{R}_p(H)N(0) = \sum_{\nu=0}^N \hat{\phi}_\nu(H)N(0)\left(\hat{\phi}_\nu(p)\frac{\hat{\rho}_N(p)}{\hat{\phi}_N(p)} - \hat{\rho}_\nu(p)\right) \tag{2. 66}$$

with

$$\hat{\rho}_n(p) = \int_R \frac{\hat{\phi}_n(p) - \hat{\phi}_n(z)}{p - z}\, d\mu_z \tag{2. 67}$$

and

$$\frac{1}{2\pi j}\int e^{pt}\tilde{R}_p(H)N(0)dp = \sum_{\nu=0}^N \hat{\phi}_\nu(H)N(0)\sum_k e^{a_k t}\left(\frac{\hat{\phi}_\nu(a_k)\hat{\rho}_N(a_k)}{\hat{\phi}_N'(a_k)}\right) = \sum_{\nu=0}^N \hat{\phi}_\nu(H)N(0)\sum_k \beta_{kN} e^{a_k t}\hat{\phi}_\nu(a_k) \tag{2. 68}$$

because

$$\frac{\hat{\rho}_N(a_k)}{\hat{\phi}_N'(a_k)} = \int_C \frac{d\mu_z}{z - a_k}\frac{\hat{\phi}_N(z) - \hat{\phi}_N(a_k)}{\hat{\phi}_N'(a_k)} = \beta_{kN}. \tag{2. 69}$$

Equation (2. 68) is nothing but the result of a Gaussian quadrature, as could be foreseen.

In case the $\{a_k\} = \{a_1, \ldots, a_N\}$ is the spectrum of the Hermitian matrix $H$, the orthogonality relation gives the expected result,

$$N(t) = \sum_l \sigma_l \psi_l \sum_{\nu=0}^N \sum_k \hat{\phi}_\nu(a_l)\hat{\phi}_\nu(a_k)\beta_{kN} e^{a_k t} = \sum_l \sigma_l \psi_l e^{a_l t}, \tag{2. 70}$$

where

$$H\psi_l = a_l\psi_l \text{ and } \sigma_l = (\psi_l, N(0)).$$

### D. General Procedure for Real Intervals

The procedure to be followed in the case of a real spectrum is stated below.

1. Evaluate the gross behavior of the solution (say, exponential decay with a constant approximately known).

2. Select a nondecreasing function $\mu(z)$ such that $\int_C e^{zt} d\mu_z$ approximates as closely as possible the gross behavior of the solution.

3. (a) If $\mu(z)$ is continuous, and is the weight function of a classical orthogonal polynomial, the $\beta_k$ and $a_k$ are known and tabulated. Therefore we choose an origin and a scale such that the greatest $a_k$, i.e., $a_1$ which commands the asymptotic behavior, approximates as closely as possible the greatest eigenvalue. However, the others $a_k$ cannot in general coincide, not even approximately, with the eigenvalues. This is a disadvantage not shared by other methods (see Sec. 3B2, 3B3, Paper I). However a notable advantage is that Eq. (2. 68) can be written at once, the $\hat{\phi}_N(a_k)$ being computed by recurrence by means of (2. 64) the $\beta_{kN} \equiv \alpha_k$ and $a_k$ being known in advance. However

the order $N$ of approximation must be fixed beforehand and if $N$ is changed the whole work must be done again, a disadvantage not shared by other methods (see Sec. 3B3, Paper I and Sec. 1).

(b) If $\mu(z)$ is continuous, and is *not* the weight function of a classical orthogonal polynomial two different courses are open.

We proceed as in 3a) with the added difficulty that $\alpha_k$ and $a_k$ are not known in advance. The polynomials $\hat{\phi}_n(z)$ are generated by the customary recurrence relation and $\alpha_k$ and $a_k$ are obtained by their definition. Unless the work can be done once for all, this is not a practical method, because we have all the disadvantages of 3a) with none of its advantages.

We disregard the rational approximation (2.58) and use a quadrature formula for

$$N(t) = \sum_\nu \hat{\phi}_\nu(H)N(0) \int_R e^{zt}\, \hat{\phi}_\nu(z)d\mu_z$$

with prescribed abcissas. We loose accuracy by comparison to 3a) since the quadrature formula is no more Gaussian and will be correct to order $N$ instead of $2N$-1. The polynomials are generated by the customary recurrence relation. Any improvement of the accuracy needs a fresh start. However we can select the $a_k$ at will as close as possible to the point spectrum of $H$.

(c) If $d\mu_z = \sum_k \alpha_k \delta(z - a_k)|dz|$ which means that $\alpha_k \equiv \beta_{kN}$ and $a_k$ are given, we can proceed as in 3a) with one added advantage—each intermediate step is optimum.

4. If $\mu(z)$ is continuous and is (or is not) the weight function of an orthogonal polynomial, it may be possible in some cases to evaluate $\int_C e^{zt}\hat{\phi}_\nu(z)d\mu_z$ analytically. It is therefore unnecessary to use the rational approximation. This is the case studied in Sec. 2B.

## 3. CONVERGENCE OF THE SOLUTION

We known from (I. 3.41) and (I. 3.42) that for a Bergman kernel,

$$\|N(t) - \tilde{N}_n(t)\|^2 \le \int_G e^{2t\,\mathrm{Re}\eta}\, d\mu_\eta^G \int_G d\mu_z^G \times \int_R |M(z,\lambda) - M_n(z,\lambda)|^2 d\mu_\lambda^R. \quad (3.1)$$

It can be easily shown that a similar expression is obtained for Szegö kernel, where $C$ is an analytic curve, boundary of the bounded domain $G$,

$$\|N(t) - \tilde{N}_n(t)\|^2 \le \int_C e^{2t\,\mathrm{Re}\eta}\, d\mu_\eta^C \int_C d\mu_z^C \times \int_R |\hat{M}(z,\lambda) - \hat{M}_n(z,\lambda)|^2 d\mu_\lambda^R. \quad (3.2)$$

A general expression has been found[12] for the asymptotic expression of $\hat{M}(z,\lambda) - \hat{M}_n(z,\lambda)$ but it is not valid for Bergman kernels. Let us examine the particular choice of Sec. 1.1:

$$\hat{\phi}_\nu(z) = [h(z)]^\nu h'^{1/2}(z)(1/\sqrt{2\pi}) \quad (3.3)$$

with $d\mu_z^C = |dz|$, and $h(z)$ the mapping function of $G$ upon the unit circle.

Since

$$J_n = \int_C |dz| \int_R |\hat{M}(z,\lambda) - \hat{M}_n(z,\lambda)|^2 d\mu_\lambda^R,$$

we have

$$J_n = \int_R \sum_{\nu=n+1}^{\infty} |h(\lambda)|^{2\nu} |h'(\lambda)|\, \frac{1}{2\pi}\, d\mu_\lambda^R. \quad (3.4)$$

and

$$\|N(t) - \tilde{N}_n(t)\|^2 \le \int_C e^{2t\,\mathrm{Re}\eta}\, d\mu_\eta^C \times \int_R \frac{|h(\lambda)|^{2(n+1)}|h'(\lambda)|}{1 - |h(\lambda)|^2}\, \frac{d\mu_\lambda^R}{2\pi}. \quad (3.5)$$

Since by assumption every point of $\bar{R}$ is at some positive distance from $C$, $|h(\lambda)| < 1$, $\lambda \in R$, and the degree of approximation is geometric. We might let $C$ approach the boundary of $R$ provided the integrals (3.5) converge; however in this case the convergence may be less than geometric.

For the Bergman kernel

$$\phi_\nu(z) = \sqrt{(\nu+1)/\pi}\, h^\nu(z)h'(z) \quad (3.6)$$

with $d\mu_z^G = dw_z$ and

$$J_n = \int_G d\omega_z \int_R |M(z,\lambda) - M_n(z,\lambda)|^2 d\mu_z^R, \quad (3.7)$$

we have

$$= \int_R \sum_{\nu=n+1}^{\infty} |h(\lambda)|^{2\nu} |h'(\lambda)|^2\, \frac{\nu+1}{\pi}\, d\mu_\lambda^R, \quad (3.8)$$

$$\|N(t) - \tilde{N}_n(t)\|^2 \le \int_G e^{2t\,\mathrm{Re}\eta} d\mu_\eta^G \int_R \frac{|h(\lambda)|^{2(n+1)}|h'(\lambda)|^2}{1 - |h(\lambda)|^2} \times [(n+2) - (n+1)|h(\lambda)|^2]\, \frac{d\mu_\lambda^R}{\pi}. \quad (3.9)$$

It is easy to show that the error norm decreases monotonically with $n$.

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## APPENDIX: RELATIONS WITH THE CONJUGATE GRADIENT METHOD

We show below the relations between the reproducing kernel formalism and the conjugate gradient method.[10,12]

Although we have used the method of reproducing kernels for solving Cauchy problems, it can be used for equations of type

$$HN - k = 0, \quad (A1)$$

where $H$ is a nonsingular matrix operator. Using Bergman kernels we have

$$N = -R_0(H)k = \sum_\nu \phi_\nu(H)k \int_G \overline{\phi}_\nu(z)\, \frac{d\mu_z}{z}. \quad (A2)$$

However we cannot have recurrence relations for $\phi_\nu(H)k$, in general, because if $H$ is not self-adjoint, $G$ cannot be reduced to a real interval. Let us write $H^{-1} = T^{-1}TH^{-1}$, where $T$ is a given nonsingular matrix.

Obviously,

$$N = \sum_\nu \phi_\nu(T)TH^{-1}k \int_G \overline{\phi}_\nu(z)\, \frac{d\mu_z}{z}. \quad (A3)$$

We show now that if $T$ has a real spectrum, the recurrence relation will give a simple algorithm to solve (A1), provided $TH^{-1}$ does involve only nonnegative powers of $H$. If we assume only first power of $H$, at most

$$TH^{-1} = C + KH^*M,$$
$$T = CH + K(H^*MH) \tag{A4}$$

with $C, K, M$ arbitrary nonsingular matrix operators.

We let $M$ be Hermitian definite positive; $H^*MH$ is also Hermitian definite positive. We select the trivial solution $C = 0$ because a proper choice of $K$ and $M$ includes the case where $C \neq 0$.

We define $N = H^*$ and $T = KN$ where $K$ is a positive definite Hermitian operator.

However, although $T$ is not in general self conjugate, the spectrum of $T$ is real.

If we write

$$T - \lambda I = KN - \lambda I = K(N - \lambda K^{-1}) = (K - \lambda N^{-1})N, \tag{A5}$$

the spectrum of $T$ is the set of values for which $K - \lambda N^{-1}$ or $N - \lambda K^{-1}$ has no inverse. Since $N^{-1}$ and $K^{-1}$ are positive definite, the pencils $K - \lambda N^{-1}$ and $N - \lambda K^{-1}$ are *regular* and the spectrum is *real*. We can thus restrict $G$ to the real axis.

We shall now write the solution as

$$N = \sum_\nu \frac{\phi_\nu(T)(KH^*Mk)}{\int_G \bar{\phi}_\nu(z)\phi_\nu(z)\,d\mu_z} \int_G \bar{\phi}_\nu(z)\frac{d\mu_z}{z}, \tag{A6}$$

where the denominator is equal to one because of the normalization. The spectrum being real, $\bar{\phi}_\nu(z) = \phi_\nu(z)$.

Let $\lambda_s$ be the $s$th eigenvalue associated with the eigenvector $|\psi_s\rangle$ of $T \equiv KN$.

Let $|\varphi_s\rangle$ and $|\pi_s\rangle$ be the eigenvectors of $K - \lambda N^{-1}$ and $N - \lambda K^{-1}$, respectively,

$$(K - \lambda_s N^{-1})|\varphi_s\rangle = 0, \qquad (N - \lambda_s K^{-1})|\pi_s\rangle = 0. \tag{A7}$$

We have also

$$(KN - \lambda_s I)|\psi_s\rangle = 0. \tag{A8}$$

Therefore the orthogonality yields $\langle\varphi_r, N^{-1}\varphi_s\rangle = \delta_s^r$, i.e., because $|\varphi_s\rangle = N|\psi_s\rangle$,

$$\langle\psi_s|N\psi_r\rangle = \delta_s^r. \tag{A9}$$

Similarly

$$\langle\pi_r|K^{-1}\pi_s\rangle = \delta_s^r. \tag{A10}$$

Let $\psi_s^*$ be the eigenvectors of $T^* = (KN)^* = NK$. We have

$$(NK - \lambda_s I)|\psi_s^*\rangle = 0, \qquad (N - \lambda_s K^{-1})|\pi_s\rangle = 0. \tag{A11}$$

Therefore,

$$|\pi_s\rangle = K|\psi_s^*\rangle, \tag{A12}$$

$$\langle\pi_r|K^{-1}\pi_s\rangle = \langle K\psi_s^*|\psi_s^*\rangle = \delta_s^r. \tag{A13}$$

We define

$$|g_0\rangle = MH^*|k\rangle,$$
$$|p_0\rangle = K|g_0\rangle,$$
$$|p_\nu\rangle = \phi_\nu(T)|p_0\rangle,$$
$$|g_\nu\rangle = |g_{\nu-1}\rangle - a_{\nu-1}N|p_{\nu-1}\rangle,$$
$$a_\nu = \langle g_\nu|p_\nu\rangle/\langle p_\nu|Np_\nu\rangle.$$

Up to now, $\mu(z)$ has been arbitrary. We choose

$$\mu(z) = \sum_s \sigma_s^2 H(z - \lambda_s). \tag{A14}$$

We have

$$\langle p_\nu|Np_\mu\rangle = \delta_\mu^\nu. \tag{A15}$$

Indeed,

$$\langle\phi_\mu(T)p_0|N\phi_\nu(T)p_0\rangle. \tag{A16}$$

can be computed if we develop

$$|p_0\rangle = K|g_0\rangle = KMH^*|k\rangle = \sum_s \sigma_s\psi_s \tag{A17}$$

$$\sum_r\sum_s \phi_\mu(\lambda_s)\phi_\nu(\lambda_r)\langle\psi_s|N\psi_r\rangle\sigma_s\sigma_r = \sum_s \phi_\mu(\lambda_s)\phi_\nu(\lambda_s)\sigma_s^2. \tag{A18}$$

The orthogonality relation yields

$$\sum_s \sigma_s^2\phi_\mu(\lambda_s)\phi_\mu(\lambda_s) = \delta_\nu^\mu, \tag{A19}$$

Therefore

$$\langle p_\mu|Np_\nu\rangle = \delta_\nu^\mu. \tag{A20}$$

The solution can be written as

$$N = \sum_\nu [\phi_\nu(T)|p_0\rangle/\langle p_\nu|Np_\nu\rangle] \sum_s \sigma_s^2\,\phi_\nu(\lambda_s)/\lambda_s. \tag{A21}$$

From (A14) and (A20), we obtain

$$\langle p_\nu|g_\nu\rangle = \langle p_\nu|g_{\nu-1}\rangle - a_\nu\langle p_\nu|Np_{\nu-1}\rangle = \langle p_\nu|g_{\nu-1}\rangle, \tag{A22}$$

Therefore

$$\langle p_\nu|g_\nu\rangle = \langle p_\nu|g_0\rangle \quad \text{and} \quad a_\nu = \langle p_\nu|Kp_0\rangle/\langle p_\nu|Np_\nu\rangle. \tag{A23}$$

We evaluate

$$\begin{aligned}\sum_s \sigma_s^2\,\phi_\nu(\lambda_s)/\lambda_s &= \sum_r\sum_s \langle[\phi_\nu(\lambda_s)/\lambda_s]\sigma_s\psi_s|N\sigma_r\psi_r\rangle \\ &= \langle\phi_\nu(T)T^{-1}p_0|Np_0\rangle = \langle T^{-1}\phi_\nu(T)p_0|Np_0\rangle \\ &= \langle p_\nu|T^{-1*}Np_0\rangle = \langle p_\nu|K^{-1}p_0\rangle \\ &= \langle p_\nu|g_0\rangle = \langle p_\nu|g_\nu\rangle.\end{aligned} \tag{A24}$$

The solution is therefore

$$N = \sum_\nu a_\nu|p_\nu\rangle. \tag{A25}$$

One easily recognizes the formalism of the conjugate gradient method. We remark that it is not necessary to know $\mu(z)$, i.e., $\sigma_s^2$ and $\lambda_s$. Indeed the vectors $|p_\nu\rangle$ are generated by a three-term relation,

$$|p_{\nu+1}\rangle = T|p_\nu\rangle - \alpha_{\nu+1}|p_\nu\rangle - \beta_\nu|p_{\nu-1}\rangle. \tag{A26}$$

From (A15) we have

$$\begin{aligned}\alpha_{\nu+1} &= \langle p_\nu|NTp_\nu\rangle/\langle p_\nu|Np_\nu\rangle, \\ \beta_\nu &= \langle p_{\nu-1}|NTp_\nu\rangle/\langle p_{\nu-1}|Np_{\nu-1}\rangle.\end{aligned} \tag{A27}$$

The finite orthogonal polynomials $\phi_\nu(z)$ satisfy a three-term recurrence relation

$$\phi_{\nu+1}(z) = (1 + b_\nu)\phi_\nu(z) - a_\nu z\phi_\nu(z) - b_{\nu-1}\phi_{\nu-1}(z), \ \nu > 0,$$
$$\phi_1(z) = (1 + b_0)\phi_0(z) - a_0 z\phi_0(z). \quad \text{(A28)}$$

The coefficient can be found in the following manner:

$$\int_G \phi_\nu(z)\phi_{\nu+1}(z)d\mu_z = 1 + b_\nu - a_\nu \int_G z\,\phi_\nu^2(z)d\mu_z = 0,$$
$$\text{i.e.,} \quad a_\nu = (1 + b_\nu)/\left(\sum_s \sigma_s^2 \lambda_s \phi_\nu^2(\lambda_s)\right) \quad \text{(A29)}$$

$$\int_G \phi_{\nu+1}^2(z)d\mu_z = -a_\nu \int_G z\phi_{\nu+1}(z)d\mu_z = 1,$$
$$\text{i.e.,} \quad a_\nu = -\left(\sum_s \sigma_s^2 \lambda_s \phi_\nu(\lambda_s)\phi_{\nu+1}(\lambda_s)\right)^{-1} \quad \text{(A30)}$$

$$a_\nu \int_G z\phi_\nu(z)\phi_{\nu-1}(z)d\mu_z - b_{\nu-1} = 0,$$
$$\text{i.e.,} \quad a_\nu = -b_{\nu-1}/\left(\sum_s \sigma_s^2 \lambda_s \phi_\nu(\lambda_s)\phi_{\nu-1}(\lambda_s)\right). \quad \text{(A31)}$$

Moreover we have the following equalities:

$$\langle p_\mu | Np_\nu\rangle = \delta_\mu^\nu = \langle \phi_\mu(T)p_0 | N\phi_\nu(T)p_0\rangle,$$
$$p_{\nu+1} = (1 + b_\nu)p_\nu - a_\nu Tp_\nu - b_{\nu-1}p_{\nu-1},$$
$$\langle p_\nu | Np_{\nu+1}\rangle = 0 = 1 + b_\nu - a_\nu\langle p_\nu | NTp_\nu\rangle, \quad \text{(A32)}$$
$$\langle p_{\nu+1} | Np_{\nu+1}\rangle = 1 = -a_\iota\langle p_{\nu-1} | NTp_\nu\rangle,$$
$$\langle p_{\nu-1} | Np_{\nu+1}\rangle = 0 = -a_\nu\langle p_{\nu-1} | NTp_\nu\rangle - b_{\nu-1},$$

and finally

$$a_\nu = -b_{\nu-1}/\langle p_{\nu+1} | NTp_{\nu}\rangle,$$
$$1 + b_\nu = a_\nu\langle p_\nu | NTp_\nu\rangle,$$
$$a_\nu/a_{\nu-1} = b_{\nu-1}.$$


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# Representations of the Invariance Group for a Bloch Electron in a Magnetic Field*


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The invariance translation-operator group for the Hamiltonian of an electron in a periodic electric field and a uniform magnetic field is examined in the context of the theory of infinite-dimensional representations. It is shown that this group is of Type I if and only if the magnetic field has rational components relative to the lattice. The case of a nonrational field along a lattice vector direction is studied in detail. Here, the group is the direct product of a factor involving the translations along the field and a factor expressible as a semidirect product in a way that depends on the choice of basic lattice vector pair for the translations across the field. For each choice, Mackey's theory of induced representations is applied to obtain an infinite set of physical irreducible representations (based on both transitive and strictly ergodic measures); it is found that for different choices the sets are different unless the vector pairs are related in a simple way. The representation carried by the state space $L^2(R^3)$ is decomposed into a direct integral of primary representations, using Landau functions for a basis in $L^2(R^3)$. These primary representations are not of Type I, for it is shown explicitly that each has an infinite number of direct integral decompositions into irreducible representations, such that representations from any two decompositions are inequivalent. Here, different decompositions involve Landau functions for propagation along different lattice vector directions. The invariance translation-operator group for a system with a uniform magnetic field only is also discussed; it is of Type I, and its physical irreducible representations are given.


## I. INTRODUCTION

The invariance groups of the Hamiltonian for an electron moving in the periodic potential of a crystal and a uniform magnetic field have been a subject of investigation in a series of recent papers.[1-5] One of the main results of these investigations has been to show that the translational symmetries of the system lead to infinite invariance groups with a very special structure, critically dependent on the direction and magnitude of the field relative to the orientation and lattice parameters of the crystal. This was first shown in the papers by Brown[1] and Zak.[2] A complete classification of these groups in so far as translational symmetry is concerned is given in the paper by Opechowski and Tam,[4] together with a discussion on their irreducible representations. This has been extended to include symmetries other than translational by Tam.[5] At the same time it has become clear that the representations of these groups possess some features not usually found in applications to solid state physics, and it is the purpose of this paper to try to set them in the context of mathematical developments in the general theory of representations of infinite groups. In fact, it turns out that these features can be characterized very well in terms of some well-known mathematical results for groups that are not of Type I, whose definition we give later. In the process, several questions that have been raised on the properties of certain infinite-dimensional representations of the invariance groups can be answered.[6]

The system under discussion consists of a single nonrelativistic electron without spin subject simultaneously to a uniform magnetic field B and an electric potential $\mathcal{U}(\mathbf{r})$ with the periodicity of an infinite three-dimensional lattice; here r denotes the position vector of the electron. The Hamiltonian is

$$\mathcal{H} = -\frac{\hbar^2}{2m}\left(\nabla - \frac{ie}{\hbar c}\mathbf{A}(\mathbf{r})\right)^2 + \mathcal{U}(\mathbf{r}), \quad (1)$$

$$\phi_{\nu+1}(z) = (1 + b_\nu)\phi_\nu(z) - a_\nu z\phi_\nu(z) - b_{\nu-1}\phi_{\nu-1}(z), \ \nu > 0,$$
$$\phi_1(z) = (1 + b_0)\phi_0(z) - a_0 z\phi_0(z). \quad \text{(A28)}$$

The coefficient can be found in the following manner:

$$\int_G \phi_\nu(z)\phi_{\nu+1}(z)d\mu_z = 1 + b_\nu - a_\nu \int_G z\,\phi_\nu^2(z)d\mu_z = 0,$$
$$\text{i.e.,} \quad a_\nu = (1 + b_\nu)/\left(\sum_s \sigma_s^2 \lambda_s \phi_\nu^2(\lambda_s)\right) \quad \text{(A29)}$$

$$\int_G \phi_{\nu+1}^2(z)d\mu_z = -a_\nu \int_G z\phi_{\nu+1}(z)d\mu_z = 1,$$
$$\text{i.e.,} \quad a_\nu = -\left(\sum_s \sigma_s^2 \lambda_s \phi_\nu(\lambda_s)\phi_{\nu+1}(\lambda_s)\right)^{-1} \quad \text{(A30)}$$

$$a_\nu \int_G z\phi_\nu(z)\phi_{\nu-1}(z)d\mu_z - b_{\nu-1} = 0,$$
$$\text{i.e.,} \quad a_\nu = -b_{\nu-1}/\left(\sum_s \sigma_s^2 \lambda_s \phi_\nu(\lambda_s)\phi_{\nu-1}(\lambda_s)\right). \quad \text{(A31)}$$

Moreover we have the following equalities:

$$\langle p_\mu | Np_\nu\rangle = \delta_\mu^\nu = \langle \phi_\mu(T)p_0 | N\phi_\nu(T)p_0\rangle,$$
$$p_{\nu+1} = (1 + b_\nu)p_\nu - a_\nu Tp_\nu - b_{\nu-1}p_{\nu-1},$$
$$\langle p_\nu | Np_{\nu+1}\rangle = 0 = 1 + b_\nu - a_\nu\langle p_\nu | NTp_\nu\rangle, \quad \text{(A32)}$$
$$\langle p_{\nu+1} | Np_{\nu+1}\rangle = 1 = -a_\iota\langle p_{\nu-1} | NTp_\nu\rangle,$$
$$\langle p_{\nu-1} | Np_{\nu+1}\rangle = 0 = -a_\nu\langle p_{\nu-1} | NTp_\nu\rangle - b_{\nu-1},$$

and finally

$$a_\nu = -b_{\nu-1}/\langle p_{\nu+1} | NTp_{\nu}\rangle,$$
$$1 + b_\nu = a_\nu\langle p_\nu | NTp_\nu\rangle,$$
$$a_\nu/a_{\nu-1} = b_{\nu-1}.$$


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# Representations of the Invariance Group for a Bloch Electron in a Magnetic Field*


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The invariance translation-operator group for the Hamiltonian of an electron in a periodic electric field and a uniform magnetic field is examined in the context of the theory of infinite-dimensional representations. It is shown that this group is of Type I if and only if the magnetic field has rational components relative to the lattice. The case of a nonrational field along a lattice vector direction is studied in detail. Here, the group is the direct product of a factor involving the translations along the field and a factor expressible as a semidirect product in a way that depends on the choice of basic lattice vector pair for the translations across the field. For each choice, Mackey's theory of induced representations is applied to obtain an infinite set of physical irreducible representations (based on both transitive and strictly ergodic measures); it is found that for different choices the sets are different unless the vector pairs are related in a simple way. The representation carried by the state space $L^2(R^3)$ is decomposed into a direct integral of primary representations, using Landau functions for a basis in $L^2(R^3)$. These primary representations are not of Type I, for it is shown explicitly that each has an infinite number of direct integral decompositions into irreducible representations, such that representations from any two decompositions are inequivalent. Here, different decompositions involve Landau functions for propagation along different lattice vector directions. The invariance translation-operator group for a system with a uniform magnetic field only is also discussed; it is of Type I, and its physical irreducible representations are given.


## I. INTRODUCTION

The invariance groups of the Hamiltonian for an electron moving in the periodic potential of a crystal and a uniform magnetic field have been a subject of investigation in a series of recent papers.[1-5] One of the main results of these investigations has been to show that the translational symmetries of the system lead to infinite invariance groups with a very special structure, critically dependent on the direction and magnitude of the field relative to the orientation and lattice parameters of the crystal. This was first shown in the papers by Brown[1] and Zak.[2] A complete classification of these groups in so far as translational symmetry is concerned is given in the paper by Opechowski and Tam,[4] together with a discussion on their irreducible representations. This has been extended to include symmetries other than translational by Tam.[5] At the same time it has become clear that the representations of these groups possess some features not usually found in applications to solid state physics, and it is the purpose of this paper to try to set them in the context of mathematical developments in the general theory of representations of infinite groups. In fact, it turns out that these features can be characterized very well in terms of some well-known mathematical results for groups that are not of Type I, whose definition we give later. In the process, several questions that have been raised on the properties of certain infinite-dimensional representations of the invariance groups can be answered.[6]

The system under discussion consists of a single nonrelativistic electron without spin subject simultaneously to a uniform magnetic field B and an electric potential $\mathcal{U}(\mathbf{r})$ with the periodicity of an infinite three-dimensional lattice; here r denotes the position vector of the electron. The Hamiltonian is

$$\mathcal{H} = -\frac{\hbar^2}{2m}\left(\nabla - \frac{ie}{\hbar c}\mathbf{A}(\mathbf{r})\right)^2 + \mathcal{U}(\mathbf{r}), \quad (1)$$

where $-i\hbar\nabla$ is the electron momentum operator, $\mathbf{A}(\mathbf{r})$ the vector potential for the magnetic field and $m, e, c$, and $\hbar$ are the electron mass, electron charge (a negative number), velocity of light, and Planck's constant $h$ divided by $2\pi$. There is of course a certain freedom of choice for $\mathbf{A}(\mathbf{r})$, and we take for convenience the so-called symmetric gauge

$$\mathbf{A}(\mathbf{r}) = \tfrac{1}{2}\mathbf{B} \times \mathbf{r}. \tag{2}$$

A change of gauge makes no essential difference from the point of view of the symmetry of the system,[4] so that there is no loss of generality in retaining (2).

The Hilbert space of states in which $\mathcal{H}$ acts is the usual space $\mathfrak{L} \equiv L^2(R^3)$ of functions square-integrable over infinite volume, and $\mathcal{H}$ itself will in general have an energy spectrum with a continuous as well as a discrete part; in fact, in the systems considered below the spectrum is entirely continuous. Periodic boundary conditions will not be applied.

Any group of unitary operators in $\mathfrak{L}$ that commute with $\mathcal{H}$ is termed an invariance operator group of $\mathcal{H}$. There is, of course, a maximal such group which is called the symmetry group of $\mathcal{H}$; but since in this paper we shall not usually be dealing with the maximal group we retain the term "invariance group." To be more explicit, we shall be concerned with the infinite "invariance translation operator group" of $\mathcal{H}$.[4] As the name implies, the only geometrical operations involved are the translations. Rotational and time-reversal symmetries will be ignored, except for a brief mention of the former at the end.

The plan of this paper is as follows. In the remaining part of the Introduction we summarize some definitions and concepts from the theory of representations of infinite groups that we need later, including a description of what is meant by groups and representations not of Type I. In Sec. II we introduce the invariance translation operator group for $\mathcal{H}$ of (1) and show that it is of Type I when and only when the magnetic field is "rational," i.e., its contravariant components, with respect to a triple of basic primitive lattice vectors for the crystal, are rational numbers in certain natural units. We also introduce the invariance translation operator group for the system with $\mathcal{V}(\mathbf{r}) \equiv 0$, i.e., an electron moving in a magnetic field only. The relationship between this group and the invariance translation operator group for $\mathcal{H}$ of (1), which it contains as a subgroup, is used in the later analysis. In Sec. III we investigate the irreducible unitary representations of the group for systems with the magnetic field parallel to a lattice vector, with particular attention to the nonrational, i.e., non-Type I case. For this case, we find a nondenumerable number of equivalence classes of irreducible unitary representations, which are given in a summary at the end of the section. (We should note that present mathematical theory does not allow us definitely to establish the complete set of irreducible representations of a non-Type I group.) The irreducible unitary representations for the $\mathcal{V}(\mathbf{r}) \equiv 0$ case are also obtained and are given in the summary. The main method used in this section is Mackey's theory for semidirect products. Finally, Sec. IV contains an analysis of the (reducible) representation of the group afforded by the state space $\mathfrak{L}$ for the systems discussed in Sec. III. The principal result here is that the representation afforded by $\mathfrak{L}$ is not of Type I when the field is irrational; the proof being by a method of explicit decomposition of the representation.

All groups referred to throughout, in particular all the invariance operator groups, are topological groups that are locally compact and separable. We shall be especially concerned with representations of infinite groups of this class, mainly those of infinite dimension, and so it is appropriate here to recall some of their properties. The following discussion will be primarily descriptive; practically all the material is drawn from the articles of Mackey[7-10] on infinite-dimensional group representations, and the reader is referred there for details and references to the mathematical literature. A review article by Coleman[11] is also useful in this regard.

We begin with some terminology. Let $G = \{g\}$ be a separable locally compact group with elements $g$. By a representation $\Gamma$ of $G$ we always mean a continuous unitary representation by operators in some separable Hilbert space $\mathfrak{M}$, and we write $\Gamma = \{\Gamma(g)\}$, where $\Gamma(g)$ is the unitary operator in $\mathfrak{M}$ representing $g$. We often refer to $\mathfrak{M}$ as the carrier space of $\Gamma$. Of course, the invariance operator groups in the carrier space $\mathfrak{L}$ of states are representations of themselves. However, in the sequel we shall sometimes talk of them in the sense of abstract groups (of which they are then faithful representations); but the meaning at the time should always be clear from the context. Two representations $\Gamma = \{\Gamma(g)\}$ and $\Gamma' = \{\Gamma'(g)\}$ of $G$ carried by the spaces $\mathfrak{M}$ and $\mathfrak{M}'$, respectively, are said to be *equivalent*, and written $\Gamma \simeq \Gamma'$, if there exists a unitary map $U$ of $\mathfrak{M}$ onto $\mathfrak{M}'$ such that $\Gamma'(g) = U^{-1}\Gamma(g)U$ for all $g \in G$. A representation $\Gamma$ carried by $\mathfrak{M}$ is said to be *irreducible* if $\mathfrak{M}$ possesses no closed subspace stable under the operations of $G$. If $\mathfrak{M}$ possesses such a subspace $\mathfrak{N}$, then $\Gamma$ is reducible; $\Gamma$ restricted to $\mathfrak{N}$ is called a *subrepresentation* of $\Gamma$. We recall that the unitary property implies that a reducible representation is decomposable, with a corresponding decomposition of its carrier space. By the decomposition of a representation we shall mean, in general, a *direct integral decomposition* and not only a direct sum, which is a special case. The precise definition can be found in the literature[12]; a direct integral decomposition of a representation $\Gamma$ and the accompanying decomposition of its carrier $\mathfrak{M}$ have the form

$$\mathfrak{M} = \oplus \int_Y \mathfrak{M}^y d\mu(y), \qquad \Gamma = \oplus \int_Y \Gamma^y d\mu(y), \tag{3}$$

where $\mathfrak{M}^y$ is the carrier space for $\Gamma^y$, for each $y$ belonging to an index space $Y$, and where $\mu$ is a measure on $Y$. The $\mathfrak{M}^y$ and $\Gamma^y$ will be termed the *constituents* of $\mathfrak{M}$ and $\Gamma$ in the given decomposition, respectively. We note that a given constituent $\Gamma^y$ is not a subrepresentation of $\Gamma$ unless the latter can be written in the direct sum form $\Gamma = \Gamma^y \oplus \Gamma'$, and a parallel statement holds for $\mathfrak{M}^y$. Two representations which have no equivalent subrepresentations are termed *disjoint*. A representation which cannot be decomposed into a direct sum of two disjoint subrepresentations is called primary.[13] Obviously, irreducible representations are primary, and so are direct multiples of irreducible representations, i.e., representations that decompose into a direct sum of

the same irreducible representation (to within equivalence) a countable number of times. We note that the term "irreducible representation" has been used in the last phrase in the sense of "equivalence class of irreducible representations" rather than that of "individual irreducible representation"; both meanings will be used without further specification when the context is clear. The same duality of meaning will occur in referring to primary representations.

Primary representations do not always have the structure of the ones mentioned above, as being direct multiples of irreducible representations; but any primary that does is said to be of *Type I*. Furthermore, any primary representation that has an irreducible subrepresentation is automatically equivalent to a uniquely-determined direct multiple of a uniquely-determined irreducible representation and so is of Type I. A non-Type-I primary representation, on the other hand, has no irreducible subrepresentation. Concerning primary representations in general, one can make the following statements: (a) Any primary representation can be decomposed into a direct integral of irreducible representations, but not necessarily in only one way; (b) For a primary representation $\Gamma$ of Type I, every decomposition (3) of $\Gamma$ into irreducible representations has the property that $\Gamma^y \simeq \gamma$ for ($\mu$-almost) all $y \in Y$, where $\gamma$ is some fixed irreducible representation independent of the decomposition; and, consequently: (c) Any primary representation exhibiting decompositions into irreducible constituents without the property in (b) is not of Type I. Indeed, in connection with (c), there are examples of non-Type-I primary representations decomposable into irreducible constituents in two or more different ways, each having no constituent in common with the others.[14] One such example, for which there is in fact an infinite number of decompositions that differ mutually in this fashion, occurs for some of the groups discussed in this paper (Sec. IV). We should add that non-Type-I primary representations can be classified further into Types II or III.[15] (One way of characterizing the difference is: A non-Type-I primary representation is of Type II or III according to whether or not it has a subrepresentation inequivalent to the whole representation, respectively.[11])

A group whose primary representations are all of Type I is called a *Type I group*; in particular all finite, compact, and commutative groups are of Type I.

For any group, the primary representations can be considered in some sense the basic "building blocks" for arbitrary representations. Indeed, there is a theorem to the effect that if $\Gamma$ is any representation of $G$, then there exists a direct integral decomposition (3) of $\Gamma$ into primary constituents $\Gamma^y$, the so-called *central decomposition*, in which the constituents are mutually disjoint (apart possibly from a subset whose indices $y$ have $\mu$-measure zero in $Y$) and form a uniquely determined set (to within certain possible reassignments of indices). For a more precise definition of the central decomposition we again refer to the literature.[7] Thus, to this extent the study of all representations can be reduced to a study of primary representations; but as the earlier remarks on primary representations imply, the next step of reducing the latter to a study of irreducible representations seems possible only for groups of Type-I. This said, the actual survey of all the primary, or even of all the irreducible, representations of a non-Type-I group is a difficult matter, and does not appear to have been completed in any explicit case.[16] It is known, however, that every non-Type-I group does have a large supply of irreducible representations.

Although we shall not be considering the energy spectrum in this paper, it is worth pointing out that a knowledge of the central decomposition of the operator invariance group of $\mathcal{K}$ in the state space $\mathcal{L}$ gives us certain information on the spectrum of $\mathcal{K}$. Accompanying the central decomposition there is a corresponding reduction of the Hamiltonian as a direct integral: The simultaneous decompositions for $\mathcal{L}$ and $\mathcal{K}$ are then

$$\mathcal{L} = \oplus \int_Y \mathcal{L}^y \, d\mu(y), \quad \mathcal{K} = \oplus \int_Y \mathcal{K}^y \, d\mu(y),$$

where the constituents $\mathcal{K}^y$ of $\mathcal{K}$ operate in the respective $\mathcal{L}^y$, and where the $\mathcal{L}^y$ are determined by the central decomposition. The problem of finding the spectrum of $\mathcal{K}$ is thus reduced to the problem of determining it for the constituents $\mathcal{K}^y$. One of the most familiar examples of this reduction procedure in solid state physics is for the system of a Bloch electron without magnetic field, where the invariance group is the ordinary translation group of the lattice, and $y$ is a Bloch wave vector and $Y$ the Brillouin zone. In this example, of course, the group is of Type I, whereas the above decomposition holds whether the group is Type I or not. Certain technical mathematical problems that we have ignored in the preceding description are considered by Scharf[17] and Mackey[18] for the Bloch-electron system without field.

## II. THE INVARIANCE GROUPS

In this section we present the invariance translation operator groups for the Hamiltonian (1) and for the potential-free Hamiltonian with $\mathcal{V}(\mathbf{r}) \equiv 0$. They are given as set forth by Opechowski and Tam,[4] and their notation will be followed as far as possible.

It is convenient to introduce coordinates with axes and scale determined by an arbitrary three-dimensional lattice, to be used for the potential-free case as well as otherwise. Denoting the three linearly independent basic primitive vectors of the lattice by $\mathbf{a}_1, \mathbf{a}_2$, and $\mathbf{a}_3$, we choose the $x_1, x_2$, and $x_3$ coordinate axes to lie along these directions, respectively, forming what will be in general an oblique coordinate system. We write

$$\mathbf{r} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3$$
$$\text{and} \quad \mathbf{v} = v_1\mathbf{a}_1 + v_2\mathbf{a}_2 + v_3\mathbf{a}_3 \quad (4)$$

for an arbitrary position and translation vector, respectively, where the triples $(x_1, x_2, x_3)$ and $(v_1, v_2, v_3)$ are dimensionless real numbers. The scaling units along the three directions are the lattice constants $|\mathbf{a}_1| = a_1$, $|\mathbf{a}_2| = a_2$, and $|\mathbf{a}_3| = a_3$. The origin of coordinates is located at a point of the lattice so that the lattice itself is the triply infinite set of points with coordinates $(n_1, n_2, n_3)$ for arbitrary integers $n_1, n_2$, and $n_3$.

The vectors $\mathbf{v}$ form the infinite group $V$ of translations in three dimensions, and for each $v \in V$ we can define a translation operator $[\mathbf{v}]$ in the state space $\mathcal{L}$,

where

$$[\mathbf{v}]f(\mathbf{r}) = f(\mathbf{r} - \mathbf{v}) \tag{5}$$

for any function $f(\mathbf{r})$ in $\mathfrak{L}$. The $[\mathbf{v}]$ form a translation operator group which we can without confusion denote by the same letter $V$. The periodic potential $\mathcal{U}(\mathbf{r})$ is assumed invariant under the subgroup T of $V$ of all primitive translation operators $[\mathbf{t}]$ with

$$\mathbf{t} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 \tag{6}$$

for an arbitrary triple $(n_1, n_2, n_3)$ of integers, where for a given $\mathcal{U}(\mathbf{r})$ the coordinate system has been chosen in the obvious way. Again the group of vectors $\mathbf{t}$ and the group of operators $[\mathbf{t}]$ will be denoted by the same letter $T$.

The group for the potential-free case will be presented first. The form of the operator depends on the gauge (2) but it can be shown that for each system discussed here, with or without potential, the groups for different choices of gauge are all isomorphic with one another.[4]

The elements of the translation operator invariance group $W(\mathbf{B})$ of (1) where $\mathcal{U}(\mathbf{r}) \equiv 0$ are the operators $[\mathbf{v}, \lambda]$ in $\mathfrak{L}$, where

$$[\mathbf{v}, \lambda] = e^{2\pi i\lambda} \exp[-(ie/2c\hbar)\ \mathbf{B}\cdot\mathbf{r} \times \mathbf{v}][\mathbf{v}] \tag{7}$$

for all $\mathbf{v} \in V$ and all real $\lambda \in [0, 1)$. It is in fact easy to verify by inspection that the operators (7) commute with $\mathfrak{H}$ when the electric potential is zero and that they form a group with multiplication law

$$[\mathbf{v}, \lambda][\mathbf{v}', \lambda'] = [\mathbf{v} + \mathbf{v}', \lambda + \lambda' + (e/2ch)\ \mathbf{B}\cdot\mathbf{v} \times \mathbf{v}'], \tag{8}$$

where the second component in the element on the right-hand side will always be understood as equal to its calculated value modulo whatever integer is necessary to reduce it to the range $[0, 1)$. If $\nu$ is any real number, we shall use the notation $(\nu)_r$ to indicate its value reduced in this way. We observe from (8) that $W(\mathbf{B})$ is not Abelian. Its center contains the circle group of operators $[\mathbf{0}, \lambda]$ for all $\lambda \in [0, 1)$, where $\mathbf{0}$ is the zero translation and $W(\mathbf{B})$ is an extension of the circle group by $V$. It is not difficult to verify that $W(\mathbf{B})$ is minimal in the sense that it has no subgroup which is an extension by $V$.

The infinite group $W(\mathbf{B})$ has all the requisite topological properties: In fact, it is obviously a separable locally compact group with respect to the natural topology generated by open sets in $R^3 \times S$, where $R^3$ is the three-dimensional Euclidean space of points $\mathbf{v} \equiv (v_1, v_2, v_3)$ and $S$ is the circle with unit circumference of points $\lambda (0 \leq \lambda < 1)$. We shall see in the next section that it is a group of Type I.

The groups $W(\mathbf{B})$ for different $\mathbf{B} \neq \mathbf{0}$ are all isomorphic,[4] a situation which is far from being true of the invariance groups when there is a potential $\mathcal{U}(\mathbf{r})$. Before giving the groups in this case, it is convenient to express $\mathbf{B}$ in the form

$$\mathbf{B} = (ch/e|\Omega|)(\eta_1\mathbf{a}_1 + \eta_2\mathbf{a}_2 + \eta_3\mathbf{a}_3), \quad \Omega = \mathbf{a}_3\cdot\mathbf{a}_1 \times \mathbf{a}_2, \tag{9}$$

where $|\Omega|$ is the volume of the lattice primitive cell. In this way, $\mathbf{B}$ is specified by a triple $(\eta_1, \eta_2, \eta_3)$ of dimensionless real numbers. Now, with a potential $\mathcal{U}(\mathbf{r})$ invariant under the group $T$ of primitive translations $[\mathbf{t}]$, it follows from (7) and (8) that the Hamiltonian (1) is invariant under the operations $[\mathbf{t}, \lambda]$; and that these operations form a group for all $\mathbf{t} \in T$ and all $\lambda \in [0, 1)$. This group is an extension of the circle group by $T$; but it is not minimal in this case: It possesses subgroups that are extensions by $T$.[4] To see this, we write down their multiplication law derived from (8):

$$[\mathbf{t}, \lambda][\mathbf{t}', \lambda'] = [\mathbf{t} + \mathbf{t}', \lambda + \lambda' + \tfrac{1}{2}\xi\boldsymbol{\eta}\cdot\mathbf{n} \times \mathbf{n}'], \tag{10}$$

where $\mathbf{t} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ and $\mathbf{t}' = n_1'\mathbf{a}_1 + n_2'\mathbf{a}_2 + n_3'\mathbf{a}_3$, and where we have used (9) for $\mathbf{B}$. The quantity $\xi \equiv \Omega/|\Omega| = \pm 1$ will be called the *sign* of the basic vector trio $(\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3)$. The quantities $\boldsymbol{\eta} = (\eta_1, \eta_2, \eta_3)$, $\mathbf{n} = (n_1, n_2, n_3)$, and $\mathbf{n}' = (n_1', n_2', n_3')$ behave like vectors with cartesian components and, by a slight abuse of terminology, will be referred to as the field $\boldsymbol{\eta}$, translation $\mathbf{n}$, etc. Consider the countably infinite set of operators

$$T(\mathbf{B}) = \{[\mathbf{t}, \tfrac{1}{2}\boldsymbol{\mu}\cdot\boldsymbol{\eta}]\} \tag{11}$$

for all $\mathbf{t} \in T$ and for all vectors $\boldsymbol{\mu} = (\mu_1, \mu_2, \mu_3)$ with arbitrary integral components leading to distinct numbers $(\tfrac{1}{2}\boldsymbol{\mu}\cdot\boldsymbol{\eta})_r \in [0, 1)$. It follows immediately from (10) that the operators of $T(\mathbf{B})$ are closed under multiplication and form a group; furthermore, we can verify that $T(\mathbf{B})$ is a minimal extension by $T$. Then, by definition, the countably infinite group $T(\mathbf{B})$ is the *invariance translation operator group* of the Hamiltonian (1)[4]; it is evidently a subgroup of the corresponding invariance group $W(\mathbf{B})$ for the potential-free system. The structure of $T(\mathbf{B})$ depends critically on the direction and magnitude of $\mathbf{B}$; in other words, on the values of $\eta_1, \eta_2$ and $\eta_3$. There are two sharply divided cases, according to whether all three of these numbers are rational, or one or more is irrational; the field $\mathbf{B}$ is said to be "rational" or "nonrational" accordingly. We discuss briefly the two cases in turn.

*(a) Rational field:* Here $\eta_i = m_i/M_i$, where $m_i$ and $M_i$ are relatively prime integers. The group $T(\mathbf{B})$ has the characteristic that the number of distinct $(\tfrac{1}{2}\boldsymbol{\mu}\cdot\boldsymbol{\eta})_r$ that appear in the operators (11) is *finite*. This case has been widely investigated,[1-4] and the details can be found in Ref. 4. The field $\boldsymbol{\eta}$ can be put in the form

$$\boldsymbol{\eta} = (m/M)\boldsymbol{l}, \tag{12}$$

where $m$ and $M$ are relatively prime integers, and $\boldsymbol{l}$ is a vector with relatively prime integral components [these are the components of the shortest lattice vector (6) along the direction of the field]. The group $T(\mathbf{B})$ consists of the operators $[\mathbf{t}, \lambda]$ for all $\mathbf{t} \in T$ and $\lambda = 0, 1, \ldots, (r-1)/r$, where $r = M$ ($m$ even) or $2M$ ($m$ odd). We observe that when $M = 1$ and $m$ is even, only $\lambda = 0$ appears, and $T(\mathbf{B})$ is Abelian and isomorphic to $T$.

*(b) Nonrational field:* Here at least one of the components of $\boldsymbol{\eta}$ is irrational, say $\eta_3$. The set of distinct $(\tfrac{1}{2}\boldsymbol{\mu}\cdot\boldsymbol{\eta})_r \in [0, 1)$ appearing in the operators (11) is now infinite, since it contains the numbers $(\tfrac{1}{2}\mu_3\eta_3)_r$ obtained by taking all $\mu$ of the form $(0, 0, \mu_3)$. Consequently $T(\mathbf{B})$ consists of the operators $[\mathbf{t}, \lambda]$ for all

$t \in T$ and an infinite number of $\lambda$; we note that it is never Abelian.

A more refined classification of these invariance groups according to the rationality or otherwise of one, two, or three of the components of $\eta$ has been made in the literature.[4] Their evidently wild variation with infinitesimal changes in the magnetic field has been commented and is reflected in the proposition in the next paragraph.

The $T(\mathbf{B})$ are all given the discrete topology (each element an open set) and are, therefore, separable and locally compact. From a theorem of Thoma[19] that a countably infinite discrete group $G$ is of Type I if and only if it has a normal Abelian subgroup $F$ such that the factor group $G/F$ is finite, we can conclude that

*Proposition 1:* The invariance translation operator group $T(\mathbf{B})$ is Type I if and only if the field $\mathbf{B}$ is rational.

For the case (a) of rational field we have then to find a normal Abelian subgroup of finite index in $T(\mathbf{B})$. To this end, we observe from (10) that two elements of $T(\mathbf{B})$, say $[t, \lambda]$ and $[t', \lambda']$, will commute when and only when

$$\eta \cdot \mathbf{n} \times \mathbf{n}' = (m/M)\boldsymbol{l} \cdot \mathbf{n} \times \mathbf{n}' = \text{integer},$$

where we have used (12) for $\eta$. Thus, for example, all operators of $T(\mathbf{B})$ of the form $[\tau, \lambda]$ for arbitrary $\lambda = \frac{1}{2}(\boldsymbol{\mu} \cdot \boldsymbol{\eta})_r$ and for $\tau = M(p_1\mathbf{a}_1 + p_2\mathbf{a}_2 + p_3\mathbf{a}_3)$ with arbitrary integers $p_1, p_2, p_3$, commute with every group element; and it is easy to verify that they form a subgroup $F$ of $T(\mathbf{B})$. This subgroup is Abelian and normal, and since the $\tau$ form a group of translations in three dimensions based on an enlarged primitive cell $M$ times the size of the original, it follows that the factor group $T(\mathbf{B})/F$ is finite. Thus $T(\mathbf{B})$ is of Type I.

When the field is nonrational as in (b), the requirement for two elements to commute, i.e., $\eta \cdot \mathbf{n} \times \mathbf{n}' =$ Integer, tells us that no Abelian subgroup can be of finite index in $T(\mathbf{B})$. For if $\eta_3$, say, is irrational, this requirement can only be satisfied for all elements of an Abelian subgroup if $(\mathbf{n} \times \mathbf{n}')_3 = 0$ for every pair of such elements, and this is only possible if the subgroup is formed of translations in one or two dimensions. The index in $T(\mathbf{B})$ of any Abelian subgroup is therefore infinite, and so $T(\mathbf{B})$ is not of Type I.

It is worth noting parenthetically that for a rational field there are infinitely many Abelian subgroups of the form $F = \{[\tau, 0]\}$, where $\tau$ runs over the translations of a three-dimensional sublattice and where each $[\tau, 0]$ commutes with all elements of $T(\mathbf{B})$. This follows from arguments similar to those used in the proof above. For subgroups $F$ that are minimal (with respect to inclusion), the primitive cell of the corresponding sublattice, whose three basic vectors are multiples of $\mathbf{a}_1, \mathbf{a}_2$, and $\mathbf{a}_3$, respectively, is called by Brown[1] a "magnetic unit cell." There will, in general, be a (finite) number of minimal subgroups $F$ with different magnetic unit cells, but in each case the idea is the same: The magnetic unit cell is a minimal domain to which we can apply periodic boundary conditions for the Hamiltonian. Thus, for any finite crystal built up by a repetition of one of these magnetic unit cells it is possible to define a system with periodic boundary conditions; then the infinite group is replaced by a finite group in similar fashion to the field-free case.

When the field is nonrational, it follows from the proof of the above proposition that it is impossible to find a magnetic unit cell; and so we are always obliged to retain infinite systems.

From now on, for the sake of simplicity we shall specialize to systems, in which the magnetic field is directed along $\mathbf{a}_3$;[20] then with $\eta_1 = \eta_2 = 0$ and $\eta_3 = \eta$,

$$\mathbf{B} = (ch/e|\Omega|)\eta\mathbf{a}_3. \tag{13}$$

We collect together some formulas for the groups $W(\mathbf{B})$ and $T(\mathbf{B})$ when B has the value (13). There are three cases:

*(A) The potential-free case:* $\mathcal{U}(\mathbf{r}) \equiv 0$. Since the $W(\mathbf{B})$ are isomorphic for all $\mathbf{B}$, it is evidently no real restriction to suppose $\mathbf{B}$ parallel to $\mathbf{a}_3$; rather, we choose the lattice so that this is true. We replace the symbol $W(\mathbf{B})$ by $W$. The elements (7) of $W$ are

$$[\mathbf{v}, \lambda] = e^{2\pi i\lambda} \exp\{-i\pi\xi\eta(v_2x_1 - v_1x_2)\}[\mathbf{v}] \tag{14}$$

for $\mathbf{v} \in V$ and all real $\lambda \in [0, 1)$. The multiplication law (8) becomes

$$[\mathbf{v}, \lambda][\mathbf{v}', \lambda'] = [\mathbf{v} + \mathbf{v}', \lambda + \lambda' + \tfrac{1}{2}\xi\eta(v_1v_2' - v_2v_1')]. \tag{15}$$

*(B) Case of periodic potential and irrational field* $\eta$: The group $T(\mathbf{B})$ for $\mathbf{B}$ of (13) will be denoted by $T_\eta$. The elements (11) will be written $[t, \lambda_j]$, where

$$[t, \lambda_j] = e^{2\pi i\lambda_j} \exp\{-i\pi\xi\eta(n_2x_1 - n_1x_2)\}[t] \tag{16}$$

for all $t \in T$ and all $\lambda_j = (\frac{1}{2}j\eta)_r$ ($j$ an integer). The multiplication law (10) becomes

$$[t, \lambda_j][t', \lambda_i] = [t + t', \lambda_j + \lambda_i + \tfrac{1}{2}\xi\eta(n_1n_2' - n_2n_1')]. \tag{17}$$

*(C) Case of periodic potential and rational field* $\eta = m/M$. Here $m$ and $M$ have the same meaning as in (12), where now $\boldsymbol{l} = (0, 0, 1)$. The group elements and multiplication law are as in case (B) with $\eta = m/M$, except that the set of $\lambda_j$ is now finite.

The invariance groups in each of the above cases can be simply expressed in terms of Abelian subgroups involving translations along three different directions, respectively. In fact, if $G$ denotes any one of the groups of (A)–(C), then it can be factored first as a direct product

$$G = P \times Q, \tag{18}$$

where

$$P = \begin{cases} \{[v_3\mathbf{a}_3, 0]\} \\ \\ \{[n_3\mathbf{a}_3, 0]\} \end{cases}, \quad Q = \begin{cases} \{[v_1\mathbf{a}_1 + v_2\mathbf{a}_2, \lambda]\} & \text{(A)} \\ \\ \{[n_1\mathbf{a}_1 + n_2\mathbf{a}_2, \lambda_j]\} & \text{(B), (C)} \end{cases} \tag{19a, 19b}$$

Here as in other places curly brackets are used to denote collections of elements, and the specifications (A), (B), and (C) refer to the three cases above. The factorization (18) separates translations along the field direction $\mathbf{a}_3$ from those in the $\mathbf{a}_1 - \mathbf{a}_2$ plane.

Further factorization of $Q$ into Abelian subgroups has the semidirect product form $Q = N \circledS H$. [We recall that for any group $Q$ to be a semidirect product of two subgroups $N$ and $H$ (Abelian or not) requires that $Q = NH$, that $N \cap H = \{\text{Unit element}\}$, and that one of them ($N$) be normal. This means, in particular, that every element $q$ of $Q$ can be written $q = nh$ where $n \in N$ and $h \in H$ are unique. The product of two elements $q$ and $q'$ being $qq' = (nhn'h^{-1})(hh')$, we observe that, given $N$ and $H$ satisfying the above three requirements, their semidirect product is characterized by the action of $H$ on $N$, i.e., the automorphisms $h: n \to hnh^{-1}$ of $N$ generated by the $h \in H$.] Indeed it is easy to see that we can write

$$Q = N \circledS H, \tag{20}$$

where

$$N = \begin{cases} \{[v_1\mathbf{a}_1, \lambda]\} \\ \\ \{[n_1\mathbf{a}_1, \lambda_j]\} \end{cases}, \quad H = \begin{cases} \{[v_2\mathbf{a}_2, 0]\} & \text{(A)} \quad (21a) \\ \\ \{[n_2\mathbf{a}_2, 0]\} & \text{(B), (C)} \quad (21b) \end{cases}.$$

The symbols specifying the various groups defined in (18)–(21) will carry labels distinguishing the different cases only when the context is not clear. Then $N_B$, for example, will refer to the group $N$ in case (B).

It should be borne in mind that there is no unique way of expressing $Q$ as a semidirect product of subgroups involving translations in different directions; we have given one instance of an infinite number of possible ways. Any two vectors $\mathbf{b}_1, \mathbf{b}_2$ for which

$$\left.\begin{aligned} &\mathbf{b}_i = \sum_{j=1}^{2} l_{ij}\mathbf{a}_j, \quad i = 1, 2 \\ &l_{ij} \text{ integral and } l_{11}l_{22} - l_{12}l_{21} = \xi^b/\xi = \pm 1 \end{aligned}\right\} \tag{22}$$

can be chosen as the basic primitive lattice vector pair for the two-dimensional $\mathbf{a}_1 - \mathbf{a}_2$ lattice. Here $\xi^b = \mathbf{a}_3 \cdot \mathbf{b}_1 \times \mathbf{b}_2 / |\mathbf{a}_3 \cdot \mathbf{b}_1 \times \mathbf{b}_2|$ is the sign of the trio $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{a}_3)$. Then for the discrete groups, for example, we can factor $Q$ as

$$\left.\begin{aligned} &Q = N(\mathbf{b}_1) \circledS H(\mathbf{b}_2) \\ &N(\mathbf{b}_1) = \{[r_1\mathbf{b}_1, \lambda_j]\}, \quad H(\mathbf{b}_2) = \{[r_2\mathbf{b}_2, 0]\} \end{aligned}\right\}, \tag{23}$$

where $r_1, r_2$ run over all integers. These different ways of expressing $Q$ are important for the study of the representations of the non-Type-I group $T_\eta$. There is a factorization (23) for each ordered choice of $(\mathbf{b}_1, \mathbf{b}_2)$; in particular, we get *complementary* factorizations on exchanging $\mathbf{b}_1$ and $\mathbf{b}_2$. Two factorizations coincide when the corresponding basic vector pairs differ in the sign of one or both vectors. To avoid this situation, we shall restrict the domain of $\mathbf{b}_1$ and $\mathbf{b}_2$. We divide the $\mathbf{a}_1 - \mathbf{a}_2$ plane into two with a line drawn through the origin at right angles to the bisector of $\mathbf{a}_1$ and $\mathbf{a}_2$. Then we allow $\mathbf{b}_1$ and $\mathbf{b}_2$ to lie only in the same half-plane as $\mathbf{a}_1$ and $\mathbf{a}_2$; if one of them lies along the dividing line, we allow only the direction which makes an acute angle with $\mathbf{a}_1$. Now each factorization (23) will be different.[32]

A word on notation is necessary at this point. We shall often write $b \equiv (\mathbf{b}_1, \mathbf{b}_2)$ as shorthand for an allowed basic vector pair, and denote the complementary pair by $\bar{b} \equiv (\mathbf{b}_2, \mathbf{b}_1)$. The original pair will be written $a \equiv (\mathbf{a}_1, \mathbf{a}_2)$. The 1- and 2-components of a fixed vector $\mathbf{t}$ depend, of course, on the basic vector pair $b$, and they will bear an appropriate label, thus: $\mathbf{t} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 = n_1^b\mathbf{b}_1 + n_2^b\mathbf{b}_2 + n_3\mathbf{a}_3$. Components $n_1, n_2$ without superscript refer to the basic vector pair $a$; the components $n_1^b, n_2^b$ are related linearly to $n_1, n_2$ through (22).

The group multiplication law (17) retains the same form on changing to the basic vector pair $b$. The only difference is that in the product of a given pair of elements, the old components must be changed to the new ones and $\xi$ to $\xi^b$; indeed it is easy to verify using (22) that $\xi(n_1n_2' - n_2n_1') = \xi^b\{n_1^b(n_2^b)' - n_2^b(n_1^b)'\}$. This form-invariance of the multiplication law will be exploited in the investigation of the irreducible representations of $T_\eta$.

Finally, we should remark that all the subgroups introduced above are topologically closed (as subsets of their respective groups). This is a necessary condition for the application of much of the theory of representations in the next section.

## III. THE IRREDUCIBLE REPRESENTATIONS

For the "rational" case (C) of the previous section we know that the group is of Type I. Its irreducible representations have been obtained by Brown,[1] Zak,[2] and Fischbeck,[3] and are also given in the paper by Opechowski and Tam.[4] This case will not, therefore, be considered further. The last paper cited gives some of the representations for the "nonrational" case (B) as well; but we shall be able to extend the analysis and find many more.

The irreducible representations of $G$ in both cases (A) and (B) will be Kronecker products of the irreducible representations of the direct factors $P$ and $Q$ in (18). For $P$, the group of translations parallel to the magnetic field, they are all one-dimensional and easily written down; those for the semidirect product $Q$ are more interesting, notably in the case (B) of periodic potential with irrational field $\eta$, and to tackle them we use the procedure developed by Mackey.[8,10] We shall describe this procedure in only so much generality as is necessary for our purpose, and apply it to the two cases as we go along.

The irreducible representations of $P$ of (19) are all one-dimensional with characters

$$\chi^{k_3} = \{e^{-2\pi i k_3 v_3}\}, \quad -\infty < k_3 < \infty, \text{ (A)} \tag{24a}$$

$$\chi^{\kappa_3} = \{e^{-2\pi i \kappa_3 n_3}\}, \quad 0 \leq \kappa_3 < 1, \quad \text{(B)} \tag{24b}$$

labeled by wave vectors for the $z$ direction. In the curly brackets, $v_3$ and $n_3$ run over all elements of their respective groups.

From here on, we fix our attention on the group $Q$. Let $Q = N \circledS H$ be for the moment *any* (separable, locally compact) group that is a semidirect product of (closed) subgroups $N$ and $H$ of which $N$ is commutative and normal in $Q$. The method to be used aims to construct irreducible representations of $Q$ from those of $N$ and of $H$. Since $N$ is commutative, its irreducible representations are all one-dimensional with characters $\chi_l = \{\chi_l(n)\}$, where $\chi_l(n)$ is a continuous function of $n \in N$ with unit modulus and where the parameter $l$ labels the representations. The set $\hat{N}$ of all $\chi_l$ for different $l$ is called the *character space* of $N$. It can be made into a Borel space, i.e., given a

collection of Borel sets,[21] in a natural and well-defined manner that we do not attempt to describe in general, but shall indicate for our two examples. The Borel structure of $\hat{N}$ is of importance later on.

For our two cases (A) and (B) the groups $N$ and $H$ are defined in (21). The elements of $\hat{N}$ are

$$\chi^{k,\zeta} = \{e^{2\pi i\zeta\lambda}\, e^{-2\pi ikv_1}\}, \quad -\infty < k,\zeta < \infty, \text{ (A)} \qquad (25a)$$

$$\chi^{\kappa,\zeta} = \{e^{2\pi i\zeta\lambda_j}\, e^{-2\pi i\kappa n_1}\}, \quad 0 \leq \kappa < 1, 0 \leq \zeta < |\frac{2}{\eta}|. \text{ (B)} \qquad (25b)$$

Here $k$ and $\kappa$ are wave vectors along the $\mathbf{a}_1$ direction. The significance of $\zeta$ will be seen later. The respective character spaces $\hat{N}$ with elements (25) are for (A) the infinite two-dimensional plane with Cartesian coordinates $(k, \zeta)$ and for (B) the surface of a torus with cyclic coordinates $\kappa$ and $\zeta$. The Borel sets in both cases are the standard ones, generated from the open sets.[21]

Returning to the general semidirect product $Q$, we observe that the action of $H$ on $N$, namely the automorphism $h: n \to hnh^{-1}$ of $N$ where $h \in H$, induces a corresponding action of $h$ on $\hat{N}$: for each $h$ we define a mapping in $\hat{N}$ given by

$$h: \chi \to \chi_h, \qquad \chi = \{\chi(n)\}, \qquad \chi_h = \{\chi(hnh^{-1})\},$$

where $\chi_h$ may or may not be the same character as $\chi$. The set of distinct $\chi_h$ generated from $\chi$ is called an orbit of $H$ in $\hat{N}$. Since the same orbit is obtained in this way from any one of its members, the action of $H$ on $\hat{N}$ partitions $\hat{N}$ into disjoint orbits. Each orbit is a Borel set in $\hat{N}$. Further, with each $\chi$ of $\hat{N}$ we associate the so-called isotropy group $H_\chi$ of $\chi$, being the subgroup of all $h \in H$ for which $\chi_h = \chi$. The $H_\chi$ are closed subgroups of $Q$; for different $\chi$ of the same orbit they are conjugate subgroups in $Q$. Using (21) for the elements of $N$ and $H$, and with the aid of the respective multiplication laws (15) and (17), we find for the two cases:

(A) the $k$ plane is partitioned into orbits $\mathcal{O}^\zeta = \{k, \zeta \mid -\infty < k < \infty\}$ and $\mathcal{O}^k = (k, 0)$, respectively, lines parallel to the $k$ axis for $\zeta \neq 0$ and points on the $k$ axis for $\zeta = 0$. The isotropy groups are $H$ (for any member of $\mathcal{O}^k$) and $E$ (for any member of $\mathcal{O}^\zeta$), where $E$ is the group consisting of the identity element $[\mathbf{0}, 0]$.

(B) The orbits on the surface of the $\kappa - \zeta$ torus are more complicated. Each orbit lies in some circle $\mathcal{S}^\zeta = \{\kappa, \zeta \mid 0 \leq \kappa < 1\}$. For $\zeta = 0$, each point on $\mathcal{S}^0$ forms an orbit $\mathcal{O}^\kappa$. The orbits on the circle $\mathcal{S}^\zeta$ for $\zeta \neq 0$ are $\mathcal{O}^{[\kappa],\zeta} = \{(\kappa + \zeta\xi\eta n_2)_\gamma, \zeta \mid \text{all } n_2; \zeta \neq 0\}$, the $n_2$ coming from the action of $[n_2\mathbf{a}_2, 0]$ of $H$. The label $[\kappa]$ stands for the set of distinct numbers $(\kappa + \zeta\xi\eta n_2)_\gamma$ as $n_2$ goes over all integers; $\kappa$ can evidently be replaced in the bracket by any other member of the set. When $|\zeta\eta|$ is a rational number, equal to $m/M$, say, in its lowest terms, each orbit in $\mathcal{O}^\zeta$ contains $M$ points. Also, the orbit label $[\kappa]$ can be conveniently replaced here by the smallest of the $M$ members of $[\kappa]$, say $\bar{\kappa}$, where $0 \leq \bar{\kappa} < 1/M$. There is one orbit in $\mathcal{S}^\zeta$ for each $\bar{\kappa}$ in this interval. On the other hand, when $|\zeta\eta|$ is irrational, each orbit consists of a countable infinity of points, dense in $\mathcal{S}^\zeta$. Furthermore, it is not possible in this case to distinguish or label the different orbits in $\mathcal{S}^\zeta$ with the $\kappa$ coordinates of a representative point from each orbit, in the sense that no such collection of coordinates can form a measurable set of the circle.[22]

The isotropy groups are $H$ (for any member of $\mathcal{O}^\kappa$), $E$ (for any member of $\mathcal{O}^{[\kappa],\zeta}$ with $|\zeta\eta|$ irrational) and $H^{\bar{\kappa}}$ (for any member of $\mathcal{O}^{\bar{\kappa},\zeta}$ with $|\zeta\eta|$ rational). Here $H^{\bar{\kappa}}$ is a subgroup of index $M$ in $H$ and consists of the elements of $H$ for which $(\bar{\kappa} + \zeta\xi\eta n_2)_\gamma = \bar{\kappa}$.

In order to define the representations of $N$ from which the irreducible representations of $Q$ are constructed, we must first introduce certain measures on the character space $\hat{N}$. Any countably additive $\sigma$-finite measure $\mu$ defined on all Borel sets of $\hat{N}$ is called a *Borel* measure on $\hat{N}$.[21] From now on, all measures will be understood to be of this kind.

The mappings of $N$ onto itself under the action of $H$, defined earlier, can be shown to be Borel isomorphisms, i.e., if $h: \mathcal{E} \to \mathcal{E}_h$, where $\mathcal{E}_h$ is the image of the set $\mathcal{E}$, then $\mathcal{E}_h$ is a Borel set whenever $\mathcal{E}$ is a Borel set and vice versa, for all $h \in H$. Thus $\mathcal{E}_h$ is always measurable when $\mathcal{E}$ is, and we can define a measure $\mathcal{E}$ to be *$H$-invariant* whenever $\mu(\mathcal{E}_h) = \mu(\mathcal{E})$ for all $h \in H$ and all Borel sets $\mathcal{E} \in \hat{N}$. An $H$-invariant measure is further said to be *ergodic*, if $\mathcal{E}_h = \mathcal{E}$ (to within a possible null set) for all $h \in H$ implies that $\mathcal{E}$ is a null set or the complement of one. (A null set for $\mu$ is a set with zero measure with respect to $\mu$.)

In the sequel, two measures will be referred to as "different" if and only if they have different null sets. Measures with the same null sets are said to belong to the same measure class, and throughout the rest of the paper the word measure will be used as a synonym for measure class; measures given explicitly are to be thought of as convenient representatives of their class. The theorems and results of the general theory presented below can be shown to be independent of the choice of measure within a given class. (We should remark that, to be quite general, $H$-invariance is defined for measure classes rather than individual measures (see, e.g., Ref. 10, p. 25). An $H$-invariant class may or may not contain individually $H$-invariant members. If it does not, small modifications are necessary in the exposition which, however, we will be able to ignore, since the situation does not arise for the measures considered in our examples.)

Let $\mathcal{F}$ be any Borel subset of $\hat{N}$. A measure $\mu$ on $\hat{N}$ is said to be *concentrated* in $\mathcal{F}$ if $\mu(\mathcal{E}) = \mu(\mathcal{E} \cap \mathcal{F})$ for all Borel sets $\mathcal{E} \in \hat{N}$; evidently then $\mu(\hat{N}) = \mu(\mathcal{F})$. If $\mathcal{F}$ is regarded as a space with Borel sets derived from those of $N$,[21] then to specify the measures on $\hat{N}$ concentrated in $\mathcal{F}$ amounts just to specifying the measures on $\mathcal{F}$. The same goes for the $H$-invariant measures concentrated in $\mathcal{F}$ whenever $\mathcal{F}$ is a subset invariant under the action of $\mathcal{H}$ (i.e., maps onto itself under the action of $H$). If $\mathcal{F}$ is transitive under the action of $H$ (i.e., the set $\{\chi_h\} = \mathcal{F}$ for any $\chi \in \mathcal{F}$), it can be shown that there exists one and only one ergodic $H$-invariant measure concentrated in $\mathcal{F}$.[8] Since the transitive Borel sets of $\hat{N}$ are just the orbits, we can divide the ergodic $H$ invariant measures on $\hat{N}$ into two kinds:

(i) the *transitive* measures: Namely, those concentrated in the orbits, one for each orbit.

(ii) the *strictly ergodic* measures: Namely those, if

they exist, that are not transitive. For $\mu$ any such, $\mu(\mathcal{O}) = 0$ for every orbit $\mathcal{O}$.

The situation is very different according to whether or not there exist any strictly ergodic measures. If not, the semidirect product $Q = N \circledS H$ is said to be *regular*,[8] and in this case the procedure for obtaining the irreducible representations of $Q$ is relatively complete when those of $H$ are known. A sufficient condition for regularity is the existence of a Borel set in $\hat{N}$ intersecting each orbit in one point.[8] There is a theorem that a regular semi-direct product $Q$ is of Type I if and only if each isotropy group $H_\chi$ is of Type I.[8] For a nonregular semidirect product, the present state of knowledge is much less satisfactory; for instance, there seems to be no known example of one for which all the strictly ergodic measures have been definitely identified.[23]

We now investigate the ergodic $H$-invariant measures on $\hat{N}$ for (A) and (B); we recall that they should be regarded as convenient representations of their respective measure classes.

(A) The semidirect product here is regular, as the Borel set consisting of the union of the $k$ axis and the $\zeta$ axis intersects each orbit just once. From the discussion above $Q$ is then, of Type I, since the isotropy groups are all either $H$ or $E$, both of Type I. The ergodic $H$-invariant measures are easily established, since they are transitive and one-to-one with the orbits. They are: On $\mathcal{O}^\zeta$ the Lebesgue linear measure and on $\mathcal{O}^k$ the measure assigning unit mass to the single point.

(B) There are strictly ergodic measures here as well as transitive ones, so that the semidirect product is not regular; and in any case we know from Sec. II that it is not of Type I. The transitive measures are: On $\mathcal{O}^\kappa$ the measure assigning unit mass to the single point and on $\mathcal{O}^{[\kappa],\zeta}$ (or on $\mathcal{O}^{\kappa,\zeta}$ for $|\zeta\eta|$ rational) the atomic measure assigning unit mass to each point of the orbit.

Consider any circle $\mathcal{S}^\zeta$ where $|\zeta\eta|$ is irrational, so that orbits are dense in the circle. Lebesgue linear measure on $\mathcal{S}^\zeta$ is $H$-invariant and strictly ergodic: the action $\kappa \to (\kappa + \zeta\xi\eta n_2)_r$ of the elements of $H$ rotates $\mathcal{S}^\zeta$ through multiples $n_2$ of an irrational fraction $|\zeta\eta|$ of $2\pi$. Lebesgue measure is well known to be ergodic relative to this action on the circle, and it is certainly not transitive since each orbit, being a countable set, has measure zero (see, e.g., Ref. 8, Sec. 7). It is not known at present whether there exist other measure classes on the circle that are strictly ergodic with respect to this action of $H$.

Circles $\mathcal{S}^\zeta$ for $|\zeta\eta|$ rational evidently do not admit strictly ergodic measures.

We return to the general theory. Given any fixed measure $\mu$ on $\hat{N}$ (ergodic $H$-invariant or not), we introduce a representation of $N$ as follows. Let $L^2(\hat{N}, \mu)$ be the Hilbert space of functions on $\hat{N}$, measurable and square integrable with respect to $\mu$. Then the representation is defined in $L^2(\hat{N}, \mu)$, and is given by

$$\left.\begin{aligned} \Lambda_\mu &= \oplus \textstyle\int_{\hat{N}} \chi \, d\mu(\chi) \\ \Lambda_\mu(n) f(\chi) &= \chi(n) f(\chi) \end{aligned}\right\} \tag{26}$$

for $n \in \hat{N}$ and $f(\chi) \in L^2(\hat{N}, \mu)$. The importance of the $\Lambda_\mu$ is revealed by the following.

*Theorem 1*[24]: If $\Delta$ is an irreducible representation of $Q$, then its restriction to $N$ is a direct multiple (finite or infinite) of some $\Lambda_\mu$, for $\mu$ an ergodic $H$-invariant measure on $\hat{N}$. We shall say that $\Delta$ is *based* on the corresponding measure. Irreducible $\Delta$ based on different measures are always inequivalent.

The aim of Mackey's method for finding the irreducible representations of $Q$ is thus: Find the ergodic $H$ invariant measures on $\hat{N}$, then find the irreducible $\Delta$ based on each of them. We have discussed the first part of this program; for the second part we take the transitive and strictly ergodic measures in turn.

Consider the transitive measure $\mu$ concentrated in the orbit $\mathcal{O}$. Let $\chi$ be any fixed member of $\mathcal{O}$ with isotropy group $H_\chi$, and let $\Omega = \{\omega(h) \,|\, h \in H_\chi\}$ be any irreducible representation of $H_\chi$, with carrier space $\mathcal{L}_\Omega$. We introduce the (closed) subgroup $L_\chi = H_\chi \circledS N$ of $Q$ called the *little group* of $\Omega$. The assignment $nh \to \chi(n)\omega(h)$ of the elements of $L_\chi$ to operators in $\mathcal{L}_\Omega$ yields an irreducible representation $\Omega_\chi$ of $L_\chi$, the so-called *allowed* representation of $L_\chi$ corresponding to $\Omega$. We construct the representation of $Q$ *induced* from $\Omega_\chi$ in the following manner. Let $Q/L_\chi = \{L_\chi s\}$ be the right coset decomposition of $Q$ with respect to $L_\chi$, where for convenience we select the coset representatives $s$ to belong to $H$. The set of characters $\chi_s = \{\chi(sns^{-1})\}$ for all $s$ describes the orbit $\mathcal{O}$ just once, by definition of $L_\chi$. It turns out that the orbit $\mathcal{O}$ (with Borel sets as a subspace of $\hat{N}$)[21] and the coset space $Q/L_\chi$ (with Borel sets as a quotient space of $Q$)[21] can be identified by the 1–1 Borel isomorphic mapping $\{L_\chi s\} \longleftrightarrow \chi_s$; by a slight abuse of terminology we can take $s$ as a parameter describing both spaces. Let $\mathcal{L}(\mathcal{O}, \mu)$ denote the Hilbert space of functions defined on $\mathcal{O}$ with values in $\mathcal{L}_\Omega$. This consists of all functions $f(s)$ from $\mathcal{O}$ (writing $s$ in abbreviation for $\chi_s$) to $\mathcal{L}_\Omega$ such that the scalar product $(\phi, f(s))$ is a $\mu$-measurable function on $\mathcal{O}$ for all $\phi \in \mathcal{L}_\Omega$ and such that $\int_{\mathcal{O}} \|f(s)\|^2 d\mu(s) < \infty$, where $\|f(s)\|$ is the norm of $f(s) \in \mathcal{L}_\Omega$. Then the representation $\Delta = \{\Delta(q)\}$ of $Q$ *induced* from $\Omega_\chi$ is carried by $\mathcal{L}(\mathcal{O}, \mu)$ and defined by

$$\Delta(q) f(s) = \Omega_\chi(sq\bar{s}^{-1}) f(\bar{s}), \qquad sq\bar{s}^{-1} \in L_\chi \tag{27}$$

for all $q \in Q$ and all $f(s)$. Here, $\bar{s}$ is the unique coset representative for which $sq\bar{s}^{-1} \in L_\chi$ for given $q$ and $s$.

*Theorem 2*:[24] Given a transitive measure $\mu$ concentrated in an orbit $\mathcal{O}$, with isotropy group $H_\chi$ for $\chi \in \mathcal{O}$. For each irreducible representation $\Omega$ of $H_\chi$, the $\Delta$ of $Q$ corresponding to $\Omega$ via (27) is irreducible and based on $\mu$. Two such representations are equivalent if and only if the corresponding $\Omega$ of $H_\chi$ are equivalent, and the representations obtained from all the inequivalent $\Omega$ form the complete set of irreducible representations of $Q$ based on $\mu$, independently of the initial choice of $\chi \in \mathcal{O}$.

Thus, the problem of finding the irreducible representations of $Q$ based on a transitive measure is reduced to the problem of finding the irreducible representations of $H$. No such practicable method exists at present for a strictly ergodic measure, although even here at least some of the representations based on it can be constructed. Suppose $\mu$ is a strictly ergodic $H$-invariant measure. Let $\Omega = \{\omega(h)\}$ be any one-di-

mensional representation of $H$. For any $q = nh \in Q$, we define a representation $\tilde{\Delta} = \{\tilde{\Delta}(q)\}$ of $Q$ in the space $L^2(\hat{N}, \mu)$ by

$$\tilde{\Delta}(q)f(\chi) = \chi(n)\omega(h)f(\chi_h) \tag{28}$$

for all $f(\chi) \in L^2(\hat{N}, \mu)$. With the aid of the $H$-invariance and the strict ergodicity of $\mu$, the following theorem about the $\tilde{\Delta}$ can be proved.

*Theorem 3*[24]: Given a strictly ergodic measure $\mu$ on $\hat{N}$. For each one-dimensional representation $\Omega$ of $H$, the representation $\tilde{\Delta}$ of $Q$ corresponding to $\Omega$ via (28) is irreducible, infinite-dimensional, and based on $\mu$. Two such representations of $Q$ for different $\Omega$ are not necessarily inequivalent. There always exists at least one such representation: Take for $\Omega$ the identity representation of $H$.

In applying the prescriptions above to Cases (A) and (B), we shall give detailed results only for a subclass of irreducible representations of $Q$. This subclass consists of the so-called *physical* representations, which we now define.

For case (A) any representation (irreducible or otherwise) of $Q$ or of $N$ in which the representatives of the operators $[\mathbf{0}, \lambda]$ are $\exp(2\pi i\lambda)I$, where $I$ is the unit operator in the carrier space of the representation, is termed *physical*.[2] For the definition in case (B), we replace $\lambda$ by $\lambda_j$. The physical representations are the only ones that can occur in the physical state space $\mathcal{L}$, since we see from definition (14) [respectively (16)] that these operators are just multiplication by the respective phase factors.

The physical irreducible representations of $N$ are those whose characters (25) have $\zeta = 1$ [or $\zeta = 1 - |2/\eta|$ in case (B) if $|2/\eta| < 1$]. They form a subset of $\hat{N}$ that we denote by $\mathcal{P}$. For case (A) the set $\mathcal{P}$ is the infinite line $\mathcal{K} = \{k, 1 \mid -\infty < k < \infty\}$ and for case (B) the circle $\mathcal{S}^1 = \{\kappa, 1 \mid 0 \leq \kappa < 1\}$. In both cases $\mathcal{P}$ is an invariant set under the action of $H$, and so consists of a union of whole orbits, the so-called *physical* orbits. For (A) we have $\mathcal{K} = \mathcal{O}^{\zeta=1}$, comprising a single physical orbit. For (B) we have $\mathcal{S}^1 = \cup_{[\kappa]}\mathcal{O}^{[\kappa],1}$; since $|\zeta\eta|$ is irrational, we know from earlier discussion that this is a union of a nonmeasurable set of (countably) infinite physical orbits. In dealing with physical representations we drop the superscript $\zeta = 1$, writing $\mathcal{S}$ for the circle and $\mathcal{O}^{[\kappa]}$ for the orbits.

The invariant set $\mathcal{P}$ is in both cases a Borel set of $\hat{N}$. Ergodic $H$-invariant measures concentrated in $\mathcal{P}$ are therefore defined, and can be classified as measures on $\mathcal{P}$ into transitive (concentrated in the physical orbits) and strictly ergodic. We call them *physical* measures. It follows easily from Theorem 1 and (26) that an irreducible representation of $Q$ is physical if and only if it is based on a physical measure. Thus we deal in detail only with physical measures. For the two cases in turn:

(A) The only physical measure is the one concentrated on the single physical orbit, i.e., Lebesgue measure $dk$ on $\mathcal{K}$. From $\mathcal{K}$ we choose $\chi = \chi^{0,1}$ of (25a); here $H_\chi = E$ and has only the trivial irreducible representation. The corresponding allowed representation of $L_\chi = N$ is $\chi^{0,1}$ itself. The coset space is $Q/N = H = \{[\bar{v}_2\mathbf{a}_2, 0]\}$ from (21a) (where $\bar{v}_2$ replaces $v_2$). The orbit is therefore parametrized by $\bar{v}_2(-\infty < \bar{v}_2 < \infty)$, which we can check is related to the earlier parameter $k$ by $k = \xi\eta\bar{v}_2$. From the prescription (27) above, the representation $\Delta$ of $Q$ induced from $\chi^{0,1}$ has carrier space $\mathcal{L}(\mathcal{K}, dk) = L^2(R)$, i.e., the space of square-integrable functions on the infinite line. Using (27) we obtain

$$\left.\begin{aligned}&\Delta[v_1\mathbf{a}_1 + v_2\mathbf{a}_2, \lambda]f(k) = g(k)\\ &g(k) = e^{2\pi i\lambda}\exp[-2\pi i(k + \tfrac{1}{2}\xi\eta v_2)v_1]f(k + \xi\eta v_2)\end{aligned}\right\} \tag{29}$$

for all $f(k) \in L^2(R)$, where we use the parameter $k$ rather than $\bar{v}_2$ for convenience. From Theorem 2, $\Delta$ is the only irreducible representation based on the measure $dk$.

There is no difficulty in constructing the induced representations for the nonphysical measures. There is one, similar to (29), based on each $\mathcal{O}^\zeta(\zeta \neq 0)$. For each $\mathcal{O}^k$, where $H_\chi = H$, there is a one-dimensional representation based on $\mathcal{O}^k$ for each one-dimensional representation of $H$.

(B) The physical orbits are $\mathcal{O}^{[\kappa]} \in \mathcal{S}$. The physical measure $\mu^{[\kappa]}$ concentrated in $\mathcal{O}^{[\kappa]}$ assigns unit mass to each point of $\mathcal{S}$ with $\kappa$-coordinate in the set $[\kappa]$: The measure of any Borel set $\mathcal{E}$ in the circle $\mathcal{S}$ is $\mu^{[\kappa]}(\mathcal{E}) =$ number of points of the orbit in $\mathcal{E}$. For $\chi = \chi^{\kappa,1} \in \mathcal{O}^{[\kappa]}$, we have $H_\chi = E$ and $L_\chi = N$, with one allowed representation $\chi^{\kappa,1}$. Since $Q/N = H = \{[m\mathbf{a}_2, 0]\}$ from (21b) (where $m$ replaces $n_2$), we can parametrize the orbit with $m$. The single induced representation for this orbit we denote by $\Delta^{[\kappa]}$; its carrier space is $\mathcal{L}(\mathcal{O}^{[\kappa]}, \mu^{[\kappa]}) = l_2$, the space of square-summable sequences $\{f(m)\}$, and using (27) we have

$$\left.\begin{aligned}&\Delta^{[\kappa]}[n_1\mathbf{a}_1 + n_2\mathbf{a}_2, \lambda_j]\{f(m)\} = \{g(m)\},\\ &g(m) = e^{2\pi i\lambda_j}\exp[-2\pi i(\kappa + \xi\eta m\\ &\qquad + \tfrac{1}{2}\xi\eta n_2)n_1]f(m + n_2).\end{aligned}\right\} \tag{30}$$

Therefore, for each physical orbit of $\mathcal{S}$ there is, from Theorem 2, one infinite-dimensional irreducible representation $\Delta^{[\kappa]}$; Theorem 1 (last sentence) ensures that the representations corresponding to different orbits are equivalent.

For the strictly ergodic Lebesgue measure $d\kappa$ on $\mathcal{S}$, we construct physical irreducible representations of $Q$ according to the prescription (28). Their carrier space $L^2(\hat{N}, \mu)$ in this instance is $L^2(\mathcal{S})$, the space of square-integrable functions on $\mathcal{S}$. The one-dimensional representations of $H$ are $\Omega^\rho = \{\exp(-2\pi i\rho n_2)\}$, $0 \leq \rho < 1$, and the corresponding representations of $Q$, which we denote $\tilde{\Delta}^{[\rho]}$, are given by

$$\left.\begin{aligned}&\tilde{\Delta}^{[\rho]}[n_1\mathbf{a}_1 + n_2\mathbf{a}_2, \lambda_j]f(\kappa) = g(\kappa),\\ &g(\kappa) = e^{2\pi i\lambda_j}\exp[-2\pi i(\kappa n_1 + \rho n_2\\ &\qquad + \tfrac{1}{2}\xi\eta m_1 n_2)]f[\kappa + \xi\eta n_2)_r],\end{aligned}\right\} \tag{31}$$

where $f(\kappa) \in L^2(\mathcal{S})$. The symbol $[\rho]$ stands for the set $\{(\rho + \xi\eta m)_r \mid \text{all integers } n\}$ in the cyclic interval $0 \leq \rho < 1$, i.e., an orbit of $\rho$-values. This labeling anticipates the fact, proved below, that $\tilde{\Delta}^{[\rho_1]} \simeq \tilde{\Delta}^{[\rho_2]}$ if and only if $\rho_1$ and $\rho_2$ belong to the same $\rho$-orbit. The representations (31) are irreducible and infinite-dimensional (Theorem 3) and are not equivalent to the representations (30) (Theorem 1).

We can find many more irreducible representations based on the measure $d\kappa$ in the following indirect manner. In Sec. II we pointed out the different ways of expressing $Q$ as a semidirect product, according to the choice of basic lattice vector pair. Let $b \equiv (\mathbf{b}_1, \mathbf{b}_2)$ be a new basic vector pair, so that $n_1\mathbf{a}_1 + n_2\mathbf{a}_2 = n_1^b\mathbf{b}_1 + n_2^b\mathbf{b}_2$ for any vector of the $\mathbf{a}_1 - \mathbf{a}_2$ lattice. For the new factorization (23), we can go right through the above procedure, obtaining sets of irreducible representations of $Q$ analogous to (30) and (31); we have only to replace $n_1, n_2$, and $\xi$ everywhere by $n_1^b, n_2^b$ and $\xi^b$, respectively. This follows from the discussion at the end of Sec. II and, in particular, from the form invariance of the multiplication law under this substitution. Explicitly, we have representations $\Delta_b^{[\kappa]}$ analogous to (30) and $\tilde{\Delta}_b^{[\rho]}$ analogous to (31), where

$$\Delta_b^{[\kappa]}[n_1\mathbf{a}_1 + n_2\mathbf{a}_2, \lambda_j]\{f(m)\} = \Delta_b^{[\kappa]}[n_1^b\mathbf{b}_1 + n_2^b\mathbf{b}_2, \lambda_j]\{f(m)\} = \{g(m)\},$$
$$g(m) = e^{2\pi i\lambda_j} \exp[-2\pi i(\kappa + \xi^b\eta m + \tfrac{1}{2}\xi^b\eta n_2^b)n_1^b] f(m + n_2^b) \tag{32}$$

for all sequences $\{f(m)\} \in l_2$ and

$$\tilde{\Delta}_b^{[\rho]}[n_1\mathbf{a}_1 + n_2\mathbf{a}_2, \lambda_j]f(\kappa) = \tilde{\Delta}_b^{[\rho]}[n_1^b\mathbf{b}_1^b + n_2^b\mathbf{b}_2, \lambda_j]f(\kappa) = g(\kappa),$$
$$g(\kappa) = e^{2\pi i\lambda_j} \exp[-2\pi i(\kappa n_1^b + \rho n_2^b + \tfrac{1}{2}\xi^b\eta n_1^b n_2^b)] f[(\kappa + \xi^b\eta n_2^b)_r] \tag{33}$$

for all functions $f(\kappa) \in L^2(\mathcal{S})$. The components $n_1^b, n_2^b$ are related to $n_1, n_2$ via (22). These representations obviously reduce to (30) and (31), respectively, when $b = a \equiv (\mathbf{a}_1, \mathbf{a}_2)$ and $\xi^b = \xi$.

We have still to justify labeling the representations (33) and (31) by orbits $[\rho]$. We shall prove that $\tilde{\Delta}_b^{[\rho_1]} \simeq \tilde{\Delta}_b^{[\rho_2]}$ if and only if $\rho_1$ and $\rho_2$ are in the same orbit. Consider the Fourier transform that maps $f(\kappa) \in L^2(\mathcal{S})$ on to the sequence $\{f(m)\} \in l_2$, where

$$f(m) = \int_0^1 f(\kappa)e^{-2\pi i\kappa m}\, d\kappa .$$

Under this unitary transformation, the representation $\tilde{\Delta}_b^{[\rho]}$ of (33) is transformed into the (equivalent) representation $\Gamma$, where

$$\Gamma[n_1^b\mathbf{b}_1 + n_2^b\mathbf{b}_2, \lambda_j]\{f(m)\} = \{g(m)\},$$
$$g(m) = e^{2\pi i\lambda_j} \exp[-2\pi i(\rho - \xi^b\eta m - \tfrac{1}{2}\xi^b\eta n_1^b)n_2^b] f(m + n_1^b).$$

On comparing $\Gamma$ with the representations defined in (32) we see that $\Gamma \simeq \Delta_{\bar{b}}^{[\rho]}$, where $\bar{b} = (\mathbf{b}_2, \mathbf{b}_1)$ is the vector pair complementary to $b$ and where we have used the fact that $\xi^{\bar{b}} = -\xi^b$. Consequently we have $\tilde{\Delta}_b^{[\rho]} \simeq \Delta_{\bar{b}}^{[\rho]}$, and since we know from Theorem 1 that $\Delta_{\bar{b}}^{[\rho_1]} \simeq \Delta_{\bar{b}}^{[\rho_2]}$ if and only if $\rho_1$ and $\rho_2$ belong to the same orbit $[\rho_1] = [\rho_2]$, the assertion is proved. We have in fact proved the following.

*Proposition 2:* Given the complementary factorizations $Q = N(\mathbf{b}_1) \circledS H(\mathbf{b}_2) = N(\mathbf{b}_2) \circledS H(\mathbf{b}_1)$ for the two choices $b \equiv (\mathbf{b}_1, \mathbf{b}_2)$ and $\bar{b} \equiv (\mathbf{b}_2, \mathbf{b}_1)$ of basic primitive lattice vector pair. Then, for the representations defined in (32) and (33) we have $\tilde{\Delta}_b^{[\kappa]} \simeq \Delta_b^{[\kappa]}$ and $\tilde{\Delta}_{\bar{b}}^{[\kappa]} \simeq \Delta_b^{[\kappa]}$ for all orbits $[\kappa] \in \mathcal{S}$. In other words, the set of representations (32) and (33) obtained from complementary factorizations is the same; but in going from one factorization to the other the role of the strictly ergodic measure is interchanged with the role of the transitive measures (on the orbits).

The next proposition establishes the equivalence relationships among the $\Delta_b^{[\kappa]}$ for varying $b$.

*Proposition 3:* Let $b \equiv (\mathbf{b}_1, \mathbf{b}_2)$ and $b' \equiv (\mathbf{b}_1', \mathbf{b}_2')$ be any two basic vector pairs. Then $\Delta_{b'}^{[\kappa']} \simeq \Delta_b^{[\kappa]}$ if and only if $\mathbf{b}_1' = \mathbf{b}_1$ and $[\kappa'] = [\kappa]$.

*Proof:* It follows from (22) that the relation between the vector pairs $b'$ and $b$ is

$$\mathbf{b}_i' = \sum_{j=1}^{2} L_{ij}\mathbf{b}_j, \quad i = 1, 2, \tag{34}$$
$$L_{ij} \text{ integral}, \quad L_{11}L_{22} - L_{12}L_{21} = (\xi^{b'}/\xi^b) = \pm 1$$

for some $L_{ij}$. Let us take the irreducible representation $\Delta_b^{[\kappa]}$ of $Q$ obtained from the factorization $Q = N(\mathbf{b}_1) \circledS H(\mathbf{b}_2)$ and defined in (32). Consider the factorization $Q = N(\mathbf{b}_1') \circledS H(\mathbf{b}_2')$. It follows from Theorem 1 that $\Delta_b^{[\kappa]}$ must be based on some ergodic $H$-invariant measure on $N(\mathbf{b}_1')$ (which will be physical), and to find this measure we determine the restriction $\Delta_b^{[\kappa]} \downarrow N(\mathbf{b}_1')$ of the representation to $N(\mathbf{b}_1')$. For any element $[r\mathbf{b}_1', \lambda_j]$ of $N(\mathbf{b}_1')$ for $r$ an integer, we have, using (32) and (34),

$$\Delta_b^{[\kappa]}[r\mathbf{b}_1', \lambda_j]\{f(m)\} = \{g(m)\},$$
$$g(m) = e^{2\pi i\lambda_j} \exp[-2\pi i(\kappa + \xi^b\eta m + \tfrac{1}{2}\xi^b\eta L_{12}r)L_{11}r] f(m + rL_{12}) \tag{35}$$

for all $\{f(m)\} \in l_2$. By inspection, we see there are two cases:

*(a) $L_{12} = 0$:* Then the only solutions of (34) consistent with the half-plane restriction on the basic vectors all have $L_{11} = 1$ and, consequently, $\mathbf{b}_1' = \mathbf{b}_1$. Furthermore, from (35) with $L_{12} = 0$ and $L_{11} = 1$, it follows that $\Delta_b^{[\kappa]} \downarrow N(\mathbf{b}_1')$ is equivalent to a representation $\Lambda_\mu$ of $N(\mathbf{b}_1')$ of the kind (26), where $\mu$ is the atomic measure $\mu^{[\kappa]}$ concentrated in the orbit $|\kappa|$. Since we know there is only one irreducible representation of $Q$ based on each orbit, we must have $\Delta_b^{[\kappa]} \simeq \Delta_{b'}^{[\kappa']}$ when (and only when) $[\kappa'] = [\kappa]$.

*(b) $L_{12} \neq 0$:* From (35), the space $l_2$ decomposes into a direct sum of $|L_{12}|$ subspaces each invariant under $N(\mathbf{b}_1')$. In fact, $l_2 = \oplus \sum_{s=1}^{|L_{12}|} l_2^{(s)}$, where $l_2^{(s)}$ consists of all those sequences $\{f(m)\}$ which have zeros everywhere except for $m = s + uL_{12}$, $s$ a fixed integer with $0 \leq s < |L_{12}|$, and $u$ running over all integers. Let us consider the operations (35) restricted to the subspace $l_2^{(s)}$. We can rewrite any vector of $l_2^{(s)}$ as a sequence $g = \{g(u)\}$ with $g(u) = f(s + uL_{12})$. Then from (35)

$$\Delta_b^{[\kappa]}[r\mathbf{b}_1', \lambda_j]\{g(u)\} = \{h(u)\},$$
$$h(u) = e^{2\pi i\lambda_j}[\alpha(u + r)/\alpha(u)]g(u + r), \tag{36}$$
$$\alpha(u) = \exp[-2\pi i L_{11}u(\kappa + \xi^b\eta s + \tfrac{1}{2}\xi^b\eta L_{12}u)].$$

Under the unitary transformation of $l_2^{(s)}$ onto $L^2(\mathcal{S})$

that maps $\{g(u)\}$ onto $g(\beta)$ with $\beta$ $(0 \leq \beta < 1)$ the cyclic coordinate for $\mathcal{S}$ and

$$g(\beta) = \sum_{u=-\infty} e^{2\pi i \beta u} \alpha(u) g(u),$$

the representation (36) of $N(\mathbf{b}_1')$ is transformed into the representation $\gamma$, where

$$\gamma[r\mathbf{b}_1', \lambda_j] g(\beta) = e^{2\pi i \lambda_j} e^{-2\pi i \beta r} g(\beta).$$

Evidently, $\gamma$ is equivalent to a representation $\Lambda_\mu$ of $N(\mathbf{b}_1')$ of the kind (26), where $\mu$ is the (strictly ergodic) Lebesgue measure $d\beta$ on $\mathcal{S}$. The argument is the same for each subspace $l_2^{(s)}$, so that altogether $\Delta_b^{[\kappa]} \downarrow N(\mathbf{b}_1') \simeq |L_{12}| \Lambda_\mu$ for $\mu = d\beta$. From the last sentence of Theorem 1 we conclude that $\Delta_b^{[\kappa]} \not\simeq \Delta_{b'}^{[\kappa']}$ for all $[\kappa']$. The two results (a) and (b) prove the proposition.

These propositions establish the equivalence relationships among all the representations of the form (32) and (33). Let us say that two basic vector pairs $b$ and $b'$ are *equivalent* if $\mathbf{b}_1 = \mathbf{b}_1'$, and write $[b]$ to denote an equivalence class of basic vector pairs. From the Proposition 3, $\Delta_b^{[\kappa]}$ and $\Delta_{b'}^{[\kappa]}$ are equivalent representations if and only if $b$ and $b'$ are equivalent vector pairs. Therefore we will write $\Delta_{[b]}^{[\kappa]}$ to denote the equivalence class of representations, individual members of which are obtained by taking any $b \in [b]$ (and any $\kappa \in [\kappa]$) in (32). As a consequence of Propositions 2 and 3 we have

*Proposition 4:* The irreducible representations $\Delta_{[b]}^{[\kappa]}$ of $Q$, for the different equivalence classes $[b]$ and the different orbits $[\kappa]$, are mutually inequivalent and form the complete set of inequivalent representations defined in (32) and (33). We note that there is one equivalence class $[b]$ for each choice of $\mathbf{b}_1$ as the shortest lattice vector in its direction (in the allowed half-plane).

Returning to the original factorization of $Q$, with normal subgroup $N = N(\mathbf{a}_1)$, we ask for the (physical) measure classes on which the different $\Delta_{[b]}^{[\kappa]}$ of Proposition 4 are based. When $[b] = [a]$, $\Delta_{[a]}^{[\kappa]}$ is, of course, the equivalence class of representations exemplified by (30) and based on the orbit $[\kappa] \in \mathcal{S}$. For any other $[b]$, we find that

$$\Delta_{[a]}^{[\kappa]} \downarrow N = |l_{12}| \Lambda_\mu, \quad \mu = d\kappa \text{ on } \mathcal{S},$$

where the integer $l_{12}$ is as in (22). This relation is obtained by the argument of part (b) of the proof of Proposition 3, with $b' = a$. Hence we have the following proposition.

*Proposition 5:* The irreducible representation $\Delta_{[b]}^{[\kappa]}$ of $Q$ is based on the transitive measure concentrated in the orbit $[\kappa]$ in $\mathcal{S}$ when $[b] = [a]$ and on the strictly ergodic measure $d\kappa$ on $\mathcal{S}$ when $[b] \neq [a]$.

Thus there is, for each $[\kappa]$, a denumerable infinity of different irreducible representations based on $d\kappa$, one for each choice of $\mathbf{b}_1 \neq \mathbf{a}_1$ in the allowed half-plane. For the particular case $\mathbf{b}_1 = \mathbf{a}_2$, i.e., $[b] = [\bar{a}]$, the equivalence class of representations $\Delta_{[\bar{a}]}^{[\kappa]}$ is the one exemplified by $\tilde{\Delta}^{[\rho]}$ of (31), for $\rho = \kappa$.

For completeness, we should say a word about the nonphysical irreducible representations of $Q$. These are based on measures concentrated in the circle $\mathcal{S}^\zeta \in \hat{N}$. For $|\zeta\eta|$ irrational, the analysis is exactly as for the physical representations. When $|\zeta\eta| = m/M$ is rational, the only measures are the transitive ones based on the orbits $\mathcal{O}^{\bar{\kappa},\zeta} (0 \leq \bar{\kappa} < 1/M)$, as we have seen. For each orbit there is, following Theorem 2, one induced representation for each irreducible representation of the isotropy group $H^{\bar{\kappa}}$. Since $H^{\bar{\kappa}}$ is commutative, its irreducible representations are one-dimensional; then the induced representations are, from definition (27), all of dimension $M$, the index of $H^{\bar{\kappa}}$ in $H$. These nonphysical representations of $Q$ for $|\zeta\eta|$ rational are isomorphic with the physical representations that one finds for a "rational" magnetic field $\eta' = \zeta\eta$.

We conclude by writing down the representations of $G = P \times Q$ for the two cases $G = W$ and $G = T_\eta$ and by summarizing the main results of the section.

*Summary:* (A) The group $W$ is of Type I. The complete set of physical irreducible representations are the Kronecker products

$$\Delta^{k_3} \equiv \chi^{k_3} \times \Delta, \quad -\infty < k_3 < \infty \tag{37a}$$

of the factors (24a) and (29). More explicitly, for the element $[\mathbf{v}, \lambda]$ we have

$$\Delta^{k_3}[\mathbf{v}, \lambda] = e^{-2\pi i k_3 v_3} \Delta[v_1\mathbf{a}_1 + v_2\mathbf{a}_2, \lambda], \tag{37b}$$

where the carrier space is $L^2(R)$ and the expression for the second factor is given in (29). All these representations are infinite-dimensional.

(B) The group $T_\eta$ is not of Type I for irrational $\eta$. The identification of *all* the irreducible representations appears to be an unsolved mathematical problem for groups that are not of Type I. In the case of $T_\eta$, this is true not only for all the irreducible representations, but also for the subset of physical ones. Of the latter, those we have found are the Kronecker products

$$\Delta_{[b]}^{\kappa_3,[\kappa]} \equiv \chi^{\kappa_3} \times \Delta_{[b]}^{[\kappa]}, \quad 0 \leq \kappa, \kappa_3 < 1 \tag{38a}$$

of the factors (24b) and (32). Here $[\kappa]$ is an orbit in the circle $\mathcal{S}$ of unit circumference, and $[b]$ is an equivalence class of basic primitive lattice vector pairs.

More explicitly, the representation $\Delta_{[b]}^{\kappa_3,[\kappa]}$ is carried by the space $l_2$ of sequences $\{f(m)\}$ and is given by

$$\Delta_{[b]}^{\kappa_3,[\kappa]}[n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \lambda_j]\{f(m)\} = \Delta_{[b]}^{\kappa_3,[\kappa]}[n_1^b\mathbf{b}_1 + n_2^b\mathbf{b}_2 + n_3\mathbf{a}_3, \lambda_j]\{f(m)\} = \{g(m)\}, \tag{38b}$$

$$g(m) = e^{2\pi i \lambda_j} e^{-2\pi i \kappa_3 n_3} \exp[-2\pi i(\kappa + \xi^b \eta m + \tfrac{1}{2}\xi^b \eta n_2^b) n_1^b] f(m + n_2^b),$$

where $n_1^b$ and $n_2^b$ are related to $n_1$ and $n_2$ via (22) and $n_3$ is the same whatever the choice of $b$. All the representations are infinite-dimensional.

If we repeat the calculation with basic vector trios $(\mathbf{c}_1, \mathbf{c}_2, \mathbf{a}_3)$, where the $\mathbf{c}_1 - \mathbf{c}_2$ plane does not coincide with the $\mathbf{a}_1 - \mathbf{a}_2$ plane, no new representations are obtained. This is shown in Appendix A.

The representations for $[b] = [a]$ and $[b] = [\bar{a}]$ in case (B) were given by Opechowski and Tam.[4] We can now

answer two questions posed by them in Ref. 4 p. 545. Question (1), in our terminology, asks whether for $[b] = [a]$ the representation (38) is independent (to within equivalence) of the member of the orbit $[\kappa]$ from which $\Delta^{[\kappa]}_{[a]}$ is induced? The answer is yes, from Theorem 2 of the general (Mackey) theory. Question (2) asks whether the set of representations (38) for $[b] = [a]$ is the same, apart from equivalence, as the set for $[b] = [\bar{a}]$. From our results (Proposition 4) the answer is no.

## IV. REPRESENTATIONS IN THE STATE SPACE

In this section we examine the nature of the representations carried by the physical state space $\mathcal{L} = L^2(R^3)$ for the two invariance groups we have been dealing with in cases (A) and (B), namely $W$ for the potential-free system and its subgroup $T_\eta$ for the system with irrational field $\eta$ along a lattice vector.[25] We should remark that Bentosela[26] has made a detailed study of this problem for case (C) of a rational field along a lattice vector, from a somewhat different point of view.

From the beginning, we shall express position and translation vectors in terms of any of the possible basic lattice vector trios $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{a}_3)$ we have introduced, the pair $b = (\mathbf{b}_1, \mathbf{b}_2)$ being related to $a = (\mathbf{a}_1, \mathbf{a}_2)$ as in (22). Thus, take an arbitrary but fixed such trio for the following. Then, as a generalization of (4) and (6), we write

$$\mathbf{r} = x_1^b \mathbf{b}_1 + x_2^b \mathbf{b}_2 + x_3 \mathbf{a}_3, \quad \mathbf{v} = v_1^b \mathbf{b}_1 + v_2^b \mathbf{b}_2 + v_3 \mathbf{a}_3, \quad \mathbf{t} = n_1^b \mathbf{b}_1 + n_2^b \mathbf{b}_2 + n_3 \mathbf{a}_3. \tag{39}$$

(The third components have no superscript since they do not depend on $b$.) A given group element $[\mathbf{v}, \lambda]$ of $W$ or $[\mathbf{t}, \lambda_j]$ of $T_\eta$ retains precisely the same form as in (14) or (16), respectively, except that we make the replacements $x_i \to x_i^b; v_i \to v_i^b; n_i \to n_i^b (i = 1, 2)$ and $\xi \to \xi^b$, wherever appropriate. The respective multiplication laws (15) and (17) also retain the same form with the same replacements, as was mentioned at the end of Sec. II.

For our purposes, the most appropriate way of decomposing $\mathcal{L}$ is in terms of the so-called Landau functions, which are continuous eigenfunctions of $\mathcal{H}$ in the potential-free case. They are not square-integrable, and the decomposition involves direct integration.

The Landau functions will be defined relative to the framework of basic vectors $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{a}_3)$, and for this purpose it is convenient to introduce an auxiliary cartesian coordinate system attached to the vectors. We write $\mathbf{r} = (x, y, z)$, with the positive $z$ axis along $\mathbf{a}_3$, the $x$ axis in the $\mathbf{a}_3 - \mathbf{b}_1$ plane directed so that $\mathbf{b}_1$ has positive $x$ projection, and the $y$ axis making the system right-handed. Then the Landau functions are denoted $|l, k_3 k\rangle_b$ and given by

$$\langle \mathbf{r} | l, k_3, k\rangle_b = A(l, k_3, k) \exp\{[(2\pi i k_3 z)/a_3] - i\chi x(\tfrac{1}{2} y - \beta)\} u_l(\chi^{1/2}(y - \beta)), \tag{40}$$

where $u_l$ is the $l$th Hermite function, $\chi = |e\mathbf{B}|/\hbar c$, $\beta = \gamma k_3 + \delta k$ with $\gamma$ and $\delta$ constants independent of the wave vectors, and $A(l, k_3, k)$ is a normalization constant. This last is chosen to give convenient normalization and transformation properties to the Landau functions. The precise definition of $\beta$ and $A(l, k_3, k)$ are found in Appendix B. Except for details depending on the lattice vectors, the functions (40) are those given by Johnson and Lippmann.[27]

Of the labels in $|l, k_3, k\rangle_b$, the first designates the Landau level $l$, and $k_3$ and $k$ are dimensionless wave vectors corresponding to propagation in the $\mathbf{a}_3$ and $\mathbf{b}_1$ directions, respectively. For any fixed $b$, the set of functions $\{|l, k_3, k\rangle_b \mid l = 0, 1 \cdots \infty; -\infty < k_3, k < \infty\}$ satisfy the relations of completeness and closure[28]

$${}_b\langle l, k_3, k | l', k_3', k'\rangle_b = \delta_{ll'} \delta(k_3 - k_3') \delta(k - k'), \tag{41a}$$

$$\sum_{l=0}^{\infty} \iint_{-\infty}^{\infty} |l, k_3, k\rangle_b \, dk_3 dk \; {}_b\langle l, k_3, k| = I, \tag{41b}$$

where, of the delta functions, $\delta_{ll'}$ is the Kronecker function and the others are Dirac functions, and $I$ is the unit operator in $\mathcal{L}$. We add to these relations the overlap integral between Landau functions defined for different basic vector pairs $b$ and $b'$:

$${}_b\langle l, k_3, k | l', k_3', k'\rangle_{b'} = \delta_{ll'} \delta(k_3 - k_3') \; {}_b\langle l, k_3, k | l, k_3, k'\rangle_{b'}. \tag{42}$$

Here (i) if $[b'] = [b]$, then the kernel ${}_b\langle l, k_3, k | l, k_3, k'\rangle_{b'}$ is equal to $\delta(k - k')$ and (42) reduces to (41a), and (ii) if $[b'] \neq [b]$, then the kernel is a bounded function continuous in $k$ and $k'$ (for each $l$ and $k_3$). Relation (42) is derived in detail in Appendix B.

In accordance with the properties (41) of the Landau functions, we can decompose $\mathcal{L}$ as

$$\mathcal{L} = \oplus \sum_{l=0}^{\infty} \int_{-\infty}^{\infty} \mathfrak{M}(l, k_3) dk_3, \tag{43a}$$

$$\mathfrak{M}(l, k_3) = \oplus \int_{-\infty}^{\infty} \{\langle \mathbf{r} | l, k_3, k\rangle_b\} \, dk, \tag{43b}$$

where $\{\langle \mathbf{r} | l, k_3, k\rangle_b\}$ is the one-dimensional space spanned by the corresponding Landau function. The constituent spaces $\mathfrak{M}(l, k_3)$ in (43a) are the eigenspaces for $\mathcal{H}$ in the potential-free case, corresponding to the continuum eigenvalues $\mathcal{E}(l, k_3) = (\hbar^2 k_3^2/2m) + \hbar\omega(l + \frac{1}{2}); \omega = |e\mathbf{B}|/mc$, respectively. The decomposition (43) is valid for any choice of $b$.

The Landau functions transform under the group elements $[\mathbf{v}, \lambda]$ of W as

$$\langle \mathbf{r} | [\mathbf{v}, \lambda] | l, k_3, k\rangle_b = e^{2\pi i \lambda} \exp[-2\pi i (k_3 v_3 + k v_1^b - \tfrac{1}{2} \xi^b \eta v_1^b v_2^b)] \times \langle \mathbf{r} | l, k_3, k - \xi^b \eta v_2^b\rangle_b, \tag{44}$$

where to obtain this expression we have used (14) adapted to the vector pair $b$ as described above, together with (5), (39), and the definition of the constants in the Landau function (40), to be found in Appendix B. The transformation under the elements $[\mathbf{t}, \lambda_j]$ of $T_\eta$ are found simply by restriction of (44) to $T_\eta$. We see from (43) and (44) that the spaces $\mathfrak{M}(l, k_3)$ are stable under the operations of $W$ and $T_\eta$, and therefore in both cases the analysis of the representation carried by $\mathcal{L}$ is reduced to study of the representations in the $\mathfrak{M}(l, k_3)$. Thus we shall be dealing in the following paragraphs with a constituent space $\mathfrak{M}(l, k_3)$ for fixed values of $l$ and $k_3$, and these two labels will be omitted wherever possible. The constituent space will be

denoted $\mathfrak{M}$, and relations (41), (42), and (43b) are replaced by

$$\mathfrak{M} = \oplus \int_{-\infty}^{\infty} \{|\mathbf{r}|k\rangle_b\}\, dk,$$
$$ {}_b\langle k|k'\rangle_b = \delta(k-k'), \qquad \int_{-\infty}^{\infty} |k\rangle_b\, dk\, {}_b\langle k| = I, \tag{45}$$

where $I$ is now the unit operator in $\mathfrak{M}$ and only the label $k$ is retained in the Landau function. Let $\langle \mathbf{r}|\phi\rangle$ be any vector in $\mathfrak{M}$; then from (45) we have

$$\langle \mathbf{r}|\phi\rangle = \int_{-\infty}^{\infty} \langle \mathbf{r}|k\rangle_b\ {}_b\langle k|\phi\rangle\, dk, \tag{46}$$

where the Fourier transform function ${}_b\langle k|\phi\rangle$ is square integrable in $k(-\infty < k < \infty)$. We shall denote the (Hilbert) space of Fourier transforms ${}_b\langle k|\phi\rangle$ by $\mathfrak{M}_b$. The Fourier transforms of the same $\langle \mathbf{r}|\phi\rangle$ in two spaces $\mathfrak{M}_b$ and $\mathfrak{M}_{b'}$ corresponding to different vector pairs $b$ and $b'$ are related by

$${}_b\langle k|\phi\rangle = \int_{-\infty}^{\infty} {}_b\langle k|k'\rangle_{b'}\, {}_{b'}\langle k'|\phi\rangle dk', \tag{47}$$

where the kernel ${}_b\langle k|k'\rangle_{b'}$ is as defined in (42) with only the labels $k$ and $k'$ retained; it is given explicitly in Appendix B. We note from (46) and (47) that the assignments $\langle \mathbf{r}|\phi\rangle \mapsto {}_b\langle k|\phi\rangle$ and ${}_b\langle k|\phi\rangle \mapsto {}_{b'}\langle k'|\phi\rangle$ for all $|\phi\rangle$ are unitary mappings of $\mathfrak{M}$ onto $\mathfrak{M}_b$ and $\mathfrak{M}_b$ onto $\mathfrak{M}_{b'}$, respectively.

Let us now take the two cases in turn:

(A) We denote by $\Gamma$ the representation of $W$ carried by $\mathfrak{M}$. It is defined directly by (44) (for fixed $l$ and $k_3$), and under the unitary mapping (46) it is transformed into the equivalent representation $\Gamma_b$ in $\mathfrak{M}_b$, given by

$$ {}_b\langle k|[\mathbf{v},\lambda]|\phi\rangle = e^{2\pi i\lambda} \exp[-2\pi i(k_3 v_3 + k v_1^b + \tfrac{1}{2}\xi^b \eta v_1^b v_2^b)]\ {}_b\langle k + \xi^b \eta v_2^b|\phi\rangle \tag{48}$$

for all ${}_b\langle k|\phi\rangle \in \mathfrak{M}_b$. The $\Gamma_b$ for different $b$ are all (unitarily) equivalent via the mappings (47), and on taking $b = a$ we see, by comparison of (48) with the representation of $W$ defined by (37) and (29), that $\Gamma \simeq \Gamma_a \simeq \Delta^{k_3}$. [We recall that in (29) the label $b = a$ is understood.] In particular, therefore, $\Gamma$ is irreducible.

(B) The representation of $T_\eta$ carried by $\mathfrak{M}$, denoted by $\gamma$, is evidently subduced from $\Gamma$ of $W$. It is, however, no longer irreducible; we shall show that it is a primary representation of $T_\eta$ and can be decomposed into irreducible constituents in an infinite number of different ways such that no two decompositions have a constituent in common. This proves it is not of Type I.[29] We first establish these different decompositions. The representation $\gamma$ is equivalent to the representation $\gamma_b$ in $\mathfrak{M}_b$ obtained by restriction of (48) to the element $[\mathbf{t},\lambda_j]$ of $T_\eta$: Thus

$$ {}_b\langle k|[\mathbf{t},\lambda_j]|\phi\rangle = e^{2\pi i\lambda_j} \exp[-2\pi i(k_3 n_3 + k n_1^b + \tfrac{1}{2}\xi^b \eta n_1^b n_2^b)]\ {}_b\langle k + \xi^b \eta n_2^b|\phi\rangle \tag{49}$$

defines $\gamma_b$. We observe that the discrete nature of the translations in (49) allows us to make the decomposition

$$\mathfrak{M}_b = \oplus \int_0^{|\eta|} \mathfrak{M}_b(k)\, dk, \qquad \gamma_b = \oplus \int_0^{|\eta|} \gamma_b(k)\, dk, \tag{50}$$

where $\mathfrak{M}_b(k)$ is the space $l_2$ of sequences $\{{}_b\langle k + \eta m|\phi\rangle\}$ for which $\sum_m |{}_b\langle k + \eta m|\phi\rangle|^2 < \infty$, and $k$ is restricted here to the interval $[0,|\eta|]$. The space $\mathfrak{M}_b(k)$ is stable under $T_\eta$ and carries the representation denoted by $\gamma_b(k)$ in (50). The form of $\gamma_b(k)$ follows from (49), and on comparing it with (38) we observe that

$$\gamma_b(k) \simeq \Delta_{[b]}^{\kappa_3,[\kappa]}, \qquad \kappa_3 = (k_3)_r, \qquad \kappa = (k)_r. \tag{51}$$

Therefore the constituent representations in the decomposition (50) are all irreducible. Furthermore, the decomposition itself depends critically on the choice of $b$, or rather on the equivalence class $[b]$. Indeed, it follows from (51) and Proposition 4 of Sec. III that no two decompositions (50) possess an irreducible constituent in common. In other words, the representation $\gamma$, which is equivalent to $\gamma_b$ for each $b$ via a unitary mapping (46), is equivalent to an infinite number of decompositions (50), one for each class $[b]$, such that the irreducible constituents in one decomposition are inequivalent to those in all the others. This nonuniqueness of decomposition into irreducible constituents is a manifestation of the fact that $T_\eta$ is not of Type I.

A further property of the decomposition (50) for a fixed $b$, is that the irreducible constituents are "inextricably mixed" in such a way that there are an infinite number of inequivalent ones contained in any interval, however small, in the integral over $k$. This is due to the erratic way in which the orbit $[\kappa]$ in (51) depends on $\kappa = (k)_r$. We cannot "disentangle" the representations by grouping the equivalent ones together, since, as we saw in Sec. II, the distinguishing labels would have to be a nonmeasurable set of the $k$.

By availing ourselves of the transformation of $\mathfrak{M}_b$ onto $\mathfrak{M}$ inverse to (46), we can find the decomposition of $\mathfrak{M}$ equivalent to (50). It has the same form as (50), the constituent space labeled by $k(0 \leq k < |\eta|)$ carrying a representation equivalent to (51), and consisting of the space of functions $\langle \mathbf{r}|\Phi\rangle$ on $R^3$ of the form

$$\langle \mathbf{r}|\Phi\rangle = \sum_{m=-\infty}^{\infty} \langle \mathbf{r}|k + \eta m\rangle_b\ {}_b\langle k + \eta m|\phi\rangle \tag{52}$$

for all sequences $\{{}_b\langle k + \eta m|\phi\rangle\} \in \mathfrak{M}_b(k)$. This constituent space is a Hilbert space, with scalar product of $|\Phi_1\rangle$ and $|\Phi_2\rangle$ defined by

$$\langle \Phi_1|\Phi_2\rangle = \sum_{m=-\infty}^{\infty} \langle \phi_1|k + \eta m\rangle_b\ {}_b\langle k + \eta m|\phi_2\rangle.$$

The proof that $\langle \mathbf{r}|\Phi\rangle$ exists as an everywhere-defined and bounded function on $R^3$ is found in Appendix B. Reintroducing all the labels for a moment, this means that the infinite set of Landau functions $\{\langle \mathbf{r}|l, k_3, k + \eta m\rangle_b | m = 0, \pm 1, \ldots, \pm\infty\}$ span a space of wavefunctions carrying the irreducible representation $\Delta_{[b]}^{\kappa_3,[\kappa]}$ of $T_\eta$, where $\kappa_3 = (k_3)_r$ and $\kappa = (k)_r$ as in (51). Opechowski and Tam[4] have made this observation for the case $b = a$ and a crystal with orthorhombic symmetry.

To prove that $\gamma$ is primary, we shall use the fact that a representation is primary if and only if its commuting algebra is a factor, i.e., has a center consisting of multiples of the identity operator.[7] (We recall that the commuting algebra of a representation is the algebra of bounded operators in the representation space that commute with each operator of the representation, and that its center consists of those operators of the algebra that commute with every operator

of the algebra.) Consider the representation $\gamma_b$ in $\mathfrak{M}_b$. Let $A$ be any multiplicative operator in $\mathfrak{M}_b$ defined by

$$ {}_b\langle k|A|\phi\rangle = \alpha(k)\ {}_b\langle k|\phi\rangle, \qquad \alpha(k+\eta)=\alpha(k) \tag{53}$$

for all ${}_b\langle k|\phi\rangle \in \mathfrak{M}_b$, where $\alpha(k)$ is a bounded Lebesgue-measurable function on the infinite line with periodicity $\eta$. It follows from (49) and (50) that $A$ belongs to the commuting algebra of $\gamma_b$. Any (bounded) operator in the centre of this algebra must therefore commute with all operators of the kind (53), as well as with $\gamma_b$; from a standard result on multiplicative operators[30] and from Schur's lemma applied with reference to the decomposition (50), it follows that such an operator is then itself of the kind (53). The center is therefore contained in the set of operators $A$. An analogous conclusion is, of course, valid for any choice of $b$. Let us take $b'$ so that $[b'] \neq [b]$. Since the center of $\gamma_b$ must be mapped onto the center of $\gamma_{b'}$, under the mapping (47) of $\mathfrak{M}_b$ onto $\mathfrak{M}_{b'}$ we have that

$$\alpha(k)\ {}_b\langle k|\phi\rangle = \int_{-\infty}^{\infty} {}_b\langle k|k'\rangle_{b'}\ \alpha'(k')\ {}_{b'}\langle k'|\phi\rangle\, dk', \tag{54}$$

for all ${}_b\langle k|\phi\rangle \in \mathfrak{M}_b$. Here $\alpha'(k')$ is a bounded Lebesgue-measurable function on the infinite line with periodicity $\eta$, which defines the image of $A$ in $\mathfrak{M}_{b'}$ via an expression analogous to (53). We now show that (47) and (54) imply that $\alpha(k) = \alpha'(k') = \text{const}$ for all $k$ and $k'$, using a particular property of the kernel ${}_b\langle k|k'\rangle_{b'}$. Consider any operator $[\mathbf{v}, 0]$ belonging to the group $W$; from unitarity we have the invariance

$$ {}_b\langle k|k'\rangle_{b'} = {}_b\langle k|[\mathbf{v},0]|[\mathbf{v},0]|k'\rangle_{b'} $$

of the scalar product. Making this substitution for the kernel in (54) and using (44) for the transformation of the Landau functions under $[\mathbf{v}, 0]$, we can rewrite (54) after a little manipulation as

$$\alpha(k-\xi^b\eta v_2^b)\ {}_b\langle k|\phi\rangle = \int_{-\infty}^{\infty} {}_b\langle k|k'\rangle_{b'} \times \alpha'(k'-\xi^{b'}\eta v_2^{b'})\ {}_{b'}\langle k'|\phi\rangle\, dk'.$$

Now choose $\mathbf{v}$ so that $v_1^{b'} = u$, $v_2^{b'} = 0$ for any real $u$; from the equality $v_1^{b'}\mathbf{b}_1' + v_2^{b'}\mathbf{b}_2' = v_1^b\mathbf{b}_1 + v_2^b\mathbf{b}_2$ and the relations (34) between $b'$ and $b$, we have $v_2^b = uL_{12}$, where $L_{12} \neq 0$ since $[b'] \neq [b]$. Comparing the last expression with (54) we obtain immediately that

$$\alpha(k-\xi^b\eta L_{12}u) = \alpha(k)$$

for all $u$. Consequently $\alpha(k)$ is a constant function, and likewise $\alpha'(k')$ is equal to the same constant function: The center consists therefore of constant functions only, and $\gamma_b \simeq \gamma_{b'} \simeq \gamma$ is primary. It is not of Type I, as we have seen, because of the nonuniqueness of its decomposition into irreducible constituents described earlier.[29]

It is interesting to note the relationship between the representations $\Gamma$ and $\gamma$ of $W$ and $T_\eta$, respectively, carried by the same space $\mathfrak{M}$. In fact, from the results under headings (A) and (B) above, we can write

$$\gamma = \Gamma\downarrow T_\eta \simeq \Delta^{k_3}\downarrow T_\eta = [\chi^{k_3}\times\Delta]\downarrow T_\eta = \chi^{\kappa_3}\times[\Delta\downarrow T_\eta], \qquad \kappa_3 = (k_3)_r,$$

where we have used (25) and (37). The representation $\chi^{k_3}$ of $P_B$ is subduced from $\chi^{k_3}$ of $P_A$, and likewise $\Delta\downarrow T_\eta$ of $Q_B$ from $\Delta$ of $Q$. We can derive from these relations, together with (50) and (51), the following:

*Proposition 6:* The representation of $T_\eta$ subduced from the irreducible representation $\Delta^{k_3}$ of $W$ is primary and not of Type I. Two such representations subduced from $\Delta^{k_3}$ and $\Delta^{k_3'}$ of $W$, respectively, are equivalent if and only if $(k_3')_r = (k_3)_r$, and we write $\Lambda^{\kappa_3} \simeq \Delta^{k_3}\downarrow T_\eta$, where $\kappa_3 = (k_3)_r$. The primary representation can be decomposed into irreducible constituent representations of $T_\eta$ as

$$\Lambda^{\kappa_3} \simeq \int_0^{|\eta|} \Delta_{[b]}^{\kappa_3,[\kappa]}\, dk, \qquad \kappa = (k)_r$$

for any choice of $b$; for $b$ and $b'$ such that $[b'] \neq [b]$ the corresponding two decompositions have no irreducible constituent in common. Furthermore, if $\Lambda = \Delta\downarrow T_\eta$ is the representation of $Q_B$ subduced from the irreducible representation $\Delta$ of $Q_A$, then $\Lambda$ is a primary representation not of Type I and

$$\Lambda \simeq \int_0^{|\eta|} \Delta_{[b]}^{[\kappa]}\, dk, \qquad \kappa = (k)_r,$$

where inequivalent $b$ give rise to different decompositions as in the last paragraph.

In Proposition 6, the decomposition of $\Lambda^{\kappa_3}$ is formal in the sense that it relates equivalence classes of representations; those of (37) and (38), respectively. That the decomposition can be realized by selecting a member from each equivalence class is exemplified by (50). The second part of the proposition, relating irreducible representation classes of the subgroups $Q$ of (19) in the two cases (A) and (B), follows directly from the first part and from the definitions $\Delta^{k_3} = \chi^{k_3}\times\Delta$ and $\Delta_{[b]}^{\kappa_3,[\kappa]} = \chi^{\kappa_3}\times\Delta_{[b]}^{[\kappa]}$ of (37) and (38).

Returning to a consideration of the whole state space $\mathfrak{L}$, we let $\Omega$ denote the representation of either group $W$ or $T_\eta$ carried by $\mathfrak{L}$. Then, we conclude from the above analysis that, corresponding to the decomposition (43a) of $\mathfrak{L}$, we have

$$\Omega = \oplus \sum_{l=0}^{\infty} \int_{-\infty}^{\infty} \Omega(l,k_3)\, dk_3, \qquad \Omega(l,k_3) \simeq \begin{cases} \Delta^{k_3} & \text{(A)} \\ \Lambda^{\kappa_3};\ \kappa_3 = (k_3)_r, & \text{(B)} \end{cases} \tag{55}$$

where $\Omega(l,k_3)$ is the representation in $\mathfrak{M}(l,k_3)$. For case (A), the constituents are the irreducible representations (37); for case (B), they are the primary representations given in Proposition 6. Whereas the set of irreducible constituents is uniquely determined in case (A), for case (B) the further decomposition of $\Omega$ into irreducible constituents is highly nonunique, as follows from the analysis in this section. However, as was remarked at the end of Sec. I, the central decomposition of $\Omega$, i.e., the decomposition into mutually inequivalent primary representations, will be unique in both cases. It is obtained from (46) and (35) by combining in a direct sum all those constituent spaces $\mathfrak{M}(l,k_3)$ carrying equivalent representations. Thus, for case (A) the central decomposition of $\Omega$ is given by

$$\mathfrak{L} = \oplus \int_{-\infty}^{\infty} \mathfrak{M}(k_3)\, dk_3, \qquad \mathfrak{M}(k_3) = \oplus \sum_{l=0}^{\infty} \mathfrak{M}(l,k_3)$$
$$\Omega = \oplus \int_{-\infty}^{\infty} \Omega(k_3)\, dk_3, \qquad \Omega(k_3) \simeq \infty\, \Delta^{k_3},$$

and for case (B) by

$$\mathfrak{L} = \oplus \int_0^1 \mathfrak{M}(\kappa_3)\, d\kappa_3,$$
$$\mathfrak{M}(\kappa_3) = \oplus \sum_{l=0}^{\infty} \sum_{m=-\infty}^{\infty} \mathfrak{M}(l, \kappa_3 + m), \quad (56)$$
$$\Omega = \oplus \int_0^1 \Omega(\kappa_3)\, d\kappa_3, \qquad \Omega(\kappa_3) \simeq \infty\, \Lambda^{\kappa_3}.$$

Here, the notation $\infty\gamma$ means an infinite direct multiple of the representation $\gamma$. Whenever $\gamma$ is primary, then $\infty\gamma$ is primary and of the same Type as $\gamma$,[9] so that the constituents in these two decompositions are indeed primary. Also, the primary constituents $\infty\Delta^{k_3}$ for case (A) are of Type I, as is to be expected, whereas the primary constituents $\infty\Lambda^{\kappa_3}$ for case (B) are not of Type I.

## V. SUMMARY AND REMARKS

The invariance translation operator groups for the Hamiltonian of a Bloch electron in a uniform magnetic field have properties that are certainly unusual for systems encountered in solid state physics. As we have found in Sec. II, they are of Type I only when the components of the magnetic field relative to the lattice vector directions are rational numbers in terms of natural flux units. For these "rational" fields with Type I groups, the group theoretical analysis presents no unfamiliar aspects.[1-4,26] The irreducible representations, for instance, can all be classified and are all finite-dimensional. For the "nonrational" fields, however, the situation is entirely different. We have confined our analysis to the case where the (nonrational) field is along a lattice vector, but the general features will be the same for the field in an arbitrary direction. It turns out that here the group has an infinite number of classes of physical irreducible representations, all of infinite dimension. They are summarized at the end of Sec. III. There may be more; since the group is not of Type I in this case, there is at present no method available for determining them all with certainty. In any case, it is just these representations of Sec. III that occur in the decomposition of the representation carried by the state space $\mathfrak{L}$ into irreducible constituents, and we are therefore able to analyze this representation explicitly (Sec. IV). The decomposition into irreducible constituents is far from unique and can be accomplished in an infinite number of different ways. This is a manifestation of the fact that the group is non-Type I and shows that the concept of irreducible representation plays a much more ambiguous role here than in the usual applications of group theory to quantum systems. By contrast, the central decomposition (56) into disjoint primary constituents is unique, in the sense that the set of different primary representations that occur is unique; and, therefore, it is the primary rather than the irreducible representations that appear to have the greater significance, in the physical as well as the mathematical context. These primary constituents in (56) are not of Type I, as is proved in Sec. IV; and, in fact, Grossmann has shown in an independent study that they are of Type II.[25] Grossmann's demonstration is an abstract one (using the properties of symplectic forms on phase space); our method is complementary to his in being more concrete, as we use explicit decompositions of the primary representation into irreducible constituents (whose carrier spaces are spanned by the well-known Landau functions for a free electron in a magnetic field).

When we come to consider the spectrum of the Hamiltonian, it is again the primary rather than the irreducible representations which appear to be the most important. For, as described at the end of Sec. I, there is a natural decomposition of $\mathfrak{K}$ that corresponds to the central decomposition of its invariance group, which for the case of (56) will have constituents which we can label $\mathfrak{K}(\kappa_3)$ $(0 \leq \kappa_3 < 1)$ in an evident notation, where $\mathfrak{K}(\kappa_3)$ is an operator in $\mathfrak{M}(\kappa_3)$. We are then left with the difficult problem of finding the spectrum of $\mathfrak{K}(\kappa_3)$; what information on this spectrum can be deduced from the fact that $\mathfrak{M}(\kappa_3)$ carries a Type II primary representation of the invariance group of $\mathfrak{K}$ remains to be investigated.

The enlargement of the invariance groups to include rotational symmetries will make no essential difference to the general features of the analysis in this paper, since the enlarged groups are only finite extensions of the original ones.

There are, of course, other physical problems besides the energy spectrum for which the implications of the unusual properties of the groups need to be studied: the behavior of the selection rules, for example. Although these physical questions are not dealt with here, this paper is intended to be a contribution to laying the necessary basis for their investigation.

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## APPENDIX A

We show that a representation of $T_\eta$ that is analogous to (38), but constructed with reference to a basic primitive lattice vector trio $(\mathbf{c}_1, \mathbf{c}_2, \mathbf{a}_3)$ where the $\mathbf{c}_1 - \mathbf{c}_2$ plane is not (necessarily) coincident with the $\mathbf{a}_1 - \mathbf{a}_2$ plane, is equivalent to one of the set (38).

The group $T_\eta$, therefore, is now factorized as

$$T_\eta = P \times Q', \qquad Q' = N(\mathbf{c}_1) \circledS H(\mathbf{c}_2) \quad (A1)$$

where $P$ is as in (19b) and $N(\mathbf{c}_1), H(\mathbf{c}_2)$ are defined analogously to (23). As in Sec. II, the domain of $\mathbf{c}_1$ and $\mathbf{c}_2$ must be restricted in order to obtain a one-to-one correspondence between the factorizations of $Q'$ and the pairs $(\mathbf{c}_1, \mathbf{c}_2)$ in the same plane. This is done as follows. For a given basic vector trio $(\mathbf{c}_1, \mathbf{c}_2, \mathbf{a}_3)$, there is always a uniquely-determined basic vector trio $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{a}_3)$ with $\mathbf{b}_1, \mathbf{b}_2$ in the $\mathbf{a}_1 - \mathbf{a}_2$ plane and

$$\mathbf{b}_1 = \mathbf{c}_1 + r_1\mathbf{a}_3, \qquad \mathbf{b}_2 = \mathbf{c}_2 + r_2\mathbf{a}_3 \quad (A2)$$

for $r_1, r_2$ uniquely determined integers. We restrict the domain of $\mathbf{c}_1$ and $\mathbf{c}_2$ so that $\mathbf{b}_1$ and $\mathbf{b}_2$ lie in the allowed half-plane defined in Sec. II. Then, to each

allowed $c \equiv (\mathbf{c}_1, \mathbf{c}_2)$, there is a unique allowed $b \equiv (\mathbf{b}_1, \mathbf{b}_2)$ and a unique pair of integers $r_1, r_2$ defined by (A2). Let

$$\mathbf{t} = n_1^c \mathbf{c}_1 + n_2^c \mathbf{c}_2 + n_3^c \mathbf{a}_3 = n_1^b \mathbf{b}_1 + n_2^b \mathbf{b}_2 + n_3 \mathbf{a}_3 \qquad \text{(A3)}$$

be any vector expressed in terms of the two vector trios (the third component with respect to the first trio bears the label $c$, because it now varies when the vector pair $c$ moves out of the $\mathbf{a}_1$–$\mathbf{a}_2$ plane). Then, using (A2) and (A3) we have

$$n_1^c = n_1^b, \quad n_2^c = n_2^b, \quad n_3^c = n_3^b + r_1 n_1^b + r_2 n_2^b, \quad \xi^c = \xi^b, \qquad \text{(A4)}$$

relating the components and signs of the two vector trios.

Applying the general procedure of Sec. III to the factorization (A1) of $T_\eta$, we construct a representation $\Delta_{[c]}^{\kappa_3,[\kappa]}$ of $T_\eta$ with carrier space $l_2$ in analogy with (38), where

$$\Delta_{[c]}^{\kappa_3,[\kappa]}[n_1^c \mathbf{c}_1 + n_2^c \mathbf{c}_2 + n_3^c \mathbf{a}_3, \lambda_j]\{f(m)\} = \{g(m)\},$$

and $g(m)$ is given by the third line of (38b) with the replacement of $n_1^b, n_2^b, n_3$ and $\xi^b$ by $n_1^c, n_2^c, n_3^c$ and $\xi^c$, respectively. If we use Eqs. (A3) and (A4) to express both sides of this relation back in terms of $n_1^b, n_2^b, n_3$ and $\xi^b$, and then make the unitary mapping $\{f(m)\} \to \{h(m)\}; h(m) = \exp(-2\pi i \kappa_3 r_2 m) f(m)$ of $l_2$ onto itself, we verify with a little algebra that $\Delta_{[c]}^{\kappa_3,[\kappa]}$ is transformed into the representation $\Delta_{[b]}^{\kappa_3,[\kappa + r_1 \kappa_3]}$ of the set (38). Here $[b]$ is the equivalence class to which the $b$ of (A2) belongs. Therefore the choice of $c$ as vector pair gives no new representation.

## APPENDIX B

Here we derive several properties of the Landau functions (40) used in Sec. IV. We repeat the definition in more detail. The Landau function $\langle \mathbf{r} | l, k_3, k \rangle_b$ is defined relative to the basic vector trio $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{a}_3)$ and expressed in terms of the cartesian coordinates $(x, y, z)$ attached to these vectors, where we recall: The $z$ axis is positive along $\mathbf{a}_3$, the $x$ axis is in the $\mathbf{a}_3 - \mathbf{b}_1$ plane directed so that $\mathbf{b}_1$ has positive $x$ projection, and the $y$ axis makes the system right-handed. This means that

$$a_{3z} = a_3 > 0, \quad a_{3x} = a_{3y} = b_{2y} = 0, \quad b_{1x} > 0, \quad b_{2y} \neq 0, \qquad \text{(B1)}$$

where $a_{3z}, b_{2y}$, etc. denote the projections of the basic vectors along the Cartesian axes, in an obvious notation. The full definition of (42) is

$$\langle \mathbf{r} | l, k_3, k \rangle_b = A(l, k_3, k) \exp\{[(2\pi i k_3 z)/a_3] - i\chi x(\tfrac{1}{2} y - \beta)\} u_l(\chi^{1/2}(y - \beta)),$$

$$\chi = |e\mathbf{B}|/(\hbar c), \quad \beta = (b_{2y}/\xi^b \eta)[(k_3 b_{1z}/a_3) - k], \qquad \text{(B2)}$$

$$A(l, k_3, k) = i^l \chi^{1/4} (2^l l! \pi^{1/2} b_{1x} a_3)^{-1/2} \exp[-i\phi(k, k_3)],$$

$$\phi(k, k_3) = (\beta/b_{2y})[\tfrac{1}{2}\chi \beta b_{2x} + (2\pi k_3 b_{2z}/a_3)].$$

All quantities in (B2) are well-defined in virtue of (B1). For the Hermite functions, we have

$$\left.\begin{aligned} u_l(\zeta) &= \exp(-\tfrac{1}{2}\zeta^2) H_l(\zeta) \\ \int_{-\infty}^{\infty} u_l(\zeta) u_{l'}(\zeta) d\zeta &= 2^l l! \pi^{1/2} \delta_{l,l'} \end{aligned}\right\}, \qquad \text{(B3)}$$

where $H_l$ is the $l$th Hermite polynomial. The magnitude of $A(l, k_3, k)$ in (B2) is chosen so that the functions are normalized as in (41a), and its phase is chosen so that they transform conveniently under the group operations as in (44). There are two parts to this Appendix.

I. We show that the functions (52), which we write here as

$$\langle \mathbf{r} | \Phi \rangle = \sum_{m=-\infty}^{\infty} a_m \langle \mathbf{r} | l, k_3, k + \eta m \rangle_b, \quad \sum_{m=-\infty}^{\infty} |a_m|^2 = c^2 < \infty,$$

exist as everywhere defined functions on $R^3$. Here $c$ is a real positive constant. From Schwartz's inequality we have

$$|\langle \mathbf{r} | \Phi \rangle| \leq c \left( \sum_{m=-\infty}^{\infty} |\langle \mathbf{r} | l, k_3, k + \eta m \rangle_b|^2 \right)^{1/2} \leq c_1 \times \left( \sum_{m=-\infty}^{\infty} u_l^2(\chi^{1/2}(y - c_2 - c_3 m)) \right)^{1/2},$$

where $c_1, c_2$, and $c_3$ are real constants depending only on $l, k_3, k$ and the basic vectors. In the second step we used (B2). The infinite sum in the square brackets is uniformly bounded in $y$, as follows from the definition of $u_l$ in (B3). Hence $\langle \mathbf{r} | \Phi \rangle$ exists for all $\mathbf{r} \in R^3$ and is uniformly bounded on $R^3$.

II. We calculate the overlap integral (42) between Landau functions $\langle \mathbf{r} | l, k_3, k \rangle_b$ and $\langle \mathbf{r} | l', k_3', k' \rangle_{b'}$ defined relative to different basic vector pairs $b$ and $b'$. The two sets of cartesian axes $(x, y, z)$ and $(x', y', z')$ attached to the trios $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{a}_3)$ and $(\mathbf{b}_1', \mathbf{b}_2', \mathbf{a}_3)$, respectively, are related by

$$x' = x \cos\theta + y \sin\theta, \quad y' = -x \sin\theta + y \cos\theta, \quad z' = z, \quad 0 \leq \theta < \pi, \qquad \text{(B4)}$$

where $\theta$ is the angle between the $\mathbf{a}_3 - \mathbf{b}_1$ and $\mathbf{a}_3 - \mathbf{b}_1'$ planes. The restriction on the range of $\theta$ arises from the half-plane restriction on the basic vectors. Note that $\theta = 0$ if and only if $\mathbf{b}_1' = \mathbf{b}_1$, i.e., $[b'] = [b]$. We shall write the overlap integral ${}_b\langle l, k_3, k | l', k_3', k' \rangle_{b'} \equiv \mathcal{J}$; on expressing the two functions in the appropriate explicit form (B2), the $z' = z$ coordinates can be integrated out immediately to give

$$\mathcal{J} = A^*(l, k_3, k) A'(l', k_3', k') a_3 \delta(k_3 - k_3') J, \qquad \text{(B5)}$$

where

$$J = \int_{R^2} \exp[\tfrac{1}{2} i\chi(xy - x'y') - i\chi(x\beta - x'\beta')] \times u_l(\chi^{1/2}(y - \beta)) u_{l'}(\chi^{1/2}(y' - \beta')) dx dy.$$

Here $x'$ and $y'$ are related to $x$ and $y$ through (B4). The star in (B5) denotes the complex conjugate; the primed functions $A'$ and $\beta'$ have the same form in the primed variables $l', k_3', k'$ and primed vectors $b'$ (whose projections $b_{1z}'$, etc, are taken with respect to the primed coordinate axes) as have $A$ and $\beta$ in the corresponding unprimed quantities in (B2). We now distinguish two cases:

(i) $[b'] = [b]$, i.e., $\theta = 0$. Then $x' = x$, $y' = y$, and, using (B3), we obtain

$$J = 2^{l+1}\, l!\, (\pi/\chi)^{3/2}\, \delta_{ll'}\, \delta(\beta - \beta').$$

Substituting in (B5) and using the definitions of the normalization constants and of $\beta$ and $\beta'$ from (B2), we have

$$\mathcal{J} = 2\pi\, |\eta|\, (\chi b_{1x} |b_{2y}|)^{-1}\, \delta_{ll'}\, \delta(k_3 - k_3')\, \delta(k - k').$$

We recover (41a) on noting that, from (B2) and (13),

$$\chi = |eB|/(\hbar c) = 2\pi a_3 |\eta/\Omega| = 2\pi\, |\eta|\, /(b_{1x} |b_{2y}|). \quad \text{(B6)}$$

Here we recall that the volume $|\Omega|$ of the unit cell is independent of the basic vector trio: $|\Omega| = |\mathbf{a}_3 \cdot \mathbf{a}_1 \times \mathbf{a}_2| = |\mathbf{a}_3 \cdot \mathbf{b}_1 \times \mathbf{b}_2| = a_3 b_{1x} |b_{2y}|$.

(ii) $[b'] \neq [b]$, i.e., $0 < \theta < \pi$. Changing the independent variables in the integral $J$ from $x, y$ to $\omega, \omega'$, where

$$\omega = \chi^{1/2}\, (y - \beta), \qquad \omega' = \chi^{1/2}\, (y' - \beta') = \chi^{1/2}\, (-x \sin\theta + y \cos\theta - \beta'),$$

we obtain, with the aid of (B4) and a little rearrangement,

$$J = \chi^{-1} \operatorname{cosec}\theta \exp\{-\tfrac{1}{2} i\chi[\beta^2 + (\beta')^2] \cot\theta + i\chi[\beta\beta' \operatorname{cosec}\theta]\} \int_{R^2} \exp\{\tfrac{1}{2} i[\omega^2 + (\omega')^2] \cot\theta - i\omega\omega' \operatorname{cosec}\theta\}\, u_l(\omega)\, u_{l'}(\omega')\, d\omega d\omega'.$$

To evaluate the integral in this expression, we need a relation between Hermite functions:

$$\int_{-\infty}^{\infty} \exp\{\tfrac{1}{2} i[\omega^2 + (\omega')^2] \cot\theta - i\omega\omega' \operatorname{cosec}\theta\}\, u_l(\omega)\, d\omega = \exp[il(\pi - \theta) + i(\tfrac{1}{4}\pi - \tfrac{1}{2}\theta)]\, (2\pi \sin\theta)^{1/2}\, u_l(\omega'), \quad \text{(B7)}$$

valid for $0 < \theta < \pi$.[31] This relation can be established by induction on $l$, for example, using the recurrence formula

$$\frac{d}{d\omega}\, [\exp(-\tfrac{1}{2}\omega^2)\, u_l(\omega)] = -\exp(-\tfrac{1}{2}\omega^2)\, u_{l+1}(\omega).$$

Via (B7) and (B3) in the last expression for $J$, and substituting the value so obtained in (B5), the overlap integral becomes

$$J = \delta_{ll'}\, \delta(k_3 - k_3')\mathcal{K},$$
$$\mathcal{K} = (2\pi \operatorname{csc}\theta/\chi b_{1x} b_{1x}')^{1/2} \exp[il(\pi - \theta) + i(\tfrac{1}{4}\pi - \tfrac{1}{2}\theta)] \times \exp\{i[\phi(k, k_3) - \phi'(k', k_3)] - \tfrac{1}{2} i\chi[\beta^2 + (\beta')^2] \cot\theta + i\chi\beta\beta' \operatorname{csc}\theta\}. \quad \text{(B8)}$$

Here the explicit expressions for the normalization constants have been inserted. On comparing with (42) we see that $\mathcal{K}$ is just the kernel ${}_b\langle l, k_3, k | l, k_3, k' \rangle_{b'}$ [written later as ${}_b\langle k | k' \rangle_{b'}$ in (47)]. Therefore Eq. (B8) proves (42), and also the assertion that the kernel is a bounded continuous function in $k$ and $k'$, since $\mathcal{K}$ evidently possesses these properties.

An interesting special case is when the crystal is orthorhombic and when $b = a \equiv (\mathbf{a}_1, \mathbf{a}_2)$, $b' = \overline{a} \equiv (\mathbf{a}_2, \mathbf{a}_1)$. Here the two Landau functions represent waves, with wave vectors $k$ and $k'$, respectively, propagating at right angles to each other along two principal crystal directions, and in a plane at right angles to the magnetic field. With the aid of (B2) and (B6) the kernel $\mathcal{K}$ reduces in this case to the Fourier transform

$$\mathcal{K} \equiv {}_b\langle k | k' \rangle_{b'} = i^l (2\pi/\chi a_1 a_2)^{1/2} \exp(-2\pi i k k'/|\eta|).$$

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21 We recall some definitions needed now and later. A collection of sets $\mathcal{E}$ in a space $\mathfrak{N}$ closed under complementation and denumerable unions and intersections and including the whole space and the empty set, are called Borel sets. Given a topology, a collection of Borel sets can be generated from the open sets by closure under these operations. If $\mathfrak{M}$ is a subspace of $\mathfrak{N}$, we can define Borel sets $\mathcal{E} \cap \mathfrak{M}$ in $\mathfrak{M}$ derived from the $\mathcal{E}$ of $\mathfrak{N}$. If $\mathcal{P}$ is a quotient space of $\mathfrak{N}$, we can define Borel sets in $\mathcal{P}$ as the images of the Borel sets in $\mathfrak{N}$ under the canonical mapping of $\mathfrak{N}$ on $\mathcal{P}$. A measure $\mu$ on $\mathfrak{N}$ which assigns a real number (measure) $\mu(\mathcal{E}) \geq 0$ to each Borel set $\mathcal{E}$, such that the measure of any countable union of disjoint Borel sets is the sum of the measures of the sets, is called countably additive; it is $\sigma$-finite if $\mathfrak{N}$ is itself the countable union of disjoint Borel sets.
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[32] *Note added in proof:* For irrational $\eta$, the different $N(\mathfrak{b}_1)$ are all maximal Abelian normal subgroups of $Q$. We remark, in this connection, that the list of maximal Abelian normal subgroups of $T_\eta$ given in Table I of Ref. 4 is incomplete.

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## 1. INTRODUCTION

Consider a self-adjoint operator $H_0$ acting in the Hilbert space $\mathcal{K}$. Assume that $V$ is another self-adjoint operator acting in $\mathcal{K}$ and that $H = H_0 + V$ is also self-adjoint. (For instance if $V$ is bounded this is always so.) A fundamental problem in linear perturbation theory is to get information about the spectrum of $H$ from a knowledge of the spectrum of $H_0$.

The standard approach is the Rayleigh–Schrödinger expansion in powers of $V$. The difficulty is that $V$ must be sufficiently small for this expansion to converge. [For instance, consider the case when $\mu_0$ is an isolated eigenvalue of $H_0$ of multiplicity one. Let $d$ be the distance from $\mu_0$ to the rest of the spectrum, and let $S$ be the circle in the complex plane with center $\mu_0$ and radius $d/2$. The projection onto the eigenspace of $H_0$ corresponding to $\mu_0$ is then $P_0 = -(2\pi i)^{-1}\int_S (H_0 - z)^{-1}dz$. If $V$ is sufficiently small (for instance if $\|V\| < d/2$), then the expansion $(H - z)^{-1} = (H_0 - z)^{-1} \sum_{n=0}^{\infty} (-V(H_0 - z)^{-1})^n$ converges for $z$ on $S$. In that case $H$ has an eigenvalue $\mu$ inside $S$ and $P = (-2\pi i)^{-1} \int_S (H - z)^{-1}dz$ is the corresponding projection. Thus $P$ depends analytically on $V$; we conclude that $\mu$ also has multiplicity one.[1]]

Any source of information about the spectrum of $H$ that does not depend on the convergence of this expansion is thus obviously of great value. One such source is the Perron–Frobenius theory, based on the notion of invariant cone. The main conclusion of this theory is that in certain circumstances (often met in quantum mechanics) the lowest eigenvalue of $H$ is of multiplicity one, that is, the ground state is unique.

The Perron–Frobenius theory has recently been applied to quantum field theory in the boson case by Glimm and Jaffe.[2] In a fundamental paper,[3] Gross has extended the theory in a direction suited for application to the fermion case. Using a representation of the fermion Fock space due to Segal,[4] he has been able to conclude uniqueness of the ground state for a class of fermion interactions.

In the present paper we develop an abstract version of the Perron–Frobenius theory in a form suited for applications to quantum mechanics. The setting is a Hilbert space and a given cone in the space; no special algebraic properties of the space or of the interaction are assumed. The main abstract results are the perturbation theorems in Sec. 4. This theory is applied to give uniqueness of the ground state for a different class of fermion interactions from that considered by Gross. The main result here is Theorem 4 in Sec. 7.

## 2. REAL HILBERT SPACES IN QUANTUM MECHANICS

In quantum mechanics one deals usually with a complex Hilbert space. However, it is worth recalling that many problems may be reduced to problems in a real Hilbert space.[5] In fact, let $\mathcal{W}$ be a complex Hilbert space and let $T: \mathcal{W} \to \mathcal{W}$ be a *conjugation*. That is, $T$ is an antilinear map with $T^2 = 1$ which is antiunitary: $(Tu, Tv) = (u, v)^*$. An element $u$ in $\mathcal{W}$ such that $Tu = u$ is called *real*. The set of all real elements forms a real Hilbert space $\mathcal{K}$.

Now if $A: \mathcal{W} \to \mathcal{W}$ is a linear operator such that $AT = TA$, then $A$ leaves the real space invariant. Such an operator is called *real* (with respect to $T$). It is easy to see that many questions concerning the spectrum of $A: \mathcal{W} \to \mathcal{W}$ may be reduced to questions about the restricted operator $A: \mathcal{K} \to \mathcal{K}$ acting in the real Hilbert space. For instance, if $Au = \lambda u$ with $\lambda$ real and $u$ in $\mathcal{W}$, then $Au_1 = \lambda u_1$ and $Au_2 = \lambda u_2$, where $u = u_1 + iu_2$ and $u_1$ and $u_2$ are in $\mathcal{K}$. Thus the multiplicity of the eigenvalue $\lambda$ may be computed in the real space.

The obvious example is $\mathcal{W} = L^2(M, \mu)$ with inner product $\langle u, v\rangle = \int_M u^* v d\mu$. Then $Tu = u^*$ defines a conjugation and $\mathcal{K}$ is the space of real functions in $L^2$.

In the nonrelativistic quantum mechanics of particles there is a conjugation which has a physical interpretation. The Hilbert space for a system of $n$ particles may be taken to be $\mathcal{W} = L^2(\mathbb{R}^{3n}, dx)$ in the position representation. The conjugation $T$ is given by $Tu(x) = u(x)^*$. The interpretation of $T$ is most easily seen in the momentum representation. Let $F: \mathcal{W} \to L^2(\mathbb{R}^{3n}, dk)$ be the Fourier transform, which gives the isomorphism with the momentum representation. Then the formula $FTF^{-1}g(k) = g(-k)^*$, $g \in L^2(\mathbb{R}^{3n}, dk)$ shows that $T$ has effect of reversing momenta. Since following a process backward in time has the effect of reversing momenta, $T$ is called the time reversal conjugation. The usual Hamiltonian operators are real with respect to time reversal.

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$$u \in \mathcal{K},\ -u \in \mathcal{K} \text{ implies } u = 0. \tag{3}$$

Let $\mathcal{H}$ be a real Hilbert space. A *Hilbert cone* $\mathcal{K} \subset \mathcal{H}$ is a cone such that

$$\mathcal{K} \text{ is closed;} \tag{4}$$

$$u \in \mathcal{K},\ v \in \mathcal{K} \text{ implies } \langle u, v\rangle \geqslant 0; \tag{5}$$

$$\text{For all } w \in \mathcal{H}, \text{ there exist } u, v \in \mathcal{K} \text{ with } w = u - v \text{ and } \langle u, v\rangle = 0. \tag{6}$$

The most important example is the case of the real Hilbert space $\mathcal{H} = L^2(M, \mu)$, where $\mu$ is a measure in the measure space $M$. The inner product is of course $\langle u, v\rangle = \int_M uv d\mu$. If $\mathcal{K} = \{u \in L^2 : u \geqslant 0 \text{ a.e.}\}$, then $\mathcal{K}$ is a Hilbert cone. It is important to notice that in general this cone has no interior points.

There exists an extensive theory of invariant cones; however, most uniqueness results are either for the case of a cone with nonempty interior or for the case of a Banach lattice.[6] While $L^2(M, \mu)$ is certainly a Banach lattice, in the application to fermion systems the space is not a lattice. In fact, already the space of self-adjoint $2 \times 2$ matrices (with the cone of positive matrices) provides an example where the space is not a lattice.

In the following we will usually write $u \geqslant 0$ when $u \in \mathcal{K}$.

*Definition 2:* Let $\mathcal{H}$ be a real Hilbert space and $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. A vector $w \geqslant 0$ is *strictly positive* if whenever $u \geqslant 0$, $u \neq 0$, then $\langle u, w\rangle > 0$.

In the example of the space $L^2(M, \mu)$ $w$ is strictly positive if and only if $w > 0$ a.e.

*Definition 3:* Let $\mathcal{H}$ be a real Hilbert space and $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $A : \mathcal{H} \to \mathcal{H}$ be a bounded linear operator. $A$ is *positivity preserving* if $u \geqslant 0$ implies $Au \geqslant 0$. $A$ is *positivity improving* if for all $u \geqslant 0$, $u \neq 0$, $Au$ is strictly positive. $A$ is *ergodic* if for all $u \geqslant 0$, $v \geqslant 0$, $u \neq 0$, $v \neq 0$, there exists an integer $n \geqslant 0$ such that $\langle u, A^n v\rangle > 0$.

If $A$ is positivity improving, then $A$ is certainly ergodic. Another relation between these two concepts is expressed in the following proposition.

*Proposition 1:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $A : \mathcal{H} \to \mathcal{H}$ be a bounded, positivity preserving linear operator. Let $\lambda > \|A\|$. Then $A$ is ergodic if and only if $(\lambda - A)^{-1}$ is positivity improving.

*Proof:* The representation $(\lambda - A)^{-1} = \lambda^{-1} \sum_n (A/\lambda)^n$ shows that $(\lambda - A)^{-1}$ is positivity preserving and that $A$ is ergodic if and only if $(\lambda - A)^{-1}$ is positivity improving.

The next result is the version of the Perron–Frobenius theorem we shall need. It should be noted in connection with the statement of the theorem that an operator on a real Hilbert space can be positive but not self-adjoint.

*Theorem 1:* Let $\mathcal{H}$ be a real Hilbert space. Let $A : \mathcal{H} \to \mathcal{H}$ be a bounded positive self-adjoint operator. Assume that $\|A\|$ is an eigenvalue of $A$. Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Assume that $A$ is positivity preserving. Then $A$ is ergodic if and only if $\|A\|$ is an eigenvalue of multiplicity one and the corresponding eigenspace is spanned by a strictly positive vector.

*Proof:* Let $\lambda = \|A\|$. Throughout the proof we take $\lambda \neq 0$.

Assume first that $A$ is ergodic. Consider $w \neq 0$ with $Aw = \lambda w$. Write $w = u - v$ with $u \geqslant 0$, $v \geqslant 0$, $\langle u, v\rangle = 0$ and set $z = u + v$. Then $z \geqslant 0$ and $\langle z, z\rangle = \langle w, w\rangle \neq 0$. Since $A^n$ is positivity preserving, $\langle w, A^n w\rangle \leqslant \langle z, A^n z\rangle$. Hence we have $\lambda^n \langle w, w\rangle = \langle w, A^n w\rangle \leqslant \langle z, A^n z\rangle \leqslant \lambda^n \langle z, z\rangle = \lambda^n \langle w, w\rangle$, that is, $\langle w, A^n w\rangle = \langle z, A^n z\rangle$. In terms of $u$ and $v$ this says $\langle u, A^n v\rangle = 0$. Since $A$ is ergodic, it follows that $u = 0$ or $v = 0$. Thus we have shown that $w \geqslant 0$ or $-w \geqslant 0$.

Next we show that if $w \geqslant 0$, then $w$ must be strictly positive. For if $u \geqslant 0$ and $u \neq 0$, then (since $A$ is ergodic) there must exist an $n \geqslant 0$ with $\lambda^n \langle u, w\rangle = \langle u, A^n w\rangle > 0$.

To show that $\lambda$ can have multiplicity at most one, assume the contrary. Then there are $w \neq 0$ and $x \neq 0$ with $Aw = \lambda w$ and $Ax = \lambda x$ and $\langle x, w\rangle = 0$. From the above we see that we may also assume that $w$ and $x$ are strictly positive. But then $\langle w, x\rangle > 0$, which is a contradiction.

For the proof of the converse, let $w$ be a strictly positive unit vector spanning the eigenspace. Let $u \geqslant 0$ and $v \geqslant 0$ be nonzero vectors. Write $v = x + \langle w, v\rangle w$, so that $\langle x, w\rangle = 0$. Then $A^n v = A^n x + \lambda^n \langle w, v\rangle w$, so $\lambda^{-n} \langle u, A^n v\rangle = \lambda^{-n} \langle u, A^n x\rangle + \langle u, w\rangle \langle w, v\rangle$. Since $x$ is orthogonal to the eigenspace corresponding to $\lambda$, and since our assumption that $A \geqslant 0$ excludes the possibility that $-\lambda$ is an eigenvalue, the spectral theorem implies that $\langle u, (A/\lambda)^n x\rangle \to 0$ as $n \to \infty$. Since $\langle u, w\rangle \langle w, v\rangle > 0$, it follows that $\lambda^{-n} \langle u, A^n v\rangle > 0$ for some $n$ sufficiently large.

*Remark:* The example of the matrix $A = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ acting in $\mathbb{R}^2$ shows that $A$ may be positivity preserving and ergodic, and yet $-\|A\|$ may be an eigenvalue. Of course, this $A$ is not positive, since its eigenvalues are $\pm 1$.

*Corollary 1.1:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $H$ be a self-adjoint operator acting in $\mathcal{H}$. Assume that there exists an eigenvalue $\mu$ of $H$ with $H \geqslant \mu$. Assume that $(H + c)^{-1}$ is positivity preserving for some $c$ with $c + \mu > 0$. Then $(H + c)^{-1}$ is ergodic if and only if $\mu$ is an eigenvalue of multiplicity one and the corresponding eigenspace is spanned by a strictly positive vector.

*Proof:* Set $A = (H + c)^{-1}$. Then $A \geqslant 0$, $\|A\| = (\mu + c)^{-1}$, and $Aw = (\mu + c)^{-1} w$ if and only if $Hw = \mu w$.

*Proposition 2:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $H$ be a self-adjoint operator which is bounded below. Then $\exp(-tH)$ is positivity preserving for all $t \geqslant 0$ if and only if $(H + c)^{-1}$ is positivity preserving for all $c$ sufficiently positive.

*Proof:* This equivalence follows from the formula

$$(H + c)^{-1} v = \int_0^\infty \exp(-ct) \exp(-tH) v dt$$

and the inversion formula

$$\exp(-tH) v = \lim_{n \to \infty} (1 + (t/n)H)^{-n} v.$$

*Definition 4:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $H$ be a self-adjoint operator acting in $\mathcal{H}$ which is bounded below. Assume that $\exp(-tH)$ is positivity preserving for all $t \geq 0$. Then the family $\exp(-tH)$, $t \geq 0$ is an *ergodic semigroup* if for all $u \geq 0$, $v \geq 0$, $u \neq 0$, $v \neq 0$, there exists $t \geq 0$ with $\langle u, \exp(-tH)v\rangle > 0$.

*Proposition 3:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $H$ be a self-adjoint operator which is bounded below. Assume that $\exp(-tH)$ is positivity preserving for all $t \geq 0$. Let $c$ be a real number such that $-c$ is less than the lower bound of $H$. Then $\exp(-tH)$ is an ergodic semigroup if and only if $(H + c)^{-1}$ is positivity improving.

*Proof:*

$$\langle u, (H + c)^{-1}v\rangle = \int_0^\infty \exp(-ct)\langle u, \exp(-tH)v\rangle\, dt.$$

*Corollary 1.2:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $H$ be a self-adjoint operator acting in $\mathcal{H}$. Assume that there exists an eigenvalue $\mu$ of $H$ with $H \geq \mu$. Assume that $\exp(-tH)$ is positivity preserving for $t \geq 0$. Then $\exp(-tH)$ is an ergodic semigroup if and only if $\mu$ is an eigenvalue of multiplicity one and the corresponding eigenspace is spanned by a strictly positive vector.

*Proof:* Set $A = \exp(-H)$. Then $0 \leq A \leq \|A\| = \exp(-\mu)$. The Perron–Frobenius theorem (Theorem 1) remains valid if the definition of ergodic is modified to allow nonintegral powers of $A$, as in the definition of ergodic semigroup. But $A^t = \exp(-tH)$.

The notion of ergodic semigroup may be used to improve Corollary 1.1.

*Corollary 1.3:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $H$ be a self-adjoint operator acting in $\mathcal{H}$. Assume that there exists an eigenvalue $\mu$ of $H$ with $H \geq \mu$. Assume that $(H + c)^{-1}$ is positivity preserving for all $c$ with $c + \mu > 0$. Then $(H + c)^{-1}$ is positivity improving if and only if $\mu$ is an eigenvalue of multiplicity one and the corresponding eigenspace is spanned by a strictly positive vector.

*Proof:* Since $(H + c)^{-1}$ is positivity preserving for all $c$ sufficiently positive, $\exp(-tH)$ is positivity preserving for $t \geq 0$, by Proposition 2.

Assume $\mu$ satisfies the multiplicity condition. Then $\exp(-tH)$ is an ergodic semigroup, by Corollary 1.2. Thus using Proposition 3 we see that $(H + c)^{-1}$ is positivity improving.

The other direction is a special case of Corollary 1.1.

## 4. PERTURBATION THEORY

*Theorem 2:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $H_0$ be a self-adjoint operator acting in $\mathcal{H}$ which is bounded below. Let $V$ be a self-adjoint operator which is relatively bounded with respect to $H_0$ with relative bound less than one. Set $H = H_0 + V$. Then $H$ is a self-adjoint operator which is bounded below. Assume that $(H_0 + c)^{-1}$ is positivity preserving and ergodic for all $c$ such that $c + \inf \text{spectrum } H_0 > 0$. Assume also that $-V$ is positivity preserving, in the sense that it sends elements of $\mathcal{K}$ which are in its domain into $\mathcal{K}$. Then $(H + c)^{-1}$ is positivity preserving and ergodic for all $c$ such that $c + \inf \text{spectrum } H > 0$. If $(H_0 + c)^{-1}$ is, in fact, positivity improving, then so is $(H + c)^{-1}$.

*Proof:* Let $\nu = \inf \text{spectrum } H_0$. We consider real numbers $c$ such that $-c < \nu$. Since $V$ is relatively bounded with respect to $H_0$ with relative bound less than one, it follows that $\|V(H_0 + c)^{-1}\| < 1$ for $c$ sufficiently large. Hence $(H + c)^{-1} = (H_0 + c)^{-1}\sum_{n=0}^{\infty} [-V(H_0 + c)^{-1}]^n$ converges for these $c$. Thus $H$ is self-adjoint and bounded below. It also follows immediately from this series representation that $(H + c)^{-1}$ is positivity preserving.

Let $\mu = \inf \text{spectrum } H$. We now know that there exists a $c$ with $-c < \mu$ and $(H + c)^{-1}$ positivity preserving. Consider a $d \leq c$ such that $-d < \mu$. Then $(c - d)(H + c)^{-1}$ has norm $(c - d)(c + \mu)^{-1} < 1$. So $(H + d)^{-1} = (H + c)^{-1}\sum_{n=0}^{\infty} [(c - d)(H + c)^{-1}]^n$ is also positivity preserving.

We next show that $(H + c)^{-1}$ is ergodic for $c$ sufficiently large. In fact, we may write

$$(H + c)^{-1} = (H_0 + c)^{-1} + T,$$

where $T = -(H_0 + c)^{-1}V(H + c)^{-1}$ is positivity preserving. Let $u$ and $v$ be nonzero vectors in $\mathcal{K}$. Then there exists $n \geq 0$ with $\langle u, (H_0 + c)^{-n}v\rangle > 0$. Since $(H + c)^{-n} = [(H_0 + c)^{-1} + T]^n$, we also have $\langle u, (H + c)^{-n}v\rangle > 0$. [In case $(H_0 + c)^{-1}$ is positivity improving, we may take $n = 1$. Thus $(H + c)^{-1}$ is also positivity improving.]

Finally, we show that $(H + d)^{-1}$ is ergodic whenever $-d < \mu$. In fact $(H + d)^{-1} = (H + c)^{-1} + S$, where $S = (c - d)(H + d)^{-2}$. If $d \leq c$ then $S$ is positivity preserving. Since $(H + c)^{-1}$ is ergodic, $(H + d)^{-1}$ is also. [And if $(H + c)^{-1}$ is positivity improving, then so is $(H + d)^{-1}$.]

*Remark:* This theorem applies in particular when $V$ is bounded, and the result is independent of the magnitude of the bound. For then $\|V(H_0 + c)^{-1}\| \leq \|V\|\|(H_0 + c)^{-1}\| = \|V\|(\nu + c)^{-1} < 1$ for $c$ sufficiently large.

The following theorem is an abstraction of results of Glimm and Jaffe[2] and Segal.[7]

*Theorem 3:* Let $\mathcal{K} \subset \mathcal{H}$ be a Hilbert cone. Let $H_0$ be a self-adjoint operator acting in $\mathcal{H}$ which is bounded below. Let $V$ be another self-adjoint operator such that $H = H_0 + V$ is essentially self-adjoint on $D = D(H_0) \cap D(V)$ and is bounded below. Assume also that the restriction of $H_0$ to $D$ is essentially self-adjoint. Let $V_k = V$ when $|V| \leq k$, 0 otherwise. Assume that $\exp(-tH_0)$ is a positivity preserving and ergodic semigroup. Assume also that $\exp(-tV_k)$ is positivity preserving for all $t$ and all $k$. Assume finally that $u \geq 0$, $v \geq 0$, $\langle u, v\rangle = 0$ implies $\langle \exp(-tV_k)u, v\rangle = 0$. Then $\exp(-tH)$ is a positivity preserving and ergodic semigroup.

*Proof:* Let $H_k = H_0 + V_k$. Then by the Trotter product formula,[8] $\exp(-tH_k)u = \lim[\exp(-t/nH_0) \times \exp(-t/nV_k)]^n u$ for $u$ in $\mathcal{H}$ as $n \to \infty$. Thus $\exp(-tH_k)$ is positivity preserving. Now $V_k u \to Vu$ for $u$ in $D$, and $D$ is a core for $H$. Thus $\exp(-tH_k)u \to \exp(-tH)u$ for $u$ in $\mathcal{H}$.[9] Hence $\exp(-tH)$ is positivity preserving.

Let $v \geq 0$, $v \neq 0$. Let $\mathcal{K}(v) = \{u \geq 0 : \langle u, \exp(-tH)v\rangle = 0 \text{ for all } t \geq 0\}$. To show $\exp(-tH)$ is an ergodic semigroup it is sufficient to show that $\mathcal{K}(v) = \{0\}$ for all such $v$.

First of all, note that $\mathcal{K}(v)$ is a closed cone and that $\exp(-tH)$ leaves $\mathcal{K}(v)$ invariant. But also $\exp(tV_k)$ leaves $\mathcal{K}(v)$ invariant. For if $u \geq 0$, $v \geq 0$, and $\langle u, \exp(-tH)v\rangle = 0$, then by assumption $\langle \exp(tV_k)u, \exp(-tH)v\rangle = 0$. Thus from $\exp[-t(H - V_k)]u = \lim_n [\exp(-t/nH)\exp(t/nV_k)]^n u$, we see that $\exp[-t(H - V_k)]$ leaves $\mathcal{K}(v)$ invariant. But $D$ is a core for $H_0$, so $\exp[-t(H - V_k)]u \to \exp(-tH_0)u$. Thus $\exp(-tH_0)$ leaves $\mathcal{K}(v)$ invariant. In particular, if $u \in \mathcal{K}(v)$, then $\langle \exp(-tH_0)u, v\rangle = 0$. Thus $u = 0$, since $\exp(-tH_0)$ is an ergodic semigroup.

In applications of Theorems 2 and 3 it is not necessary that $H_0$ has an eigenvalue. In fact it is often possible to see that $\exp(-tH_0)$ and $(H_0 + c)^{-1}$ are ergodic by inspection.

As an example of this perturbation theory we may take the quantum mechanics of $n$ nonrelativistic particles. This application has previously been considered by Simon and Høegh-Krohn[10] and the author.[11] In this case $\mathcal{K} = L^2(\mathbb{R}^{3n}, dx)$ and $\mathcal{K}$ is the cone of positive functions. We take $H_0 = -\Delta$; an explicit computation shows that $\exp(-tH_0)$ is convolution by a Gaussian for $t > 0$. Thus $\exp(-tH_0)$ is positivity improving for $t > 0$. It follows that $(H_0 + c)^{-1}$ is positivity improving for all $c > 0$.

For the interaction term we take a real function $V$ on $\mathbb{R}^{3n}$ which is a finite sum of functions $V_\alpha$ of the form $V_\alpha(x_1, \ldots, x_n) = W_\alpha(z_1)$, where the coordinates $z_1, \ldots, z_n$ are related to $x_1, \ldots, x_n$ by an affine transformation. The function $W_\alpha$ is required to be in $L^p(\mathbb{R}^3)$ for some $p$ with $2 \leq p \leq \infty$. It is known that in this case $V$ is relatively bounded with respect to $H_0$ with relative bound zero.[8,12]

Set $H = H_0 + V$. If $V$ is bounded above, then there exists a constant $b$ such that $H - b = H_0 + (V - b)$ and $V - b$ is negative. Thus we may apply Theorem 2 and conclude that if $H$ has a ground state, it is unique. This argument would generalize easily to perturbations which are given by an integral operator with negative kernel. In order to remove the restriction that $V$ is bounded above, we may use Theorem 3 in place of Theorem 2. However, this argument would not generalize to perturbations given by integral operators.

## 5. THE SEGAL REPRESENTATION OF THE ANTICOMMUTATION RELATIONS

In the application of the Perron–Frobenius theory to quantum field theory,[2,7,10] the natural representation of the boson Fock space is the $L^2$ representation in which the field operators are multiplication operators. The cone is then taken to be the cone of positive functions in $L^2$. For the fermion case the situation is not so simple; the fermion field operators do not commute. However Segal[4] has given a representation of the Fock space for a fermion system in which the field operators become left multiplication operators on a Clifford algebra. This turns out to be the natural analog of the boson representation.

Let $E$ be a complex Hilbert space. The *$C^*$-algebra of the canonical anticommutation relations* is the $C^*$-algebra generated by elements 1 and $A(x)$, $x \in E$, with the relations

$$A(x)A(y) + A(y)A(x) = 0$$

and

$$A(x)A(y)^* + A(y)^*A(x) = (x, y).$$

Here $A(y)^*$ depends linearly on $y \in E$. [The inner product is taken to be linear in the right factor. Thus $A(x)$ is conjugate linear in $x$.]

The norm on a $C^*$-algebra is uniquely determined: The norm of an element $u$ is the spectral radius of $(u^*u)^{1/2}$. The $C^*$-algebra of the anticommutation relations is discussed in detail by Shale and Stinespring.[13]

Let $J : E \to E$ be a conjugation. Write $Q(x) = A(Jx) + A(x)^*$ and $iP(x) = A(Jx) - A(x)^*$. Then

$$Q(x)Q(y) + Q(y)Q(x) = 2\langle x, y\rangle,$$

$$Q(x)P(y) + P(y)Q(x) = 0,$$

$$P(x)P(y) + P(y)P(x) = 2\langle x, y\rangle,$$

where $\langle x, y\rangle = (Jx, y)$. Also $Q(x)^* = Q(Jx)$ and $P(x)^* = P(Jx)$. Thus the $C^*$-algebra of the anticommutation relations may also be viewed as the Clifford algebra $\mathcal{C}(E \oplus E)$ generated by the $Q(x)$ and $P(y)$. (In Shale and Stinespring's treatment[13] the algebra is taken as the Clifford algebra over the real subspace of $E \oplus E$ defined by $J$. Their conjugation $\Lambda$ is not $J$; it is the one reversing the roles of $Q$ and $P$.)

Let $e_1, e_2, e_3, \cdots$ be an orthonormal basis of $E$ consisting of real elements. Let $Q(i) = Q(e_i)$ and $P(j) = P(e_j)$. The anticommutation relations then read $Q(i)Q(l) + Q(l)Q(i) = 2\delta_{il}$, etc. The Clifford algebra $\mathcal{C}(E \oplus E)$ is generated by 1 and the self-adjoint elements $Q(i)$ and $P(j)$.

For the construction of the Segal representation we need some facts about states on $C^*$-algebras. Let $\mathfrak{A}$ be a $C^*$-algebra with identity. If $u \in \mathfrak{A}$, $u$ is said to be *positive* if there exists $v$ in $\mathfrak{A}$ with $u = v^*v$. Though it is not obvious from this definition, the positive elements of $\mathfrak{A}$ form a cone.[14] A linear form $\omega$ on $\mathfrak{A}$ is called *positive* if $u \geq 0$ implies $\omega(u) \geq 0$. A *state* on $\mathfrak{A}$ is a positive linear form such that $\omega(1) = 1$. A state is called a *central state* (or trace state) if $\omega(uv) = \omega(vu)$ for all $u, v \in \mathfrak{A}$. A central state is called *faithful* if $u \geq 0$, $\omega(u) = 0$ implies $u = 0$.

There is a standard way of representing an algebra by linear transformations, which applies in particular to the case of a $C^*$-algebra $\mathfrak{A}$. If $u \in \mathfrak{A}$, define the linear transformation $L_u : \mathfrak{A} \to \mathfrak{A}$ by $L_u v = uv$. Similarly, define $R_u : \mathfrak{A} \to \mathfrak{A}$ by $R_u v = vu$. Let $\omega$ be a state on $\mathfrak{A}$ and consider the form $\langle u, v\rangle = \omega(u^*v)$. Then the adjointness relation $\langle L_u v, w\rangle = \langle v, L_u^* w\rangle$ is valid. The corresponding statement for $R_u$ is false in general. But if $\omega$ is a central state, then $\langle R_u v, w\rangle = \langle v, R_u^* w\rangle$ holds.

If we write $\|v\|_2^2 = \langle v, v\rangle$, then $\|L_u v\|_2 \leq \|u\|_\infty \|v\|_2$, where $\|u\|_\infty$ is the norm in the $C^*$-algebra $\mathfrak{A}$. [In fact, $\omega(v^*u^*uv) \leq \omega(v^*\|u\|_\infty^2 v) = \|u\|_\infty^2 \omega(v^*v)$.] If $\omega$ is central then we also have $\|R_u v\|_2 \leq \|u\|_\infty \|v\|_2$.

We apply this construction to the Clifford algebra $\mathcal{C}(E)$ generated by 1 and the $Q(x)$, $x \in E$. [This algebra is in fact generated by 1 and the $Q(i)$.]

*Proposition 4*[13]: If the dimension of $E$ is even or infinite, there is a unique central state $\omega$ on $\mathcal{C}(E)$.

It is not difficult to see why this is so. Consider the elements $Q(I) = Q(i_1)\cdots Q(i_k)$ of $\mathcal{C}(E)$, where $I = (i_1, \ldots, i_k)$ and $i_1 < \cdots < i_k$. The convention here is that $Q(\emptyset) = 1$, where $\emptyset$ is the empty sequence of integers. It is enough to show that $\omega$ is determined on the $Q(I)$. Of course $\omega(Q(\emptyset)) = \omega(1) = 1$.

If $I \neq \emptyset$, let $I' = (i_2, \ldots, i_k)$. If $k$ is even, then $Q(I) = Q(i_1)Q(I') = -Q(I')Q(i_1)$. Since $\omega$ is central, $\omega(Q(I)) = 0$. If $k$ is odd, and the dimension of $E$ is even or infinite, there exists an index $j$ which does not belong to $I$. Then $Q(I) = -Q(j)Q(I)Q(j)$. Since $\omega$ is central, again $\omega(Q(I)) = 0$. From this we see that if $u = \sum c_I Q(I)$, then $\omega(u) = c_\varphi$. It follows easily that $\omega(u^*u) = \sum_I |c_I|^2 \geq 0$.

*Definition 5:* The *principal automorphism* of $\mathcal{C}(E)$ is the unique automorphism $B$ such that $BQ(x) = Q(-x)$.

The automorphism $B$ is $+1$ on the even elements and $-1$ on the odd elements of the algebra. Clearly $B^2 = 1$.

From now on we assume that the dimension of $E$ is even or infinite. Let $\omega$ be the central state of $\mathcal{C}(E)$. Define the inner product $\langle u, v\rangle = \omega(u^*v)$ on $\mathcal{C}(E)$. Let $\mathcal{W}$ be the Hilbert space which is the completion of $\mathcal{C}(E)$ with respect to this inner product. The operators $L_u$ and $R_u[u \in \mathcal{C}(E)]$ extend to this completion.

The principal automorphism $B$ leaves $\omega$ invariant. Thus $B$ extends to a unitary transformation $B: \mathcal{W} \to \mathcal{W}$. Since $B^* = B^{-1} = B$, $B$ is also self-adjoint.

*Definition 6:* The *Segal representation* $\pi$ of $\mathcal{C}(E \oplus E)$ is the representation by operators on the Hilbert space $\mathcal{W}$ [the completion of $\mathcal{C}(E)$ given by the central state $\omega$] determined by

$$\pi(Q(x)) = L_{Q(x)}$$

and

$$\pi(P(x)) = iR_{Q(x)}B.$$

Note that $BL_{Q(x)} = -L_{Q(x)}B$, $BR_{Q(x)} = -R_{Q(x)}B$, and $B^2 = 1$, so this is indeed a representation. Since also $B = B^*$, it is in fact a $*$ representation.

*Proposition 5:* The Segal representation is unitarily equivalent to the Fock representation.

*Proof:* Let $\Omega_0 \in \mathcal{W}$ be the element 1. Let $\omega_0$ be the state of $\mathcal{C}(E \oplus E)$ defined by $\omega_0(u) = \langle \Omega_0, \pi(u)\Omega_0\rangle$. We use the identities (valid for $x$ real) $A^*(x)A(x) = \frac{1}{2}[\|x\|^2 - iP(x)Q(x)]$ and $Q(x)^2 = \|x\|^2$ to evaluate $\omega_0(A^*(x)A(x))$. We obtain $\omega_0(A^*(x)A(x)) = \langle \Omega_0, \pi(A^*(x)A(x))\Omega_0\rangle = \frac{1}{2}\omega(\|x\|^2 - Q(x)^2) = 0$. Thus, by a theorem of Shale and Stinespring,[13] $\omega_0$ is the Fock vacuum state of the canonical anticommutation relations.

## 6. THE GROSS CONE

The Segal representation allows us to exhibit a certain cone, one which is not a cone of positive functions. The discovery of Gross was that this cone may be used to obtain spectral properties of operators acting in the fermion Fock space.

Let $\mathfrak{A}$ be a $C^*$-algebra with identity and let $\omega$ be a faithful central state on $\mathfrak{A}$. Define the inner product $\langle u, v\rangle = \omega(u^*v)$ on $\mathfrak{A}$. Let $\mathcal{W}$ be the Hilbert space which is the completion of $\mathfrak{A}$ with respect to this inner product.

Since $\omega$ is central, $\langle u^*, v^*\rangle = \omega(uv^*) = \omega(v^*u) = \langle v, u\rangle$. Thus the adjoint $^*$ is anti-unitary and extends to a conjugation on $\mathcal{W}$.

Let $\mathcal{K}$ be the real subspace of $\mathcal{W}$ corresponding to this conjugation. Then $\mathcal{K}$ is the closure of the self-adjoint elements of the $C^*$-algebra $\mathfrak{A}$.

*Definition 7:* Let $\mathfrak{A}$ be a $C^*$-algebra with identity, and let $\omega$ be a faithful central state on $\mathfrak{A}$. Let $\mathcal{K}$ be the associated real Hilbert space. The *positive cone* $\mathcal{K} \subset \mathcal{K}$ is the closure of the cone of positive elements of $\mathfrak{A}$.

In the case where $\mathfrak{A}$ is the $C^*$-algebra of the canonical anticommutation relations, we will call $\mathcal{K}$ the *Gross cone*.

*Proposition 6:* Let $\mathfrak{A}$ be a $C^*$-algebra with identity, and let $\omega$ be a faithful central state on $\mathfrak{A}$. Let $\mathcal{K}$ be the associated real Hilbert space and let $\mathcal{K} \subset \mathcal{K}$ be the positive cone. Then $\mathcal{K}$ is a Hilbert cone.

*Proof:* We must show that properties (5) and (6) of the definition of a Hilbert cone are satisfied.

Property (5) states that if $u \in \mathcal{K}$, $v \in \mathcal{K}$, then $\langle u, v\rangle \geq 0$. This is obvious if $u, v \in \mathfrak{A}$, since then the centrality of $\omega$ implies that $\langle u, v\rangle = \omega(uv) = \omega(v^{1/2}uv^{1/2}) \geq 0$. The result extends by continuity to all $u, v \in \mathcal{K}$.

Property (6) is the decomposition property. It is known[14] that if $u$ is a self-adjoint element of a $C^*$-algebra $\mathfrak{A}$, then there are positive elements $u^+$ and $u^-$ in $\mathfrak{A}$ with $u = u^+ - u^-$ and $u^+u^- = 0$. We set $|u| = u^+ + u^-$.

*Lemma 1:* $\omega(uv) \leq \omega(|u|\,|v|)$, for all self-adjoint elements $u, v \in \mathfrak{A}$.

*Proof:* Set $u = pq$ and $v = rs$, where $|u| = p^2 = q^2$ and $|v| = r^2 = s^2$. Then

$$\omega(uv) = \omega(pqrs) = \omega(spqr)$$
$$\leq \omega(pssp)^{1/2}\omega(rqqr)^{1/2} = \omega(p^2s^2)^{1/2}\omega(q^2r^2)^{1/2}$$
$$= \omega(|u|\,|v|).$$

*Lemma 2:* Set $\|u\|_2^2 = \omega(u^2)$. Then $\|\,|u| - |v|\,\|_2 \leq \|u - v\|_2$ for all self-adjoint elements $u, v \in \mathfrak{A}$.

*Proof:* This follows immediately from Lemma 1.

Thus we have shown that $|u|$ depends continuously on $u$ in the Hilbert space sense. It follows that $u^+$ and $u^-$ depend continuously on $u$. Thus the decomposition property extends from the space of self-adjoint elements of $\mathfrak{A}$ to its closure $\mathcal{K}$.

*Proposition 7:* The vector 1 is strictly positive.

*Proof*[15]: Consider a vector $u \geq 0$ such that $\langle u, 1\rangle = 0$. We must show that $u = 0$.

Since $u \in \mathcal{K}$, $u \geq 0$, there exists a sequence of $u_n \in \mathfrak{A}$ with $u_n \geq 0$ such that $u_n \to u$. We have $\langle u_n, u_m\rangle = \omega(u_n u_m) = \omega(u_m^{1/2}u_n u_m^{1/2}) \leq \|u_n\|_\infty \omega(u_m) = \|u_n\|_\infty \langle u_m, 1\rangle$. Fix $n$ and let $m \to \infty$. We see that $\langle u_n, u\rangle \leq 0$. Now let $n \to \infty$. It follows that $\langle u, u\rangle \leq 0$, so $u = 0$.

## 7. A CLASS OF FERMION INTERACTIONS

In quantum field theory a system is described by a Hamiltonian $H = H_0 + V$, where $H_0$ is the kinetic energy of the particles that are present, and $V$ is an operator which creates or destroys particles. In the case when the particles are fermions, the creation and destruction operators obey the canonical anticommutation relations.

The operator $H_0$ may be characterized as follows. Let $\mathfrak{A}$ be the $C^*$-algebra of the anticommutation relations [generated by 1 and the $A(x)$, $x \in E$] represented by operators on the Hilbert space $\mathfrak{W}$. Assume the representation is unitarily equivalent to the Fock representation. Let $\Omega_0 \in \mathfrak{W}$ be the Fock vacuum. If $\mu$ is a self-adjoint operator acting in $E$, then there is a unique self-adjoint operator $H_0$ acting in $\mathfrak{W}$ such that $\exp(itH_0)A(x)^* \exp(-itH_0) = A(\exp(it\mu)x)^*$ and $H_0\Omega_0 = 0$. If $\mu$ is positive, then so is $H_0$.

One important example is when $\mu$ has discrete spectrum. Let $\mu = \sum_k \mu_k x_k \langle x_k|$, where for each $k$ $\mu_k$ is a real number and $x_k \langle x_k|$ is the projection onto the space spanned by the vector $x_k \in E$. (The $x_k$ are taken to be orthogonal.) Then the corresponding $H_0$ is given explicitly by $H_0 = \sum_k \mu_k A(k)^*A(k)$. [In this equation and in the following we write $A(k)$ for $A(x_k)$. Similarly we will write $Q(k)$ for $Q(x_k)$ and $P(k)$ for $P(x_k)$.]

*Proposition 8*[3]: Let $J: E \to E$ be a conjugation. Let $\mu$ be a positive self-adjoint operator acting in $E$ which is real (that is, commutes with $J$). Assume that zero is not an eigenvalue of $\mu$. Let $H_0$ be the corresponding self-adjoint operator acting in $\mathfrak{W}$. Then $\exp(-tH_0)$, $t \geq 0$ preserves the Gross cone and is an ergodic semigroup.

It follows from this proposition that $(H_0 + c)^{-1}$ is positivity improving when $c > 0$.

The first part of Proposition 8 is easy to verify explicitly when $\mu$ has discrete spectrum. In that case $\exp(-tH_0) = \Pi_k \exp[-t\mu_k A(k)^*A(k)]$. It is thus sufficient to show that $\exp[-tN(k)]$ is positivity preserving, where $N(k) = A(k)^*A(k)$. Since $N(k)^2 = N(k)$, we may evaluate $\exp[-tN(k)] = 1 + [\exp(-t) - 1]N(k)$. But $N(k) = A(k)^*A(k) = \frac{1}{2}[1 + iQ(k)P(k)]$. Thus in the Segal representation

$$\exp[-tN(k)]u = u + [\exp(-t) - 1]\tfrac{1}{2}[u - Q(k)(Bu)Q(k)]$$
$$= \tfrac{1}{2}[1 + \exp(-t)]u + \tfrac{1}{2}[1 - \exp(-t)]Q(k)(Bu)Q(k).$$

From this expression it is evident that if $u \geq 0$, then $\exp[-tN(k)]u \geq 0$. The general case follows by an approximation argument.[3]

The second part of Proposition 8 follows from Corollary 1.2. In fact, since zero is not an eigenvalue of $\mu$, it follows that zero is an eigenvalue of $H_0$ of multiplicity one with eigenvector $\Omega_0$. In the Segal representation, $\Omega_0 = 1$. But 1 is a strictly positive vector, by Proposition 7. So $\exp(-tH_0)$ is an ergodic semigroup.

*Theorem 4:* Let $\mathfrak{A}$ be the $C^*$-algebra of the anticommutation relations in the Segal representation by operators on the Hilbert space $\mathfrak{W}$. Let $\mathfrak{K}$ be the real subspace of $\mathfrak{W}$ and let $\mathfrak{K} \subset \mathfrak{K}$ be the Gross cone.

Let $u$ be a self-adjoint element of $\mathfrak{A}$ and let $V = -L_uR_u$. Set $H = H_0 + V$. Then if $H \geq \lambda$ and $H\Omega = \lambda\Omega$, $\Omega \neq 0$, then some complex multiple of $\Omega$ is strictly positive and $\lambda$ is an eigenvalue of multiplicity one.

*Proof:* Since $(H_0 + c)^{-1}$ is positivity improving and $-V$ is positivity preserving, it follows that $(H + c)^{-1}$ is positivity improving for $c$ sufficiently large. Thus $\lambda$ is an eigenvalue of multiplicity one and the corresponding eigenspace is spanned by a strictly positive vector.

In the work of Gross[3] a similar result is obtained for $V$ of the form $V = L_u + R_u$, $u = u^*$. In applications these results state that the ground state for a fermion system described in Fock space in unique. In the case of an interaction $V$ which leaves unchanged the number of particles the ground state of $H = H_0 + V$ would be the no-particle state $\Omega_0$. (The Hamiltonian $H$ restricted to an $n$-particle space may well have a degenerate ground state!) Thus these results are significant only when the interaction creates or destroys particles.

It is thus fortunate that the interactions considered here may create and destroy particles. For example, let $x_k$ be mutually orthogonal real unit vectors in $E$, and set $u = ai\,Q(x_1)Q(x_2) + b$, where $a$ and $b$ are real numbers. We shall see that the operator $V = -L_uR_u$ contains pair creation and annihilation terms.

In the Segal representation $Q(k)$ is represented by $L_{Q(k)}$ and $P(k)$ is represented by $iR_{Q(k)}B$. [Here again we write $Q(k)$ for $Q(x_k)$, etc.] Thus $L_u$ represents $aiQ(1)Q(2) + b$, and $R_u$ represents $aiP(2)P(1) + b$. So $V = -L_uR_u$ represents

$$a^2Q(1)Q(2)P(1)P(2) - iab[Q(1)Q(2) + P(2)P(1)] - b^2$$
$$= a^2[2A(2)^*A(2) - 1][2A(1)^*A(1) - 1]$$
$$- 2iab[A(1)^*A(2)^* + A(1)A(2)] - b^2.$$

Notice that the pair creation and annihilation terms are the same as those arising in quantum field theory. In fact, Gross was able to apply his theory to the Hamiltonian $H = H_0 + \lambda i[A(1)^*A(2)^* + A(1)A(2)]$ and derive a uniqueness result for a field theory Hamiltonian with cutoffs but for arbitrary coupling constant $\lambda$.

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# An Analytic Approximation Method for the One-Dimensional Schrödinger Equation. I

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A mathematical method for approximating the solutions of the one-dimensional Schrödinger equation is suggested which leads to a classification scheme identical to that of "classical turning points." In this paper problems with at most two classical turning points are studied. Physical examples are chosen in such a way as to clarify especially the role of complex conjugate turning points and of others which do not belong to the physical region of the position variable. It is shown that, in general, those turning points must be taken into account and can be neglected only if their distances from the physical region of the position variable, as measured in units of a local wavelength, is large. The problem with three classical turning points, which turns out to be of special importance for intermolecular and internuclear forces will be treated in a later paper.

## 1. GENERAL PROBLEM

The solutions of the one-dimensional Schrödinger equation

$$\frac{d^2\psi}{d\xi^2} + K^2(\xi)\psi = 0, \qquad K^2(\xi) = E - V_{\text{eff}}(\xi) \tag{1}$$

shall be approximated by functions of the form

$$\hat{v}(\xi) = \left(\frac{dx}{d\xi}\right)^{-1/2} v(x), \qquad x = x(\xi), \tag{2}$$

where the position variable is called $\xi$. It is the purpose of the approximation method to construct $v(x)$ as a solution to another differential equation

$$\frac{d^2v}{dx^2} + [\rho_1(x) + \rho_2(x)]v = 0 \tag{3}$$

with appropriately chosen functions $\rho_1(x)$, $\rho_2(x)$. Upon inserting (2), (3) transforms into

$$\frac{d^2\hat{v}}{d\xi^2} + \left[\left(\frac{dx}{d\xi}\right)^2 \rho_1(x) + \left(\frac{dx}{d\xi}\right)^2 \rho_2(x) + \tfrac{1}{2}\langle x;\xi\rangle\right]\hat{v} = 0 \tag{3a}$$

which can directly be compared with (1). The term

$$\langle x;\xi\rangle = -2\left(\frac{dx}{d\xi}\right)^{1/2} \frac{d^2}{d\xi^2}\left[\left(\frac{dx}{d\xi}\right)^{-1/2}\right] \tag{4}$$

is called a Schwarz derivative and tends to infinity as $(dx/d\xi)$ tends to zero. In order to get suitable approximations, the following requirements are imposed:

(a) (3) should be exactly solvable;

(b) $\left(\frac{dx}{d\xi}\right)^2 \rho_1(x) = K^2(\xi)$;

(c) $\left(\frac{dx}{d\xi}\right)^2 \rho_2(x) + \frac{1}{2}\langle x;\xi\rangle$ should be free of poles in $\xi$.

These will be discussed in the following. First of all the zeros of $K^2(\xi)$, which from now on are called classical turning points (or simpler turning points) and the choice of $\rho_1(x)$ determine the zeros of $(dx/d\xi)$ [see requirement (b)] which lead to poles of the Schwarz derivative. The choice of $\rho_1(x)$ moreover defines, through requirement (b), the variable $x$ in terms of $\xi$. The function $\rho_2(x)$ should then be chosen so as to fulfill requirements (c) and (a). The approximation method will first be tested on problems with 0, 1, or 2 turning points.

## 2. PROBLEMS WITH 0 AND 1 CLASSICAL TURNING POINTS

All requirements (a), (b), (c) can be satisfied by choosing

$$\rho_1(x) \equiv 1, \qquad x = \int_{\xi_0}^{\xi} K(s)\,ds,$$

$$\rho_2(x) \equiv 0, \qquad \text{or } \rho_2(x) = [(\alpha^2 + 4\alpha)/4(\alpha+2)^2]\,(1/x^2).$$

$\alpha$ = order of the zero of $K^2(\xi)$

for problems with, respectively, no (or one, located at $\xi_0$) classical turning point. The differential equation (3) in this case has no (or one, located at $x = 0$) regular singular point and one irregular singular point at $x = \infty$. The approximation equation (2) becomes identical to the WKB-approximation in the first case (no classical turning point) and to Langer's extension in the second case (one classical turning point of order $\alpha$). These approximations will not be discussed further in this context because they have been treated extensively in the literature (see, for ex., Refs. 1–3).

## 3. PROBLEMS WITH CLASSICAL TURNING POINTS AT $\xi_1$ AND $\xi_2$

Accepting the form

$$\rho_2(x) = (1 - \mu^2 - c^2)/4x^2 \tag{5}$$

for $\rho_2(x)$ and choosing

$$\rho_1(x) = 1 + (2i\kappa/x) + (c^2/4x^2), \tag{6}$$

Eq. (3) becomes the most general differential equation with one regular singular point at $x = 0$ and one irregular singular point at $x = \infty$:

$$\frac{d^2v}{dx^2} + \left(1 + \frac{2i\kappa}{x} + \frac{1-\mu^2}{4x^2}\right)v = 0 \tag{7}$$

which explicitly satisfies requirement (a).

The constants are chosen so as to make this equation identical with Kummer's equation as given in Ref. 4. The case of a single second-order zero of $K^2(\xi)$ ($\alpha = 2$), that is, two coinciding turning points, can be obtained again by choosing

$$\kappa = c = 0, \qquad x(\xi_1) = x(\xi_2) = 0, \qquad \mu^2 = \tfrac{1}{4}, \qquad \xi_1 = \xi_2 = \xi_0.$$

For the case of two turning points it is, therefore, tempting to try now the ansatz

$$\kappa \neq 0, \qquad c = 0, \qquad x(\xi_1) = x(\xi_2) = -2i\kappa, \qquad \mu^2 = \tfrac{1}{4}, \qquad \xi_1 \neq \xi_2 \tag{8}$$

which, through requirement (b), would satisfy requirement (c) as can be seen from the fact, that the only zero of $(dx/d\xi)$ and, therefore, the only pole of the term $\frac{1}{2}\langle x;\xi\rangle$ is located at $x = 0$, cancelling the pole of $(dx/d\xi)^2\rho_2(x)$. It is not yet proved, that the values $x(\xi_1), x(\xi_2)$ as fixed by Eq. (8) coincide with the values $x(\xi_1), x(\xi_2)$ as fixed by the function $x(\xi)$, which again is determined by $\rho_1(x)$ through requirement (b) [see also Eq. (17) below].

The mathematical goal, stated by (a)–(c) would thus be reached for this case too, if the above formulas could be made compatible with (b). That this is possible will be shown by working out physical examples. These will be chosen so as to get further insight into the physical content of the aforementioned concepts and the usefulness of the approximation method.

First, for the special cases $V(r) \equiv 0$ and $V(r) = \text{const}/r$, $l \neq 0$ (both problem with exactly two turning points if $l \neq 0$), requirements (a)–(c) could be fulfilled and would lead to the exact solution of the corresponding radial Schrödinger equations by simply taking $c \neq 0$. However, in order to calculate the harmonic oscillator exactly (also a problem with exactly two classical turning points), energies of bound states, the penetration through potential barriers and the example below approximately, we shall use Eqs. (8). In all these cases it is necessary to fix the branch of the multivalued function $K(\xi)$ which shall be done by taking

$$\arg K(\xi) = \left.\begin{matrix} -\frac{1}{2}\pi \\ +\frac{1}{2}\pi \end{matrix}\right\} \text{ for } \begin{cases} \xi > \xi_2 \\ \xi < \xi_1 \end{cases} \tag{9}$$

for the case of Fig. 1 (energies of bound states).

In a similar manner we take

$$\arg K(\xi) = \left.\begin{matrix} 0 \\ \pi \end{matrix}\right\} \text{ for } \begin{cases} \xi > \xi_2 \\ \xi < \xi_1 \end{cases}, \quad E \leq V_{\max} \tag{10}$$

for the case of Fig. 2 (penetration through potential barriers). The last formula is valid for the case $E \leq V_{\max}$ only, which guarantees real classical turning points.

The opposite case $E > V_{\max}$ leads to complex conjugate turning points and brings in a new difficulty which will first be discussed by specializing $K^2(\xi)$ to be

$$\begin{aligned} K^2(\xi) &= \varphi(\xi - \xi_1)\cdot(\xi - \xi_2) \\ &\equiv \varphi \cdot [(\xi - \bar{\xi})^2 + (\xi - \bar{\xi})(2\bar{\xi} - \xi_1 - \xi_2) \\ &\quad + (\bar{\xi} - \xi_1)(\bar{\xi} - \xi_2)] \end{aligned} \tag{11}$$

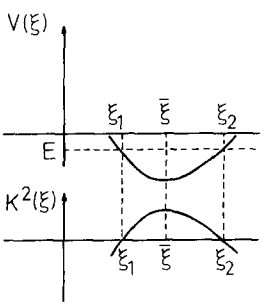


FIG. 1. Energies of bound states.

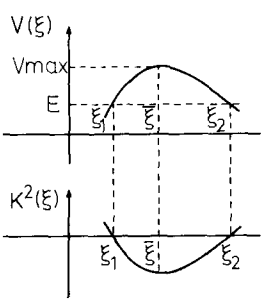


FIG. 2. Penetration through potential barriers.

with constant (or slowly varying) $\varphi$ and an arbitrary constant $\bar{\xi}$. The function $K(\xi)$ then has a branch cut in the complex $\xi$ plane running from $\xi_1$ to $\xi_2$. Requirement (b),

$$\left(\frac{dx}{d\xi}\right)^2 \left(1 + \frac{2i\kappa}{x}\right) = K^2(\xi),$$

can then be satisfied by choosing

$$x = \tfrac{1}{2}\sqrt{\varphi}\,(\xi - \bar{\xi})^2, \tag{12}$$

$$2i\kappa = \tfrac{1}{2}\sqrt{\varphi}\,(\bar{\xi} - \xi_1)(\bar{\xi} - \xi_2), \tag{13}$$

$$\bar{\xi} - \tfrac{1}{2}(\xi_1 + \xi_2) = \pm 0. \tag{14}$$

Equations (12) and (13) automatically satisfy $x(\xi_1) = x(\xi_2) = -2i\kappa$ [see Eqs. (8)]. A distinction has been made in Eq. (14) which is relevant for complex conjugate turning points only, that is, for $E > V_{\max}$. The new situation can be studied by taking

$$\begin{aligned} \arg(\xi - \xi_1) &= \left.\begin{matrix} -\frac{1}{2}\pi \\ +\frac{3}{2}\pi \end{matrix}\right\} \text{for} \begin{cases} \xi - \frac{1}{2}(\xi_1 + \xi_2) = +0 \\ \xi - \frac{1}{2}(\xi_1 + \xi_2) = -0 \end{cases}; \\ \arg(\xi - \xi_2) &= \begin{matrix} +\frac{1}{2}\pi \\ +\frac{1}{2}\pi \end{matrix} \text{ for } \xi - \tfrac{1}{2}(\xi_1 + \xi_2) = \pm 0, \end{aligned} \tag{15}$$

which leads to the following choice of signs of $K(\xi)$ on the two rims of its cut:

$$\arg K(\xi) = \left.\begin{matrix} 0 \\ \pi \end{matrix}\right\} \text{ for } \begin{cases} \xi - \frac{1}{2}(\xi_1 + \xi_2) = +0 \\ \xi - \frac{1}{2}(\xi_1 + \xi_2) = -0 \end{cases}, \quad E > V_{\max} \tag{10'}$$

instead of (10). Since $\kappa$ is defined in terms of $\bar{\xi}$ which according to Eq. (14) may be situated on either side of the cut, it seems quite natural to now choose the upper or lower sign in Eq. (14) according to whether $\kappa$ is inserted into a wavefunction with coordinate $\xi$ on the right or on the left side of the cut, respectively.

Summing up, (9), (10), and (10′) finally lead to the assignments

$$\kappa = \begin{cases} e^{-i\pi/2}\,|\kappa| \\ e^{(3/2)i\pi}\,|\kappa| \end{cases} \text{ for a wave with } \begin{cases} \xi > \frac{1}{2}(\xi_1 + \xi_2) \\ \xi < \frac{1}{2}(\xi_1 + \xi_2) \end{cases}$$

$$\kappa = e^{i\pi/2}\,|\kappa| \quad \text{if } E \leq V_{\max} \tag{16}$$

which, together with (10′) remain valid also in the general case where $\varphi$ is allowed to be any regular function of $\xi$ without zeros. Formula (12) then becomes a special case of the integrated form of requirement (b),

$$\begin{aligned} &\int_0^x [1 + (2i\kappa/u)]^{1/2}\, du = (x^2 + 2i\kappa x)^{1/2} \\ &\quad + i\kappa \ln\left(1 + \{[x + (x^2 + 2i\kappa x)^{1/2}]/i\kappa\}\right) = \int_{\bar{\xi}}^{\xi} K(s)\,ds, \end{aligned} \tag{17}$$

where the multivalued functions are fixed according to (9), (10), (10′) and

$$\ln(e^{i\alpha}) = i\alpha, \quad \sqrt{e^{i\alpha}} = e^{i\alpha/2}. \tag{18}$$

The generalization of (13) can be obtained by inserting

$$x(\xi_1) = e^{i\pi}(2i\kappa), \quad x(\xi_2) = e^{-i\pi}(2i\kappa) \tag{19}$$

into (17). This remains true in the case $E > V_{\max}$ only if $\kappa$ appears in a wavefunction with $\xi > \frac{1}{2}(\xi_1 + \xi_2)$

otherwise Eq. (19) should be replaced by

$$x(\xi_1) = e^{-i\pi}(2i\kappa), \qquad x(\xi_2) = e^{i\pi}(2i\kappa). \tag{20}$$

None of the formulas (19), (20) therefore contradict requirement (b). They also check with Eqs. (8), even in the general case, and, therefore, automatically satisfy requirement (c). Inserting either one of them, (17) finally lead to

$$|\kappa| = \frac{1}{\pi}\left|\int_{\bar{\xi}}^{\xi_1}|K(s)|ds\right| = \frac{1}{\pi}\left|\int_{\bar{\xi}}^{\xi_2}|K(s)|ds\right| = \left|\int_{\xi_1}^{\xi_2}\frac{1}{|\lambda(s)|}\,ds\right| \tag{21}$$

which should be read in connection with (16). The constant $|\kappa|$ can thus be interpreted as a distance between the two classical turning points, measured in units of an "effective wavelength" which itself depends on $\xi$.

Arguments quite analogous to these given in Sec. 4 (see the following example) now lead to the well-known transmission coefficient

$$D = \left[1 + \exp\left(\pm 2\left|\int_{\xi_1}^{\xi_2}|K(s)|ds|\right|\right)\right]^{-1} \quad \text{for } E \gtrless V_{\max}$$

and to a formula for energies of bound states

$$\int_{\xi_1}^{\xi_2} K(s)ds = \pi(n + \tfrac{1}{2}), \qquad n = 0, 1, 2, \ldots,$$

which can also be inferred from Langer's method. Inspite of the fact that new aspects of these approximations could be obtained (based on the new mathematical method used here), they will not be discussed further in this context.

As a preliminary result, it can be stated that there are "classical turning points" which are not contained in the physical region of $\xi$ and which nevertheless play an important role for the above approximation method. In order to discuss this point further, another problem with two classical turning points will be examined.

## 4. $s$-WAVE SCATTERING FROM REPULSIVE POTENTIALS WITH ZERO SLOPE AT THE ORIGIN

For the function now required

$$K^2(r) = 2m/\hbar^2[E - V(r)], \qquad E > 0,$$

a figure can be drawn which agrees with the right side of Fig. 2, the physical region $r \geq 0$ corresponding to the region $\xi \geq \bar{\xi}$ in Fig. 2. At first sight there seems to be no reason for taking into account the region $\xi < \bar{\xi}$ too, corresponding to the "unphysical" region $r < 0$. Remembering that there is a classical turning point in this region it nevertheless seems tempting to use the above formulas, valid for problems with exactly two turning points. A full justification for doing so will be given by the discussion below.

In order to get the regular wavefunction from the general solution

$$\hat{v}(r) = \left(\frac{dx}{d\xi}\right)^{-1/2}[AW_{\kappa,1/4}(2ix) + BW_{-\kappa,1/4}(2ixe^{-i\pi})] \tag{22}$$

which can be inferred from Eqs. (2) and (7), the constants A, B must be chosen so as to get

$$\hat{v}(0) = 0, \qquad \frac{d\hat{v}}{dr}(0) = 1. \tag{23}$$

From the asymptotic expansion

$$\hat{v}(r) \simeq (1/2ik)[\mathfrak{L}_-(k)\,e^{ikr} - \mathfrak{L}_+(k)\,e^{-ikr}], \tag{24}$$

one may then read off the Jost function

$$\mathfrak{L}_+(k) = |\mathfrak{L}_+(k)|\,e^{-i\delta(k)} \tag{25}$$

which can be used to get the $s$-wave phase shift $\delta(k)$. [We are using Jost functions with the phase convention of Newton (see Ref. 5)]. The relevant calculations are made in the Appendix which lead to

$$\mathfrak{L}_+(k) = \sqrt{2\pi}\,[((\kappa)^{\kappa+1/4}e^{-\kappa})/\Gamma(\tfrac{3}{4} + \kappa)]\mathfrak{L}_+(k)^{\mathrm{WKB}}. \tag{26}$$

In this result, we have denoted by

$$\begin{aligned}\mathfrak{L}_+(k)^{\mathrm{WKB}} &= |\mathfrak{L}_+(k)^{\mathrm{WKB}}|\,\exp[-i\delta(k)^{\mathrm{WKB}}] \\ &= \lim_{R\to\infty}(K(\infty)/K(0))^{1/2} \\ &\quad \times \exp\left[-i\left(\int_0^R K(s)\,ds - K(\infty)R\right)\right]\end{aligned} \tag{27}$$

the Jost function [and by $\delta(k)^{\mathrm{WKB}}$ the corresponding $s$-wave phase shift] which is obtained in the WKB approximation for $E > V_{\max}$ and from Langer's extension for $E < V_{\max}$.

As a special result it turns out that the difference $\delta(k) - \delta(k)^{\mathrm{WKB}}$, which can be inferred from (26) is a function of $\kappa$ only (independently of other characteristics of the potential and in contrast to the following example) and tends to zero as $|\kappa| \to \infty$.

The phase $\delta(k)^{\mathrm{WKB}}$ does not take into account the turning point ($s$) outside the physical region of the coordinate. Interpreting the above result we may say that the turning points lying in the unphysical region of the position variable can be neglected if their "distance" to the physical region of the position variable becomes large.

It is interesting to test Eq. (26) on the special example

$$V(r) = (\hbar^2/2m)\,[\alpha^2(\tfrac{1}{4} + b^2)/\cosh^2\alpha r], \qquad \alpha, b = \text{const}, \tag{28}$$

which can be solved exactly (Ref. 6). The Jost function in this case.

$$\frac{\mathfrak{L}_+(K)^{\mathrm{exact}}}{\mathfrak{L}_+(K)^{\mathrm{WKB}}} = \frac{\sqrt{2\pi}\,\exp[-\frac{1}{2}i(b - \sqrt{\frac{1}{4} + b^2}) - \kappa](\kappa)^{\kappa+1/4}\;\sqrt{2\pi}\,\exp[\frac{1}{2}i(b + \sqrt{\frac{1}{4} + b^2}) - \kappa]\cdot[e^{-i\pi/2}\sqrt{\frac{1}{4} + b^2} + \kappa]^{-i\sqrt{(1/4)+b^2}+\kappa+(1/4)}}{\Gamma[\frac{3}{4} + \kappa + \frac{1}{2}i(b - \sqrt{\frac{1}{4} + b^2})]\,\Gamma[\frac{3}{4} + \kappa - \frac{1}{2}i(b + \sqrt{\frac{1}{4} + b^2})]}$$

$$\times \frac{\Gamma(2\kappa - i\sqrt{\frac{1}{4} + b^2})}{\sqrt{2\pi}\,\exp[i\sqrt{\frac{1}{4} + b^2} - 2\kappa]\cdot[2\kappa + e^{-i\pi/2}\sqrt{\frac{1}{4} + b^2}]^{2\kappa - i\sqrt{(1/4)+b^2}-(1/2)}} \tag{29a}$$

$$i\kappa = (k/\alpha) - \sqrt{\tfrac{1}{4} + b^2} \tag{29b}$$

contains terms which depend on $\kappa$ *and* on the potential characteristic $b$. It is thus difficult to compare with the approximation formula (26).

However, until now, we have not taken into account the fact that besides the classical turning points

$$r_{1/2} = \pm r_0, \tag{30}$$

which are real for $E \leq V_{\max}$, there are infinitely many others, located at

$$\pm r_0 + in\pi/\alpha, \quad n = \pm 1, \pm 2, \ldots, \tag{31}$$

which are always complex for real $\alpha$ (these come in through the periodicity of $\cosh\alpha r$). Therefore, strictly speaking, the potential (28) cannot be used as an example for problems with exactly two classical turning points.

Still, remembering the above result, we may try to eliminate the influence of the additional turning points. It is easy to see that their distance $d$ to the physical region of the position variable tends to infinity if $|\alpha|$ tends to zero. However, in order to keep $\kappa$ fixed we then must choose $b$ appropriately, namely $b^2 \gg \frac{1}{4}$ [see Eq. (29b)]. In this way, the special example (28) should reduce to a problem with exactly two turning points. This is confirmed by the fact that the exact formula (29) tends to the approximation formula (26) if $b$ tends to infinity (for $b \gg \frac{1}{2}$ we can insert the asymptotic formula for the $\Gamma$-function).

To sum up, suitable approximation formulas for solutions of the one-dimensional Schrödinger equation can be obtained by taking into account only those classical turning points which are located "nearest" to the physical region of the coordinate variable. This general statement shall be further discussed in later publications, where problems with more than two turning points will be treated.

## APPENDIX

The relation

$$\begin{aligned}\Gamma\left(\frac{1+\mu}{2} - \kappa\right)\Gamma(1-\mu)\, W_{\kappa,\mu/2}(x) - e^{\mp i(\pi/2)(1-\mu)} \\ \times\ \Gamma\left(\frac{1+\mu}{2} + \kappa\right)\Gamma(1-\mu)\, W_{-\kappa,\mu/2}(xe^{\pm i\pi}) \\ = -\frac{\pi}{\sin\pi\mu}\, x^{(1+\mu)/2}\left[\frac{\Gamma(\frac{1}{2}(1+\mu)-\kappa)\Gamma(1-\mu)}{\Gamma(\frac{1}{2}(1-\mu)-\kappa)\Gamma(1+\mu)}\right. \\ \left. - e^{\mp i\pi/2}\cdot\frac{\Gamma(\frac{1}{2}(1+\mu)+\kappa)\Gamma(1-\mu)}{\Gamma(\frac{1}{2}(1-\mu)+\kappa)\Gamma(1+\mu)}\right]\end{aligned} \tag{A1}$$

valid for $|x| \to 0$, can be inferred from Buchholz (Ref. 4). Together with

$$x^{1/2}(\xi) = \tfrac{1}{2}(2i\kappa)^{-1/2}\cdot K(0)\cdot\xi \quad \text{for } \xi \to \bar{\xi} = 0,$$

which can be inferred from Eq. (17), requirement (23) leads to

$$\hat{v}(r) = -\frac{\kappa^{1/4}}{\sqrt{2i\pi K(0)}}\left(\frac{dx}{dr}\right)^{-1/2}\frac{\Gamma(\frac{3}{4}-\kappa)\, W_{\kappa,1/4}(2ix) - e^{i\pi/4}\Gamma(\frac{3}{4}+\kappa)\, W_{-\kappa,1/4}(2ixe^{-i\pi})}{\Gamma(\frac{3}{4}-\kappa)\Gamma(\frac{1}{4}+\kappa) - e^{i\pi/2}\Gamma(\frac{3}{4}+\kappa)\Gamma(\frac{1}{4}-\kappa)}\cdot\ \Gamma(\tfrac{1}{4}-\kappa)\,\Gamma(\tfrac{1}{4}+\kappa) \tag{A2}$$

as regular solution. The Jost function (26) can be read off by inserting the asymptotic expansion of the Whittaker function for the special case of Eqs. (10), (10′)

$$W_{\kappa,1/4}(2ix) \simeq (e^{i\pi}\kappa)^{\kappa}\ \exp\left(-i\int_0^r K(s)ds\right) \tag{A3}$$

$$W_{-\kappa,1/4}(2ixe^{-i\pi}) \simeq e^{i\pi\kappa}(\kappa e^{i\pi})^{-\kappa}\ \exp\left(i\int_0^r K(s)ds\right) \tag{A4}$$

$r \to \infty$.

Here, the asymptotic expansions

$$(2ix)^{\mp\kappa}e^{\pm ix} \simeq (\kappa e^{i\pi})^{\mp\kappa}\ \exp\left(\pm i\int_{\bar{\xi}}^{\xi} K(s)ds\right), \quad \xi \to \infty, \tag{A5}$$

which too can be taken from Eq. (17) has been used.

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