The three-body time-delay operator*

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Using Faddeev's form of time-dependent scattering theory, we give an abstract definition of time delay valid for multichannel scattering. For the three-body scattering problem we find an explicit relation, that is valid on the energy shell, between the time-delay operator and the S operators and their energy derivatives.

I. INTRODUCTION

This paper studies the time-delay problem as it occurs in three-body scattering.[1] Roughly speaking, the time-delay effect is the advancement or retardation of wavepacket motion due to the presence of interactions not contained in the asymptotic Hamiltonians. In the following we first give a rigorous definition of multichannel time delay. This definition is an extension to the multichannel case of the one employed by Goldberger and Watson.[2] Using then Faddeev's[3] results in time-dependent scattering theory, together with the primary singularity structure[4,5] of the exact stationary wavefunction, we construct an explicit solution of the time-delay problem by following an approach similar to Jauch and Marchand's treatment[6] of two-body time delay. Specifically, we obtain a relation between the time-delay operator and the different S operators and their energy derivatives, that is valid on the energy shell. It is the proof of this relation that is the main objective of this paper.

The physical interpretation of the time-delay operator we define is only touched upon very briefly. Because of the controversy that clearly exists already for two-particle time delay regarding the different definition,[2,6,7] which might or might not be equivalent,[8] that are given in the literature, and because of the length of the present paper, we prefer to discuss the physical aspects of the problem elsewhere.

This paper is organized into five sections. Section II introduces those features of three-body time-dependent scattering theory which are necessary in this problem. In Sec. III we define a set of reduced S operators which have an explicit energy dependence because the solution of the time-delay problem cannot be expressed directly in terms of the usual S operators. In Sec. IV we construct the time-delay operator starting from first principles and state the problem we want to solve. Section V gives the main body of the derivation of the time-delay relation. Finally, Appendix A contains a discussion of the projection operators and their momentum–space representations. Appendix B collects some of the details needed in Sec. V. Appendix C discusses a class of terms which vanish and do not contribute to the result derived in Sec. V.

II. TIME-DEPENDENT SCATTERING THEORY

This section gives an outline of the aspects of three-body time-dependent theory that are necessary in the analysis of our problem. The physical scattering problem is taken to be that studied by Faddeev, namely the scattering of three distinct nonrelativistic particles interacting via short range forces. Furthermore, the interaction in each two-body channel is assumed to be such that there is only one two-body boundstate.

Let us briefly describe the coordinate systems we employ. After the center-of-mass motion has been eliminated from our problem there remain six degrees of freedom. In coordinate space we choose the Jacobi variables[9] $\mathbf{x}_\alpha, \mathbf{y}_\alpha$ to describe these. The variable $\mathbf{x}_\alpha$ is the separation of particle α from the center-of-mass of the $(\beta\gamma)$ cluster. The independent variable $\mathbf{y}_\alpha$ gives the vector separation of the constituents of the α cluster namely the spatial separation of particles β and γ. The canonically conjugate momenta related to $\mathbf{x}_\alpha$ and $\mathbf{y}_\alpha$ are denoted by $\mathbf{p}_\alpha$ and $\mathbf{q}_\alpha$. The momenta $\mathbf{p}_\alpha$ describes the relative motion of particle α and cluster α. The kinetic energy of this motion is given by $\mathbf{p}_\alpha^2/2n_\alpha$ where $n_\alpha = m_\alpha(m_\beta+m_\gamma)/(m_\alpha+m_\beta+m_\gamma)$ represents the reduced mass of particle α and cluster α. The internal momentum of cluster α is just $\mathbf{q}_\alpha$. The kinetic energy associated with this motion is $\mathbf{q}_\alpha^2/2\mu_\alpha$ where $\mu_\alpha = m_\beta m_\gamma/(m_\beta+m_\gamma)$ is now the reduced mass for particles β and γ relative to their own center-of-mass system. It is clear that we have three distinct ($\alpha = 1, 2, 3$) Jacobi coordinate systems each of which provides a complete description of the degrees of freedom.

The behavior of any physical system is determined by its Hamiltonian. The free Hamiltonian related to the total kinetic energy is given by

$$H_0 = \frac{\mathbf{p}_\alpha^2}{2n_\alpha} + \frac{\mathbf{q}_\alpha^2}{2\mu_\alpha}, \quad \alpha = 1, 2, 3. \tag{2.1}$$

We shall employ an abbreviated notation for these kinetic energies, viz.

$$\tilde{p}_\alpha^2 = \frac{\mathbf{p}_\alpha^2}{2n_\alpha}, \quad \tilde{q}_\alpha^2 = \frac{\mathbf{q}_\alpha^2}{2\mu_\alpha}. \tag{2.2}$$

The right-hand side of Eq. (2.1) is independent of the index α. We shall take notational advantage of this in-

variance of H_0 by frequently omitting the α label. There is a similar invariant quantity in coordinate space. If we define

$$\tilde{x}_\alpha^2 = 2n_\alpha \mathbf{x}_\alpha^2, \quad \tilde{y}_\alpha^2 = 2\mu_\alpha \mathbf{y}_\alpha^2, \tag{2.3a}$$

and

$$\tilde{\rho}^2 = \tilde{x}_\alpha^2 + \tilde{y}_\alpha^2, \tag{2.3b}$$

then $\tilde{\rho}$ is a coordinate space invariant for all α.

The complete Hamiltonian is then obtained by adding to H_0 all the interactions possible in the system. So for the system Faddeev studies we get

$$H = H_0 + \sum_{\alpha=1}^{3} V_\alpha \tag{2.4}$$

where V_α is the potential acting between the particles β and γ. The Hamiltonians H and H_0 are operators acting in the Hilbert space of square integrable functions of our six degrees of freedom, i.e., $L^2(\mathbf{p}_\alpha, \mathbf{q}_\alpha)$. We shall denote this Hilbert space by $\mathcal{H}$, the inner product related to $\mathcal{H}$ by $(,)$ and the identity operator on $\mathcal{H}$ by E. Acting on $\mathcal{H}$, H_0 and H are both self-adjoint operators.[3]

We next want to consider the different kinds of asymptotic motion because these will finally specify the solutions of the scattering problem. Because of the short-range nature of the forces we may expect that as $t \to \pm\infty$ the three-body problem is characterized by freely moving clusters. We have two distinct types of cluster motion. First, there are three possible cases of motion involving two clusters, each of which can be labeled by the index α, indicating the particle that moves in isolation. Secondly, there is a single motion involving three clusters, labeled by the index $\alpha = 0$, namely when all three particles move independently. With each cluster description of the asymptotic motion there is an associated asymptotic Hamiltonian, determined by including all the intracluster potentials and omitting the intercluster potentials. For the two-cluster type of motion these Hamiltonians are given by

$$H_\alpha = H_0 + V_\alpha. \tag{2.5}$$

For the three-cluster motion the asymptotic Hamiltonian is clearly H_0.

At this point we recall that each two-body interaction is capable of supporting only one boundstate. We shall let $\psi_\alpha(\mathbf{q}_\alpha)$ be this unit normalized two-body boundstate wavefunction in the space of square integrable functions of $\mathbf{q}_\alpha$, i.e., $L^2(\mathbf{q}_\alpha)$. The corresponding boundstate energy is $-\chi_\alpha^2$. So we have

$$(\tilde{q}_\alpha^2 + v_\alpha)\psi_\alpha = -\chi_\alpha^2 \psi_\alpha, \quad \alpha = 1, 2, 3. \tag{2.6}$$

The symbol v_α represents the potential found in the two-body problem involving the particles β and γ. As we know V_α and v_α are integral operators in momentum space whose kernels are related in the following way:

$$V_\alpha(\mathbf{p}_\alpha, \mathbf{q}_\alpha; \mathbf{p}'_\alpha, \mathbf{q}'_\alpha) = v_\alpha(\mathbf{q}_\alpha, \mathbf{q}'_\alpha)\,\delta(\mathbf{p}_\alpha - \mathbf{p}'_\alpha). \tag{2.7}$$

Because of this fact that there is only one boundstate for a pair, each of the different cluster geometries will specify a scattering channel. We now want to describe the wavepackets that characterize the asymptotic channel motion. Let us consider, e.g., the α channel ($\alpha \neq 0$). The cluster $(\beta\gamma)$ will be described by the boundstate wavefunction $\psi_\alpha(\mathbf{q}_\alpha)$. To describe the relative motion of α and the center-of-mass of the pair $(\beta\gamma)$ we shall need the appropriate wavepacket indicated by $f_\alpha(\mathbf{p}_\alpha)$. In effect this function f_α is like a two-particle wavepacket except that one of the particles is a cluster. So for f_α to be an acceptable wavepacket it must lie in the Hilbert space of square integrable function of $\mathbf{p}_\alpha$, i.e., $L^2(\mathbf{p}_\alpha)$ which we denote by $\mathcal{H}_\alpha$. The inner product for this space will be $(,)_\alpha$ and E_α will be the identity operator. So the α channel motion is described by $f_\alpha(\mathbf{p}_\alpha)\psi_\alpha(\mathbf{q}_\alpha)$ and since ψ_α is a known function, all the nontrivial information about this channel is given by f_α. For the three free particle cluster we have all six degrees of freedom present and the related wavepacket will have the form $f_0(\mathbf{p}, \mathbf{q})$. The space for f_0 will be $L^2(\mathbf{p}, \mathbf{q}) = \mathcal{H}_0$, its inner product $(,)_0$ and its identity E_0. Of course, $\mathcal{H}_0$ is mathematically identical with $\mathcal{H}$.

It is useful now to construct Hamiltonians that act in the channel spaces $\mathcal{H}_\alpha$. These new Hamiltonians are suggested by utilizing Eqs. (2.5), (2.6), and (2.7) to get

$$\begin{aligned} H_\alpha f_\alpha(\mathbf{p}_\alpha)\psi_\alpha(\mathbf{q}_\alpha) &= (\tilde{p}_\alpha^2 + \tilde{q}_\alpha^2 + V_\alpha) f_\alpha(\mathbf{p}_\alpha)\psi_\alpha(\mathbf{q}_\alpha) \\ &= (\tilde{p}_\alpha^2 - \chi_\alpha^2) f_\alpha(\mathbf{p}_\alpha)\psi_\alpha(\mathbf{q}_\alpha), \quad \alpha > 0. \end{aligned} \tag{2.8}$$

Eliminating the multiplicative factor $\psi_\alpha(\mathbf{q}_\alpha)$, we are lead to define the channel Hamiltonian $\tilde{H}_\alpha$ by

$$\tilde{H}_\alpha f_\alpha = (\tilde{p}_\alpha^2 - \chi_\alpha^2) f_\alpha \in \mathcal{H}_\alpha, \quad \alpha > 0. \tag{2.9}$$

For the $\alpha = 0$ case the channel Hamiltonian $\tilde{H}_0$ does not differ from the asymptotic Hamiltonian H_0. Thus

$$\tilde{H}_0 f_0 = (\tilde{p}^2 + \tilde{q}^2) f_0 \in \mathcal{H}_0. \tag{2.10}$$

We then introduce a single Hilbert space to describe all these possible asymptotic motions of the three-body system. This space, denoted by $\hat{\mathcal{H}}$, must clearly be the following product space:

$$\hat{\mathcal{H}} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3. \tag{2.11}$$

The inner product of $\hat{\mathcal{H}}$ will be $(,)_\wedge$, its identity will be $\hat{E}$. This inner product is given in terms of previous inner products as

$$(f, f')_\wedge = \sum_{\alpha=0}^{3} (f_\alpha, f'_\alpha)_\alpha. \tag{2.12}$$

An important remark we have to make here is that for multichannel scattering this Hilbert space describing free asymptotic motion, namely $\hat{\mathcal{H}}$, is different from the Hilbert space describing the exact solution, namely $\mathcal{H}$. So, if the channel functions f_α are set in $\mathcal{H}$ by writing $f_\alpha\psi_\alpha$, then the channels are not orthogonal, viz. $(f_\alpha\psi_\alpha, f'_\beta\psi_\beta) \neq 0$ $(\alpha, \beta > 0)$.

To conclude this part, we first define a projection operator P_α from $\mathcal{H}$ into $\mathcal{H}$ by

$$P_\alpha f = f_\alpha \psi_\alpha \in \mathcal{H}, \quad \alpha > 0, \tag{2.13a}$$

where

$$f_\alpha(\mathbf{p}_\alpha) = \int \psi_\alpha(\mathbf{q}_\alpha)^* f(\mathbf{p}_\alpha, \mathbf{q}_\alpha)\, d\mathbf{q}_\alpha. \tag{2.13b}$$

The subspace associated with the range of P_α consists of all separable functions in $\mathbf{p}_\alpha$ and $\mathbf{q}_\alpha$ where the function of $\mathbf{q}_\alpha$ is ψ_α. Secondly, we define an operator I_α from $\mathcal{H}$ onto $\mathcal{H}_\alpha$ by

$$I_\alpha f = f_\alpha \in \mathcal{H}_\alpha. \tag{2.14}$$

We now turn to the discussion of the Moller operators $U_\alpha^{(\pm)}$ which are the basic elements of scattering theory. Faddeev's work[3] establishes that $U_\alpha^{(\pm)}$ may be constructed from the solutions of a Fredholm integral equation that contains the same physics as the three-body time-independent Schrödinger equation, with the supplementary advantage that the boundary conditions are built into the structure of the equation.

The $U_\alpha^{(\pm)}$ operators which map $\mathcal{H}_\alpha$ into $\mathcal{H}$, have the following three properties:

$$(1)\quad U_\alpha^{(\pm)\dagger} U_\beta^{(\pm)} = \delta_{\alpha\beta} E_\beta \quad : \mathcal{H}_\beta \to \mathcal{H}_\alpha, \tag{2.15}$$

$$(2)\quad \sum_{\alpha=0}^{3} U_\alpha^{(\pm)} U_\alpha^{(\pm)\dagger} = E - P_d \quad : \mathcal{H} \to \mathcal{H}, \tag{2.16}$$

$$(3)\quad H U_\alpha^{(\pm)} = U_\alpha^{(\pm)} \tilde{H}_\alpha \quad : \mathcal{H}_\alpha \to \mathcal{H}. \tag{2.17}$$

We shall refer to these basic statements as the fundamental theorem. Property (1) is a statement of the channel orthogonality of the exact wavefunction solution, when $\alpha = \beta$ it becomes a statement of probability conservation. Property (2) is the asymptotic completeness of the exact scattering states. P_d is the projection operator onto the subspace spanned by the eigenfunctions of the discrete spectrum of H. Property (3) is the intertwining property and states that the exact wavefunction will have the same energy as the incident wavefunction, i. e., energy conservation. Furthermore, the function $\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | U_\alpha^{(\pm)} | \mathbf{p}'_\alpha \rangle$ has the following structure:

$$\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | U_\alpha^{(\pm)} | \mathbf{p}'_\alpha \rangle = \psi_\alpha(\mathbf{q}_\alpha)\delta(\mathbf{p}_\alpha - \mathbf{p}'_\alpha) - \langle \mathbf{p}_\alpha \mathbf{q}_\alpha | K_\alpha^{(\pm)} | \mathbf{p}'_\alpha \rangle. \tag{2.18}$$

The first term on the right represents the unscattered portion of the wavefunction. The second term is the scattered wave and can be written as

$$\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | K_\alpha^{(\pm)} | \mathbf{p}'_\alpha \rangle = \frac{\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | \beta_{0\alpha}^{(\mp)} | \mathbf{p}'_\alpha \rangle}{\tilde{p}_\alpha^2 + \tilde{q}_\alpha^2 - \tilde{p}_\alpha'^2 + \chi_\alpha^2 \pm i0} \tag{2.19}$$

where

$$\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | \beta_{0\alpha}^{(\pm)} | \mathbf{p}'_\alpha \rangle = -\sum_{\gamma=1}^{3} \left(\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | G_{\gamma\alpha}^{(\pm)} | \mathbf{p}'_\alpha \rangle - \frac{\phi_\gamma(\mathbf{q}_\gamma) \langle \mathbf{p}_\gamma | H_{\gamma\alpha}^{(\pm)} | \mathbf{p}'_\alpha \rangle}{\tilde{p}_\alpha^2 - \chi_\gamma^2 - \tilde{p}_\alpha'^2 + \chi_\alpha^2 \mp i0} \right). \tag{2.20}$$

Here the functions $\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | G_{\gamma\alpha}^{(\pm)} | \mathbf{p}'_\alpha \rangle$, $\langle \mathbf{p}_\alpha | H_{\gamma\alpha}^{(\pm)} | \mathbf{p}'_\alpha \rangle$ are the half-on-shell solutions of the well-known Faddeev integral equations,[10] viz.

$$\langle \mathbf{p}_\gamma | H_{\gamma\alpha}^{(\pm)} | \mathbf{p}'_\alpha \rangle = H_{\gamma\alpha}(\mathbf{p}_\gamma; \mathbf{p}'_\alpha; \tilde{p}_\alpha'^2 - \chi_\alpha^2 \pm i0), \tag{2.21}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | G_{\gamma\alpha}^{(\pm)} | \mathbf{p}'_\alpha \rangle = G_{\gamma\alpha}(\mathbf{p}_\gamma, \mathbf{q}_\gamma; \mathbf{p}'_\alpha; \mathbf{p}_\alpha'^2 - \chi_\alpha^2 \pm i0). \tag{2.22}$$

The function ϕ_γ is the vertex function defined by $\phi_\gamma(\mathbf{q}_\gamma) = (\tilde{q}_\gamma^2 + \chi_\gamma^2)\psi_\gamma(\mathbf{q}_\gamma)$. In the same way, the wavefunction for three to three scattering is

$$\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | U_0^{(\pm)} | \mathbf{p}'_\alpha \mathbf{q}'_\alpha \rangle = \delta(\mathbf{q}_\alpha - \mathbf{q}'_\alpha)\delta(\mathbf{p}_\alpha - \mathbf{p}'_\alpha) - \langle \mathbf{p}_\alpha \mathbf{q}_\alpha | K_0^{(\pm)} | \mathbf{p}'_\alpha \mathbf{q}'_\alpha \rangle \tag{2.23}$$

where the matrix elements of $K_0^{(\pm)}$ are related to Faddeev's $M_{\alpha\beta}$ operators[3,5]

$$\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | K_0^{(\pm)} | \mathbf{p}'_\alpha \mathbf{q}'_\alpha \rangle = \frac{\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | T^{(\mp)} | \mathbf{p}'_\alpha \mathbf{q}'_\alpha \rangle}{\tilde{p}_\alpha^2 + \tilde{q}_\alpha^2 - \tilde{p}_\alpha'^2 - \tilde{q}_\alpha'^2 \pm i0}, \tag{2.24}$$

$$\langle \mathbf{p}_\alpha \mathbf{q}_\alpha | T^{(\pm)} | \mathbf{p}'_\alpha \mathbf{q}'_\alpha \rangle = \sum_{\alpha,\beta} M_{\alpha\beta}(\mathbf{p}_\alpha, \mathbf{q}_\alpha; \mathbf{p}'_\alpha \mathbf{q}'_\alpha; \tilde{p}_\alpha'^2 + \tilde{q}_\alpha'^2 \pm i0). \tag{2.25}$$

In concluding this section we recall that Faddeev proves the above described results with the assumption that the two-body potentials satisfy a boundedness property and a Holder continuity requirement. Using these assumptions, e. g., the half-on-shell two-body t-matrix satisfies[11]

$$|\langle \mathbf{p} | t^{(\pm)} | \mathbf{p} \rangle| \leq C/(1 + |\mathbf{p} - \mathbf{p}'|)^{1+\theta}, \tag{2.26}$$

$$|\langle \mathbf{p} + \Delta\mathbf{p} | t^{(\pm)} | \mathbf{p}' + \Delta\mathbf{p}' \rangle - \langle \mathbf{p} | t^{(\pm)} | \mathbf{p}' \rangle| \leq C/(1 + |\mathbf{p} - \mathbf{p}'|)^{1+\theta}[|\Delta\mathbf{p}|^\nu + |\Delta\mathbf{p}'|^\nu], \quad \nu < \tfrac{1}{2}, \tag{2.27}$$

where $|\Delta\mathbf{p}| < 1$, $|\Delta\mathbf{p}'| < 1$, and ν may be taken as close to $\frac{1}{2}$ as desired. In our time-delay proof we shall have to construct derivatives of the half-on-shell amplitudes with respect to the momentum arguments. It is clear that the estimate (2. 27) is not strong enough to claim that $\langle \mathbf{p} | t^{(\pm)} | \mathbf{p}' \rangle$ is differentiable with respect to p or p'. We have not investigated the necessary modifications needed to ensure differentiability of $t^{(\pm)}$ and the other half-on-shell matrix elements $H_{\alpha\beta}^{(\pm)}$, $\beta_{0\beta}^{(\pm)}$, $T^{(\pm)}$. However, it is likely that the original potential must be differentiable and that this derivative of the potential must also satisfy a Holder continuity requirement.

III. REDUCED S-MATRIX ELEMENTS

In this section we describe the essential features of the S matrix and introduce the reduced S-matrix elements needed in our derivation. The S matrix is defined to be a mapping between the initial experimentally determined wavepacket f_α and the observed post-scattering wavepackets f'_β. We know[3] that, in terms of the Moller wave operators, this mapping looks like

$$f'_\beta = U_\beta^{(+)\dagger} U_\alpha^{(-)} f_\alpha, \tag{3.1}$$

so

$$S_{\beta\alpha} = U_\beta^{(+)\dagger} U_\alpha^{(-)} \quad : \mathcal{H}_\alpha \to \mathcal{H}_\beta. \tag{3.2}$$

This S matrix is even simpler when written down as an operator on the asymptotic channel space $\hat{\mathcal{H}}$. In this case the information in Eq. (3. 1) can be expressed as

$$\hat{f}' = S\hat{f} \quad : \hat{\mathcal{H}} \to \hat{\mathcal{H}}. \tag{3.3}$$

Let us now recall the basic properties of the S matrix because it will turn out that the time-delay operator has properties which parallel those of the S matrix. The first basic property of the S matrix is that it is a unitary operator when acting on the channel space $\hat{\mathcal{H}}$, viz.

$$S^\dagger S = S S^\dagger = \hat{E}. \tag{3.4}$$

In component form the equivalent of Eq. (3. 4) is

$$\sum_{\gamma=0}^{3} S_{\gamma\alpha}^\dagger S_{\gamma\beta} = E_\beta \delta_{\alpha\beta}. \tag{3.5}$$

This unitarity is an immediate consequence of the statements (1) and (2) in the fundamental theorem.

The second basic property of S we want to stress is the intertwining property with the channel Hamiltonians $\tilde{H}_\alpha$,

$$S_{\alpha\beta} \tilde{H}_\beta = \tilde{H}_\alpha S_{\alpha\beta}. \tag{3.6}$$

This intertwining feature is the direct consequence of statement (3) in the fundamental theorem.

We now shall turn to the definition of the reduced matrix elements of S. In order to carry out this definition we first require the known[4,5] representations of the kernels of S in terms of $T^{(+)}$, $\beta_{0\beta}^{(+)}$, and $H_{\alpha\beta}^{(+)}$ introduced in Sec. II. For a rearrangement scattering process one has

$$S_{\alpha\beta}(\mathbf{p}_\alpha;\mathbf{p}'_\beta)=\delta_{\alpha\beta}\delta(\mathbf{p}_\alpha-\mathbf{p}'_\beta)-2\pi i\delta(\tilde{p}_\alpha^2-\chi_\alpha^2-\tilde{p}_\beta'^2+\chi_\beta^2)\times\langle\mathbf{p}_\alpha|H_{\alpha\beta}^{(+)}|\mathbf{p}'_\beta\rangle. \tag{3.7}$$

The S matrices involving three free particles in either the initial or final state are given by

$$S_{0\beta}(\mathbf{p},\mathbf{q};\mathbf{p}'_\beta)=-2\pi i\delta(\tilde{p}^2+\tilde{q}^2-\tilde{p}_\beta'^2+\chi_\beta^2)\langle\mathbf{pq}|\beta_{0\beta}^{(+)}|\mathbf{p}'_\beta\rangle, \tag{3.8}$$

and

$$S_{\alpha0}(\mathbf{p}_\alpha;\mathbf{p}',\mathbf{q}')=-2\pi i\delta(\tilde{p}_\alpha^2-\chi_\alpha^2-\tilde{p}'^2-\tilde{q}'^2)\langle\mathbf{p}_\alpha|\beta_{\alpha0}^{(+)}|\mathbf{p}'\mathbf{q}'\rangle. \tag{3.9}$$

The amplitude $\beta_{\alpha0}^{(+)}$ is related to $\beta_{0\alpha}^{(-)}$ by

$$\langle\mathbf{p}_\alpha|\beta_{\alpha0}^{(+)}|\mathbf{p}'\mathbf{q}'\rangle=\langle\mathbf{p}'\mathbf{q}'|\beta_{0\alpha}^{(-)}|\mathbf{p}_\alpha\rangle^*. \tag{3.10}$$

The $*$ indicates complex conjugation. Finally the three-to-three S matrix is

$$S_{00}(\mathbf{p},\mathbf{q};\mathbf{p}'\mathbf{q}')=\delta(\mathbf{p}-\mathbf{p}')\delta(\mathbf{q}-\mathbf{q}')-2\pi i\delta(\tilde{p}^2+\tilde{q}^2-\tilde{p}'^2-\tilde{q}'^2)\langle\mathbf{pq}|T^{(+)}|\mathbf{p}'\mathbf{q}'\rangle. \tag{3.11}$$

We want to construct S matrices related to the expression above but with the energy delta function removed. We will use a lower case s to denote these new S matrices. Consider, in the first instance, $S_{\alpha\beta}$. Defining $E=\tilde{p}_\alpha^2-\chi_\alpha^2$ and $E'=p_\beta'^2-\chi_\beta^2$ and employing the relation

$$\delta_{\alpha\beta}\delta(\mathbf{p}_\alpha-\mathbf{p}'_\beta)=\delta_{\alpha\beta}\frac{\delta(E-E')\delta(\hat{p}_\alpha-\hat{p}'_\beta)}{(n_\alpha p_\alpha n_\beta p'_\beta)^{1/2}}, \tag{3.12}$$

we may write Eq. (3.7) in the form

$$S_{\alpha\beta}(\mathbf{p}_\alpha;\mathbf{p}'_\beta)=\frac{\delta(E-E')}{(n_\alpha p_\alpha n_\beta p'_\beta)^{1/2}}\times[\delta_{\alpha\beta}\delta(\hat{p}_\alpha-\hat{p}'_\beta)-2\pi i(n_\alpha p_\alpha n_\beta p'_\beta)^{1/2}\times\langle\mathbf{p}_\alpha|H_{\alpha\beta}^{(+)}|\mathbf{p}'_\beta\rangle]. \tag{3.13}$$

In these expressions $\hat{p}$ indicates the unit direction vector associated with $\mathbf{p}$. Thus we are lead to define $s_{\alpha\beta}(E)$ by

$$\langle\hat{p}_\alpha|s_{\alpha\beta}(E)|\hat{p}'_\beta\rangle\equiv\delta_{\alpha\beta}\delta(\hat{p}_\alpha-\hat{p}'_\beta)-2\pi i(n_\alpha p_\alpha n_\beta p'_\beta)^{1/2}\times\langle\mathbf{p}_\alpha|H_{\alpha\beta}^{(+)}|\mathbf{p}'_\beta\rangle. \tag{3.14}$$

The energy dependence E appears on the right-hand side of Eq. (3.14) by virtue of the fact that $p_\alpha=[2n_\alpha(E+\chi_\alpha^2)]^{1/2}$ and $p'_\beta=[2n_\beta(E+\chi_\beta^2)]^{1/2}$. The kernel $\langle\hat{p}_\alpha|s_{\alpha\beta}(E)|\hat{p}'_\beta\rangle$ represents an operator that will map square integrable functions with respect to the measure $d\Omega_{\hat{p}'_\beta}$, i.e., $L^2(\hat{p}'_\beta)$, into $L^2(\hat{p}_\alpha)$. When $\alpha=\beta$ the leading factor on the right of Eq. (3.14) is the identity operator on the space $L^2(\hat{p}_\alpha)$. The energy dependence indicated on the left of Eq. (3.14) means that for each $S_{\alpha\beta}$ operator we have a one-parameter family of operators $s_{\alpha\beta}(E)$.

We consider next S matrices involving three free particles in the initial or final state. The kinematic relation $E=\tilde{p}_\alpha^2+\tilde{q}_\alpha^2$ suggests we define the angle ω_α such that

$$\tilde{p}_\alpha=\sqrt{E}\cos\omega_\alpha,\quad \tilde{q}_\alpha=\sqrt{E}\sin\omega_\alpha,\quad 0\le\omega_\alpha\le\pi/2. \tag{3.15}$$

Using this convention the six-dimension delta function appearing in (3.11) may be written

$$\delta(\mathbf{p}_\alpha-\mathbf{p}'_\alpha)\delta(\mathbf{q}_\alpha-\mathbf{q}'_\alpha)=\frac{\delta(E-E')\delta(\omega_\alpha-\omega'_\alpha)\delta(\hat{p}_\alpha-\hat{p}'_\alpha)\delta(\hat{q}_\alpha-\hat{q}'_\alpha)}{p_\alpha q_\alpha p'_\alpha q'_\alpha(\mu_\alpha n_\alpha)^{1/2}}. \tag{3.16}$$

Then using Eq. (3.11) we find that the reduced matrix operator $s_{00}(E)$ is

$$\langle\omega_\alpha\hat{p}_\alpha\hat{q}_\alpha|s_{00}(E)|\omega'_\alpha\hat{p}'_\alpha\hat{q}'_\alpha\rangle\equiv\delta(\omega_\alpha-\omega'_\alpha)\delta(\hat{p}_\alpha-\hat{p}'_\alpha)\delta(\hat{q}_\alpha-\hat{q}'_\alpha)-2\pi i(\mu_\alpha n_\alpha)^{1/2}p_\alpha q_\alpha p'_\alpha q'_\alpha\langle\mathbf{p}_\alpha\mathbf{q}_\alpha|T^{(+)}|\mathbf{p}'_\alpha\mathbf{q}'_\alpha\rangle. \tag{3.17}$$

Here the operator $s_{00}(E)$ takes a function from $L^2(\omega'_\alpha,\hat{q}'_\alpha,\hat{p}'_\alpha)$ into $L^2(\omega_\alpha,\hat{q}_\alpha,\hat{p}_\alpha)$. In this case the Hilbert space is defined relative to the measure $\frac{1}{2}(2\mu_\alpha 2n_\alpha)^{3/2}\times\cos^2\omega_\alpha\sin^2\omega_\alpha d\omega_\alpha d\hat{p}_\alpha d\hat{q}_\alpha$. This measure is independent of α. From now on, we will denote this space by L_0^2 and L_α^2 will indicate the space $L^2(\hat{p}_\alpha)$.

The reduced S-operator related to $S_{0\beta}$ and $S_{\alpha0}$ are defined in the same way, e.g.,

$$S_{0\beta}(\mathbf{p}_\alpha,\mathbf{q}_\alpha;\mathbf{p}'_\beta)\equiv\delta(E-E')\frac{\langle\omega_\alpha\hat{p}_\alpha\hat{q}_\alpha|s_{0\beta}(E)|\hat{p}'_\beta\rangle}{(\mu_\alpha n_\alpha)^{1/4}p_\alpha q_\alpha(n_\beta p'_\beta)^{1/2}} \tag{3.18}$$

and, using Eq. (3.8)

$$\langle\omega_\alpha\hat{p}_\alpha\hat{q}_\alpha|s_{0\beta}(E)|\hat{p}'_\beta\rangle=-2\pi i(\mu_\alpha n_\alpha)^{1/4}p_\alpha q_\alpha(n_\beta p'_\beta)^{1/2}\langle\mathbf{p}_\alpha\mathbf{q}_\alpha|\beta_{0\beta}^{(+)}|\mathbf{p}'_\beta\rangle \tag{3.19}$$

where p_α and q_α are the momenta determined by E.

The momentum and reduced mass factors are chosen such that the operator relations S obeys on $\hat{H}$ are also valid for $s(E)$ on a reduced space. To illustrate this consider the kernel form of the unitarity Eq. (3.5) for $\alpha,\beta>0$

$$\delta^3(\mathbf{p}_\alpha-\mathbf{p}'_\beta)\delta_{\alpha\beta}=\sum_{\gamma=1}^{3}\int S_{\gamma\alpha}(\mathbf{p}''_\gamma,\mathbf{p}_\alpha)^*S_{\gamma\beta}(\mathbf{p}''_\gamma,\mathbf{p}'_\beta)\,d\mathbf{p}''_\gamma+\int S_{0\alpha}(\mathbf{p}''_\alpha,\mathbf{q}''_\alpha;\mathbf{p}_\alpha)^*S_{0\beta}(\mathbf{p}''_\alpha\mathbf{q}''_\alpha;\mathbf{p}'_\beta)\,d\mathbf{p}''_\alpha\,d\mathbf{q}''_\alpha. \tag{3.20}$$

If we now use

$$d\mathbf{p}''_\alpha\,d\mathbf{q}''_\alpha=(n_\alpha\mu_\alpha)^{1/2}p''^2_\alpha q''^2_\alpha\,dE''\,d\omega''_\alpha\,d\hat{p}''_\alpha\,d\hat{q}''_\alpha \tag{3.21}$$

together with Eq. (3.12) and we equate the coefficient of $\delta(E-E')$ appearing on both sides we obtain for Eq. (3.20)

$$\delta_{\alpha\beta}\delta(\hat{p}_\alpha-\hat{p}'_\beta)=\sum_{\gamma=1}^{3}\int\langle\hat{p}''_\gamma|s_{\gamma\alpha}(E)|\hat{p}_\alpha\rangle^*\langle\hat{p}''_\gamma|s_{\gamma\beta}(E)|\hat{p}'_\beta\rangle\,d\hat{p}''_\gamma+\int\langle\omega''_\alpha\hat{p}''_\alpha\hat{q}''_\alpha|s_{0\alpha}(E)|\hat{p}_\alpha\rangle^*\times\langle\omega''_\alpha\hat{p}''_\alpha\hat{q}''_\alpha|s_{0\beta}(E)|\hat{p}'_\beta\rangle\,d\omega''_\alpha\,d\hat{p}''_\alpha\,d\hat{q}''_\alpha. \tag{3.22}$$

This result is the kernel form of the operator equation

$$\delta_{\alpha\beta}1_\alpha = \sum_{\gamma=0}^{3} s^\dagger_{\gamma\alpha}(E)s_{\gamma\beta}(E). \tag{3.23}$$

A similar demonstration shows that this equation is valid for all values of α and β. The operator 1_α stands for the identity operator on the space L^2_α, 1_0 is the identity operator on L^2_0.

Note that we can introduce a reduced channel space defined by

$$\hat{H}_r \equiv L^2_0 \oplus L^2_1 \oplus L^2_2 \oplus L^2_3. \tag{3.24}$$

Acting on this space, the Eq. (3.23) is the component form of the first part of

$$\hat{1}_r = s^\dagger(E)s(E) = s(E)s^\dagger(E) \tag{3.25}$$

where 1_r is the identity on $\hat{H}_r$. The second equality here is obtained in the same way as the first. Clearly Eq. (3.25) is a one parameter family of operator relations on $\hat{H}_r$ which are equivalent to the relation (3.4) on the channel space $\hat{H}$. It shall turn out that the three-body time-delay operator will also have two forms—one on $\hat{H}$ and one on $\hat{H}_r$.

IV. DEFINITION OF TIME DELAY AND STATEMENT OF THE PROBLEM

Let us now describe the definition of the time-delay operator. Consider the exact wavepacket given by

$$\Psi_\alpha(t) = \exp(-iHt)U^{(-)}_\alpha f_\alpha, \quad f_\alpha \in H_\alpha, \quad \Psi_\alpha(t) \in H. \tag{4.1}$$

This is the wavepacket that evolves from the asymptotic channel wavepacket f_α. Likewise consider

$$\Psi'_\beta(t) = \exp(-iHt)U^{(-)}_\beta f'_\beta, \quad f'_\beta \in H_\beta, \quad \Psi'_\beta(t) \in H.$$

If we recall that $\tilde{\rho} = (\tilde{x}^2_\alpha + \tilde{y}^2_\alpha)^{1/2}$ is independent of $\alpha = 1, 2, 3$, then we can use the distance $\tilde{\rho}$ to define the radius of a sphere in the six-dimensional space $\mathbf{x}_\alpha, \mathbf{y}_\alpha$. We will associate a projection operator $\bar{P}(R)$ on H with this sphere:

$$\begin{aligned} \bar{P}(R)f(\mathbf{x}_\alpha, \mathbf{y}_\alpha) &= f(\mathbf{x}_\alpha, \mathbf{y}_\alpha) \quad \text{if } |\tilde{x}^2_\alpha + \tilde{y}^2_\alpha|^{1/2} \le R \\ &= 0 \qquad\qquad \text{if } |\tilde{x}^2_\alpha + \tilde{y}^2_\alpha|^{1/2} > R. \end{aligned} \tag{4.2}$$

The inner product $(\Psi_\alpha(t), \bar{P}(R)\Psi_\alpha(t))$ is the likelihood of finding the state Ψ_α inside the sphere of radius R at time t. Now if we form the integral

$$\int_{-t_0}^{t_0} (\Psi_\alpha(t), \bar{P}(R)\Psi_\alpha(t))\, dt, \tag{4.3}$$

its physical interpretation is the fraction of time between $-t_0$ and t_0 that the state Ψ_α spends inside the sphere of radius R. If we perform the limit $t_0 \to \infty$ then the integral represents the total time Ψ_α spends inside the sphere. In association with the integral above we can form the more general integral which gives the overlap within the sphere of two distinct states Ψ_α and Ψ'_β. We define

$$T^E_{\alpha\beta}(R, t_0) \equiv \int_{-t_0}^{t_0} (\Psi_\alpha(t), \bar{P}(R)\Psi'_\beta(t))\, dt. \tag{4.4}$$

In the notation for the complex number $T^E_{\alpha\beta}$ we have indicated some but not all the factors that it depends on. For example, the value of $T^E_{\alpha\beta}$ will depend on f_α and f'_β as well as R and t_0. In the circumstance $\alpha = \beta$ and $f_\alpha = f'_\alpha$, $T^E_{\alpha\beta}$ is real and has the interpretation we have given for the expression (4.3). Our notation for $T^E_{\alpha\beta}$ carries a superscript E in order to specify that the times associated with $T^E_{\alpha\beta}$ relate to the exact wavefunctions $\Psi(t)$.

We may also write down similar definitions that pertain to the evolution of the asymptotic solutions in the absence of the intercluster potentials. For example, these wavepackets are given by

$$\Phi_\alpha(t) = \exp(-iH_\alpha t)I^\dagger_\alpha f_\alpha, \quad f_\alpha \in H_\alpha, \quad \Phi_\alpha(t) \in H, \tag{4.5}$$

$$\Phi'_\beta(t) = \exp(-iH_\beta t)I^\dagger_\beta f'_\beta, \quad f'_\beta \in H_\beta, \quad \Phi'_\beta(t) \in H. \tag{4.6}$$

The absence of the intercluster potentials means that the corresponding evolution may be thought of as "free" since the interaction between the target and the incident wave has no effect on the evolution of the wavepacket. The "free" equivalent of the integral (4.3) is

$$\int_{-t_0}^{t_0} (\Phi_\alpha(t), \bar{P}(R)\Phi_\alpha(t))\, dt. \tag{4.7}$$

This gives the fraction of the time interval $(-t_0, t_0)$ that the "free" system spends in the sphere. The numerical value of the "free" integral will differ from that of the integral for the exact wavepacket. This time difference is entirely due to the effect of the intercluster interaction on the evolution of the wavepacket. As above we write down a general matrix element that has the form (4.7) as its diagonal element:

$$T^F_{\alpha\beta}(R, t_0) \equiv \delta_{\alpha\beta} \int_{-t_0}^{t_0} (\Phi_\alpha(t), \bar{P}(R)\Phi'_\beta))\, dt. \tag{4.8}$$

The Kronecker delta function appears in the definition (4.8) of the free transit time for the following reason. In the α channel free scattering there is no interaction between the target cluster and the incident particle. Thus any scattering which begins in the α-channel must remain in the α-channel. Since the asymptotic forms $\Phi_\alpha(t)$ and $\Phi'_\beta(t)$ are not orthogonal, the Kronecker delta is necessary to preserve the diagonality of the free scattering. Taking the difference of $T^E_{\alpha\beta}$ and $T^F_{\alpha\beta}$ gives us the time-delay for the time interval $(-t_0, t_0)$ and a sphere of radius R.

Now we would like to construct an operator whose expectation value gives us the time-difference described above. We define

$$(f_\alpha, Q_{\alpha\beta}(R, t_0)f'_\beta) \equiv T^E_{\alpha\beta}(R, t_0) - T^F_{\alpha\beta}(R, t_0). \tag{4.9}$$

For each f_α and f'_β the quantities $T^E_{\alpha\beta}$ and $T^F_{\alpha\beta}$ have unique values so that $Q_{\alpha\beta}(R, t_0)$ is defined by Eq. (4.9). It is useful to have an explicit form for $Q_{\alpha\beta}$. This may be obtained as follows. One can write $T^F_{\alpha\beta}$ as

$$\begin{aligned} T^F_{\alpha\beta}(R, t_0) &= \delta_{\alpha\beta} \int_{-t_0}^{t_0} (\exp(-iH_\alpha t)I^\dagger_\alpha f_\alpha, \bar{P}(R)\exp(-iH_\beta t)I^\dagger_\beta f'_\beta)\, dt \\ &= \delta_{\alpha\beta} \int_{-t_0}^{t_0} (I^\dagger_\alpha \exp(-i\tilde{H}_\alpha t)f_\alpha, \bar{P}(R)I^\dagger_\beta \exp(-i\tilde{H}_\beta t)f'_\beta)\, dt \\ &= \delta_{\alpha\beta} \int_{-t_0}^{t_0} (f_\alpha, \exp(i\tilde{H}_\alpha t)\bar{P}_\alpha(R)\exp(-i\tilde{H}_\beta t)f'_\beta)\, dt \end{aligned} \tag{4.10}$$

where the operator $\bar{P}_\alpha(R)$ is

$$\bar{P}_\alpha(R) = I_\alpha \bar{P}(R) I^\dagger_\alpha \quad : H_\alpha \to H_\alpha. \tag{4.11}$$

From the definition (4.11) it at once follows that $\bar{P}_\alpha(R)$ is a bounded self-adjoint operator. It is however not a

projection operator since the idempotent property is not valid. This is seen from

$$\bar{P}_\alpha^2(R) = I_\alpha \bar{P}(R) I_\alpha^\dagger I_\alpha \bar{P}(R) I_\alpha^\dagger \quad : \mathcal{H}_\alpha \to \mathcal{H}_\alpha$$
$$= I_\alpha \bar{P}(R) P_\alpha \bar{P}(R) I_\alpha^\dagger \tag{4.12}$$

where we have used $I_\alpha^\dagger I_\alpha = P_\alpha$ which follows from the definition of I_α, Eq. (2.14). However, in the limit $R \to \infty$, $\bar{P}_\alpha^2(R)$ becomes the identity operator E_α since $\bar{P}(R) \to E$ and

$$I_\alpha E P_\alpha E I_\alpha^\dagger = I_\alpha P_\alpha I_\alpha^\dagger = I_\alpha I_\alpha^\dagger = E_\alpha. \tag{4.13}$$

The last equality again follows from the definition (2.14).

We continue with the explicit construction of $Q_{\alpha\beta}$ by treating $T^E_{\alpha\beta}$ in a fashion parallel to that of $T^F_{\alpha\beta}$. The term $T^E_{\alpha\beta}$ can be written as

$$T^E_{\alpha\beta}(R, t_0) = \int_{-t_0}^{t_0} (\exp(-iHt) U_\alpha^{(-)} f_\alpha, \bar{P}(R) \exp(-iHt) U_\beta^{(-)} f'_\beta)\, dt$$
$$= \int_{-t_0}^{t_0} (U_\alpha^{(-)} \exp(-i\tilde{H}_\alpha t) f_\alpha, \bar{P}(R) U_\beta^{(-)} \times \exp(-i\tilde{H}_\beta t) f'_\beta)\, dt$$
$$= \int_{-t_0}^{t_0} (f_\alpha, \exp(+i\tilde{H}_\alpha t) U_\alpha^{(-)\dagger} \bar{P}(R) U_\beta^{(-)} \times \exp(-i\tilde{H}_\beta t) f'_\beta)_\alpha\, dt. \tag{4.14}$$

In the second version of (4.14) we have employed the intertwinning relation (2). In the third version we have employed the adjoint operation. The difference of Eq. (4.10) and Eq. (4.14) is

$$(f_\alpha, Q_{\alpha\beta}(R, t_0) f'_\beta)$$
$$= \int_{-t_0}^{t_0} (f_\alpha, \exp(i\tilde{H}_\alpha t)[U_\alpha^{(-)\dagger} \bar{P}(R) U_\beta^{(-)} - \delta_{\alpha\beta} \bar{P}_\alpha(R)] \times \exp(-i\tilde{H}_\beta t) f'_\beta)\, dt. \tag{4.15}$$

This defines the operator $Q_{\alpha\beta}(R, t_0)$. The expression above is defined for all $f_\alpha \in \mathcal{H}_\alpha$ and $f'_\beta \in \mathcal{H}_\beta$ since all the operators in the inner product on the right are bounded and the integral is over a finite time interval. So the operator $Q_{\alpha\beta}(R, t_0)$ given by

$$Q_{\alpha\beta}(R, t_0) = \int_{-t_0}^{t_0} \exp(i\tilde{H}_\alpha t)[U_\alpha^{(-)\dagger} \bar{P}(R) U_\beta^{(-)} - \delta_{\alpha\beta} \bar{P}_\alpha(R)] \times \exp(-i\tilde{H}_\beta t)\, dt \tag{4.16}$$

is a bounded operator for finite R, t_0.

Eventually to obtain the physical time delay we will take the limit $t_0 \to \infty$ and follow it by the limit $R \to \infty$. However, some of the interesting properties of the time-delay operator are already present in form (4.16). First, we see that $Q_{\alpha\beta}$ is the component form of an operator on the channel space $\hat{\mathcal{H}}$. Its channel structure is identical to that of the S matrix. The next property is that

$$Q_{\alpha\beta}(R, t_0) = Q^\dagger_{\beta\alpha}(R, t_0). \tag{4.17}$$

This follows directly from the structure of (4.16). In fact, Eq. (4.17) is just the component form of the self-adjoint property for operators on $\hat{\mathcal{H}}$. Thus for any $\hat{f} \in \hat{\mathcal{H}}$ which describes the state of the three-body system in terms of the asymptotic channel wavefunctions the time-delay operator Q will have real matrix elements. Since Q represents an observable this must be the case. However, off-diagonal component forms of Q, i.e., $Q_{\alpha\beta}$, will not generally be real.

It is desirable to take the limits $t_0 \to \infty$ and $R \to \infty$ in the definition of our operator $Q_{\alpha\beta}(R, t_0)$. In the following section we shall construct an operator $Q_{\alpha\beta}$ defined by a kernel composed of generalized functions such that

$$(f_\alpha, Q_{\alpha\beta} f'_\beta)_\alpha = \lim_{R\to\infty} \lim_{t_0\to\infty} (f_\alpha, Q_{\alpha\beta}(R, t_0) f'_\beta)_\alpha. \tag{4.18}$$

The functions f_α and f'_β need to be smooth enough so that the generalized functions appearing in the representation of $Q_{\alpha\beta}$ are well-defined. This restricted set of functions, defined in Appendix A, for which Eq. (4.18) is valid are dense in the space $\hat{\mathcal{H}}$.

One effect of taking the limit $t_0 \to \infty$ in the representation (4.16) is that the $Q_{\alpha\beta}$ operators will now intertwine with the channel Hamiltonians. By changing the variable of integration in Eq. (4.16) it easily follows that

$$\exp(i\tilde{H}_\alpha t) Q_{\alpha\beta}(R, \infty) = Q_{\alpha\beta}(R, \infty) \exp(i\tilde{H}_\beta t) \tag{4.19}$$

or, equivalently,

$$\tilde{H}_\alpha Q_{\alpha\beta}(R, \infty) = Q_{\alpha\beta}(R, \infty) \tilde{H}_\beta. \tag{4.20}$$

This property mirrors the intertwining relation (3.6) valid for the S matrix $S_{\alpha\beta}$.

Before proceeding further we pause to contrast our definition of the time-delay operator with those that exist in the current literature. The main novelty of Eq. (4.16) and the limit process in Eq. (4.18) is of course its multichannel character. However the type of limit in Eq. (4.18) is simpler than that previously introduced by Smith[12] and also adopted by Jauch and Marchand[6] and others.[7] These papers employ an average over R before the $R \to \infty$ limit is taken. This average is used to get rid of oscillatory terms in R. Here we shall find that treating the behavior of the projection operators $\bar{P}_\beta(R)$ and $\bar{P}(R)$ carefully enough shows that these oscillating terms all vanish when evaluated between appropriately smooth wavepackets f_α and f'_β.

Let us now resume the development of the problem. At this point we shall utilize the approach found in Jauch and Marchand's[6] treatment of time-delay in the two-body case. Since the inverse of S exists one can find Q by determining SQ. An element of this product takes the form

$$S_{\gamma\alpha} Q_{\alpha\beta}(R, t_0)$$
$$= \int_{-t_0}^{t_0} S_{\gamma\alpha} \exp(i\tilde{H}_\alpha t)[U_\alpha^{(-)\dagger} \bar{P}(R) U_\beta^{(-)} - \delta_{\alpha\beta} \bar{P}_\beta(R)] \times \exp(-i\tilde{H}_\beta t)\, dt \tag{4.21}$$
$$= \int_{-t_0}^{t_0} \exp(i\tilde{H}_\gamma t) S_{\gamma\alpha}[U_\alpha^{(-)\dagger} \bar{P}(R) U_\beta^{(-)} - \delta_{\alpha\beta} \bar{P}_\beta(R)] \times \exp(-i\tilde{H}_\beta t)\, dt. \tag{4.22}$$

The first term in the square brackets may be simplified by noting that

$$\sum_{\alpha=0}^{3} S_{\gamma\alpha} U_\alpha^{(-)\dagger} = \sum_{\alpha=0}^{3} U_\gamma^{(+)\dagger} U_\alpha^{(-)} U_\alpha^{(-)\dagger} = U_\gamma^{(+)\dagger}(1 - P_d) = U_\gamma^{(+)\dagger}. \tag{4.23}$$

The second equality is the asymptotic completeness of

the U's and the third equality follows from orthogonality properties of bound and scattering states. So

$$\sum_{\alpha=0}^{3} S_{\gamma\alpha}Q_{\alpha\beta}(R,t_0) = \int_{-t_0}^{t_0} \exp(i\tilde{H}_\gamma t)U_\gamma^{(+)\dagger}[\bar{p}(R)U_\beta^{(-)} - U_\beta^{(-)}\bar{p}_\beta(R)]\exp(-i\tilde{H}_\beta t)\,dt. \tag{4.24}$$

Our problem is now reduced to evaluating the right-hand side Eq. (4.24). Let us take matrix elements of Eq. (4.24) and let the $t_0 \to \infty$. For $\gamma \neq 0$ and $\beta \neq 0$ one has

$$\left(f_\gamma, \sum_{\alpha=0}^{3} S_{\gamma\alpha}Q_{\alpha\beta}(R,\infty)f'_\beta\right)_\gamma = \int_{-\infty}^{\infty} (f_\gamma, \exp(i\tilde{H}_\gamma t)U_\gamma^{(+)\dagger}[\bar{p}(R)U_\beta^{(-)} - U_\beta^{(-)}\bar{p}_\beta(R)] \times \exp(-i\tilde{H}_\beta t)f'_\beta)_\gamma\,dt. \tag{4.25}$$

We now assume that f_γ and f'_β are well enough behaved so we may interchange the order of integration in Eq. (4.25). Thus we can rewrite our equation in the following form:

$$\left(f_\gamma, \sum_{\alpha=0}^{3} S_{\gamma\alpha}Q_{\alpha\beta}(R,\infty)f'_\beta\right)_\gamma = \int f_\gamma(\mathbf{p}_\gamma)^*\left(\int_{-\infty}^{\infty}\exp[it(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2)]\,dt\right) \times\langle \mathbf{p}_\gamma | U_\gamma^{(+)\dagger}[\bar{p}(R)U_\beta^{(-)} - U_\beta^{(-)}\bar{p}_\beta(R)]|\mathbf{p}'_\beta\rangle f'_\beta(\mathbf{p}'_\beta)\,d\mathbf{p}_\gamma\,d\mathbf{p}'_\beta. \tag{4.26}$$

The integral in the curly brackets in $2\pi\delta(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2)$ and physically enforces energy conservation between an asymptotic state in the β channel and one in the γ channel. Since Eq. (4.26) holds for a dense set of functions f_γ and f'_β, we can associate it with the following kernel in momentum space:

$$\left\langle \mathbf{p}_\gamma \middle| \sum_{\alpha=0}^{3} S_{\gamma\alpha}Q_{\alpha\beta}(R,\infty)\middle|\mathbf{p}'_\beta\right\rangle = 2\pi\delta(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2)\langle \mathbf{p}_\gamma | U_\gamma^{(+)\dagger}[\bar{p}(R)U_\beta^{(-)} - U_\beta^{(-)}\bar{p}_\beta(R)]|\mathbf{p}'_\beta\rangle, \quad \gamma > 0, \quad \beta > 0. \tag{4.27}$$

For values of the indices γ and β where either one or both are zero, one can repeat an evaluation similar to the one above. We find that

$$\left\langle \mathbf{pq} \middle| \sum_{\alpha=0}^{3} S_{0\alpha}Q_{\alpha\beta}(R,\infty)\middle|\mathbf{p}'_\beta\right\rangle = 2\pi\delta(\tilde{p}^2 + \tilde{q}^2 - \tilde{p}_\beta'^2 + \chi_\beta^2)\langle \mathbf{pq} | U_0^{(+)\dagger}[\bar{p}(R)U_\beta^{(-)} - U_\beta^{(-)}\bar{p}_\beta(R)]|\mathbf{p}'_\beta\rangle, \quad \beta > 0, \tag{4.28}$$

$$\left\langle \mathbf{pq} \middle| \sum_{\alpha=0}^{3} S_{0\alpha}Q_{\alpha 0}(R,\infty)\middle|\mathbf{p}'\mathbf{q}'\right\rangle = 2\pi\delta(\tilde{p}^2 + \tilde{q}^2 - \tilde{p}'^2 - \tilde{q}'^2)\langle \mathbf{pq} | U_0^{(+)\dagger}[\bar{p}(R)U_0^{(-)} - U_0^{(-)}\bar{p}(R)]|\mathbf{p}'\mathbf{q}'\rangle. \tag{4.29}$$

The remaining portions of the paper are concerned with evaluating the matrix elements appearing in these last three equations.

V. DERIVATION OF THE TIME-DELAY RELATION

The previous section has demonstrated that if we can evaluate the matrix element $U_\gamma^{(+)\dagger}[\bar{p}(R)U_\beta^{(-)} - U_\beta^{(-)}\bar{p}_\beta(R)]$, then we know the product SQ. This is equivalent to knowing Q since S^{-1} exists. We now shall compute the *on-shell* values of the above matrix element. Let us define

$$X_\beta(R) \equiv \bar{p}(R)U_\beta^{(-)} - U_\beta^{(-)}\bar{p}_\beta(R) \quad : \mathcal{H}_\beta \to \mathcal{H}. \tag{5.1}$$

We note that the operator form of Eq. (2.18) may be written

$$U_\gamma^{(\pm)} = I_\gamma^\dagger - K_\gamma^{(\pm)}. \tag{5.2}$$

The kernel associated with K_γ is that given by Eq. (2.19). Physically K_γ contains all features of the wavefunction related to the scattered parts of the wavefunction. We note that Eq. (5.1) can be expanded as the sum of two terms, which we may treat separately:

$$X_\beta(R) = \bar{p}(R)(I_\beta^\dagger - K_\beta^{(-)}) - (I_\beta^\dagger - K_\beta^{(-)})\bar{p}_\beta(R) \tag{5.3}$$

$$= [\bar{p}(R) - P_\beta\bar{p}(R)]I_\beta^\dagger + [K_\beta^{(-)}\bar{p}_\beta(R) - \bar{p}(R)K_\beta^{(-)}]. \tag{5.4}$$

Here we have used $I_\beta^\dagger I_\beta = P_\beta$. Now we observe that the first term in expression (5.4) for $X_\beta(R)$ vanishes strongly as $R \to \infty$. That this is so may be seen as follows.

Let f_β be any function in $\mathcal{H}_\beta$. Then

$$\|[\bar{p}(R) - P_\beta\bar{p}(R)]I_\beta^\dagger f_\beta\| = \|[\bar{p}(R) - P_\beta(\bar{p}(R) - E) - P_\beta E]I_\beta^\dagger f_\beta\| \leq \|(\bar{p}(R) - P_\beta)I_\beta^\dagger f_\beta\| + \|P_\beta(\bar{p}(R) - E)I_\beta^\dagger f_\beta\|; \tag{5.5}$$

using $P_\beta I_\beta^\dagger = I_\beta^\dagger$ and $\|P_\beta\| = 1$, our inequality becomes

$$\leq 2\|(\bar{p}(R) - E)I_\beta^\dagger f_\beta\|. \tag{5.6}$$

This last expression goes to zero since $\bar{p}(R)$ strongly converges to unity. Thus we need only compute the value of $U_\gamma^{(+)\dagger}Y_\beta(R)$, where $Y_\beta(R)$ is defined as

$$Y_\beta(R) \equiv K_\beta^{(-)}\bar{p}_\beta(R) - \bar{p}(R)K_\beta^{(-)}. \tag{5.7}$$

A lengthy and detailed analysis is needed to evaluate the expectation values of $U_\gamma^{(+)\dagger}Y_\beta(R)$. Most of the terms entering the computation turn out to be zero. We shall deal with this complexity by placing in the appendices the evaluation of the zero terms. Thus the detail exhibited in this section is somewhat more important since it leads directly to the desired matrix element values. For example we show in Appendix C that $K_\gamma^{(+)\dagger}Y_\beta(R) \to 0$ in the $R \to \infty$ limit. Thus our problem is simplified to computing

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma | U_\gamma^{(+)\dagger}[\bar{p}(R)U_\beta^{(-)} - U_\beta^{(-)}\bar{p}_\beta(R)]|\mathbf{p}'_\beta\rangle = \lim_{R\to\infty}\langle \mathbf{p}_\gamma | I_\gamma Y_\beta(R)|\mathbf{p}'_\beta\rangle. \tag{5.8}$$

Our expression for $Y_\beta(R)$ has two terms. We treat the operator $K_\beta^{(-)}\bar{p}_\beta(R)$ first. Using the Eqs. (2.19) and (2.20) for $K_\beta^{(-)}$, we may write $K_\beta^{(-)}\bar{p}_\beta(R)$ as

$$\langle \mathbf{p}_\gamma\mathbf{q}_\gamma | K_\beta^{(-)}\bar{p}_\beta(R)|\mathbf{p}'_\beta\rangle = \int \sum_{\alpha=1}^{3}\left(-\langle \mathbf{p}_\gamma\mathbf{q}_\gamma | G_{\alpha\beta}^{(+)}|\mathbf{p}''_\beta\rangle + \frac{\phi_\alpha(\mathbf{q}_\alpha)\langle \mathbf{p}_\alpha | H'^{(+)}_{\alpha\beta}|\mathbf{p}''_\beta\rangle}{\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta''^2 + \chi_\beta^2 - i0}\right) \times \frac{\langle \mathbf{p}''_\beta | \bar{p}_\beta(R)|\mathbf{p}'_\beta\rangle\,d^3p''_\beta}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2 - i0}. \tag{5.9}$$

We further expand this by expressing the singular denominators in terms of their delta-function and principal-value parts. We shall denote a principal-value in-

tegral by writing the denominator terms without the customary $\pm i0$ notation. Our expansion of Eq. (5.9) now reads

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | K_\beta^{(-)} \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle \equiv \left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=1}^{6} B_i(R) \middle| \mathbf{p}'_\beta \right\rangle \tag{5.10}$$

where the kernels $B_i(R)$ are given by

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_1(R) | \mathbf{p}'_\beta \rangle \equiv -\int \sum_{\alpha=1}^{3} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | G_{\alpha\beta}^{(+)} | \mathbf{p}''_\beta \rangle \frac{\langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} \, d^3p''_\beta, \tag{5.11}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_2(R) | \mathbf{p}'_\beta \rangle \equiv \int \sum_{\alpha=1}^{3} \frac{\phi_\alpha(\mathbf{q}_\alpha) \langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}''_\beta \rangle}{\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} \frac{\langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} \, d^3p''_\beta, \tag{5.12}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_3(R) | \mathbf{p}'_\beta \rangle \equiv \int \sum_{\alpha=1}^{3} i\pi \delta(\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta''^2 + \chi_\beta^2) \phi_\alpha(\mathbf{q}_\alpha) \times \frac{\langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}''_\beta \rangle \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} \, d^3p''_\beta, \tag{5.13}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_4(R) | \mathbf{p}'_\beta \rangle \equiv -\int \sum_{\alpha=1}^{3} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | G_{\alpha\beta}^{(+)} | \mathbf{p}''_\beta \rangle i\pi \delta(\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2) \times \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle \, d^3p''_\beta, \tag{5.14}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_5(R) | \mathbf{p}'_\beta \rangle \equiv \int \sum_{\alpha=1}^{3} \frac{\phi_\alpha(\mathbf{q}_\alpha) \langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}''_\beta \rangle}{\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} i\pi \delta(\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2) \times \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle \, d^3p''_\beta, \tag{5.15}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_6(R) | \mathbf{p}'_\beta \rangle \equiv \int \sum_{\alpha=1}^{3} i\pi \delta(\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta''^2 + \chi_\beta^2) \phi_\alpha(\mathbf{q}_\alpha) \langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}''_\beta \rangle \times i\pi \delta(\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2) \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle \, d^3p''_\beta. \tag{5.16}$$

It is now appropriate to examine the operator $\bar{P}(R)K_\beta^{(-)}$. The kernel representation of $\bar{P}(R)K_\beta^{(-)}$ is

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) K_\beta^{(-)} | \mathbf{p}'_\beta \rangle = \int \frac{\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle}{\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2 - i0} \sum_{\alpha=1}^{3} \left(-\langle \mathbf{p}''_\gamma \mathbf{q}''_\gamma | G_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle + \frac{\phi_\alpha(\mathbf{q}''_\alpha) \langle \mathbf{p}''_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle}{\tilde{p}_\alpha''^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2 - i0} \right) d^3p''_\gamma \, d^3q''_\gamma. \tag{5.17}$$

As before, we expand this in terms of its principal-value and delta-function parts. We have

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) K_\beta^{(-)} | \mathbf{p}'_\beta \rangle \equiv \left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=1}^{6} A_i(R) \middle| \mathbf{p}'_\beta \right\rangle, \tag{5.18}$$

where the operators $A_i(R)$ are given by

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_1(R) | \mathbf{p}'_\beta \rangle \equiv -\int \frac{\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle}{\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \sum_{\alpha=1}^{3} \langle \mathbf{p}''_\gamma \mathbf{q}''_\gamma | G_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle \, d^3p''_\gamma \, d^3q''_\gamma, \tag{5.19}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_2(R) | \mathbf{p}'_\beta \rangle \equiv +\int \frac{\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle}{\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \sum_{\alpha=1}^{3} \frac{\phi_\alpha(\mathbf{q}''_\alpha) \langle \mathbf{p}''_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle}{\tilde{p}_\alpha''^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \, d^3p''_\gamma \, d^3q''_\gamma \tag{5.20}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_3(R) | \mathbf{p}'_\beta \rangle \equiv +\int \frac{\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle}{\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \sum_{\alpha=1}^{3} i\pi \delta(\tilde{p}_\alpha''^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \phi_\alpha(\mathbf{q}''_\alpha) \times \langle \mathbf{p}''_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle \, d^3p''_\gamma \, d^3q''_\gamma, \tag{5.21}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_4(R) | \mathbf{p}'_\beta \rangle \equiv -\int \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle \sum_{\alpha=1}^{3} \langle \mathbf{p}''_\gamma \mathbf{q}''_\gamma | G_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle \times i\pi \delta(\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \, d^3p''_\gamma \, d^3q''_\gamma, \tag{5.22}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_5(R) | \mathbf{p}'_\beta \rangle \equiv \int \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle \sum_{\alpha=1}^{3} \frac{\phi_\alpha(\mathbf{q}''_\alpha) \langle \mathbf{p}''_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle}{\tilde{p}_\alpha''^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \times i\pi \delta(\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \, d^3p''_\gamma \, d^3q''_\gamma, \tag{5.23}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_6(R) | \mathbf{p}'_\beta \rangle \equiv \int \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle \sum_{\alpha=1}^{3} i\pi \delta(\tilde{p}_\alpha''^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \phi_\alpha(\mathbf{q}''_\alpha) \times \langle \mathbf{p}''_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle i\pi \delta(\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \, d^3p''_\gamma \, d^3q''_\gamma. \tag{5.24}$$

We now proceed to evaluate the matrix element given in Eq. (5.8). We show in Appendix B that

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma | I_\gamma (B_i(R) - A_i(R)) | \mathbf{p}'_\beta \rangle = 0, \quad \text{all } i \neq 2. \tag{5.25}$$

When this result is combined with Eq. (5.8) we have

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma | U_\gamma^{(+)\dagger} [\bar{P}(R) U_\beta^{(-)} - U_\beta^{(-)} \bar{P}_\beta(R)] | \mathbf{p}'_\beta \rangle = \lim_{R\to\infty} \langle \mathbf{p}_\gamma | I_\gamma (B_2(R) - A_2(R)) | \mathbf{p}'_\beta \rangle \tag{5.26}$$

for $\gamma > 0$. When $\gamma = 0$ this equation becomes

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | U_0^{(+)\dagger} [\bar{P}(R) U_\beta^{(-)} - U_\beta^{(-)} \bar{P}_\beta(R)] | \mathbf{p}'_\beta \rangle = \lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_2(R) - A_2(R) | \mathbf{p}'_\beta \rangle. \tag{5.27}$$

At this point we stress that we have to evaluate the above matrix element only for on-shell values of the momentum arguments. This on-shell requirement is a consequence of the delta function appearing in Eq. (4.27) and Eq. (4.28).

We continue by considering the evaluation of the operator $I_\gamma B_2(R)$. Examining $B_2(R)$ we see that it is the sum of three terms. Defining $B_{2\alpha}(R)$ by

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_{2\alpha}(R) | \mathbf{p}'_\beta \rangle \equiv \phi_\alpha(\mathbf{q}_\alpha) \int \frac{\langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}''_\beta \rangle \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle}{(\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta''^2 + \chi_\beta^2)(\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2)} \, d^3p''_\beta, \tag{5.28}$$

then

$$B_2(R) = \sum_{\alpha=1}^{3} B_{2\alpha}(R). \tag{5.29}$$

We shall demonstrate in Appendix B that only the term $I_\gamma B_{2\gamma}$ in the above sum contributes to the nonzero matrix elements. So in this section we examine only $I_\gamma B_{2\gamma}$. Setting $\alpha = \gamma$ in Eq. (5.28) gives us

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_{2\gamma}(R) | \mathbf{p}'_\beta \rangle = 2n_\beta \phi_\gamma(\mathbf{q}_\gamma) \int \frac{\langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}''_\beta \rangle}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} \frac{\langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle}{(p'_\beta + p''_\beta)(p'_\beta - p''_\beta)} \, d^3p''_\beta. \tag{5.30}$$

We now use a property of $\bar{P}_\beta(R)$ established in Appendix A, namely, for $f(\mathbf{p}_\beta)$ a smooth function in $\mathcal{H}_\beta$ and differentiable in $|\mathbf{p}_\beta|$ the following limiting relation is valid:

$$\lim_{R\to\infty}\int \frac{\langle \mathbf{p}_\beta|\bar{P}_\beta(R)|\mathbf{p}''_\beta\rangle f(\mathbf{p}''_\beta)}{p_\beta - p''_\beta}\, d^3p''_\beta = -\frac{d}{dp''_\beta}\left(\frac{p''_\beta}{p_\beta} f(p''_\beta\hat{p}_\beta)\right)\Big|_{p''_\beta=p_\beta}. \tag{5.31}$$

In obtaining the form of Eq. (5.30) we have exploited the on-shell condition $\tilde{p}_\gamma^2 - \chi_\gamma^2 = \tilde{p}_\beta'^2 - \chi_\beta^2$ to write the first denominator solely in terms of the β momentum. The distinctive feature of this term which prevents it from cancelling against the corresponding term $I_\gamma A_2(R)$ is the fact that the singular surface occurring at $p_\beta = p''_\beta$ changes the character of the $R\to\infty$ limit. Without such a singularity $\bar{P}_\beta(R)\to E_\beta$. If this were the case then $B_{2\gamma}(R) - A_{2\gamma}(R)$ would go to zero.

We are permitted to use Eq. (5.31) in evaluating the $R\to\infty$ limit in Eq. (5.30), since the portion of the integrand excluding $\langle \mathbf{p}''_\beta|\bar{P}_\beta(R)|\mathbf{p}'_\beta\rangle/p'_\beta - p''_\beta$ is a smooth function of p''_β. This is a consequence of our assumptions in Sec. II about the physical amplitude $\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}''_\beta\rangle$, namely it is differentiable function of its arguments. The remaining ingredient of the integrand in Eq. (5.30) is the denominator $\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}''^2_\beta + \chi_\beta^2$. We need only estimate its behavior in the neighborhood of $p''^2_\beta = p'^2_\beta$. So one has that

$$\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}'^2_\beta + \chi_\beta^2 = \tilde{q}_\gamma^2 + \chi_\gamma^2 \geq \chi_\gamma^2. \tag{5.32a}$$

Thus for $|\tilde{p}'^2_\beta - \tilde{p}''^2_\beta| < \chi_\gamma^2$ we have the estimate

$$\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - p''^2_\beta + \chi_\beta^2 > 0, \quad \text{all } \mathbf{q}_\gamma. \tag{5.32b}$$

Employing Eq. (5.31) in Eq. (5.30) now gives us

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma\mathbf{q}_\gamma|B_{2\gamma}(R)|\mathbf{p}'_\beta\rangle = -2n_\beta\phi_\gamma(\mathbf{q}_\gamma)\frac{d}{dp''_\beta} \times\left(\frac{\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}''\rangle p''_\beta}{(\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}''^2_\beta + \chi_\beta^2)(p'_\beta + p''_\beta)p'_\beta}\right)\Big|_{p''_\beta=p'_\beta} \tag{5.32c}$$

where $\mathbf{p}''_\beta = p''_\beta\hat{p}'_\beta$. If we use

$$\frac{d}{dp''_\beta}\,\frac{p''_\beta}{(p'_\beta + p''_\beta)p'_\beta}\Big|_{p''_\beta=p'_\beta} = \frac{1}{4p'^2_\beta}, \tag{5.33}$$

our expression for the right-hand side of Eq. (5.32c) becomes

$$-\frac{n_\beta}{p'_\beta}\psi_\gamma(\mathbf{q}_\gamma)\frac{d}{dp''_\beta}\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}''_\beta\rangle\Big|_{p''_\beta=p'_\beta} - \frac{n_\beta}{2p'^2_\beta}\psi_\gamma(\mathbf{q}_\gamma)\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle - \frac{\psi_\gamma(\mathbf{q}_\gamma)}{\tilde{q}_\gamma^2 + \chi_\gamma^2}\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle. \tag{5.34}$$

In order to find $I_\gamma B_{2\gamma}(R)$ we must integrate this last set of terms with $\int \psi_\gamma(\mathbf{q}_\gamma)^* d^3q_\gamma$. Since ψ_γ is a unit normalized boundstate wavefunction, one has at once that

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma|I_\gamma B_{2\gamma}(R)|\mathbf{p}'_\beta\rangle = -\frac{n_\beta}{p'_\beta}\frac{d}{dp'_\beta}\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle - \frac{n_\beta}{2p'^2_\beta}\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle - \langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle\int\frac{|\psi_\gamma(\mathbf{q}_\gamma)|^2}{\tilde{q}_\gamma^2 + \chi_\gamma^2}\, d^3q_\gamma. \tag{5.35}$$

This completes the evaluation of $I_\gamma B_{2\gamma}(R)$.

Let us now study the companion terms of $I_\gamma B_{2\gamma}(R)$ that occur in Eq. (5.26), namely $I_\gamma A_2(R)$. As in the case of $B_2(R)$ we can decompose $A_2(R)$ into a sum of three terms. From the form (5.20) for $A_2(R)$ we can define

$$A_2(R) = \sum_{\alpha=1}^{3} A_{2\alpha}(R) \tag{5.36}$$

where $A_{2\alpha}(R)$ is given by

$$\langle \mathbf{p}_\gamma\mathbf{q}_\gamma|A_{2\alpha}(R)|\mathbf{p}'_\beta\rangle = \int \frac{\langle \mathbf{p}_\gamma\mathbf{q}_\gamma|\bar{P}(R)|\mathbf{p}''_\gamma\mathbf{q}''_\gamma\rangle}{(\tilde{p}''^2_\alpha - \chi_\alpha^2 - \tilde{p}'^2_\beta + \chi_\beta^2)}\,\frac{\phi_\alpha(\mathbf{q}''_\alpha)\langle \mathbf{p}''_\alpha|H^{(+)}_{\alpha\beta}|\mathbf{p}'_\beta\rangle}{(\tilde{p}''^2_\gamma + \tilde{q}''^2_\gamma - \tilde{p}'^2_\beta + \chi_\beta^2)}\, d^3p''_\gamma\, d^3q''_\gamma. \tag{5.37}$$

Again we demonstrate in Appendix B that

$$\lim_{R\to\infty}\sum_{\alpha\neq\gamma}\langle \mathbf{p}_\gamma|I_\gamma(B_{2\alpha}(R) - A_{2\alpha}(R))|\mathbf{p}'_\beta\rangle = 0. \tag{5.38}$$

So here we need consider only the term $A_{2\gamma}(R)$. Using the on-shell condition $\tilde{p}_\gamma^2 - \chi_\gamma^2 = \tilde{p}'^2_\beta - \chi_\beta^2$, we may write Eq. (5.37) as

$$\langle \mathbf{p}_\gamma\mathbf{q}_\gamma|A_{2\gamma}(R)|\mathbf{p}'_\beta\rangle = 2n_\gamma\int\frac{\langle \mathbf{p}_\gamma\mathbf{q}_\gamma|\bar{P}(R)|\mathbf{p}''_\gamma\mathbf{q}''_\gamma\rangle}{p''_\gamma - p_\gamma}\,\frac{\phi_\gamma(\mathbf{q}''_\gamma)\langle \mathbf{p}''_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle}{(p''_\gamma + p_\gamma)(\tilde{p}''^2_\gamma + \tilde{q}''^2_\gamma - \tilde{p}'^2_\gamma + \chi_\gamma^2)} \times d^3p''_\gamma\, d^3q''_\gamma. \tag{5.39}$$

We now quote another feature of the operator $\bar{P}(R)$ demonstrated in Appendix A. For $f\in\mathcal{H}_0$ and $f(\mathbf{p}''_\beta, \mathbf{q}''_\beta)$ differentiable in the $|\mathbf{p}''_\beta|$ variable we have the limiting relation

$$\lim_{R\to\infty}\int\frac{\langle \mathbf{p}_\beta\mathbf{q}_\beta|\bar{P}(R)|\mathbf{p}''_\beta\mathbf{q}''_\beta\rangle}{p_\beta - p''_\beta} f(\mathbf{p}''_\beta, \mathbf{q}''_\beta)\, d^3p''_\beta\, d^3q''_\beta = -\frac{d}{dp''_\beta}\left(\frac{p''_\beta}{p_\beta} f(p''_\beta\hat{p}_\beta, \mathbf{q}_\beta)\right)\Big|_{p''_\beta=p_\beta}. \tag{5.40}$$

In the neighborhood of $p''_\gamma = p_\gamma$ the last denominator in Eq. (5.39) never vanishes. Thus we are justified in using relation (5.40) to evaluate Eq. (5.39). The limit that Eq. (5.39) takes is

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma\mathbf{q}_\gamma|A_{2\gamma}(R)|\mathbf{p}'_\beta\rangle = 2n_\gamma\phi_\gamma(\mathbf{q}_\gamma)\frac{d}{dp''_\gamma}\left(\frac{\langle \mathbf{p}''_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle p''_\gamma}{p_\gamma(p''_\gamma + p_\gamma)(\tilde{p}''^2_\gamma - \tilde{p}'^2_\gamma + \tilde{q}''^2_\gamma + \chi_\gamma^2)}\right)\Big|_{p''_\gamma=p_\gamma} \tag{5.41}$$

where $\mathbf{p}''_\gamma = p''_\gamma\hat{p}_\gamma$. Of course the value of $\mathbf{p}_\gamma$ is on-shell. If we write out the derivative term and perform the integration with respect to $\int\psi(\mathbf{q}_\gamma)^* d^3q_\gamma$, then Eq. (5.41) becomes

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma|I_\gamma A_{2\gamma}(R)|\mathbf{p}'_\beta\rangle = \frac{n_\gamma}{p_\gamma}\frac{d}{dp_\gamma}\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle + \frac{n_\gamma}{2p_\gamma^2}\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle - \langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle\int\frac{|\psi_\gamma(\mathbf{q}_\gamma)|^2}{\tilde{q}_\gamma^2 + \chi_\gamma^2}\, d^3q_\gamma. \tag{5.42}$$

By combining Eq. (5.42) with Eq. (5.35) we can determine $I_\gamma[B_2(R) - A_2(R)]$. We have

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma|I_\gamma(B_2(R) - A_2(R))|\mathbf{p}'_\beta\rangle = -\frac{n_\gamma}{p_\gamma}\frac{d}{dp_\gamma}\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle - \frac{n_\beta}{p'_\beta}\frac{d}{dp'_\beta}\langle \mathbf{p}_\gamma|H^{(+)}_{\gamma\beta}|\mathbf{p}'_\beta\rangle$$

$$- \frac{n_\beta}{2p_\beta'^2}\langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle - \frac{n_\gamma}{2p_\gamma^2}\langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle . \tag{5.43}$$

The sum of the first two terms is just the total energy derivative since $E = \mathbf{p}_\beta'^2/2n_\beta - \chi_\beta^2 = \mathbf{p}_\gamma^2/2n_\gamma - \gamma_\gamma^2$. So we can simplify Eq. (5.43) to read

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma | I_\gamma (B_2(R) - A_2(R)) | \mathbf{p}_\beta' \rangle = - \frac{d}{dE}\langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle - \left(\frac{n_\beta}{2p_\beta'^2} + \frac{n_\gamma}{2p_\gamma^2} \right) \langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle . \tag{5.44}$$

If we use this result together with Eq. (5.26) and Eq. (4.27), we obtain part of our desired solution:

$$\lim_{R\to\infty}\left\langle \mathbf{p}_\gamma \middle| \sum_{\alpha=0}^{3} S_{\gamma\alpha} Q_{\alpha\beta}(R,\infty) \middle| \mathbf{p}_\beta' \right\rangle \equiv \left\langle \mathbf{p}_\gamma \middle| \sum_{\alpha=0}^{3} S_{\gamma\alpha} Q_{\alpha\beta} \middle| \mathbf{p}_\beta' \right\rangle = 2\pi\delta(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \left[- \frac{d}{dE}\langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle - \left(\frac{n_\beta}{2p_\beta'^2} + \frac{n_\gamma}{2p_\gamma^2} \right) \langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right] . \tag{5.45}$$

This equation is valid for all $\gamma > 0$. The case with $\gamma = 0$ must be treated separately since the number of degrees of freedom in the final state is five instead of two as in Eq. (5.45).

It is at this stage of solution that it is profitable to introduce the reduced matrix elements discussed in Sec. III. As noted before Q is an operator that maps $\hat{\mathcal{H}}$ into $\hat{\mathcal{H}}$. Also from Eqs. (4.27), (4.28), and (4.29) we see that Q has the same energy conserving delta functions that characterize S. This means we can define reduced Q-matrix elements in the same manner that we have used to construct the reduced S matrices. For example, take $\alpha > 0$, $\beta > 0$; then in analogy of Eq. (3.13) and Eq. (3.14), we have

$$\langle \mathbf{p}_\alpha | Q_{\alpha\beta} | \mathbf{p}_\beta' \rangle \equiv \frac{\delta(E - E')}{(n_\alpha p_\alpha n_\beta p_\beta')^{1/2}} \langle \hat{p}_\alpha | q_{\alpha\beta}(E) | \hat{p}_\beta' \rangle . \tag{5.46}$$

In a like manner the remaining reduced $q_{\alpha\beta}(E)$'s are defined by the same process that we employed to construct the $s_{\alpha\beta}(E)$. Furthermore, the general $q(E)$ operator maps $\hat{\mathcal{H}}_\tau$ into $\hat{\mathcal{H}}_\tau$ just as the operator $s(E)$ does. In this new notation Eq. (5.45) may be expressed as

$$\left\langle \mathbf{p}_\gamma \middle| \sum_{\alpha=0}^{3} S_{\gamma\alpha} Q_{\alpha\beta} \middle| \mathbf{p}_\beta' \right\rangle = \frac{\delta(E - E')}{(n_\gamma p_\gamma n_\beta p_\beta')^{1/2}} \left\langle \hat{p}_\gamma \middle| \sum_{\alpha=0}^{3} s_{\gamma\alpha}(E) q_{\alpha\beta}(E) \middle| \hat{p}_\beta' \right\rangle \tag{5.47}$$

where

$$\left\langle \hat{p}_\gamma \middle| \sum_{\alpha=0}^{3} s_{\gamma\alpha}(E) q_{\alpha\beta}(E) \middle| \hat{p}_\beta' \right\rangle = - 2\pi (p_\gamma n_\gamma p_\beta' n_\beta)^{1/2} \left[\frac{d}{dE}\langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle + \left(\frac{n_\beta}{2p_\beta'^2} + \frac{n_\gamma}{2p_\gamma^2} \right) \langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right] . \tag{5.48}$$

In this equation it is understood that all the momenta on the right-hand side are on-shell and thus determined by knowing E. Let us form the energy derivative of the reduced $s_{\gamma\beta}(E)$ defined by Eq. (3.14). We obtain

$$\frac{d}{dE}\langle \hat{p}_\gamma | s_{\gamma\beta}(E) | \hat{p}_\beta' \rangle = - 2\pi i (p_\gamma n_\gamma p_\beta' n_\beta)^{1/2} \left[\frac{d}{dE}\langle \hat{p}_\gamma | H_{\gamma\beta}^{(+)} | \hat{p}_\beta' \rangle + \left(\frac{n_\gamma}{2p_\gamma^2} + \frac{n_\beta}{2p_\beta'^2} \right) \langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right] . \tag{5.49}$$

These last two equations allow us to write

$$\left\langle \hat{p}_\gamma \middle| \sum_{\alpha=0}^{3} s_{\gamma\alpha}(E) q_{\alpha\beta}(E) \middle| \hat{p}_\beta' \right\rangle = - i \frac{d}{dE}\langle \hat{p}_\gamma | s_{\gamma\beta}(E) | \hat{p}_\beta' \rangle , \quad \gamma > 0. \tag{5.50}$$

Stated in operator form this is simply

$$\sum_{\alpha=0}^{3} s_{\gamma\alpha}(E) q_{\alpha\beta}(E) = - i \frac{d}{dE} s_{\gamma\beta}(E), \tag{5.51}$$

valid for $\gamma > 0$.

The next step in our analysis is to extend the result given in Eq. (5.51) to the case $\gamma = 0$. The details of the computation in this case are quite different than those described above since the final state has five degrees of freedom. The on-shell requirement here takes the form $\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 = \tilde{p}_\beta'^2 - \chi_\beta^2$. So we need to evaluate the following on-shell matrix element

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | U_0^{(+)\dagger} [\bar{P}(R) U_\beta^{(-)} - U_\beta^{(-)} \bar{P}_\beta(R)] | \mathbf{p}_\beta' \rangle = \lim_{R\to\infty}\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | Y_\beta(R) | \mathbf{p}_\beta' \rangle . \tag{5.52}$$

Again many of the terms in $Y_\beta(R)$ do not contribute to the solution. In Appendix B it is shown that

$$\lim_{R\to\infty}\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=4}^{6} (B_i(R) - A_i(R)) \middle| \mathbf{p}_\beta' \right\rangle = 0. \tag{5.53}$$

In both of the above equations it is understood that the momentum arguments in the ket on the left and the bra on the right are those given by the on-shell condition. Let us first find the contribution to Eq. (5.52) coming from $\sum_{i=1}^{3} B_i(R)$. Using definitions Eqs. (5.11), (5.12), and (5.13) we can write

$$\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=1}^{3} B_i(R) \middle| \mathbf{p}_\beta' \right\rangle = \int \frac{\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta'' \rangle \langle \mathbf{p}_\beta'' | \bar{P}_\beta(R) | \mathbf{p}_\beta' \rangle}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} \, d^3 p_\beta'' . \tag{5.54}$$

Although $\beta_{0\beta}^{(+)}$ contains singularities, only the exhibited denominator is singular in the neighborhood where $\bar{P}_\beta(R)$ acquires support in the limit $R \to \infty$. Using the on-shell condition, Eq. (5.54) becomes

$$\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=1}^{3} B_i(R) \middle| \mathbf{p}_\beta' \right\rangle = 2n_\beta \int \frac{\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta'' \rangle}{(p_\beta' + p_\beta'')} \frac{\langle \mathbf{p}_\beta'' | \bar{P}_\beta(R) | \mathbf{p}_\beta' \rangle}{p_\beta' - p_\beta''} \, d^3 p_\beta'' . \tag{5.55}$$

Using the limiting result Eq. (5.31) we find that

$$\lim_{R\to\infty}\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=1}^{3} B_i(R) \middle| \mathbf{p}_\beta' \right\rangle = - 2n_\beta \frac{d}{dp_\beta''} \left(\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta'' \rangle \frac{p_\beta''}{p_\beta'(p_\beta' + p_\beta'')} \right) \Bigg|_{p_\beta'' = p_\beta'} = - 2n_\beta \left(\frac{1}{2p_\beta'} \frac{d}{dp_\beta'} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle + \frac{1}{4p_\beta'^2} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right) . \tag{5.56}$$

In the first of these two equations $\mathbf{p}_\beta'' = p_\beta'' \hat{p}_\beta'$. In going to the last form we have employed Eq. (5.33).

It remains to evaluate $\sum_{i=1}^3 A_i(R)$. Combining Eqs. (5.19), (5.20), and (5.21) one has

$$\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \left| \sum_{i=1}^3 A_i(R) \right| \mathbf{p}_\beta' \right\rangle = \int \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}_\gamma'' \mathbf{q}_\gamma'' \rangle \frac{\langle \mathbf{p}_\gamma'' \mathbf{q}_\gamma'' | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle}{\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} d^3 p_\gamma'' \, d^3 q_\gamma''. \tag{5.57}$$

In accordance with the angle convention introduced in Eq. (3.15) we define a generalized momentum-like variable suitable for the radius coordinate in the six-dimensional space p, q,

$$\tilde{K} \equiv \sqrt{E} = (\tilde{p}_\alpha^2 + \tilde{q}_\alpha^2)^{1/2}, \quad \alpha = 1, 2, 3. \tag{5.58}$$

In the coordinate set associated with $\tilde{K}$ the point $\mathbf{p}_\alpha, \mathbf{q}_\alpha$ has the representation $(\tilde{K}, \omega_\alpha, \hat{p}_\alpha, \hat{q}_\alpha)$. If we set $\tilde{K}^2 = \tilde{p}_\beta'^2 - \chi_\beta^2 = \tilde{p}_\gamma^2 + \tilde{q}_\gamma^2$, then the integrand of Eq. (5.57) has a term of the structure $\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}_\gamma'' \mathbf{q}_\gamma'' \rangle / (\tilde{K}'' - \tilde{K})$. For integrals of this type we show in Appendix A that for sufficiently smooth $f \in H$

$$\lim_{R\to\infty} \int \frac{\langle \mathbf{p}_\beta \mathbf{q}_\beta | \bar{P}(R) | \mathbf{p}_\beta'' \mathbf{q}_\beta'' \rangle}{\tilde{K} - \tilde{K}''} f(\mathbf{p}_\beta'', \mathbf{q}_\beta'') \, d^3 p_\beta'' \, d^3 q_\beta'' = -\frac{d}{d\tilde{K}''} \left[\left(\frac{\tilde{K}''}{\tilde{K}} \right)^{5/2} f(\tilde{K}'', \omega_\beta, \hat{p}_\beta, \hat{q}_\beta) \right] \Big|_{\tilde{K}''=\tilde{K}}. \tag{5.59}$$

Employing Eq. (5.59) to evaluate Eq. (5.57) gives us

$$\begin{aligned} \lim_{R\to\infty} \left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \left| \sum_{i=1}^3 A_i(R) \right| \mathbf{p}_\beta' \right\rangle &= \frac{d}{d\tilde{K}''} \left[\left(\frac{\tilde{K}''}{\tilde{K}} \right)^{5/2} \frac{\langle \tilde{K}'' \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle}{(\tilde{K}'' + \tilde{K})} \right] \Big|_{\tilde{K}''=\tilde{K}} \\ &= \frac{1}{\tilde{K}^2} \langle \tilde{K} \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle + \frac{1}{2\tilde{K}} \frac{d}{d\tilde{K}} \langle \tilde{K} \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle. \end{aligned} \tag{5.60}$$

In this equation we have written the bra portion of $\beta_{0\beta}^{(+)}$ in the variables $\tilde{K}\omega_\gamma \hat{p}_\gamma \hat{q}_\gamma$ instead of the original coordinate system $\mathbf{p}_\gamma \mathbf{q}_\gamma$. Here as in the treatment of $\sum_{i=1}^3 B_i(R)$ the on-shell requirement $\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 = \tilde{p}_\beta'^2 - \chi_\beta^2$ is possible only for initial scattering energies $E = \tilde{p}_\beta'^2 - \chi_\beta^2$ which are positive. The S matrix $s_{0\beta}(E)$ is of course zero for negative scattering energies, $E < 0$.

Now it is appropriate to combine Eqs. (5.60) and (5.56). Utilizing Eq. (5.53), this leads to

$$\begin{aligned} \lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \, U_0^{(+)\dagger} [\bar{P}(R) U_\beta^{(-)} - U_\beta^{(-)} \bar{P}_\beta(R)] | \mathbf{p}_\beta' \rangle &= \left[-\frac{d}{d(p_\beta'^2/2n_\beta)} \langle \tilde{K} \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right. \\ &\quad - \frac{d}{d(\tilde{K}^2)} \langle \tilde{K} \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle - \left(\frac{n_\beta}{2p_\beta'^2} \right. \\ &\quad \left. \left. + \frac{1}{p_\gamma^2/2n_\gamma + q_\gamma^2/2\mu_\gamma} \right) \langle \tilde{K} \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right]. \end{aligned} \tag{5.61}$$

We note in the above expression that the first derivative term is the derivative with respect to the energy of the ket $|\mathbf{p}_\beta'\rangle$ while the second derivative is with respect to the energy of the bra $\langle \tilde{K} \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma |$. The sum of the first two terms is then the total energy derivative of the on-shell breakup amplitude $\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle$.

At this stage we introduce the reduced matrix element description. Recalling Eq. (3.18) we see that we need to define

$$\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \left| \sum_{\alpha=0}^3 S_{0\alpha} Q_{\alpha\beta} \right| \mathbf{p}_\beta' \right\rangle = \frac{\delta(E - E')}{(\mu_\gamma n_\gamma)^{1/4} p_\gamma q_\gamma (n_\beta p_\beta')^{1/2}} \left\langle \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma \left| \sum_{\alpha=0}^3 s_{0\alpha}(E) q_{\alpha\beta}(E) \right| \hat{p}_\beta' \right\rangle. \tag{5.62}$$

Because of Eq. (4.28) we can write using Eq. (5.61)

$$\begin{aligned} \left\langle \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma \left| \sum_{\alpha=0}^3 s_{0\alpha}(E) q_{\alpha\beta}(E) \right| \hat{p}_\beta' \right\rangle &= -2\pi (\mu_\gamma n_\gamma)^{1/4} p_\gamma q_\gamma (n_\beta p_\beta')^{1/2} \left[\frac{d}{dE} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right. \\ &\quad \left. + \left(\frac{n_\beta}{2p_\beta'^2} + \frac{1}{E} \right) \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right] \end{aligned} \tag{5.63}$$

where the magnitudes of the momenta in the bra and the ket of $\beta_{0\beta}^{(+)}$ are related to E by the on-shell condition.

Let us consider the matrix element of $s_{0\beta}(E)$. If we form the energy derivative of Eq. (3.19) putting $\alpha = \gamma$, we get

$$\begin{aligned} \frac{d}{dE} \langle \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | \, s_{0\beta}(E) | \hat{p}_\beta' \rangle &= -2\pi i (\mu_\gamma n_\gamma)^{1/4} p_\gamma q_\gamma (n_\beta p_\beta')^{1/2} \left[\frac{d}{dE} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right. \\ &\quad \left. + \left(\frac{n_\beta}{2p_\beta'^2} + \frac{1}{E} \right) \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right]. \end{aligned} \tag{5.64}$$

This result substituted into Eq. (5.63) yields

$$\left\langle \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma \left| \sum_{\alpha=0}^3 s_{0\alpha}(E) q_{\alpha\beta}(E) \right| \mathbf{p}_\beta' \right\rangle = -i \frac{d}{dE} \langle \omega_\gamma \hat{p}_\gamma \hat{q}_\gamma | \, s_{0\beta}(E) | \hat{p}_\beta' \rangle. \tag{5.65}$$

So we have established the validity of Eq. (5.51) for all values of γ.

In all the foregoing derivations we effectively took $\beta \neq 0$. In a similar way, however, one expects that the relation (5.51) is also valid for $\beta = 0$. The solution of the time-delay problem will be completed if we use the unitarity relation Eq. (3.23) in order to move the S matrix from the left of relation (5.51) to the right. Specifically, we have

$$\sum_{\gamma=0}^3 s_{\gamma\delta}^\dagger(E) \sum_{\alpha=0}^3 s_{\gamma\alpha}(E) q_{\alpha\beta}(E) = \sum_{\alpha=0}^3 \left(\sum_{\gamma=0}^3 s_{\gamma\delta}^\dagger(E) s_{\gamma\alpha}(E) \right) q_{\alpha\beta}(E) = \sum_{\alpha=0}^3 \delta_{\delta\alpha} 1_\alpha q_{\alpha\beta}(E) = q_{\delta\beta}(E). \tag{5.66}$$

Thus Eq. (5.51) becomes

$$q_{\delta\beta}(E) = -i \sum_{\gamma=0}^3 s_{\gamma\delta}^\dagger(E) \frac{d}{dE} s_{\gamma\beta}(E). \tag{5.67}$$

This is our principal result. Equation (5.67) is an operator relation that maps $L_\beta^2 \to L_\delta^2$. If it is viewed as a

relation on the space $\hat{H}_r$ then it has a simpler appearance, namely

$$q(E) = -is^\dagger(E)\frac{d}{dE}s(E) \quad : \hat{H}_r \to \hat{H}_r. \tag{5.68}$$

We recall that the operator we began with $Q(R, t_0)$ was a bounded symmetric operator on $\hat{H}$ [see Eq. (4.17)]. Here it is easy to see that $q(E)$ retains the symmetry property. We first note

$$q^\dagger(E) = +i\left(\frac{d}{dE}\, s^\dagger(E)\right)s(E). \tag{5.69}$$

However, if we take the derivative of Eq. (3.25)—the unitarity relation for $s(E)$—we have

$$0 = \left(\frac{d}{dE}\, s^\dagger(E)\right)s(E) + s^\dagger(E)\frac{d}{dE}s(E). \tag{5.70}$$

Thus

$$q^\dagger(E) = -is^\dagger(E)\frac{d}{dE}s(E) = q(E). \tag{5.71}$$

So one expects that $q(E)$ is a self-adjoint operator acting on the space $\hat{H}_r$.

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APPENDIX A

This appendix studies the nature of projection operators on an n-dimensional space. Particularly, we investigate the behavior of the projection operators when acting on the types of generalized function encountered in this problem. Our general method of attack is to obtain momentum—space representations of the projections. These representations are always expressed in terms of simple Bessel functions. We determine the effect of the operators on generalized functions by using a combination of explicit calculation and the Riemann—Lebesque lemma. It is the detailed results obtained in this appendix which allows us to discard the average limit in R used in previous works[6,12] on time delay.

Throughout the remainder of this appendix we assume that our operators act on the following dense set of functions. For an n-dimensional space we assume the functions and their first n-derivatives belong to $L^2(\mathbb{R}^n)$. We are interested in the $R \to \infty$ limit of the projection operators $P(R)$. For a limit of this kind we establish convergence of our results in the weak sense.

We shall first establish that

$$\lim_{R\to\infty}(f', P(R)f) = (f', f) \tag{A1}$$

where f' and f are any functions in the above dense set. This is, of course, an immediate consequence of $P(R)$ converging to the identity in the strong sense. However our proof of (A1) allows us to state certain useful properties of the momentum space representations of $P(R)$.

If we express $(f', P(R)f)$ in momentum—space we have at once

$$(f', P(R)f) = \int f'(\mathbf{k}')^*\langle \mathbf{k}' | P(R) | \mathbf{k}\rangle f(\mathbf{k})\, d^n\mathbf{k}\, d^n\mathbf{k}'. \tag{A2}$$

We have used $P(R)$ as the symbol for the n-dimensional projection operator. Primarily we are interested here in the cases when $n = 6$ or $n = 3$. For $n = 6$ then $P(R)$ is equivalent to $\bar{P}(R)$. The kernel for $P(R)$ given in formula (A2) is

$$\langle \mathbf{k}' | P(R) | \mathbf{k}\rangle = \int_{|\mathbf{x}|<R} \frac{\exp[i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}]}{(2\pi)^n}\, d^n\mathbf{x}. \tag{A3}$$

In order to evaluate this integral one may introduce an n-dimensional spherical coordinate system. A straightforward computation gives

$$\langle \mathbf{k}' | P(R) | \mathbf{k}\rangle = \left(\frac{R}{2\pi|\mathbf{k}-\mathbf{k}'|}\right)^{n/2} J_{n/2}(|\mathbf{k}-\mathbf{k}'|R) \tag{A4}$$

where J is the Bessel function of the first kind.

We now want to study the $R \to \infty$ limit of the right-hand side of (A2). If we introduce the change of variables $\mathbf{z} = R(\mathbf{k}-\mathbf{k}')$, we have after (A4) is substituted into (A2)

$$\int f'(\mathbf{k}')^* f\left(\mathbf{k}' + \frac{\mathbf{z}}{R}\right)\frac{|\mathbf{z}|^{n/2-1}}{(2\pi)^{n/2}} J_{n/2}(|\mathbf{z}|)\, d|\mathbf{z}|\, d\hat{z}\, d^n\mathbf{k}' \tag{A5}$$

where $\hat{z} = \mathbf{z}/|\mathbf{z}|$. Since f possesses a derivative we may integrate (A5) by parts employing the identity

$$\frac{1}{z}\frac{d}{dz}\left(z^{-n/2+1}J_{n/2-1}(z)\right) = -z^{-n/2}J_{n/2}(z). \tag{A6}$$

Denoting $|\mathbf{z}|$ by z the surface term arising after the integration by parts is

$$-\frac{z^{n/2-1}}{(2\pi)^{n/2}} J_{n/2-1}(z)\int f'(\mathbf{k}')^* f\left(\mathbf{k}' + \frac{\mathbf{z}}{R}\right) d\hat{z}\, d^n\mathbf{k}'\Bigg|_{z=0}^{z=\infty}. \tag{A7}$$

It may be easily seen that for $n \geq 3$ this surface term vanishes. The structure of the integral over $d^n\mathbf{k}'$ is that of a convolution of two square integrable functions. The resulting function of $\mathbf{z}/R$ is absolutely integrable with respect to $d^n\mathbf{z}$. Thus the contribution to the surface term for $z = \infty$ is zero. For $z = 0$ the term is trivally zero. For the case $n < 3$ one can prove the weak convergence (A1) without employing this integration by parts.

So after one integration by parts (A5) takes the form

$$\int f'(\mathbf{k}')^*\frac{z^{n/2-2}}{(2\pi)^{n/2}} J_{n/2-1}(z)\left[(n-2)f\left(\mathbf{k}' + \frac{\mathbf{z}}{R}\right) + z\frac{df}{dz}\left(\mathbf{k}' + \frac{\mathbf{z}}{R}\right)\right] d^n\mathbf{k}'\, d\hat{z}\, dz. \tag{A8}$$

If we continue the partial integration m times, where $m < n$, then we have that (A5) may be written as

$$\int f'(\mathbf{k}')^*\frac{z^{n/2-1-m}}{(2\pi)^{n/2}} J_{n/2-m}(z)\left[(n-2)(n-4)\cdots(n-2m)\times f\left(\mathbf{k}' + \frac{\mathbf{z}}{R}\right) + \sum_{l=1}^{m} a_l z^l \frac{d^l f}{dz^l}\left(\mathbf{k}' + \frac{\mathbf{z}}{R}\right)\right] d^n\mathbf{k}'\, d\hat{z}\, dz. \tag{A9}$$

In formula (A9) the a_l that appear are constants obtained from sequence of partial integrations. Since it is not necessary to know what they are we do not bother to write them out.

In order to show (A1) consider the cases of n even

and n odd separately. Start with n odd. Here take $m = n/2 - \frac{1}{2}$. Then, if we set $\mathbf{x} = \mathbf{z}/R$, (A9) becomes

$$\int f'(\mathbf{k}')^* \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{(2\pi)^{n/2}} \frac{\sin Rx}{x} \left[(n-2)!!\, f(\mathbf{k}'+\mathbf{x}) + \sum_{l=1}^{n/2-1/2} a_l x^l \frac{d^l f(\mathbf{k}'+\mathbf{x})}{dx^l}\right] d^n\mathbf{k}'\, d\hat{x}\, dx. \tag{A10}$$

We now consider the $R \to \infty$ limit of (A10). By applying the Riemann–Lebesque lemma[13] to (A10) we see that only the $x = 0$ point contributes to the value of the limit. So the set of terms with derivatives all vanish. We are left with just the first term. Since an n-dimensional unit sphere has a surface area

$$\int d\hat{x} = \frac{2\pi^{n/2}}{\Gamma(n/2)}, \tag{A11}$$

we have that the $R \to \infty$ value of (A10) is just

$$\int f'(\mathbf{k}')^* f(\mathbf{k}')\, d^n\mathbf{k}' = (f', f). \tag{A12}$$

This establishes the validity of (A1). A parallel argument works for n even.

Let us now turn to the evaluation of the singular kernel $\langle \mathbf{k}' | P(R) | \mathbf{k}\rangle/(k^2 - k'^2)$. The divisor here, which vanishes in the domain of integration, is given a well-defined sense by the definition of the singular integral as a principal value integral. We shall prove

Property I:

$$\lim_{R\to\infty} \int f'(\mathbf{k}')^* \frac{\langle \mathbf{k}' | P(R) | \mathbf{k}\rangle}{\mathbf{k}^2 - \mathbf{k}'^2} f(\mathbf{k})\, d^n\mathbf{k}'\, d^n\mathbf{k} = \int f'(\mathbf{k}')^* \frac{d}{dk}\left[\left(\frac{k}{k'}\right)^{(n-1)/2} \frac{f(k, \hat{k}')}{k+k'}\right]_{k=k'} d^n\mathbf{k}'. \tag{A13}$$

In our three-body problem the case $n = 6$ is of most interest to us; however, $n = 3$ is also useful in the study of the two-body problem.

Introduce the coordinate $\mathbf{z} = \mathbf{R}(\mathbf{k} - \mathbf{k}')$; then

$$R^2(k^2 - k'^2) = z(z + 2Rk'\cos\theta_{k'z}) \tag{A14}$$

where $\theta_{k'z}$ is the angle between vector $\mathbf{k}'$ and $\mathbf{z}$. Using the form (A4) for the projection operator, the integral on the left of (A13) is

$$\int f'(\mathbf{k}')^* \frac{f(\mathbf{k}' + \mathbf{z}/R)}{(z/R)[(z/R) + 2k'\cos\theta_{k'z}]} \frac{J_{n/2}(z)}{(2\pi z)^{n/2}}\, d^n\mathbf{k}'\, d^n\mathbf{z}. \tag{A15}$$

Our method of evaluating (A15) is based on the observation that we can reduce this problem to the previous problem, i. e., the demonstration of (A1). Let us introduce an n-dimensional spherical coordinate system to describe the vector $\mathbf{z}/R$. We choose the z axis of this coordinate system parallel to $\mathbf{k}'$. Denoting the coordinates by $\{(z/R), \theta_1, \theta_2, \ldots, \theta_{n-1}\}$ we have that $\theta_1 = \theta_{k'z}$. We note that if we perform the integration over $d\hat{z}$ first the denominator vanishes only when the θ_1 integration is carried out. So we are motivated to write (A15) as

$$\int f'(\mathbf{k}')^* \frac{J_{n/2}(z)}{(2\pi z)^{n/2}} F_{z/R}(\mathbf{k}')\, d^n\mathbf{z}\, d^n\mathbf{k}', \tag{A16}$$

where $F_{z/R}$ is defined as

$$F_{z/R}(\mathbf{k}') = \frac{1}{2}\int_{-1}^{1} d\cos\theta_1 \frac{\sin^{n-3}\theta_1}{(z/R)(z/R + 2k'\cos\theta_1)} \times \bar{f}_{z/R}(\mathbf{k}', \cos\theta_1), \tag{A17}$$

$$\bar{f}_{z/R}(\mathbf{k}', \cos\theta_1) = \frac{\Gamma(n/2)}{\pi^{n/2}} \int_0^{\pi} \sin^{n-3}\theta_2\, d\theta_2 \cdots \int_0^{2\pi} d\theta_{n-1} f\left(\mathbf{k}' + \frac{\mathbf{z}}{R}\right). \tag{A18}$$

Examination of these formula indicate that $F_{z/R}$ is the average value of the function $f(\mathbf{k}' + \mathbf{z}/R)(k^2 - k'^2)^{-1}$ summed over the surface of a sphere centered at $\mathbf{k}'$ with radius z/R. The $\bar{f}(\mathbf{k}', \cos\theta_1)$ is the nonsingular part of the average and integral (A17) is the integral over the singular part.

We shall show that $F_{z/R}(\mathbf{k}')$ is continuous in z/R. That $F_{z/R}$ is integrable with respect to $d^n z$ follows from (A18) and the fact that $f(\mathbf{k}' + \mathbf{z}/R)$ is integrable with respect to $d^n z$. Thus we shall be justified in using (A1) to conclude that

$$\lim_{R\to\infty} \int f'(\mathbf{k}')^* \frac{J_{n/2}(z)}{(2\pi z)^{n/2}} F_{z/R}(\mathbf{k}')\, d^n\mathbf{z}\, d^n\mathbf{k} = \int f'(\mathbf{k}')^* F_0(\mathbf{k}')\, d^n\mathbf{k}'. \tag{A19}$$

Let us investigate the behavior of $F_{z/R}(\mathbf{k}')$ as $z/R \to 0$. If we define

$$x = \frac{z}{R}\cos\theta_1 + \frac{z^2}{2k'R^2}, \tag{A20}$$

then (A17) becomes

$$F_{z/R}(\mathbf{k}') = \frac{1}{2}\frac{R}{2kz}\int_{-z/R+z^2/2k'R^2}^{z/R+z^2/2k'R^2} \left(1 - \frac{z^2}{4k'^2R^2} - \frac{R^2x^2}{z^2} + \frac{x}{k'}\right)^{(n-3)/2} \times \bar{f}(\mathbf{k}', x)\frac{dx}{x}. \tag{A21}$$

This principal value integral here is of the general form

$$\frac{1}{b+a}\int_{-a}^{b} h(x)\frac{dx}{x} = \frac{1}{b+a}\int_{-a}^{b} \frac{h(x) - h(0)}{x}\, dx + \frac{h(0)}{b+a}\int_{-a}^{b}\frac{dx}{x}, \quad a > 0, \quad b > 0 \tag{A22}$$

where h is a differentiable function. On the right of (A22) we have written the integral by adding and substracting

$$\frac{h(0)}{a+b}\int_{-a}^{b}\frac{dx}{x}.$$

We need to find the value of (A22) when $a \to 0$ and $b \to 0$. Since the integrand of the first integral on the left of of (A22) is continuous, we may use the mean value theorem to write

$$\frac{1}{b+a}\int_{-a}^{b} h(x)\frac{dx}{x} = \left(\frac{h(x_1) - h(0)}{x_1}\right) + \frac{h(0)}{b+a}\ln\frac{b}{a} \tag{A23}$$

where x_1 is some point in the interval $(b, -a)$. As the interval size goes to zero the factor in the square brackets becomes the derivative of h at $x = 0$. The second factor is just a constant times $h(0)$.

If we apply formula (A23) to (A21), we obtain

$$F_0(\mathbf{k}') = \frac{n-2}{4}\frac{1}{k'^2}f(\mathbf{k}') + \frac{1}{2k'}\frac{df(k',\hat{k}')}{dk'} = \frac{d}{dk}\left[\left(\frac{k}{k'}\right)^{(n-1)/2}\frac{f(k,\hat{k}')}{k+k'}\right]\Bigg|_{k=k'}. \tag{A24}$$

When this result is substituted into (A19) we obtain (A13). In the text we require the result of $\langle \mathbf{k}' | P(R) | \mathbf{k}\rangle/(k-k')$. This is obtained from (A13) just by setting $f(\mathbf{k}) = (k'+k)g(\mathbf{k})$, so the denominator in $(k+k')$ in (A24) is now absent.

We turn to the next important property of the $P(R)$ that we have used in our derivation. Choose n to be even and the n-dimensional vector $\mathbf{k}$ may be represented as the pair of vectors $(\mathbf{p},\mathbf{q})$ where $\mathbf{p}$ and $\mathbf{q}$ are $(n/2)$-dimensional vectors. Let us determine the effect of $\langle \mathbf{k}' | P(R) | \mathbf{k}\rangle/(p-p')$. This problem is trivally related to that of determining $\langle \mathbf{k}' | P(R) | \mathbf{k}\rangle/(p^2-p'^2)$, so we shall solve this last problem. We need to calculate the $R\to\infty$ limit of

$$\int \frac{f'(\mathbf{k}')^* f(\mathbf{k})}{p^2-p'^2}\frac{R^{n/2}}{(2\pi|\mathbf{k}-\mathbf{k}'|)^{n/2}}J_{n/2}(|\mathbf{k}-\mathbf{k}'|R)\,d^n\mathbf{k}\,d^n\mathbf{k}'. \tag{A25}$$

Introducing the variables

$$\mathbf{z} = R(\mathbf{k}-\mathbf{k}'),\quad \mathbf{x} = R(\mathbf{p}-\mathbf{p}'),\quad \mathbf{y} = R(\mathbf{q}-\mathbf{q}'),$$

where $\mathbf{x}$ and $\mathbf{y}$ are $(n/2)$-dimensional vectors, one has

$$z = (x^2+y^2)^{1/2},\quad p^2-p'^2 = \frac{x}{R}\left(\frac{x}{R}+2p'\cos\theta_{p'x}\right)$$

where $\theta_{p'x}$ is the angle between $\mathbf{p}'$ and $\mathbf{x}$. So expression (A25) may be written

$$\int f'(\mathbf{k}')^*\frac{J_{n/2}(z)}{(2\pi z)^{n/2}}\frac{f(\mathbf{p}'+\mathbf{x}/R,\mathbf{q}'+\mathbf{y}/R)}{(x/R)(x/R+2p'\cos\theta_{p'x})}d^n\mathbf{k}'\,d^n\mathbf{z}. \tag{A26}$$

The structure of this integral is similar in nature to that evaluated in (A19)—(A24) so we may utilize the same technique to show that

Property II:

$$\lim_{R\to\infty}\int f'(\mathbf{k}')^*\frac{\langle \mathbf{k}'|P(R)|\mathbf{k}\rangle}{p-p'}f(\mathbf{k})\,d^n\mathbf{k}'\,d^n\mathbf{k} = \int f'(\mathbf{k}')^*\frac{d}{dp}\left[\left(\frac{p}{p'}\right)^{(n-2)/4}f(p\hat{p}',\mathbf{q}')\right]\Bigg|_{p=p'}d^n\mathbf{k}'. \tag{A27}$$

We wish now to deduce a related property for the operators $\bar{P}_\beta(R)$. Namely we establish

Property III:

$$\lim_{R\to\infty}\int f'(\mathbf{p}'_\beta)\frac{\langle \mathbf{p}'_\beta|\bar{P}_\beta(R)|\mathbf{p}_\beta\rangle}{p_\beta-p'_\beta}f(\mathbf{p}_\beta)\,d^3\mathbf{p}_\beta\,d^3\mathbf{p}'_\beta = \int f'(\mathbf{p}'_\beta)\frac{d}{dp_\beta}\left[\left(\frac{p_\beta}{p'_\beta}\right)f(p_\beta\hat{p}'_\beta)\right]\Bigg|_{p_\beta=p'_\beta}d^3p'_\beta. \tag{A28}$$

That III is a consequence of II is seen as follows. Recall that

$$\langle \mathbf{p}'_\beta|\bar{P}_\beta(R)|\mathbf{p}_\beta\rangle = \int \psi_\beta(\mathbf{q}'_\beta)^*\langle \mathbf{p}'_\beta\mathbf{q}'_\beta|\bar{P}(R)|\mathbf{p}_\beta\mathbf{q}_\beta\rangle\psi_\beta(\mathbf{q}_\beta)\,d^3q'_\beta\,d^3q_\beta. \tag{A29}$$

In (A27) set $f(\mathbf{p}_\beta,\mathbf{q}_\beta) = f(\mathbf{p}_\beta)\psi(\mathbf{q}_\beta)$ and $f'(\mathbf{p}'_\beta,\mathbf{q}'_\beta) = f'(\mathbf{p}'_\beta)\psi(\mathbf{q}'_\beta)$; then (A28) follows at once.

Property IV:

$$\lim_{R\to\infty}\Big(\int \delta(\tilde{p}'^2_\beta-\tilde{p}''^2_\beta)\langle \mathbf{p}''_\beta|\bar{P}_\beta(R)|\mathbf{p}'_\beta\rangle\,d^3p''_\beta - \int\delta(\tilde{K}^2-\tilde{K}''^2)\,\langle \mathbf{p}_\gamma\mathbf{q}_\gamma|\bar{P}(R)|\mathbf{p}''_\gamma\mathbf{q}''_\gamma\rangle\,d^3q''_\gamma\,d^3p''_\gamma\Big) = 0 \tag{A30}$$

where $\tilde{K}^2 = \tilde{p}^2_\gamma+\tilde{q}^2_\gamma = \tilde{p}'^2_\beta-\chi^2_\beta$. The physical meaning of this property can be understood by looking at expression (4.10) for the free transit time. The meaning of the term on the left is the free transit time for a planewave in channel β having an energy $\tilde{K}^2 = \tilde{p}'^2_\beta-\chi^2_\beta$. The second expression in Eq. (A30) is the free transit time for an incident state composed of three free particles having energy $\tilde{K}^2$. Then (A30) claims these free transit times are the same in the limit $R\to\infty$.

After a prolonged examination we are unable to give a general proof of this property. Thus we are forced to add it as an ansatz to our list assumptions detailed at the end of Sec. II. The problem in the proof is that the integral expression for $\langle \mathbf{p}''_\beta|\bar{P}_\beta(R)|\mathbf{p}'_\beta\rangle$ involves Bessel functions of complicated arguments and this makes an explicit evaluation of the integral unusually difficult. We note that in the two-dimensional static coupled channel problem that Celenza and Toboman[14] studied that they required the free transit time to be independent of the channel.

The role of Property IV in our demonstration of Eq. (5.67) is restricted to showing various collections of terms, like Eq. (B1) are zero.

Property V:

$$\lim_{R\to\infty}\Big(\int \delta(\tilde{p}'^2_\alpha-\tilde{p}''^2_\alpha)\langle \mathbf{p}''_\alpha|\bar{P}_\alpha(R)|\mathbf{p}'_\alpha\rangle d^3p''_\alpha - \int\delta(\tilde{p}'^2_\beta-\tilde{p}''^2_\beta)\langle \mathbf{p}''_\beta|\bar{P}_\beta(R)|\mathbf{p}'_\beta\rangle\,d^3p''_\beta\Big) = 0 \tag{A31}$$

where $\tilde{p}'^2_\beta-\chi^2_\beta = \tilde{p}'^2_\alpha-\chi^2_\alpha$. This property is a consequence of Property IV obtained by allowing β to take on its various different nonzero values.

APPENDIX B

We collect in this appendix a number of the results claimed valid in Sec. V. Let us consider the different problems in the same order that they arise in Sec. V. We first examine the validity of

$$\lim_{R\to\infty}\langle \mathbf{p}_\gamma|I_\gamma(B_i(R)-A_i(R))|\mathbf{p}'_\beta\rangle = 0,\quad i\neq 2, \tag{B1}$$

for on-shell values of $\mathbf{p}_\gamma$ and $\mathbf{p}'_\beta$, i.e., $\tilde{p}^2_\gamma-\chi^2_\gamma = \tilde{p}'^2_\beta-\chi^2_\beta$. Most of the relations contained in Eq. (B1) are true for trivial reasons. For example, if $i\neq 2,3$, then the integrands appearing in the definitions (5.11), (5.14), (5.15), (5.16), (5.19), (5.22), (5.23), and (5.24) have smooth behaviors in the regions where the momentum space representations of $\bar{P}(R)$ and $\bar{P}_\alpha(R)$ are singular. Thus we can use $\bar{P}(R)\to E$ and $\bar{P}_\alpha(R)\to E_\alpha$. When this relation is employed Eq. (B1) is shown valid for $i\neq 2,3$.

We turn to a more complicated case $i=3$. We define

component forms of $B_3(R)$ and $A_3(R)$ given by

$$B_3(R) \equiv \sum_{\alpha=1}^{3} B_{3\alpha}(R), \tag{B2}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_{3\alpha}(R) | \mathbf{p}'_\beta \rangle \equiv i\pi \int \delta(\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta''^2 + \chi_\beta^2) \times \frac{\phi_\alpha(\mathbf{q}_\alpha)\langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}''_\beta \rangle \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} \, d^3p''_\beta \tag{B3}$$

and

$$A_3(R) \equiv \sum_{\alpha=1}^{3} A_{3\alpha}(R), \tag{B4}$$

$$\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_{3\alpha}(R) | \mathbf{p}'_\beta \rangle \equiv i\pi \int \frac{\langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle}{\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \times \delta(\tilde{p}_\alpha''^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \times \phi_\alpha(\mathbf{q}''_\alpha)\langle \mathbf{p}''_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle \, d^3p''_\gamma \, d^3q''_\gamma. \tag{B5}$$

First, let us investigate the case $\alpha \neq \gamma$. Then the denominator in (B3) takes the form

$$\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2 = \tilde{p}_\alpha^2 + \tilde{q}_\alpha^2 - \tilde{p}_\alpha^2 + \chi_\alpha^2 = \tilde{q}_\alpha^2 + \chi_\alpha^2 > 0. \tag{B6}$$

The basic behavior of $\langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle$ is that it is a convolution dependent on the difference $\mathbf{p}''_\beta - \mathbf{p}'_\beta$. As $R \to \infty$ this convolution becomes a delta function when acting on sufficient smooth functions. The exception to this situation is when p''_β is forced to always be equal to p'_β; then $\langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle$ has a constant value depending on R and β. In the case under study here $\alpha \neq \gamma$ and the delta function in Eq. (B3) does not force $p''_\beta = p'_\beta$, so we have

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_{3\alpha}(R) | \mathbf{p}'_\beta \rangle = i\pi \psi_\alpha(\mathbf{q}_\alpha)\langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle \delta(\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2). \tag{B7}$$

The vectors $\mathbf{p}_\alpha \mathbf{q}_\alpha$ are determined by $\mathbf{p}_\gamma \mathbf{q}_\gamma$.

Turning to $A_{3\alpha}(R)$ given by Eq. (B5), the denominator appearing there assumes the form

$$\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2 = \tilde{p}_\alpha''^2 + \tilde{q}_\alpha''^2 - \tilde{p}_\alpha''^2 + \chi_\alpha^2 = \tilde{q}_\alpha''^2 + \chi_\alpha^2 > 0. \tag{B8}$$

As in the case above the delta function in Eq. (B5) does not force $p_\gamma = p''_\gamma$ or $q_\gamma = q''_\gamma$, so $\bar{P}(R) \to E$ here. Thus for Eq. (B5) we obtain the limit

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_{3\alpha}(R) | \mathbf{p}'_\beta \rangle = i\pi \psi_\alpha(\mathbf{q}_\alpha)\langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle \delta(\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2), \tag{B9}$$

so $A_{3\alpha}(R) - B_{3\alpha}(R) \to 0$ as $R \to \infty$.

Consider the remaining term in A_3, B_3—that for $\alpha = \gamma$. Here one has for $I_\gamma B_{3\gamma}(R)$

$$\begin{aligned}\langle \mathbf{p}_\gamma | I_\gamma B_{3\gamma}(R) | \mathbf{p}'_\beta \rangle &= i\pi \int |\psi_\gamma(\mathbf{q}_\gamma)|^2 d^3q_\gamma \int \delta(\tilde{p}_\gamma^2 - \chi_\gamma^2 - \tilde{p}_\beta''^2 + \chi_\beta^2) \times \langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}''_\beta \rangle \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle \, d^3p''_\beta \\ &= i\pi \langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}'_\beta \rangle \int \delta(\tilde{p}_\beta'^2 - \tilde{p}_\beta''^2) \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle \, d^3p''_\beta. \end{aligned} \tag{B10}$$

For $I_\gamma A_{3\gamma}(R)$ we have

$$\begin{aligned}\langle \mathbf{p}_\gamma | I_\gamma A_{3\gamma}(R) | \mathbf{p}'_\beta \rangle &= i\pi \int \Big(\int \psi_\gamma(\mathbf{q}_\gamma)^* \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{P}(R) | \mathbf{p}''_\gamma \mathbf{q}''_\gamma \rangle \psi_\gamma(\mathbf{q}''_\gamma) \, d^3q_\gamma \, d^3q''_\gamma \Big) \\ &\quad \times \delta(\tilde{p}_\gamma''^2 - \tilde{p}_\gamma^2)\langle \mathbf{p}''_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}'_\beta \rangle \, d^3p''_\gamma \\ &= i\pi \langle \mathbf{p}_\gamma | H_{\gamma\beta}^{(+)} | \mathbf{p}'_\beta \rangle \int \langle \mathbf{p}_\gamma | \bar{P}_\gamma(R) | \mathbf{p}''_\gamma \rangle \delta(\tilde{p}_\gamma''^2 - \tilde{p}_\gamma^2) \, d^3p''_\gamma. \end{aligned} \tag{B11}$$

In Appendix A we discuss the relationship

$$\lim_{R\to\infty} \Big(\int \langle \mathbf{p}_\gamma | \bar{P}_\gamma(R) | \mathbf{p}''_\gamma \rangle \delta(\tilde{p}_\gamma''^2 - \tilde{p}_\gamma^2) \, d^3p_\gamma - \int \langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle \delta(\tilde{p}_\beta''^2 - \tilde{p}_\beta'^2) \, d^3p''_\beta \Big) = 0 \tag{B12}$$

where $\tilde{p}_\gamma^2 - \chi_\gamma^2 = \tilde{p}_\beta'^2 - \chi_\beta^2$. With the result of Eq. (B12) we obtain that $I_\gamma B_{3\gamma}(R) - I_\gamma A_{3\gamma}(R)$ vanishes as $R \to \infty$. So altogether we have shown that Eq. (B1) is correct.

The next result, employed in Sec. V, that one needs to prove is

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma | I_\gamma (B_{2\alpha}(R) - A_{2\alpha}(R)) | \mathbf{p}'_\beta \rangle = 0, \quad \alpha \neq \gamma, \tag{B13}$$

where $B_{2\alpha}(R)$ is given by Eq. (5.28) and $A_{2\alpha}(R)$ is given by Eq. (5.37). Consider $B_{2\alpha}(R)$ first. The integral in Eq. (5.28) is well defined if the denominators do not simultaneously vanish. That the singularities are always separate can be demonstrated by attempting to set $\tilde{p}_\alpha^2 - \chi_\alpha^2$ equal to $\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2$. Using $\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 = \tilde{p}_\alpha^2 + \tilde{q}_\alpha^2$ this equality is equivalent to $-\chi_\alpha^2 = \tilde{q}_\gamma^2$, which cannot be satisfied for any value of $\mathbf{q}_\gamma$. Secondly, we note that $\langle \mathbf{p}''_\beta | \bar{P}_\beta(R) | \mathbf{p}'_\beta \rangle \to \delta^3(\mathbf{p}''_\beta - \mathbf{p}'_\beta)$, unless it is divided by a term of the type $p''_\beta - p'_\beta$. Such a term could in principle come from either of the two denominators in (5.28). If the second denominator is to behave like $p'_\beta - p''_\beta$, we require

$$\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 = \tilde{p}_\beta'^2 - \chi_\beta^2 = \tilde{p}_\gamma^2 - \chi_\gamma^2. \tag{B14}$$

Again this is impossible since it is equivalent to $\tilde{q}_\gamma^2 = -\chi_\gamma^2$. So the second denominator will not effect the behavior of the $R \to \infty$ limit. The first denominator will behave as $p'_\beta - p''_\beta$ if

$$\tilde{p}_\alpha^2 - \chi_\alpha^2 = \tilde{p}_\beta'^2 - \chi_\beta^2. \tag{B15}$$

This condition may be stated as a condition on $\mathbf{q}_\gamma$ since $\mathbf{p}_\alpha$ is a function of the on-shell vector $\mathbf{p}_\gamma$ and the vector $\mathbf{q}_\gamma$. So if $\mathbf{q}_\gamma$ is such that (B15) is *not* satisfied,

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_{2\alpha}(R) | \mathbf{p}'_\beta \rangle = \frac{\phi_\alpha(\mathbf{q}_\alpha)}{\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \frac{\langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2}. \tag{B16}$$

In the case where (B15) is satisfied, then we must use Eq. (5.31) to evaluate the integral in Eq. (5.28). The result which we do not bother to write out will clearly be finite.

Let us now turn to the evaluation of $A_{2\alpha}(R)$. Again if (B15) is not satisfied we can show the $\bar{P}(R) \to E$ in Eq. (5.37), so that we have

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_{2\alpha}(R) | \mathbf{p}'_\beta \rangle = \frac{\phi_\alpha(\mathbf{q}_\alpha)}{\tilde{p}_\alpha^2 - \chi_\alpha^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \frac{\langle \mathbf{p}_\alpha | H_{\alpha\beta}^{(+)} | \mathbf{p}'_\beta \rangle}{\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 - \tilde{p}_\beta'^2 + \chi_\beta^2}. \tag{B17}$$

When (B15) is true then we need to employ Eq. (5.40) to evaluate the integral in (5.37). The result is a finite constant. Thus

$$\lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | B_{2\alpha}(R) | \mathbf{p}'_\beta \rangle = \lim_{R\to\infty} \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | A_{2\alpha}(R) | \mathbf{p}'_\beta \rangle \tag{B18}$$

for $\mathbf{q}_\gamma$ such that (B15) is not satisfied. However, in passing to the form (B13) we need to integrate (B18) by $\int \psi_\gamma(\mathbf{q}_\gamma) \, d^3q_\gamma$. The set of points in q_γ such that (B15) is true are of measure zero with respect to $q_\gamma^2 dq_\gamma$, so the

exceptional points satisfying (B15) do not contribute to the d^3q_γ integration. So we may conclude that relation (B13) is true.

We conclude this section by examining the case $\gamma = 0$. Here the on-shell condition takes the form $\tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 = \tilde{p}_\beta'^2 - \chi_\beta^2$. Referring to Sec. V we see that we have to prove relation (5.53). Looking at the $B_i(R)$ terms first we note that their sum may be expressed as

$$\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=4}^{6} B_i(R) \middle| \mathbf{p}_\beta' \right\rangle = \int \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta'' \rangle i\pi \delta(\tilde{p}_\beta'^2 - \tilde{p}_\beta''^2) \langle \mathbf{p}_\beta'' | \bar{\rho}_\beta(R) | \mathbf{p}_\beta' \rangle \, d^3p_\beta''. \tag{B19}$$

Because $\bar{\rho}_\beta(R)$ becomes diagonal in $\hat{p}_\beta''$ and $\hat{p}_\beta'$ we can write this as

$$\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=4}^{6} B_i(R) \middle| \mathbf{p}_\beta' \right\rangle = i\pi \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \int \delta(\tilde{p}_\beta'^2 - \tilde{p}_\beta''^2) \langle \mathbf{p}_\beta'' | \bar{\rho}_\beta(R) | \mathbf{p}_\beta' \rangle \, d^3p_\beta''. \tag{B20}$$

If we turn to the related terms in $A_i(R)$ their on-shell matrix elements are

$$\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=4}^{6} A_i(R) \middle| \mathbf{p}_\beta' \right\rangle = \int \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{\rho}(R) | \mathbf{p}_\gamma'' \mathbf{q}_\gamma'' \rangle \langle \mathbf{p}_\gamma'' \mathbf{q}_\gamma'' | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \times i\pi \delta(\tilde{p}_\gamma''^2 + \tilde{q}_\gamma''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \, d^3q_\gamma'' \, d^3p_\gamma''. \tag{B21}$$

Since $\bar{\rho}(R)$ becomes diagonal in the five-dimensional angle variables $\omega_\gamma \hat{p}_\gamma \hat{q}_\gamma$, we may refashion Eq. (B21) as

$$\left\langle \mathbf{p}_\gamma \mathbf{q}_\gamma \middle| \sum_{i=4}^{6} A_i(R) \middle| \mathbf{p}_\beta' \right\rangle = i\pi \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \int \delta(\tilde{K}^2 - \tilde{K}''^2) \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{\rho}(R) | \mathbf{p}_\gamma'' \mathbf{q}_\gamma'' \rangle \times d^3p_\gamma'' \, d^3q_\gamma''. \tag{B22}$$

As a result of the following relation for our projection operators, the terms (B20) cancel those of (B22):

$$\lim_{R\to\infty} \left(\int \delta(\tilde{p}_\beta'^2 - \tilde{p}_\beta''^2) \langle \mathbf{p}_\beta'' | \bar{\rho}_\beta(R) | \mathbf{p}_\beta' \rangle \, d^3p_\beta'' - \int \delta(\tilde{K}^2 - \tilde{K}''^2) \langle \mathbf{p}_\gamma \mathbf{q}_\gamma | \bar{\rho}(R) | \mathbf{p}_\gamma'' \mathbf{q}_\gamma'' \rangle \, d^3q_\gamma'' \, d^3p_\gamma'' \right) = 0 \tag{B23}$$

where $\tilde{K}^2 = \tilde{p}_\gamma^2 + \tilde{q}_\gamma^2 = \tilde{p}_\beta'^2 - \chi_\beta^2$ in this relation.

APPENDIX C

In this appendix we prove that the on-shell matrix elements of the operator $K_\gamma^{(+)\dagger} Y_\beta(R)$ vanish in the $R \to \infty$ limit. We stress that the analysis we present below only allows us to conclude that the on-shell matrix element vanishes. In fact, it is quite likely that the operator $K_\gamma^{(+)\dagger} Y_\beta(R)$ does not vanish (in any norm) as $R \to \infty$. The matrix element we need to evaluate is

$$\langle \mathbf{p}_\gamma^0 | K_\gamma^{(+)\dagger} Y_\beta(R) | \mathbf{p}_\beta' \rangle = \int \langle \mathbf{p}_\gamma^0 | K_\gamma^{(+)\dagger} | \mathbf{pq} \rangle \langle \mathbf{pq} | Y_\beta(R) | \mathbf{p}_\beta' \rangle \, d^3p \, d^3q, \tag{C1}$$

where the initial and final momentum are related by

$$\tilde{p}_\gamma^{02} - \chi_\gamma^2 = \tilde{p}_\beta'^2 - \chi_\beta^2 \equiv \tilde{K}^{02}. \tag{C2}$$

Using Eq. (2.19) for the kernel of $K_\gamma^{(+)\dagger}$ and Eq. (5.7) for the kernel of $Y_\beta(R)$, our matrix element assumes the form

$$\int d^3p \, d^3q \frac{\langle \mathbf{pq} | \beta_{0\gamma}^{(-)} | \mathbf{p}_\gamma^0 \rangle^*}{\tilde{p}^2 + \tilde{q}^2 - \tilde{p}_\gamma^{02} + \chi_\gamma^2 - i0} \times \left(\int d^3p_\beta'' \frac{\langle \mathbf{pq} | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta'' \rangle \langle \mathbf{p}_\beta'' | \bar{\rho}_\beta(R) | \mathbf{p}_\beta' \rangle}{\tilde{p}^2 + \tilde{q}^2 - \tilde{p}_\beta''^2 + \chi_\beta^2 - i0} - \int d^3p'' \, d^3q'' \frac{\langle \mathbf{pq} | \bar{\rho}(R) | \mathbf{p}''\mathbf{q}'' \rangle \langle \mathbf{p}''\mathbf{q}'' | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle}{\tilde{p}''^2 + \tilde{q}''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2 - i0} \right). \tag{C3}$$

We must show that this expression becomes zero as $R \to \infty$. We recall that the $\beta_{0\gamma}^{(-)}$ and $\beta_{0\beta}^{(+)}$ have according to Eq. (2.20) additional singular denominators which are related to the various two cluster kinds of asymptotic motion that the three-body system can produce. It turns out that the contribution to (C3) from the explicitly exhibited singularities vanishes. The contribution from the additional primary singularities in Eq. (2.20) also separately vanishes. Here we shall only bother to write down in detail the contribution to (C3) from the exhibited singular denominators.

One may evaluate expression (C3) by expanding the singular denominators into delta function plus principal-value parts. Thus we have three types of terms. First we encounter those terms having the product of two delta functions in each factor. These terms become zero as $R \to \infty$ as an immediate consequence of Property IV of the projection operators. Likewise it is easy to show that the terms involving the product of two principal-value factors are zero. For such terms we may use the delta-function properties of our projection operators and the argument employed by Jauch and Marchand[15] to show that the result is zero. Thus the nonzero terms that remain are of a mixed type involving one principal-value term times a delta-function term. The cancellations between these remaining terms is surprisingly complex. These terms are

$$\int d^3p \, d^3q \frac{\langle \mathbf{pq} | \beta_{0\gamma}^{(-)} | \mathbf{p}_\gamma^0 \rangle^*}{\tilde{p}^2 + \tilde{q}^2 - \tilde{p}_\gamma^{02} - \chi_\gamma^2} \left(\int d^3p_\beta'' \langle \mathbf{pq} | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta'' \rangle \times \langle \mathbf{p}_\beta'' | \bar{\rho}_\beta(R) | \mathbf{p}_\beta' \rangle i\pi \delta(\tilde{p}^2 + \tilde{q}^2 - \tilde{p}_\beta''^2 + \chi_\beta^2) - \int d^3p'' \, d^3q'' \times \langle \mathbf{pq} | \bar{\rho}(R) | \mathbf{p}''\mathbf{q}'' \rangle i\pi \delta(\tilde{p}''^2 + \tilde{q}''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2) \langle \mathbf{p}''\mathbf{q}'' | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle \right) + \int d^3p \, d^3q \langle \mathbf{pq} | \beta_{0\gamma}^{(-)} | \mathbf{p}_\gamma^0 \rangle^* i\pi \delta(\tilde{p}^2 + \tilde{q}^2 - \tilde{p}_\gamma^{02} + \chi_\gamma^2) \times \left(\int d^3p_\beta'' \frac{\langle \mathbf{pq} | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta'' \rangle \langle \mathbf{p}_\beta'' | \bar{\rho}_\beta(R) | \mathbf{p}_\beta' \rangle}{\tilde{p}^2 + \tilde{q}^2 - \tilde{p}_\beta''^2 + \chi_\beta^2} - \int d^3p'' \, d^3q'' \frac{\langle \mathbf{pq} | \bar{\rho}(R) | \mathbf{p}''\mathbf{q}'' \rangle \langle \mathbf{p}''\mathbf{q}'' | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle}{\tilde{p}''^2 + \tilde{q}''^2 - \tilde{p}_\beta'^2 + \chi_\beta^2} \right). \tag{C4}$$

We now eliminate the delta functions by performing the integrals over the relevant variable. After this (C4) becomes

$$i\pi \int d^3p_\beta'' \, d^5\hat{K} \frac{\langle \mathbf{p}_\beta'' | \bar{\rho}_\beta(R) | \mathbf{p}_\beta' \rangle}{p_\beta'' - p_\beta'} \left(\frac{2n_\beta(\tilde{p}_\beta''^2 + \chi_\beta^2)^2}{2(p_\beta'' + p_\beta')} \times \langle \sqrt{\tilde{p}_\beta''^2 - \chi_\beta^2} \hat{K} | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta'' \rangle \langle \sqrt{\tilde{p}_\beta''^2 - \chi_\beta^2} \hat{K} | \beta_{0\gamma}^{(-)} | \mathbf{p}_\gamma^0 \rangle^* \right) - i\pi \int \tilde{K}^5 \, d\tilde{K} \, d^5\hat{K} \, d^5\hat{K}'' \tilde{K}''^4 \langle \tilde{K}^0 \hat{K}'' | \beta_{0\beta}^{(+)} | \mathbf{p}_\beta' \rangle$$

$$\times\frac{\langle\tilde{K}\hat{K}|\bar{\rho}(R)|\tilde{K}^0\hat{K}''\rangle}{\tilde{K}-\tilde{K}^0}\left(\frac{\langle\tilde{K}\hat{K}|\beta_{0\gamma}^{(-)}|\mathbf{p}_\gamma^0\rangle^*}{2(\tilde{K}+\tilde{K}^0)}\right)$$

$$+i\pi\int d^3p_\beta''\,d^5\hat{K}\tilde{K}^{04}\langle\tilde{K}_0\hat{K}|\beta_{0\gamma}^{(-)}|\mathbf{p}_\gamma^0\rangle^*\frac{\langle\mathbf{p}_\beta''|\bar{\rho}_\beta(R)|\mathbf{p}_\beta'\rangle}{p_\beta'-p_\beta''}$$

$$\times\left(\frac{2n_\beta\langle\tilde{K}^0\hat{K}|\beta_{0\beta}^{(+)}|\mathbf{p}_\beta''\rangle}{2(p_\beta'+p_\beta'')}\right)-i\pi\int\tilde{K}''^5\,d\tilde{K}''\,d^5\hat{K}''\,d^5\hat{K}$$

$$\times\langle\tilde{K}_0\hat{K}|\beta_{0\gamma}^{(-)}|\mathbf{p}_\gamma^0\rangle^*\tilde{K}^{04}\langle\tilde{K}_0\hat{K}|\bar{\rho}(R)|\tilde{K}''\hat{K}''\rangle$$

$$\times\left(\frac{\langle\tilde{K}''\hat{K}''|\beta_{0\beta}^{(+)}|\mathbf{p}_\beta'\rangle}{2(\tilde{K}''+\tilde{K}^0)}\right). \tag{C5}$$

In expression (C5) our convention for the five-dimensional angle differential is given by the definition $d^3\tilde{p}\,d^3\tilde{q}\equiv\tilde{K}^5\,d\tilde{K}\,d^5\hat{K}$. We take the limit $R\to\infty$ and use Properties I and II of the projection operators to show that (C5) becomes

$$+\frac{i\pi}{2}\int d^5\hat{K}\frac{d}{dp_\beta''}\left((2n_\beta)\frac{p_\beta''(\tilde{p}_\beta''^2-\chi_\beta^2)^2}{p_\beta'(p_\beta'+p_\beta'')}\langle\sqrt{\tilde{p}_\beta''^2-\chi_\beta^2}\hat{K}|\beta_{0\gamma}^{(-)}|\mathbf{p}_\gamma^0\rangle^*\right.$$

$$\left.\times\langle\sqrt{\tilde{p}_\beta''^2-\chi_\beta^2}\hat{K}|\beta_{0\beta}^{(+)}|p_\beta''p_\beta'\rangle\right)\Big|_{p_\beta''=p_\beta'}-\frac{i\pi}{2}\int\tilde{K}^{04}\,d^5\hat{K}$$

$$\times\langle\tilde{K}^0\hat{K}|\beta_{0\beta}^{(+)}|\mathbf{p}_\beta'\rangle\frac{d}{d\tilde{K}''}\left[\left(\frac{\tilde{K}''}{\tilde{K}^0}\right)^{5/2}\frac{\langle\tilde{K}''\hat{K}|\beta_{0\gamma}^{(-)}|\mathbf{p}_\gamma^0\rangle^*}{\tilde{K}''+\tilde{K}^0}\right]\Big|_{\tilde{K}''=\tilde{K}^0}$$

$$-\frac{i\pi}{2}\int\tilde{K}^{04}\,d^5\hat{K}\langle\tilde{K}^0\hat{K}|\beta_{0\gamma}^{(-)}|\mathbf{p}_\gamma^0\rangle^*\frac{d}{dp_\beta''}$$

$$\times\left(2n_\beta\frac{p_\beta''}{p_\beta'}\frac{\langle\tilde{K}^0\hat{K}|\beta_{0\beta}^{(+)}|p_\beta''\hat{p}_\beta'\rangle}{p_\beta'+p_\beta''}\right)\Big|_{p_\beta''=p_\beta'}-\frac{i\pi}{2}\int\tilde{K}^{04}\,d^5\hat{K}$$

$$\times\langle\tilde{K}^0\hat{K}|\beta_{0\gamma}^{(-)}|\mathbf{p}_\gamma^0\rangle^*\frac{d}{d\tilde{K}''}\left[\left(\frac{\tilde{K}''}{\tilde{K}^0}\right)^{5/2}\frac{\langle\tilde{K}''\hat{K}|\beta_{0\beta}^{(+)}|\mathbf{p}_\beta'\rangle}{\tilde{K}''+\tilde{K}^0}\right]\Big|_{\tilde{K}''=\tilde{K}^0}. \tag{C6}$$

It is now a straightforward although somewhat lengthy algebraic task to compute all the derivative terms in (C6). The result one gets is that all of the terms cancel giving us zero for the evaluation of (C6).

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Irreducible Cartesian tensor expansions of scalar fields

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It is shown how a scalar function $V(|\mathbf{R} + \Sigma_{i=1}^{n} \mathbf{a}_i|)$ of a sum of $n + 1$ vectors can be expanded as a multiple Cartesian tensor series in the vectors $\mathbf{a}_i$. This expansion is a rearrangement of the multiple Taylor series expansion of such a function. In order to prove the fundamental theorem, Eq. (3.1) below, generalized Cartesian Legendre polynomials are defined. The theorem is applied to the eigenfunctions of the Laplace operator and to inverse powers. The expansions of the latter type of function leads to forms involving generalized hypergeometric functions in several variables. As a special case, the Cartesian form of the multipole expansion of the electrostatic potential between two linear molecules is derived. A number of sum rules for hypergeometric functions and addition formulas for (standard and modified) spherical Bessel functions are proved using a reduction property of the generalized Legendre polynomials. The case of the expansion of a tensorial function is also briefly discussed.

1. INTRODUCTION

In many problems of physics, for example the calculation of the nonspherical intermolecular potential between two or more molecules as a sum over spherical potentials between force centers in the molecules[1] and in the theory of heavy-ion transfer reactions,[2] it is necessary to have explicit expressions for scalar functions of the form

$$V\left(\left|\mathbf{R}+\sum_{i=1}^{n} \mathbf{a}_i\right|\right) \tag{1.1}$$

in terms of the vectors $\mathbf{a}_i$. A standard Taylor series expansion of (1.1) is

$$\sum_{m_1,\ldots,m_n}\left(\prod_{i=1}^{n} m_i!\right)^{-1}\prod_{i=1}^{n}(\mathbf{a}_i)^{m_i}\odot^{\Sigma m_i}(\nabla)^{\Sigma m_i} V(R) \tag{1.2}$$

where $R = |\mathbf{R}|$, the symbol $\odot^q$ means q-fold contraction of nearest Cartesian indices, and the $(\mathbf{a}_i)^{m_i}$ are tensors of rank m_i:

$$(\mathbf{a}_i)^{m_i} = \mathbf{a}_i\mathbf{a}_i\cdots\mathbf{a}_i\mathbf{a}_i \quad (m_i \text{ times}). \tag{1.3}$$

This is not very useful, since it does not arrange the terms in irreducible tensors. Indeed, the tensor (1.3) is reducible for all $m_i > 1$. It would be much more useful to rearrange (1.2) in such a way that the irreducible Cartesian tensors[3,4]

$$[\mathbf{a}_i]^{(m_i)} = (\mathbf{a}_i)^{m_i}\odot^{m_i}\mathbf{E}^{(m_i)} \tag{1.4}$$

appear explicitly. Here $\mathbf{E}^{(m)}$ is the $2m$th rank tensor which projects out the irreducible part of any mth rank tensor.[3,4]

In this article, this rearrangement is given in Sec. 3. In Sec. 2, generalized Cartesian Legendre polynomials are defined and some properties of these which are needed later on are proved. In later sections a number of applications is considered in some detail.

2. GENERALIZED LEGENDRE POLYNOMIALS

As is well known, a scalar function of two unit vectors $\hat{\mathbf{u}}$ and $\hat{\mathbf{v}}$ can be expanded in terms of Legendre polynomials (see Ref. 5 for the Cartesian tensor form):

$$Pl(\hat{\mathbf{u}},\hat{\mathbf{v}}) = (2l)!\,2^{-l}(l!)^{-2}[\hat{\mathbf{u}}]^{(l)}\odot^{l}[\hat{\mathbf{v}}]^{(l)}. \tag{2.1}$$

It would, therefore, seem natural to try to find a generalization of (2.1) for the problem posed in the introduction. To this end the following Cartesian tensors are defined first:

$$\mathbf{S}(l_1,l_2,\ldots,l_n) = q(l_1,l_2,\ldots,l_n)(4\pi)^{-1}\int d\hat{\mathbf{u}}\,[\hat{\mathbf{u}}]^{(l_1)}\cdots[\hat{\mathbf{u}}]^{(l_n)}, \tag{2.2}$$

where the normalization factor $q(l_1,l_2,\ldots,l_n)$ is given by

$$q(l_1,l_2,\ldots,l_n) = \prod_{i=1}^{n}\{(2l_i+1)!!/l_i!\}. \tag{2.3}$$

Generalized Cartesian Legendre polynomials may then be defined by

$$P_{l_1,l_2,\ldots,l_n}(\hat{\mathbf{u}}_1,\hat{\mathbf{u}}_2,\ldots,\hat{\mathbf{u}}_n) = [\hat{\mathbf{u}}_n]^{(l_n)}[\hat{\mathbf{u}}_{n-1}]^{(l_{n-1})}\cdots[\hat{\mathbf{u}}_1]^{(l_1)} \odot^{\Sigma l_i}\mathbf{S}(l_1,l_2,\ldots,l_n). \tag{2.4}$$

It should be noted at this point that the $\mathbf{S}(l_1,\ldots,l_n)$ are, for $n > 3$, *not* the most general Cartesian tensors of the symmetry $l_1,l_2,\ldots,l_n$. It is, therefore, not trivial that the functions defined by Eq. (2.4) are adequate for the problem at hand. That this is the case is proved in the next section. In the rest of this section, some properties of the generalized Legendre functions are considered.

Since the integral (2.2) is nonzero only if $l_1 + l_2 + \cdots + l_n$ is even, the functions (2.4) are only defined for such sets of indices. In particular, it is easily seen that

$$P_{l_1}(\hat{\mathbf{u}}_1) = \delta_{l_1,0}, \tag{2.5}$$

where $\delta_{p,q}$ is the Kronecker delta. For $n = 2$, Eq. (2.4) reduces to

$$P_{l_1,l_2}(\hat{\mathbf{u}},\hat{\mathbf{v}}) = \delta_{l_1,l_2}(2l_1+1)P_{l_1}(\hat{\mathbf{u}}\cdot\hat{\mathbf{v}}) \tag{2.6}$$

as can easily be seen from the formula[5,6]

$$(4\pi)^{-1}\int d\hat{\mathbf{u}}\,[\hat{\mathbf{u}}]^{(l_1)}[\hat{\mathbf{u}}]^{(l_1)} = [l_1!/(2l_1+1)!!]\,\mathbf{E}^{(l_1)}. \tag{2.7}$$

For $n=3$, the $\mathbf{S}(l_1, l_2, l_3)$ must be proportional to the Cartesian $(3-j)$-tensors defined by Coope,[7] since these are unique. With the formula[6]

$$\int d\hat{\mathbf{u}}\,[\hat{\mathbf{u}}]^{(l_1)}[\hat{\mathbf{u}}]^{(l_2)}[\hat{\mathbf{u}}]^{(l_3)} = \mu(l_1, l_2, l_3)\,\mathbf{T}(l_1, l_2, l_3), \quad (2.8)$$

where $\mathbf{T}(l_1, l_2, l_3)$ is a $(3-j)$-tensor and $\mu(l_1, l_2, l_3)$ is a numerical coefficient given by[6]

$$\mu(l_1, l_2, l_3) = (4\pi) l_1!\, l_2!\, l_3!\, \{(l_1+l_2+l_3+1)!\,!\,[\tfrac{1}{2}(l_1+l_2-l_3)]!\times[\tfrac{1}{2}(l_1-l_2+l_3)]!\,[\tfrac{1}{2}(-l_1+l_2+l_3)]!\}^{-1} \quad (2.9)$$

$[l_1+l_2+l_3$ even and l_1, l_2, l_3 satisfy $|l_1-l_2| \le l_3 \le l_1+l_2$, otherwise $\mu(l_1, l_2, l_3)=0]$, it is found that

$$\mathbf{S}(l_1, l_2, l_3) = (4\pi)^{-1}\,\mu(l_1, l_2, l_3)\,q(l_1, l_2, l_3)\,\mathbf{T}(l_1, l_2, l_3). \quad (2.10)$$

From this and the Cartesian $(3-j)$-reduction of a product of two irreducible tensors,[5] it follows immediately that

$$q(l_1, l_2)\,[\hat{\mathbf{u}}]^{(l_1)}[\hat{\mathbf{u}}]^{(l_2)} = \sum_{l_3} \mathbf{S}(l_1, l_2, l_3) \odot^{l_3} [\hat{\mathbf{u}}]^{(l_3)}. \quad (2.11)$$

This can also be proved directly by multiplying both sides with a $[\hat{\mathbf{u}}]^{(l_3)}$ and integrating over the angles of $\hat{\mathbf{u}}$ using Eqs. (2.2) and (2.7). Combination of Eqs. (2.11) and (2.2) yields the useful relation

$$\mathbf{S}(l_1, l_2, \ldots, l_n) = \sum_{l'} q(l')^{-1}\,\mathbf{S}(l_1, l_2, l')\odot^{l'}\mathbf{S}(l', l_3, \ldots, l_n), \quad (2.12)$$

and, finally, combining (2.11) and (2.12) it is found by induction that

$$q(l_1, l_2, \ldots, l_n)[\hat{\mathbf{u}}]^{(l_1)}[\hat{\mathbf{u}}]^{(l_2)}\cdots[\hat{\mathbf{u}}]^{(l_n)} = \sum_{L} \mathbf{S}(l_1, l_2, \ldots, l_n, L)\odot^{L}[\hat{\mathbf{u}}]^{(L)}, \quad (2.13)$$

which is the generalization of the Clebsch–Gordan reduction for unit vectors.

Another important relation may be derived from Eq. (2.12), namely a reduction formula for the generalized Legendre polynomials. If two of the arguments, say $\hat{\mathbf{u}}_1$ and $\hat{\mathbf{u}}_2$, are equal, then the result

$$P_{l_1, l_2, \ldots, l_n}(\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_1, \hat{\mathbf{u}}_3, \ldots, \hat{\mathbf{u}}_n) = \sum_{l'} \gamma_{l_1, l_2, l'} P_{l', l_3, \ldots, l_n}(\hat{\mathbf{u}}_1, \hat{\mathbf{u}}_3, \ldots, \hat{\mathbf{u}}_n) \quad (2.14)$$

may easily be derived with $\gamma_{l_1, l_2, l'}$ given by

$$\gamma_{l_1, l_2, l'} = (4\pi)^{-2}[\mu(l_1, l_2, l')]^2\, q(l_1, l_2, l')\,\Omega(l_1, l_2, l'), \quad (2.15)$$

where $\Omega(l_1, l_2, l_3)$ is the complete contraction of $\mathbf{T}(l_1, l_2, l_3)$; in the present case ($l_1+l_2+l_3$ even) it is given as[7]

$$\Omega(l_1, l_2, l_3) = \mathbf{T}(l_1, l_2, l_3)\odot^{l_1+l_2+l_3}\mathbf{T}(l_3, l_2, l_1) = (l_1+l_2+l_3+1)!\,(l_1+l_2-l_3)!\,(l_1-l_2+l_3)!\times(-l_1+l_2+l_3)!\times[(2l_1)!\,(2l_2)!\,(2l_3)!\,!]^{-1}. \quad (2.16)$$

3. THE FUNDAMENTAL THEOREM

The basic result can now be stated:

$$V\left(\left|\mathbf{R}+\sum_{i=1}^{n}\mathbf{a}_i\right|\right) = \sum_{l_1,\ldots,l_n,L} P_{l_1,\ldots,l_n,L}(\hat{\mathbf{a}}_1, \ldots, \hat{\mathbf{a}}_n, \nabla)\times(\nabla^2)^{(\Sigma l_i - L)/2}\times\prod_{i=1}^{n}\left(a_i^{l_i}\sum_{m_i=0}^{\infty}[m_i!(2l_i+2m_i+1)!\,!]^{-1}(\tfrac{1}{2}a_i^2\nabla^2)^{m_i}\right)V(R). \quad (3.1)$$

Here the argument ∇ in the generalized Legendre polynomial is a symbolic notation, defined formally as in Eq. (2.4) with one of the unit vectors replaced by ∇. In the following, a proof of Eq. (3.1) is given for a special class of functions $V(R)$, namely those which have a Fourier transform. Since Eq. (3.1) is only a rearrangement of Eq. (1.1), this result is of considerably wider applicability.

Proof of Eq. (3.1). Let $\tilde{V}(k)$ be the Fourier transform of $V(R)$:

$$\tilde{V}(k) = \int d\mathbf{R}\,\exp(-i\mathbf{k}\cdot\mathbf{R})\,V(R). \quad (3.2)$$

Then the Fourier transform of the left-hand side of Eq. (3.1) is

$$\int d\mathbf{R}\,\exp(-i\mathbf{k}\cdot\mathbf{R})\,V\left(\left|\mathbf{R}+\sum_{i=1}^{n}\mathbf{a}_i\right|\right) = \prod_{i=1}^{n}\exp(i\mathbf{k}\cdot\mathbf{a}_i)V(k). \quad (3.3)$$

Using the expansion of $\exp(i\mathbf{k}\cdot\mathbf{a})$ in spherical Bessel functions[6]

$$\exp(i\mathbf{k}\cdot\mathbf{a}) = \sum_{l=0}^{\infty} q(l)\,i^l j_l(ka)\,[\hat{\mathbf{k}}]^{(l)}\odot^{l}[\hat{\mathbf{a}}]^{(l)}, \quad (3.4)$$

Eq. (3.3) can be rewritten as

$$\prod_{i=1}^{n}\exp(i\mathbf{k}\cdot\mathbf{a}_i)\,\tilde{V}(k) = \sum_{l_1,\ldots,l_n}[\hat{\mathbf{a}}_n]^{(l_n)}\cdots[\hat{\mathbf{a}}_1]^{(l_1)}\odot^{\Sigma l_i}[\hat{\mathbf{k}}]^{(l_1)}\cdots[\hat{\mathbf{k}}]^{(l_n)}\,q(l_1, \ldots, l_n)\,i^{\Sigma l_i}\left[\prod_{i=1}^{n} j_{l_i}(ka_i)\right]\tilde{V}(k), \quad (3.5)$$

which, using Eqs. (2.13) and (2.4) may be seen to be equal to

$$\sum_{l_1,\ldots,l_n,L} P_{l_1,\ldots,l_n,L}(\hat{\mathbf{a}}_1, \ldots, \hat{\mathbf{a}}_n, \hat{\mathbf{k}})\,(ik)^{\Sigma l_i}\prod_{i=1}^{n}\left(a_i^{l_i}\times\sum_{m_i=0}^{\infty}(-1)^{m_i}(\tfrac{1}{2}a_i^2k^2)^{m_i}[m_i!(2l_i+2m_i+1)!\,!]^{-1}\right)\tilde{V}(k), \quad (3.6)$$

where the power series of the spherical Bessel functions have also been inserted. The inverse Fourier transform of Eq. (3.6) is obtained by making the substitutions

$$i\mathbf{k}\to\nabla, \quad -k^2\to\nabla^2, \quad \tilde{V}(k)\to V(R); \quad (3.7)$$

and is seen to be equal to Eq. (3.1). QED

Since $V(R)$ is a scalar function, Eq. (3.1) can be simplified further by noting that ∇^2 can be replaced by

the operator D_2 defined by

$$D_2 = R^{-1}\frac{d^2}{dR^2}R, \tag{3.8}$$

and the operator $[\nabla]^{(L)}$ occurring in the generalized Legendre polynomial can be eliminated by means of the identity

$$[\nabla]^{(L)} f(R) = [\hat{\mathbf{R}}]^{(L)} R^L D_1^L f(R) \tag{3.9}$$

where D_1 stands for $R^{-1}(d/dR)$. Equation (3.1) then reduces to

$$V\left(\left|\mathbf{R}+\sum_{i=1}^{n}\mathbf{a}_i\right|\right) = \sum_{l_1,\ldots,l_n,L} \rho_{l_1,\ldots,l_n,L}(\hat{\mathbf{a}}_1,\ldots,\hat{\mathbf{a}}_n,\hat{\mathbf{R}}) R^L D_1^L \times D_2^{(\sum l_i - L)/2} \prod_{i=1}^{n}[a_i^{l_i} W_{l_i}(a_i)]\, V(R). \tag{3.10}$$

Here the operator $W_l(a)$ is defined by

$$\begin{aligned} W_l(a) &= \sum_{m=0}^{\infty} [m!(2l+2m+1)!!]^{-1} (\tfrac{1}{2}a^2 D_2)^m \\ &= [(2l+1)!!]^{-1} \sum_{m=0}^{\infty} [m!(l+\tfrac{3}{2})_m]^{-1} (\tfrac{1}{4}a^2 D_2)^m \\ &= [(2l+1)!!]^{-1}\, {}_0F_1(l+\tfrac{3}{2};\ \tfrac{1}{4}a^2 D_2), \end{aligned} \tag{3.11}$$

where $(p)_q$ is Pochhammer's symbol, $(p)_q = \Gamma(p+q)/\Gamma(p)$, and ${}_0F_1$ is a generalized hypergeometric function.

4. SPECIAL CASES

Since the functions

$$\begin{aligned} &j_0(\alpha R) = (\alpha R)^{-1}\sin(\alpha R),\quad y_0(\alpha R) = -(\alpha R)^{-1}\cos(\alpha R), \\ &\tilde{j}_0(\alpha R) = (\alpha R)^{-1}\sinh(\alpha R),\quad \tilde{y}_0(\alpha R) = (\alpha R)^{-1}\cosh(\alpha R) \end{aligned} \tag{4.1}$$

are eigenfunctions of the Laplace operator D_2, the first two with eigenvalue $-\alpha^2$, the last two with eigenvalue α^2, the result of the previous section is particularly simple when applied to these. Using some of the standard properties[8] of the normal and modified spherical Bessel functions, the results may be summarized in the following formulas:

$$\begin{Bmatrix} j_0 \\ y_0 \end{Bmatrix}\left(\alpha\left|\mathbf{R}+\sum_{i=1}^{n}\mathbf{a}_i\right|\right) = \sum \rho\,(-1)^{(\sum l_i + L)/2} \prod_{i=1}^{n} j_{l_i}(\alpha a_i) \begin{Bmatrix} j_L \\ y_L \end{Bmatrix}(\alpha R), \tag{4.2}$$

$$\begin{Bmatrix} \tilde{j}_0 \\ \tilde{y}_0 \end{Bmatrix}\left(\alpha\left|\mathbf{R}+\sum_{i=1}^{n}\mathbf{a}_i\right|\right) = \sum \rho \prod_{i=1}^{n} \tilde{j}_{l_i}(\alpha a_i) \begin{Bmatrix} \tilde{j}_L \\ \tilde{y}_L \end{Bmatrix}(\alpha R). \tag{4.3}$$

Here the symbols $\sum\rho$ denote the sum over the l_i and L with the generalized Legendre polynomial as weight factor as in Eq. (3.10). The $j_l(z)$ and $y_l(z)$ are spherical Bessel functions of the first and second kinds, respectively, while the $\tilde{j}_l(z)$ and $\tilde{y}_l(z)$ are modified spherical Bessel functions of the first and second kinds. [In the notation of Ref. 8, $\tilde{j}_l(z) = (\pi/2z)^{1/2} I_{l+1/2}(z)$ and $\tilde{y}_l(z) = (\pi/2z)^{1/2} I_{-l-1/2}(z)$.] For $n=1$, the results (4.2) and (4.3) are standard.[8]

For the calculation of the nonspherical potential between two molecules,[1] two functions which may easily be derived from the above may be of importance, namely the Yukawa potential $(\alpha R)^{-1}\exp(-\alpha R)$ and the exponential potential $\exp(-\alpha R)$. For the Yukawa potential it follows immediately that

$$\left(\alpha\left|\mathbf{R}+\sum_{i=1}^{n}\mathbf{a}_i\right|\right)^{-1}\exp\left(-\alpha\left|\mathbf{R}+\sum_{i=1}^{n}\mathbf{a}_i\right|\right) = \sum \rho \prod_{i=1}^{n} \tilde{j}_{l_i}(\alpha a_i) \times [\tilde{y}_L(\alpha R) - \tilde{j}_L(\alpha R)]. \tag{4.4}$$

The result for the exponential potential follows by applying the operator $1+\alpha\partial/\partial\alpha$ to both sides of Eq. (4.4). The result may be simplified by making use of the recursion relations of the modified spherical Bessel functions.[8]

A second special case of great importance for the problem of calculating nonspherical potentials is the case of an inverse power of R (Lennard–Jones type potentials). Setting $V(R) = R^{-s}$ and using the formulas

$$D_2^q R^{-s} = (\tfrac{1}{2}s - \tfrac{1}{2})_q (\tfrac{1}{2}s)_q 2^{2q} R^{-s-2q} \tag{4.5}$$

and

$$R^L D_1^L R^{-t} = (-2)^L (\tfrac{1}{2}t)_L R^{-t-L}, \tag{4.6}$$

the result finally obtained may be written in the form

$$\begin{aligned} \left|\hat{\mathbf{R}}+\sum_{i=1}^{n}\hat{\mathbf{a}}_i x_i\right|^{-s} = \sum \rho\,(-1)^L \prod_{i=1}^{n} [(2x_i)^{l_i}/(2l_i+1)!!] \\ \times (\tfrac{1}{2}s - \tfrac{1}{2})_{(\sum l_i - L)/2} \\ \times (\tfrac{1}{2}s)_{(\sum l_i + L)/2} F^{(n)}(\tfrac{1}{2}s - \tfrac{1}{2} + \tfrac{1}{2}(\textstyle\sum l_i - L), \\ \tfrac{1}{2}s + \tfrac{1}{2}(\textstyle\sum l_i + L);\ l_1 + \tfrac{3}{2},\ldots,l_n+\tfrac{3}{2};\ x_1^2,\ldots,x_n^2). \end{aligned} \tag{4.7}$$

Here the x_i are the ratios a_i/R and the function $F^{(n)}$ is a generalized n-variable hypergeometric function defined by

$$\begin{aligned} F^{(n)}(a,b;c_1,\ldots,c_n;z_1,\ldots,z_n) = \sum_{m_1,\ldots,m_n} (a)_M (b)_M \\ \times \prod_{i=1}^{n} [z_i^{m_i}/m_i!(c_i)_{m_i}] \\ (M = m_1 + \cdots + m_n). \end{aligned} \tag{4.8}$$

For $n=1$ and $n=2$, these functions are well-known. Indeed, $F^{(1)}(a,b;c;z)$ is the Gauss hypergeometric function[8,9] $F(a,b;c;z)$ and for $n=2$, $F^{(2)}(a,b;c_1,c_2;z_1,z_2)$ is Appell's generalized hypergeometric function F_4 of two variables.[9,10] The functions with more than two variables have been much less studied, but see Ref. 10 for some results.

Of most importance here is the question of the convergence of the multiple power series (4.8). As a generalization of Horn's result[9] for F_4, it is easily seen that (4.8) converges if

$$\sum_{i=1}^{n} z_i^{1/2} < 1. \tag{4.9}$$

This means that the functions occurring in Eq. (4.7) are well-defined only if

$$\sum_{i=1}^{n} a_i < R. \tag{4.10}$$

If $n=1$, this will always be the case if $a_1 \neq R$ by interchanging, if necessary, the names of the two vectors. For $a_1 = R$, there will, in general, be a singularity. The nature of this singularity can be derived for the case s = integer from the explicit form of the Gauss hypergeometric function in terms of elementary functions, see Appendix A.

A special case of great interest of Eq. (4.7) is $s=1$, since it will show up in problems concerning electrostatic or gravitational potentials. Since $\frac{1}{2}s - \frac{1}{2} = 0$ for this case, Eq. (4.7) makes sense only if $L = \sum l_i$. The generalized hypergeometric function $F^{(n)}$ occurring in Eq. (4.7) has then its first index [a in Eq. (4.8)] equal to zero, so that it is equal to 1 for all x_i. Further, the generalized Legendre polynomial reduces in the case $L = \sum l_i$, since it follows from Eqs. (2.2) and (2.7) that

$$\mathbf{S}(l_1, \ldots, l_n, \textstyle\sum l_i) = q(l_1, \ldots, l_n)\mathbf{E}^{(\sum l_i)}. \tag{4.11}$$

The generalized multipole expansion is then

$$\Big|\mathbf{R} + \sum_{i=1}^{n} \mathbf{a}_i\Big|^{-1} = \sum_{l_1, \ldots, l_n} [\mathbf{a}_1]^{(l_1)} \cdots [\mathbf{a}_n]^{(l_n)} \odot^{\sum l_i} [\hat{\mathbf{R}}]^{(\sum l_i)} R^{-\sum l_i - 1} (-1)^{\sum l_i} (2\textstyle\sum l_i - 1)!! \, (\prod l_i!)^{-1}. \tag{4.12}$$

The special case $n=2$ may be used to obtain the electrostatic potential between two linear molecules as

$$V_m(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2, \mathbf{R}) = \sum_{l_1, l_2} [\hat{\mathbf{r}}_1]^{(l_1)} [\hat{\mathbf{r}}_2]^{(l_2)} \odot^{l_1+l_2} [\hat{\mathbf{R}}]^{(l_1+l_2)} (-1)^{l_1} (2l_1 + 2l_2 - 1)!! \, (l_1! l_2!)^{-1} \mu_{l_1}^{(1)} \mu_{l_2}^{(2)} R^{-l_1-l_2-1}, \tag{4.13}$$

where $\hat{\mathbf{r}}_1$ and $\hat{\mathbf{r}}_2$ are unit vectors along the axes of the molecules and $\mathbf{R}$ is the vector joining their centers of mass. The $\mu_l^{(i)}$ are the multipole moments of molecule i defined by

$$\mu_l^{(i)} = \int \rho_i(x) x^l \, dx, \tag{4.14}$$

where the integral is extended over the length of molecule i, which has the charge density $\rho_i(x)$ per unit length, and the variable x is chosen in such a way that $x=0$ at the center of mass. These multipole moments with respect to the center of mass may differ from the ones defined with respect to another point, e.g., the geometrical center, for $l \geq 2$ (for neutral molecules). Special cases of Eq. (4.13) have already been used in connection with the calculation of kinetic theory collision integrals for linear molecules and symmetric tops[11] and in connection with the phase transition in solid orthohydrogen.[12] Equation (4.13), when rewritten in terms of spherical harmonics (see Ref. 5 for the connection with the irreducible Cartesian tensors) is identical to the well-known results of Carlson and Rushbrooke[13] and Buehler and Hirschfelder[14] for the case of nonoverlapping charge distributions.

Another, rather trivial, case for which Eq. (4.7) may be evaluated directly is the case $s = -2m$, $m = 0, 1, 2, \cdots$, i.e., the expansion of a positive, even power. In this case $\frac{1}{2}(\sum l_i + L)$ should be less than m and for such values of the l_i and L, the second index in $F^{(n)}$ [b in Eq. (4.8)] is a negative integer, so that $F^{(n)}$ reduces to a polynomial in the x_i^2.

5. REDUCTION FORMULAS AND SUM RULES

If two of the vectors $\mathbf{a}_i$ are parallel, the fundamental theorem (3.10) may be written in two separate ways. Either the formula is used for n vectors $\mathbf{a}_i$, two of which (say $\mathbf{a}_1$ and $\mathbf{a}_2$) are parallel, so that the generalized Legendre polynomial reduces via Eq. (2.14) to a sum involving only $n-1$ vectors, or the theorem is directly applied for $n-1$ vectors, the first one being $\mathbf{a}_1 + \mathbf{a}_2$, the rest the set $\mathbf{a}_3, \ldots, \mathbf{a}_n$. In this way, reduction formulas and sum rules for the coefficient functions may be derived. In the following, the special cases of the previous section will be considered.

First, consider j_0. If $\hat{\mathbf{a}}_1 = \hat{\mathbf{a}}_2$, Eq. (4.2) reduces, using Eq. (2.14), to (suppressing the argument)

$$j_0(\cdot) = \sum_{\substack{l_1, l_2, l' \\ l_3, \ldots, l_n, L}} \gamma_{l_1, l_2, l'} \, \rho_{l', l_3, \ldots, l_n, L}(\hat{\mathbf{a}}_1, \hat{\mathbf{a}}_3, \ldots, \hat{\mathbf{a}}_n, \hat{\mathbf{R}}) (-1)^{(\sum_{i=1}^{n} l_i + L)/2} \prod_{i=1}^{n} j_{l_i}(\alpha a_i) j_L(\alpha R). \tag{5.1}$$

On the other hand, writing Eq. (4.2) directly for $n-1$ vectors $\mathbf{a}_1 + \mathbf{a}_2, \mathbf{a}_3, \ldots, \mathbf{a}_n$ gives

$$j_0(\cdot) = \sum_{l', l_3, \ldots, l_n, L} \rho_{l', l_3, \ldots, l_n, L}(\hat{\mathbf{a}}_1, \hat{\mathbf{a}}_3, \ldots, \hat{\mathbf{a}}_n, \hat{\mathbf{R}}) (-1)^{(l' + \sum_{i=3}^{n} l_i + L)/2} j_{l'}(\alpha a_1 + \alpha a_2) \prod_{i=3}^{n} j_{l_i}(\alpha a_i) j_L(\alpha R). \tag{5.2}$$

Equating these results yields the addition theorems

$$\left.\begin{matrix} j_{l'} \\ y_{l'} \end{matrix}\right\}(z_1 + z_2) = \sum_{l_1, l_2} \gamma_{l_1, l_2, l'} (-1)^{(l_1 + l_2 - l')/2} j_{l_1}(z_1) \left\{\begin{matrix} j_{l_2} \\ y_{l_2} \end{matrix}\right\}(z_2), \tag{5.3}$$

where the analogous result for y_0 has also been included. Equation (4.3) gives, in a similar way, rise to the addition theorems

$$\left.\begin{matrix} \tilde{j}_{l'} \\ \tilde{y}_{l'} \end{matrix}\right\}(z_1 + z_2) = \sum_{l_1, l_2} \gamma_{l_1, l_2, l'} \tilde{j}_{l_1}(z_1) \left\{\begin{matrix} \tilde{j}_{l_2} \\ \tilde{y}_{l_2} \end{matrix}\right\}(z_2). \tag{5.4}$$

Addition theorems of this type are well-known, especially for $l' = 0$.[8] [Note that $\gamma_{l_2, 0} = \delta_{l_1, l_2}(2l_1 + 1)$.]

Similar expressions may be obtained for the generalized hypergeometric functions by applying the above procedure to the inverse power expansions. These are, in general, rather complicated and are therefore given in Appendix B. Here two special cases will be mentioned, one involving the Gauss hypergeometric function

and one involving Appell's F_4. These relations are in the form of generating functions:

$$(1+x)^{-s} = \sum_{l=0}^{\infty} (-2x)^l [(2l-1)!!]^{-1} (\tfrac{1}{2}s)_l \, F(\tfrac{1}{2}s - \tfrac{1}{2}, \tfrac{1}{2}s + l; l + \tfrac{3}{2}; x^2) \quad (|x| < 1), \tag{5.5}$$

and

$$(1+x_1+x_2)^{-s} = \sum_{l_1, l_2, L} (-1)^L \gamma_{l_1, l_2, L} \, (2L+1) (2x_1)^{l_1} (2x_2)^{l_2} \times [(2l_1+1)!!(2l_2+1)!!]^{-1} (\tfrac{1}{2}s - \tfrac{1}{2})_{(l_1+l_2-L)/2} (\tfrac{1}{2}s)_{(l_1+l_2+L)/2} \times F_4([s-1+l_1+l_2-L]/2, [s+l_1+l_2+L]/2; l_1 + \tfrac{3}{2}, l_2 + \tfrac{3}{2}; x_1^2, x_2^2) \quad (|x_1 + x_2| < 1). \tag{5.6}$$

6. EXPANSION OF A TENSORIAL FUNCTION

The results of the foregoing sections may be directly applied to the problem of the calculation of the nonspherical potential between two molecules.[1] For some other problems, the same type of expansion is needed for a tensorial function, e.g., in the heavy-ion transfer reaction problem.[2] In this case the function is of the form

$$\sum_{t=0}^{\infty} [\mathbf{b}]^{(t)} \odot^t [\mathbf{R}]^{(t)} f_t(R), \tag{6.1}$$

where b is a fixed vector. This expression has to be evaluated for **R** replaced by $\mathbf{R} + \sum_{i=1}^{n} \mathbf{a}_i$; since the coefficient functions $f_t(R)$ are scalar, they may be expanded as in the previous sections, so that the problem left is the expansion of $[\mathbf{R}]^{(t)}$. Here the following equality holds:

$$[\mathbf{R} + \sum_{i=1}^{n} \mathbf{a}_i]^{(t)} = \sum_{m_1, \cdots, m_n} t! \left[\prod_{i=1}^{n} 1/m_i!\right] \left[(t - \sum_{i=1}^{n} m_i)\right]^{-1} \times [\mathbf{a}_1]^{(m_1)} \cdots [\mathbf{a}_n]^{(m_n)} \times [\mathbf{R}]^{(t - \sum m_i)} \odot^t \mathbf{E}^{(t)}, \tag{6.2}$$

where the summation is restricted so that $\sum_{i=1}^{n} m_i \leq t$. The product of Eq. (6.2) with the expansion of $f_t(R)$ leads to a double series involving products of two irreducible tensors built from the same vector; these may be reduced to single irreducible tensors by means of Eq. (2.11). The resulting expansion does not, in general, contain only the generalized Legendre polynomials but more complicated tensorial contractions as well. Since these general expressions are very complicated, these will not be given here. The very special cases of the Dirac delta functions $\delta(\mathbf{b} + \mathbf{R})$ and $\delta(\mathbf{b} + \mathbf{R} + \mathbf{a})$ have been treated by Elbaz *et al.*[15] in a similar fashion.

DISCUSSION

In this section some applications of the formalism described before will be discussed. In the first place, analytic expressions for nonspherical potentials derived by the method of summing spherical potentials between force-centers in the molecules[1] may be obtained. This is, of course, more satisfactory for many purposes than are numerical methods. Also, if the magnitudes of the vectors $\mathbf{a}_i$ are small compared to R, a perturbation series to any order is easily derived. This is of importance for the calculation of equilibrium and nonequilibrium properties of polyatomic fluids and liquid crystals. In these applications the number of vectors $\mathbf{a}_i$ will be one (atom—molecule interaction) or two (molecule—molecule interaction) if the molecules are rigid. For nonrigid molecules, more than two vectors are necessary since the equilibrium position of the center of force and its instantaneous deviation from this position have to be described. Of course, the potential so-obtained then has to be averaged over the vibration periods of the moelcules. These questions are treated in more detail in a separate publication.

Another possible application is, as already mentioned, in the field of heavy-ion transfer reactions.[2] The general method outlined in Sec. 6 may be easier to apply than the delta function methods proposed by Elbaz *et al.*[15] and by Anni and Taffara.[2]

Other applications of this method of expansion, which can also be regarded as a Cartesian tensor generalization of the method of invariant expansions,[16] will be found in any field of physics where expressions of the form (1.1) show up.

APPENDIX A: REDUCTION OF EQ. (4.7) FOR s = INTEGER, n = 1

In case $n = 1$, Eq. (4.7) becomes

$$|\hat{\mathbf{R}} + x\hat{\mathbf{a}}|^{-s} = \sum_{l=0}^{\infty} P_l(\hat{\mathbf{a}} \cdot \hat{\mathbf{R}}) (-2x)^l [(2l-1)!!]^{-1} (\tfrac{1}{2}s)_l \times F(\tfrac{1}{2}s - \tfrac{1}{2}, \tfrac{1}{2}s + l; l + \tfrac{3}{2}; x^2). \tag{A1}$$

If s is an integer, the hypergeometric function occurring here always reduces to an elementary function. First, the relation[8,9]

$$F(\tfrac{1}{2}s - \tfrac{1}{2}, \tfrac{1}{2}s + l; l + \tfrac{3}{2}; x^2) = (1-x^2)^{-s+2} \times F(l + 2 - \tfrac{1}{2}s, \tfrac{3}{2} - \tfrac{1}{2}s; l + \tfrac{3}{2}; x^2) \tag{A2}$$

is noted and the fact that F reduces to a polynomial of degree m in x^2 if one of the first two indices equals $-m$ ($m = 0, 1, 2, \cdots$). Therefore, Eq. (A2) gives for $s = 2m + 3$ (the case $s = 1$ is treated in the text):

$$F(m+1, m+l+\tfrac{3}{2}; l+\tfrac{3}{2}; x^2) = (1-x^2)^{-2m-1} \sum_{n=0}^{m} (-m)_n (l + \tfrac{1}{2} - m)_n [(l+\tfrac{3}{2})_n]^{-1} x^{2n}. \tag{A3}$$

This covers the case for s equal to an odd integer.

For $s = 2m + 2$, two cases can be distinguished. If $l + 1 - m$ is negative or zero, Eq. (A2) can again be used to find a form similar to Eq. (A3). This, however, is only possible for low values of l. Of more use is the general relation[8] between the hypergeometric function occurring in Eq. (A1) and the associated Legendre func-

tions of the second kind, Q_l^m. This relation is, for the case at hand,

$$F(m+l+1, m+\tfrac{1}{2}; l+\tfrac{3}{2}; x^2) = \Gamma(l+\tfrac{3}{2})(-1)^m \times [(l+m)!\,\pi^{1/2}(1-x^2)^m x^{l+1}]^{-1} \times Q_l^m(1+x^2/2x). \quad \text{(A4)}$$

These Q_l^m may always be expressed in terms of elementary functions by means of the recursion relations

$$Q_l^m(z) = (z^2-1)^{m/2}\,\frac{d^m Q_l}{dz^m}(z), \quad \text{(A5)}$$

$$(l+1)Q_{l+1}(z) = (2l+1)zQ_l(z) - lQ_{l-1}(z) \quad (l=1, 2, \cdots) \quad \text{(A6)}$$

$$Q_0(z) = \tfrac{1}{2}\ln(z+1/z-1), \quad Q_1(z) = zQ_0(z) - 1. \quad \text{(A7)}$$

APPENDIX B: GENERAL SUM RULES FOR THE FUNCTION $F^{(n)}$

Two types of sum rules for the functions $F^{(n)}$ follow from Eq. (4.7). If two of the vectors $\mathbf{a}_i$ are parallel (say $\mathbf{a}_1$ and $\mathbf{a}_2$) it is found that

$$\sum_{l_1, l_2} \gamma_{l_1, l_2, l'} (2x_1)^{l_1} (2x_2)^{l_2} [(2l_1+1)!!\,(2l_2+1)!!]^{-1} (2l'+1)!! \times \left(\left[s-1+l'+\sum_{i=3}^{n} l_i - L\right]/2\right)_{(l_1+l_2-l')/2} \times \left(\left[s+l'+\sum_{i=3}^{n} l_i + L\right]/2\right)_{(l_1+l_2-l')/2} \times F^{(n)}\left(\left[s-1+\sum_{i=1}^{n} l_i - L\right]/2,\ \left[s+\sum_{i=1}^{n} l_i + L\right]/2;\ l_1+\tfrac{3}{2}, l_2+\tfrac{3}{2}, \ldots, l_n+\tfrac{3}{2}; x_1^2, x_2^2, \ldots, x_n^2\right)$$

$$= [2(x_1+x_2)]^{l'} F^{(n-1)}\left(\left[s-1+l'+\sum_{i=3}^{n} l_i - L\right]/2,\ \left[s+l'+\sum_{i=3}^{n} l_i + L\right]/2;\ l'+\tfrac{3}{2}, l_3+\tfrac{3}{2}, \ldots, l_n+\tfrac{3}{2}; (x_1+x_2)^2, x_3^2, \ldots, x_n^2\right). \quad \text{(B1)}$$

In case one of the $\mathbf{a}_i$, say $\mathbf{a}_1$, is parallel to $\mathbf{R}$, another relation is found:

$$\sum_{l_1, L} \gamma_{l_1, L, l'} (-1)^{L-l'} (2x_1)^{l_1} [(2l_1+1)!!]^{-1} \times \left(\left[s-1+\sum_{i=2}^{n} l_i - l'\right]/2\right)_{(l'+l_1-L)/2} \left(\left[s+\sum_{i=2}^{n} l_i + l'\right]/2\right)_{(l'+l_1+L)/2} F^{(n)}\left(\left[s-1+\sum_{i=1}^{n} l_i - L\right]/2,\ \left[s+\sum_{i=1}^{n} l_i + L\right]/2;\ l_1+\tfrac{3}{2}, l_2+\tfrac{3}{2}, \ldots, l_n+\tfrac{3}{2}; x_1^2, x_2^2, \ldots, x_n^2\right)$$

$$= (1+x_1)^{-s-\sum_{i=2}^{n} l_i} F^{(n-1)}\left(\left[s-1+\sum_{i=2}^{n} l_i - l'\right]/2,\ \left[s+\sum_{i=2}^{n} l_i + l'\right]/2;\ l_2+\tfrac{3}{2}, l_3+\tfrac{3}{2}, \ldots, \times l_n+\tfrac{3}{2};\ x_2^2(1+x_1)^{-2}, x_3^2(1+x_1)^{-2}, \ldots, x_n^2(1+x_1)^{-2}\right). \quad \text{(B2)}$$

Equation (5.5) of the text results from Eq. (B2) by taking $n=1$. Equation (5.6) follows from Eq. (B1) for $n=2$ and subsequent use of Eq. (5.5), or, equivalently, from Eq. (B2) for $n=2$ and again subsequent use of Eq. (5.5). Many more sum rules may be derived from repeated applications of Eqs. (B1) and (B2).

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Decompositions of gravitational perturbations*

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We consider the Brill–Deser decomposition of the perturbations of a flat spacetime with compact Cauchy hypersurfaces. We propose a generalization of the Brill–Deser splitting which may be applied to the perturbations of arbitrary vacuum spacetimes with compact Cauchy slices. We split the space of perturbations of any allowed Cauchy data set into three subspaces which, with suitable inner product, are mutually orthogonal. Two of these subspaces comprise the solution set of the perturbed constraint equations, and one of these two subspaces represents pure gauge perturbations. Some possible applications of these splittings to the study of the vacuum perturbation equations and to the linearization stability problem for the Einstein equations are briefly discussed.

1. INTRODUCTION

Brill and Deser[1] have defined a useful orthogonal decomposition of the perturbations of a flat spacetime with compact Cauchy hypersurfaces. Their splitting corresponds, in the compact case, to the Arnowitt, Deser, and Misner[2] splitting of the perturbations of Minkowski space. In this paper we propose a generalization of the Brill–Deser decomposition which applies to the perturbations of arbitrary vacuum spacetimes with compact Cauchy surfaces. Restricted to the flat case our decomposition reduces to the Brill–Deser decomposition.

To generalize the Brill–Deser result, we must first abstract the essential features of their splitting. They introduce a suitable inner product and split the space of perturbed Cauchy data into three mutually orthogonal subspaces. Two of these subspaces comprise the solution set of the linearized constraint equations. One of these two subspaces consists of pure gauge perturbations (which always satisfy the perturbed constraints). The second contains all solutions of the perturbed constraints which are orthogonal to the gauge perturbations. Gauge perturbations are physically trivial since they merely represent deformations of the hypersurface within the background spacetime.

We consider the space of Cauchy data for an arbitrary compact three-manifold and the constraint subset of this space. The tangent space at any point of the constraint subset represents possible perturbations of the Cauchy data represented by that point. Using a convenient L^2 inner product, we split each such tangent space into three mutually orthogonal subspaces. We first split each tangent space into the solution set of the perturbed constraint equations and an orthogonal complement. We next refine the splitting by decomposing the kernel of the perturbed constraints into the subspace of pure gauge perturbations and its orthogonal complement. Finally we specialize our results to the flat case and recover the Brill–Deser decomposition. In the conclusion we discuss the application of our results to the study of the vacuum perturbation equations.

The splittings defined here may prove useful in studying the geometry of the constraint subset and in understanding the linearization stability problem for the vacuum Einstein equations. Fischer and Marsden[3] have recently derived conditions upon the Cauchy data which, if satisfied, ensure that:

(i) the constraint subset is a smooth submanifold on a neighborhood of the given point and

(ii) all solutions of the linearized constraints are tangent to the constraint submanifold at the given point.

When the Fischer–Marsden conditions fail to hold, the linearized constraints admit spurious solutions which are not tangent to any curve of exact solutions of the constraint equations. We shall refer to those Cauchy data which satisfy the Fischer–Marsden conditions as the regular points of the constraint subset. The remaining points of the constraint subset will be called the irregular points.

In a recent paper[4] it was shown that Cauchy data for a vacuum spacetime admitting one or more Killing vector fields is always an irregular point of the constraint subset. It was also shown that an irregular point always admits a Cauchy development with one or more Killing vector fields. The number of independent Killing vectors which occur was shown to equal the dimension of the kernel of a certain linear map (the adjoint map) defined by Marsden and Fischer. The regular points of the constraint subset have an injective adjoint map. An interesting feature of the splitting defined here is that it has a different character at irregular points from that at regular points. Certain elliptic equations which must be solved in effecting the decomposition admit unique solutions only at regular points. At irregular points the solutions are no longer unique but the splitting itself remains unique. Some possible applications of our decomposition to the linearization stability problem are discussed in the conclusion.

2. NOTATION AND BASIC EQUATIONS

Let M be a compact, oriented, C^∞ three-manifold without boundary and define the following spaces of C^∞ tensor fields over M:

C^∞ = space of scalar fields over M,

$\mathcal{X}^1$ = space of vector fields over M,

$\mathcal{M}$ = space of Riemannian metrics of M,

$\mathcal{S}_2$ ($\mathcal{S}_2^*$) = space of symmetric, covariant second rank tensors (tensor densities) over M,

$\mathcal{S}^2$($\mathcal{S}_*^2$) = space of symmetric, contravariant second rank tensors (tensor densities) over M.

In addition write $\mathcal{P} = \mathcal{M} \times \mathcal{S}_*^2 \approx T^*\mathcal{M}$ for the gravitational phase space of Cauchy data for M. The constraint subset $\mathcal{C} \subset \mathcal{P}$ is defined by

$$\mathcal{C} = \{(g,\pi) \in \mathcal{P} \mid \Phi(g,\pi) = 0\}, \tag{2.1}$$

where

$$\Phi : \mathcal{M} \times \mathcal{S}_*^2 \to \mathcal{C}^\infty \times \mathcal{X}^1;\ (g,\pi) \to (\mathcal{H}(g,\pi), \delta(g,\pi)) \tag{2.2}$$

with

$$\mathcal{H}(g,\pi) = (\det g)^{-1}[\pi^{ij}\pi_{ij} - \tfrac{1}{2}(g_{ij}\pi^{ij})^2] - R(g),$$
$$\delta(g,\pi) = 2(\det g)^{-1/2}\pi^{ij}{}_{|j}, \tag{2.3}$$

in which $R(g)$ is the curvature scalar of g. The vertical bar signifies covariant differentiation with respect to g.

Let $T_{(g,\pi)}\mathcal{P} \approx \mathcal{S}_2 \times \mathcal{S}_*^2$ be the tangent space at a point $(g,\pi) \in \mathcal{P}$ and define the inner product (,) by

$$((h,p),(h',p')) = \int_M d^3x\, (\det g)^{1/2} \langle (h,p),(h',p') \rangle, \tag{2.4}$$

where (h,p) and $(h',p') \in \mathcal{S}_2 \times \mathcal{S}_*^2$ and in which

$$\langle (h,p),(h',p') \rangle = [h^{ij}h'_{ij} + (\det g)^{-1} p^{ij}p'_{ij}] \in \mathcal{C}^\infty. \tag{2.5}$$

Similarly write

$$((C,X),(C',X')) = \int_M d^3x\, (\det g)^{1/2} \langle (C,X),(C',X') \rangle, \tag{2.6}$$

where (C,X) and $(C',X') \in \mathcal{C}^\infty \times \mathcal{X}^1$ and in which

$$\langle (C,X),(C',X') \rangle = C \circ C' + X^i X'_i \in \mathcal{C}^\infty. \tag{2.7}$$

The derivative $D\Phi(g,\pi)$ of Φ at a point $(g,\pi) \in \mathcal{C} = \Phi^{-1}(0)$ is given by[3,4]

$$\begin{aligned} &D\Phi(g,\pi) : \mathcal{S}_2 \times \mathcal{S}_*^2 \to \mathcal{C}^\infty \times \mathcal{X}^1; \\ &(h,p) \to \{(\det g)^{-1}[-\tfrac{1}{2}(\pi\cdot\pi - \tfrac{1}{2}(\mathrm{tr}\pi)^2)\mathrm{tr}h \\ &\quad + 2(\pi\cdot p - \tfrac{1}{2}\mathrm{tr}\pi\,\mathrm{tr}p) \\ &\quad + 2(\pi\times\pi - \tfrac{1}{2}(\mathrm{tr}\pi)\pi)\cdot h] \\ &\quad - \{\delta\delta h - \Delta(\mathrm{tr}h) - [\mathrm{Ric}(g) - \tfrac{1}{2}gR(g)]\cdot h\}; \\ &\quad (\det g)^{-1/2}[2p^{ij}{}_{|j} + \pi^{jk}(h^i{}_{j|k} \\ &\quad + h^i{}_{k|j} - h_{jk}{}^{|i})]\}, \end{aligned} \tag{2.8}$$

where $\circ$ signifies contraction (e.g., $\pi\cdot h = \pi^{ij}h_{ij}$) and tr signifies trace ($\mathrm{tr}h = g^{ij}h_{ij}$). Also $\pi\times\pi = \pi^{ik}\pi_k{}^j$, $\delta\delta h = h_{ij}{}^{|ij}$, $\Delta(\mathrm{tr}h) = (\mathrm{tr}h)_{|i}{}^{|i}$ and $\mathrm{Ric}(g)$ is the Ricci tensor of g. The adjoint map $D\Phi(g,\pi)^*$ defined through

$$((C,X), D\Phi(g,\pi)\circ(h,p)) = (D\Phi(g,\pi)^*\circ(C,X),(h,p)) \tag{2.9}$$

is given explicitly by[3,4]

$$\begin{aligned} &D\Phi(g,\pi)^* : \mathcal{C}^\infty \times \mathcal{X}^1 \to \mathcal{S}_2 \times \mathcal{S}_*^2; \\ &(C,X) \to \{(\det g)^{-1}[-\tfrac{1}{2}(\pi\cdot\pi - \tfrac{1}{2}(\mathrm{tr}\pi)^2)gC \\ &\quad + 2(\pi\times\pi - \tfrac{1}{2}\pi(\mathrm{tr}\pi))_* C] \\ &\quad - [\mathrm{Hess}C - g\Delta C - (\mathrm{Ric}(g) - \tfrac{1}{2}gR(g))C] \\ &\quad + (\det g)^{-1/2}(L_X\pi)_*; \\ &\quad 2C(\pi - \tfrac{1}{2}(\mathrm{tr}\pi)g^{-1}) - (L_X g)^{-1}(\det g)^{1/2}\}, \end{aligned} \tag{2.10}$$

where $\mathrm{Hess}C = C_{|ij}$, L_X = Lie derivative with respect to X, $^{-1}$ indicates the contravariant form of a tensor [$(L_X g)^{-1} = X^{i|j} + X^{j|i}$] and $_*$ indicates the covariant form of a tensor [$(L_X\pi)_* = (\pi_{ij}X^k)_{|k} - X_{i|k}\pi^k{}_j - X_{j|k}\pi^k{}_i$]. This notation differs somewhat from that of Ref. 4. The previous expression for the adjoint may be obtained from that here by reexpressing the first slot in contravariant density form and the second slot in covariant tensor form. The expressions given here for $D\Phi(g,\pi)$ and $D\Phi(g,\pi)^*$ are complete only at points of the constraint subset. At arbitrary points there are additional terms proportional to $\mathcal{H}(g,\pi)$ and $\delta(g,\pi)$ which vanish at $\mathcal{C}$. Our notation, with only minor modifications, is the same as that of Fischer and Marsden.[3]

3. THE FIRST SPLITTING

In this section we establish the orthogonal decomposition

$$T_{(g,\pi)}\mathcal{M} \times \mathcal{S}_*^2 \approx \mathcal{S}_2 \times \mathcal{S}_*^2 = \ker D\Phi(g,\pi) \oplus \mathrm{range}\ D\Phi(g,\pi)^* \tag{3.1}$$

for any point $(g,\pi) \in \mathcal{C}$. The orthogonality of the two subspaces is straightforward to check. If $(\bar{h},\bar{p}) \in \ker D\Phi(g,\pi)$ and $(C,X) \in \mathcal{C}^\infty \times \mathcal{X}^1$, then

$$((\bar{h},\bar{p}), D\Phi(g,\pi)^*\circ(C,X)) = (D\Phi(g,\pi)\circ(\bar{h},\bar{p}),(C,X)) = 0. \tag{3.2}$$

To show that an arbitrary tangent vector (h,p) may be uniquely split as

$$(h,p) = (\bar{h},\bar{p}) + D\Phi(g,\pi)^*\circ(C,X) \tag{3.3}$$

with $(\bar{h},\bar{p}) \in \ker D\Phi(g,\pi)$, we use elliptic theory as in Berger and Ebin[5] and Fischer and Marsden.[3] Applying $D\Phi(g,\pi)$ to Eq. (3.3), we obtain

$$D\Phi(g,\pi)\circ(h,p) = D\Phi(g,\pi)\circ[D\Phi(g,\pi)^*\circ(C,X)], \tag{3.4}$$

which are partial differential equations for C and X. Fischer and Marsden proved that $\alpha(g,\pi) \equiv D\Phi(g,\pi)\circ D\Phi(g,\pi)^*$ is elliptic by showing that $D\Phi(g,\pi)^*$ has injective symbol and applying Theorem (4.4) of Berger and Ebin.[5] Therefore, from Theorem (4.3) of Berger and Ebin, we have the orthogonal decomposition

$$\begin{aligned} \mathcal{C}^\infty \times \mathcal{X}^1 &= \mathrm{range}\ \alpha(g,\pi) \oplus \ker\alpha(g,\pi) \\ &= \mathrm{range}\ \alpha(g,\pi) \oplus \ker D\Phi(g,\pi)^*. \end{aligned} \tag{3.5}$$

The last equality follows from the observation that if $(\bar{C},\bar{X}) \in \ker\alpha(g,\pi)$, then

$$\begin{aligned} 0 &= ((\bar{C},\bar{X}), D\Phi(g,\pi)\circ[D\Phi(g,\pi)^*\cdot(\bar{C},\bar{X})) \\ &= (D\Phi(g,\pi)^*\circ(\bar{C},\bar{X}), D\Phi(g,\pi)^*\cdot(\bar{C},X)), \end{aligned} \tag{3.6}$$

which implies that $D\Phi(g,\pi)^*\circ(\bar{C},\bar{X}) = 0$. Thus $\ker\alpha(g,\pi) = \ker D\Phi(g,\pi)^*$.

The regular points of $\mathcal{C}$ are precisely those at which $D\Phi(g,\pi)^*$ is injective. Therefore, at regular points of $\mathcal{C}$, Eq. (3.5) reduces to

$$\mathcal{C}^\infty \times \mathcal{X}^1 = \mathrm{range}\,\alpha(g,\pi). \tag{3.7}$$

Thus a solution of Eq. (3.4) always exists and, since $\alpha(g,\pi)$ is injective, is unique.

At an irregular point of C a solution of Eq. (3.4) still exists provided the source term $D\Phi(g,\pi)\circ(h,p)$ lies in the space orthogonal to $\ker D\Phi(g,\pi)^*$ [and thus in the range of $\alpha(g,\pi)$]. To see that this is always the case, let $(\bar{C},\bar{X})\in\ker D\Phi(g,\pi)^*$ and compute

$$((\bar{C},\bar{X}),D\Phi(g,\pi)\cdot(h,p))=(D\Phi(g,\pi)^*\cdot(\bar{C},\bar{X}),(h,p))=0. \tag{3.8}$$

However, the solution (C,X) of Eq. (3.4) is not unique since one may always add any element of the kernel of $D\Phi(g,\pi)^*$. Nevertheless, the splitting

$$(h,p)=(\bar{h},\bar{p})+D\Phi(g,\pi)^*\circ(C,X) \tag{3.9}$$

is unique since, of course, $D\Phi(g,\pi)^*$ annihilates any element of its kernel. Our fist splitting is thus a fairly immediate consequence of the Fischer–Marsden result for $\alpha(g,\pi)$ and the Berger–Ebin analysis.

It is important to remember that, although the decomposition is defined even at irregular points of C, its geometrical significance is different from that at regular points. At an irregular point C may not be a smooth submanifold of $\mathcal{M}\times\mathcal{S}^2$. But even if it is, its tangent space is only a subset of $\ker D\Phi(g,\pi)$.[3]

It may be useful here to recall how consideration of the operator $\alpha(g,\pi)=D\Phi(g,\pi)\cdot D\Phi(g,\pi)^*$ arose in the Fischer–Marsden analysis. Part of their linearization stability theorem consists of showing that $D\Phi(g,\pi)$ is surjective if and only if $D\Phi(g,\pi)^*$ is injective. Upon deriving Eq. (3.5) they conclude at once that if $D\Phi(g,\pi)^*$ is injective, then $D\Phi(g,\pi)$ is surjective since, in fact, it maps the range of its adjoint onto $C^\infty\times X^1$. If, however, the adjoint has nontrivial kernel, then $D\Phi(g,\pi)$ is not surjective since, in fact, it cannot map to any nonzero element in the kernel of $D\Phi(g,\pi)^*$. To see this, assume $(\bar{C},\bar{X})\in\ker D\Phi(g,\pi)^*$ and suppose a tangent vector (h,p) exists for which

$$(\bar{C},\bar{X})=D\Phi(g,\pi)\circ(h,p). \tag{3.10}$$

Then

$$\begin{aligned}((\bar{C},\bar{X}),(\bar{C},\bar{X}))&=((\bar{C},\bar{X}),D\Phi(g,\pi)\cdot(h,p))\\&=(D\Phi(g,\pi)^*\circ(\bar{C},\bar{X}),(h,p))\\&=0,\end{aligned} \tag{3.11}$$

which forces $\bar{C}=\bar{X}=0$.

4. GAUGE PERTURBATIONS AND A REFINED SPLITTING

We now refine the decomposition of the previous section by splitting the kernel of $D\Phi(g,\pi)$ into two orthogonal subspaces. To explain this refinement, we first recall some results obtained in Ref. 4. There it was shown that if ${}^{(4)}X$ is a vector field on a Cauchy development of the initial data $(g',\pi')\in C$, then ${}^{(4)}X$ induces at each Cauchy surface of the development a tangent vector $(h,p)_{{}^{(4)}X}$ representing the infinitesimal diffeomorphism generated by ${}^{(4)}X$. Furthermore, this gauge perturbation of the Cauchy data (g,π) of the hypersurface may be simply expressed in terms of the adjoint map $D\Phi(g,\pi)^*$. If $\overset{\circ}{C}=n^\mu\,{}^{(4)}X_\mu=N^{-1}({}^{(4)}X_0-g^{ij}N_i\,{}^{(4)}X_j)$ and $g_{ij}\overset{\circ}{X}^j=\overset{\circ}{X}_i=$ $={}^{(4)}X_i$ are respectively the normal and tangential projections of ${}^{(4)}X$ at the hypersurface (M,g,π), then the induced tangent vector $(h,p)_{{}^{(4)}X}\equiv(\overset{\circ}{h},\overset{\circ}{p})\in T_{(g,\pi)}\mathcal{M}\times\mathcal{S}^2$ is given by

$$((\det g)^{-1/2}\overset{\circ}{p}_*,-(\det g)^{1/2}\overset{\circ}{h}^{-1})=D\Phi(g,\pi)^*\circ(\overset{\circ}{C},\overset{\circ}{X}), \tag{4.1}$$

where $\overset{\circ}{p}_*=\overset{\circ}{p}_{ij}$, $\overset{\circ}{h}^{-1}=\overset{\circ}{h}^{ij}$ and, as we have mentioned, the notation here differs slightly from that of Ref. 4.

It is convenient to define an alternative form of the adjoint in which the first slot is replaced by its contravariant density form and the second slot by its covariant tensor form. Thus, if $(\overset{\circ}{h},\overset{\circ}{p})$ are given as in Eq. (4.1), write

$$(\overset{\circ}{p},-\overset{\circ}{h})=D\Phi(g,\pi)^\dagger\cdot(\overset{\circ}{C},\overset{\circ}{X}). \tag{4.2}$$

This equation is equivalent to

$$(\overset{\circ}{h},\overset{\circ}{p})=\left(\begin{smallmatrix}0&-1\\1&0\end{smallmatrix}\right)D\Phi(g,\pi)^\dagger\cdot(\overset{\circ}{C},\overset{\circ}{X})\equiv\gamma(g,\pi)\cdot(\overset{\circ}{C},\overset{\circ}{X}), \tag{4.3}$$

where, for convenience, we regard $(\overset{\circ}{h},\overset{\circ}{p})$ and $D\Phi(g,\pi)^\dagger\cdot(\overset{\circ}{C},\overset{\circ}{X})$ as two component column vectors.

The aim is now to split the kernel of $D\Phi(g,\pi)$ into the range of $\left(\begin{smallmatrix}0&-1\\1&0\end{smallmatrix}\right)D\Phi(g,\pi)^\dagger$ and an orthogonal subspace. For this to be meaningful it is of course necessary that the range of $\gamma(g,\pi)\equiv\left(\begin{smallmatrix}0&-1\\1&0\end{smallmatrix}\right)D\Phi(g,\pi)^\dagger$ be contained in the kernel of $D\Phi(g,\pi)$. The proof is a straightforward computation.

Theorem 4.1: If $(g,\pi)\in C$, then range $\gamma(g,\pi)\subset\ker D\Phi(g,\pi)$.

Proof: Let $(\overset{\circ}{C},\overset{\circ}{X})$ be any element of $C^\infty\times X^1$ and evaluate $D\Phi(g,\pi)\circ[\gamma(g,\pi)\circ(\overset{\circ}{C},\overset{\circ}{X})]$ using the explicit expressions given by Eqs. (2.8), (2.10), (4.1), and (4.3). The result is

$$\begin{aligned}&D\Phi(g,\pi)\circ[\gamma(g,\pi)\cdot(\overset{\circ}{C},\overset{\circ}{X})]\\&\quad=\{2\overset{\circ}{C}_{|i}\delta^i(g,\pi)+\overset{\circ}{C}(\delta^i(g,\pi))_{|i}+\overset{\circ}{X}^i{}_{|i}\mathcal{H}(g,\pi)\\&\qquad+\overset{\circ}{X}^i(\mathcal{H}(g,\pi))_{|i};\\&\qquad\overset{\circ}{C}^{|i}\mathcal{H}(g,\pi)+\delta^j(g,\pi)[2\overset{\circ}{C}(\det g)^{-1/2}(\pi^i{}_j-\tfrac{1}{2}\delta^i{}_j\operatorname{tr}\pi)]\\&\qquad+(\overset{\circ}{X}^k\delta^i(g,\pi))_{|k}-\overset{\circ}{X}^i{}_{|k}\delta^k(g,\pi)\}=0\end{aligned} \tag{4.4}$$

since $\delta^i(g,\pi)=2(\det g)^{-1/2}\,\pi^{ij}{}_{|j}$ and $\mathcal{H}(g,\pi)$ vanish for any $(g,\pi)\in C$.

To identify the subspace within $\ker D\Phi(g,\pi)$ which is orthogonal to the range of $\gamma(g,\pi)$, let $(\tilde{h},\tilde{p})\in\ker D\Phi(g,\pi)$ and require, for arbitrary $(\overset{\circ}{C},\overset{\circ}{X})\in C^\infty\times X^1$, that

$$((\tilde{h},\tilde{p}),\gamma(g,\pi)\circ(\overset{\circ}{C},\overset{\circ}{X}))=0. \tag{4.5}$$

This is equivalent to

$$\begin{aligned}0&=((\tilde{p},-\tilde{h})_\dagger,D\Phi(g,\pi)^*\circ(\overset{\circ}{C},\overset{\circ}{X}))\\&=(D\Phi(g,\pi)\circ(\tilde{p},-\tilde{h})_\dagger,(\overset{\circ}{C},\overset{\circ}{X}))\end{aligned} \tag{4.6}$$

in which we have defined $(\ ,\ )_\dagger$ by

$$(\tilde{p},-\tilde{h})_\dagger=((\det g)^{-1/2}\tilde{p}_*,-(\det g)^{1/2}\tilde{h}^{-1}), \tag{4.7}$$

where, as before, $\tilde{p}_*=\tilde{p}_{ij}$, $\tilde{h}^{-1}=\tilde{h}^{ij}$. Thus a vector $(\tilde{h},\tilde{p})\in\ker D\Phi(g,\pi)$ is orthogonal to the range of $\gamma(g,\pi)$

provided that

$$D\Phi(g,\pi)\circ(\tilde{p},-\tilde{h})_\dagger=0. \tag{4.8}$$

We now attempt to split an arbitrary vector $(\bar{h},\bar{p})\in\ker D\Phi(g,\pi)$ as

$$(\bar{h},\bar{p})=(\tilde{h},\tilde{p})+\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}D\Phi(g,\pi)^\dagger\circ(\overset{\circ}{C},\overset{\circ}{X}) \tag{4.9}$$

with

$$D\Phi(g,\pi)\circ(\tilde{p},-\tilde{h})_\dagger=0. \tag{4.10}$$

Equation (4.9) is equivalent to

$$\begin{aligned}(\bar{p},-\bar{h})_\dagger&=(\tilde{p},-\tilde{h})_\dagger+[D\Phi(g,\pi)^\dagger\circ(\overset{\circ}{C},\overset{\circ}{X})]_\dagger\\&=(\tilde{p},-\tilde{h})_\dagger+D\Phi(g,\pi)^*\cdot(\overset{\circ}{C},\overset{\circ}{X}),\end{aligned} \tag{4.11}$$

where the last equality follows from the definitions of $(\ ,\ )_\dagger$ and $D\Phi(g,\pi)^\dagger$. Applying $D\Phi(g,\pi)$ and using Eq. (4.10), we obtain

$$D\Phi(g,\pi)\circ(\bar{p},-\bar{h})_\dagger=D\Phi(g,\pi)\cdot[D\Phi(g,\pi)^*\circ(\overset{\circ}{C},\overset{\circ}{X})], \tag{4.12}$$

which are partial differential equations for $(\overset{\circ}{C},\overset{\circ}{X})$. However, the operator $\alpha(g,\pi)=D\Phi(g,\pi)\cdot D\Phi(g,\pi)^*$ is the same as that treated in Sec. III. Therefore, at regular points of $\mathcal{C}$ the solution to Eq. (4.12) exists and is unique. For irregular points one shows, just as before, that the source term $D\Phi(g,\pi)\cdot(\bar{p},-\bar{h})_\dagger$ is orthogonal to $\ker D\Phi(g,\pi)^*$ so that a solution of Eq. (4.12) still exists. Again the solution $(\overset{\circ}{C},\overset{\circ}{X})$ fails to be unique as one may add any element of $\ker D\Phi(g,\pi)^*$. Nevertheless, the decomposition (4.9) is unique since $D\Phi(g,\pi)^\dagger$, which is just another form of the adjoint, annihilates any element of $\ker D\Phi(g,\pi)^*$.

To summarize the results of the preceding sections, we introduce the notation

$$\gamma(g,\pi)^*\circ(h,p)=D\Phi(g,\pi)\circ(p,-h)_\dagger, \tag{4.13}$$

which is natural since, from its definition, $\gamma(g,\pi)^*$ is the L^2 adjoint of $\gamma(g,\pi)$. Thus the splitting defined in this section may be written

$$\ker D\Phi(g,\pi)=\text{range}\gamma(g,\pi)\oplus(\ker\gamma(g,\pi)^*\cap\ker D\Phi(g,\pi)). \tag{4.14}$$

Combining this result with that of the previous section, we obtain

Theorem 4.2: If $(g,\pi)\in\mathcal{C}$, the tangent space $T_{(g,\pi)}\mathcal{M}\times\mathcal{S}_*{}^2$ may be expressed as the direct sum of three mutually orthogonal subspaces:

$$\begin{aligned}T_{(g,\pi)}\mathcal{M}\times\mathcal{S}_*{}^2=&\,\text{range}D\Phi(g,\pi)^*\oplus\text{range}\gamma(g,\pi)\\&\oplus(\ker\gamma(g,\pi)^*\cap\ker D\Phi(g,\pi)).\end{aligned}$$

At a regular point of $\mathcal{C}$ the last two spaces form the tangent space of $\mathcal{C}$ at (g,π). The second member [range $\gamma(g,\pi)$] contains all vectors representing pure gauge perturbations of (g,π). The last member represents deformations of (g,π) towards Cauchy data for vacuum spacetimes distinct from that determined by (g,π).

5. THE BRILL-DESER DECOMPOSITION

In this section we specialize the results of the previous sections to recover the Brill–Deser decomposition of perturbations at a point with $\pi=0$ and g flat. We must assume, of course, that M admits a flat metric.

If $\pi=0$ and g is flat, we have from Eqs. (2.8) and (2.10)

$$D\Phi(g,0)\cdot(h,p)=\{-h_{ij}{}^{|ij}+(\text{tr}h)_{|i}{}^{|i};2(\det g)^{-1/2}p^{ij}{}_{|j}\} \tag{5.1}$$

and

$$\begin{aligned}&D\Phi(g,0)^*\circ(C,X)\\&\quad=\{-C_{|ij}+g_{ij}C_{|k}{}^{|k};-(\det g)^{1/2}(X^{i|j}+X^{j|i})\}.\end{aligned} \tag{5.2}$$

Therefore,

$$\begin{aligned}\gamma(g,0)\circ(\overset{\circ}{C},\overset{\circ}{X})&=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}D\Phi(g,0)^\dagger\circ(\overset{\circ}{C},\overset{\circ}{X})\\&=\{\overset{\circ}{X}_{i|j}+\overset{\circ}{X}_{j|i};-(\det g)^{1/2}[\overset{\circ}{C}{}^{|ij}-g^{ij}\overset{\circ}{C}_{|k}{}^{|k}]\}\end{aligned} \tag{5.3}$$

and

$$\begin{aligned}&\gamma(g,0)^*\circ(h,p)\\&\quad=\{-(\det g)^{-1/2}[p_{ij}{}^{|ij}-(\text{tr}p)_{|i}{}^{|i}];-2h^{ij}{}_{|j}\}.\end{aligned} \tag{5.4}$$

Thus any tangent vector (h,p) may be expressed as

$$\begin{aligned}h_{ij}&=\tilde{h}_{ij}+\overset{\circ}{X}_{i|j}+\overset{\circ}{X}_{j|i}-(C_{|ij}-g_{ij}\Delta C),\\p^{ij}&=\tilde{p}^{ij}-(\det g)^{1/2}(\overset{\circ}{C}{}^{|ij}-g^{ij}\Delta\overset{\circ}{C})-(\det g)^{1/2}(X^{i|j}+X^{j|i}),\end{aligned} \tag{5.5}$$

in which $(\tilde{h},\tilde{p})$ obey

$$\tilde{h}_{ij}{}^{|j}=\tilde{p}_{ij}{}^{|j}=0 \tag{5.6}$$

and

$$\Delta(\text{tr}\tilde{h})=\Delta(\text{tr}\tilde{p})=0. \tag{5.7}$$

Since M is compact, Eqs. (5.7) imply that $\text{tr}\tilde{h}=\alpha$ and $\text{tr}\tilde{p}=(\det g)^{1/2}\beta$, where α and β are constants. Since $\tilde{h}$ and $\tilde{p}$ are both transverse, we may therefore write

$$\begin{aligned}\tilde{h}_{ij}&=\tilde{h}_{ij}{}^{\text{TT}}+\tfrac{1}{3}g_{ij}\alpha\\\tilde{p}^{ij}&=\tilde{p}^{ij\,\text{TT}}+\tfrac{1}{3}(\det g)^{1/2}g^{ij}\beta,\end{aligned} \tag{5.8}$$

where TT signifies transverse and traceless. Equations (5.5) and (5.8) are equivalent to the splitting defined by Brill and Deser.

6. DISCUSSION

Given Cauchy data $(g,\pi)\in\mathcal{C}$, one may choose a (time dependent) lapse function and shift vector field and integrate the Einstein evolution equations to determine a Ricci-flat metric ${}^{(4)}g$ on $(-\epsilon,\epsilon)\times M$. In particular, one gets a curve $(g(t),\pi(t))\in\mathcal{C}$ with $(g,\pi)=(g(0),\pi(0))$ and $t\in(-\epsilon,\epsilon)$. The Cauchy problem for the corresponding linearized equations is similar. One chooses initial data $(h,p)\in T_{(g,\pi)}\mathcal{M}\times\mathcal{S}_*{}^2$ obeying $D\Phi(g,\pi)\cdot(h,p)=0$ and specifies a (time dependent) perturbation of the lapse function and shift vector field. Integration of the perturbed evolution equations gives $(h(t),p(t))\in T_{(g(t),\pi(t))}\mathcal{M}\times\mathcal{S}_*{}^2$ with $(h,p)=(h(0),p(0))$ and $t\in(-\epsilon,\epsilon)$. Since the linearized constraints are preserved by the linearized

evolution equations, the perturbations obey

$$(h(t), p(t)) \in \ker D\Phi(g(t), \pi(t)) \tag{6.1}$$

for all $t \in (-\epsilon, \epsilon)$.

Now consider applying the decomposition theorems derived here to a solution of the perturbation equations. Since $(h(t), p(t))$ satisfies Eq. (6.1), we may split the perturbations as in Eq. (4.14):

$$(h(t), p(t)) = (\tilde{h}(t), \tilde{p}(t)) + \gamma(g(t), \pi(t)) \cdot (C(t), X(t)) \tag{6.2}$$

with

$$(\tilde{h}(t), \tilde{p}(t)) \in (\ker\gamma(g(t), \pi(t))^* \cap \ker D\Phi(g(t), \pi(t))). \tag{6.3}$$

Both terms are uniquely determined at each instant [even though $C(t)$ and $X(t)$ may not be].

We claim that $(\tilde{h}(t), \tilde{p}(t))$ are unchanged by an arbitrary gauge transformation whereas both $(C(t), X(t))$ and the perturbed lapse and shift functions are in general changed by a gauge transformation. As shown in Ref. 4, any vector field ${}^{(4)}X'$ on $((-\epsilon, \epsilon) \times M, {}^{(4)}g)$ induces, on the Cauchy surface $(M, g(t), \pi(t))$, the gauge perturbation $(h'(t), p'(t)) = \gamma(g(t), \pi(t)) \cdot (C'(t), X'(t))$, where $C'(t)$ and $X'(t)$ are the normal and tangential projections of ${}^{(4)}X'$ at that hypersurface. It follows, from the uniqueness of the decomposition, that the gauge transformed perturbations split according to

$$(h(t) + h'(t), p(t) + p'(t))$$
$$= (\tilde{h}(t), \tilde{p}(t)) + \gamma(g(t), \pi(t)) \cdot (C(t) + C'(t), X(t) + X'(t)) \tag{6.4}$$

with no change in $(\tilde{h}(t), \tilde{p}(t))$. Thus $(\tilde{h}(t), p(t))$ have a unique time development, independent of the choice of gauge, whereas the orthogonal term $[\in \text{range}\gamma(g(t), \pi(t))]$ and the perturbations of the lapse and shift functions are gauge dependent.

One may apply the decompositions defined here to the linearization stability problem for the vacuum Einstein equations precisely as Brill and Deser did for the special case of a flat spacetime. As explained in the Introduction, any vacuum spacetime (with compact Cauchy slices) which admits a Killing vector field fails to be linearization stable. For these cases some solutions of the perturbation equations should be excluded since they do not approximate any curve of exact solutions. In a subsequent paper (the sequel to Ref. 4) we shall derive the additional (nonlinear) restrictions upon the perturbations which are necessary to exclude spurious perturbation solutions. These restrictions are equivalent to demanding that the conserved quantity associated with each linearly independent Killing vector field must be constrained to vanish.

Each such conserved quantity may be evaluated on any spacelike hypersurface through the spacetime and is expressible as the integral (over that hypersurface) of a function quadratic in the perturbations. When constrained to vanish these integrals impose nontrivial restrictions upon the perturbed Cauchy data. The conservation laws ensure that these new constraints are independent of the choice of initial surface at which they are imposed.

An important feature of these conserved integrals is that they are necessarily gauge invariant (since otherwise they could not be conserved). Therefore, if one should apply the decomposition (6.2) to the perturbations, he would find that the conserved integrals are cyclic in the gauge dependent terms and thus, when required to vanish, impose restrictions only upon the gauge invariant contributions $(\tilde{h}(t), \tilde{p}(t))$. This result would be a natural generalization of that due to Brill and Deser for flat spacetimes.

Since the new constraints are nonlinear restrictions upon the perturbed Cauchy data, the set of perturbations which satisfy them is not likely to form a vector space. Thus the allowed solutions of the perturbation equations would not obey a superposition principle even though the perturbation equations themselves are linear. This observation suggests that the constraint subset C could not be a smooth submanifold of P on any neighborhood of an irregular point. If C were smooth at an irregular point, its tangent space would coincide with the set of allowed perturbations whereas the latter does not seem to form a vector space. The decompositions defined in this paper may prove useful in giving a more precise characterization of the geometry of the constraint subset near its irregular points.

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Onsager symmetry and the diagonalizability of the hydrodynamic matrix

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The diagonalizability of the hydrodynamic matrix in the case that one of the variables is odd under time reversal is investigated. The implications for a normal mode analysis and for the spectral density elements are considered.

1. INTRODUCTION

The macroscopic description of nonequilibrium processes in fluids is normally based on conservation equations such as those for total mass and for individual species and on conservation equations for momentum and for energy. One obtains, following what are now well established procedures (see, for example, Landau and Lifshitz[1]) a set of coupled nonlinear equations

$$\frac{\partial}{\partial t}A_j(\vec{r},t)=f(\{A_i(\vec{r},t),\nabla A_i(\vec{r},t),\cdots\ldots\}),\quad j=1\cdots(m+n) \tag{1}$$

where the $A_j(\vec{r},t)$ indicate field variables, e.g., $T(\vec{r},t)P(\vec{r},t)$, $v(\vec{r},t)$, etc., ∇ denotes the gradient operator, the $\cdots$ represents more complex terms, $m+n$ is the number of variables required to specify the state of the system, and m is the number of thermodynamic variables. The solution of these equations, in one form or another, forms the basis for the analysis of many physical problems of interest.

We shall be concerned with the set of equations obtained from Eq. (1) by linearizing in the small deviations $\alpha_j(\vec{r},t)=A_j(\vec{r},t)-A_j(\text{equil})$. We write the resulting linearized equations as

$$\frac{\partial}{\partial t}\underline{\alpha}(\vec{r},t)=\underline{M}\underline{\alpha}(\vec{r},t), \tag{2}$$

where $\underline{\alpha}$ is a vector whose components are the $\alpha_j(\vec{r},t)$ and $\underline{M}$ denotes a matrix whose entries express the coupling between the variables $A_j(\vec{r},t)$. Equation (2) may then be spacially decoupled by a suitable Fourier transform giving a set of equations for each Fourier component as in

$$\frac{\partial}{\partial t}\underline{\alpha}(\vec{k},t)=\underline{M}(\vec{k})\,\underline{\alpha}(\vec{k},t). \tag{3}$$

Although there are alternatives, one commonly finds the $\alpha_j(\vec{k},t)$ via a normal mode decomposition.[2] In order to carry this out, we first find the eigenvectors V_f and eigenvalues λ_f of the hydrodynamic matrix $M(\vec{k})$, i.e., we obtain the matrix $\underline{V}$ which diagonalizes $\underline{M}$ as in

$$\underline{V}^{-1}\,\underline{M}\,\underline{V}=\underline{\Lambda} \tag{4}$$

where $\Lambda=\text{diag}\{\lambda_1\cdots\lambda_f\cdots\}$ and $\underline{V}$ is a matrix whose columns are the eigenvectors V_f. Given this, one can then write

$$\underline{\alpha}(\vec{k},t)=V\underline{\gamma}(\vec{k},t),$$

where γ is a matrix whose columns are the normal modes $\gamma_f(\vec{k},t)$ defined by

$$\gamma_f(\vec{k},t)=\gamma_f(\vec{k},0)\,e^{\lambda_f t} \tag{5}$$

If the $\alpha_j(\vec{r},t)$ are taken to be random fluctuations in an isotropic fluid, then the system may be characterized, using Onsager's assumption concerning the regression of fluctuations, by the correlation matrix elements

$$R_{jl}(r,t)=\langle\alpha_j(\vec{r}'+\vec{r},t'+t)\alpha_l^*(\vec{r}',t')\rangle,$$

where $\langle\cdots\rangle$ denotes the appropriate average. Alternatively, on invoking the Weiner–Khinchin theorem, one can characterize the process by the spectral density matrix elements $S_{jl}(k,\omega)$ given by the Fourier–Laplace transform of the correlation $R_{jl}(r,t)$. To facilitate the analysis of the spectral density matrix elements, the normal mode decomposition of the preceding paragraph may be employed. One writes $S_{jl}(k,\omega)$ as

$$S_{jl}(k,\omega)=(k_BTV/2\pi)\,\text{Re}\textstyle\sum_f Z^f_{lj}/(\lambda_f+i\omega)$$

where Z^f_{lj} is an element of the "constituent" matrix $\underline{Z}^f$ defined by $\underline{Z}^f=\underline{G}\underline{\chi}(k)$. Here $\underline{G}=V_f(V_f^{-1})'$, where V_f is the fth column of $\underline{V}$, $(V_f^{-1})'$ is the fth row of $\underline{V}^{-1}$, and $\underline{\chi}(k)$ is the Fourier transform of the one-time correlation (variance) matrix with elements

$$\chi_{jl}(k)=\langle\alpha_j(\vec{k})\,\alpha_l^*(\vec{k})\rangle \tag{6}$$

Clearly, *both the eigenvalues and eigenvectors* of the Fourier transformed hydrodynamic matrix $\underline{M}(\vec{k})$ are required in the analyses described in the preceding paragraphs. The inherent symmetry of the hydrodynamic matrix has been used recently to establish the distribution of the eigenvalues λ_f in the complex plane.[3,4] This is of some significance since the number of complex eigenvalues gives the number of peaks in the spectral function which have their maximum at $\omega\neq0$. The same analysis has also allowed progress in establishing the relation between the diagonalizing matrices $\underline{V}^{-1}$ and $\underline{V}$ in the cases where the λ_f are all distinct. However, heretofore the question of diagonalizability of the hydrodynamic matrix when not all λ_f are distinct has not been widely investigated.[5] It is this question and the implications of the results that shall be our concern here. Since the results referred to above for λ_f, $\underline{V}$, and $\underline{V}^{-1}$ will be of some assistance, we shall briefly review their development using this as an opportunity to introduce required notation.

2. SYMMETRY OF THE HYDRODYNAMIC MATRIX

The development[3,4] begins with rewriting the Fourier transformed hydrodynamic equations of Eq. (2) in terms

of statistically independent normalized variables $\underline{\beta}(\vec{k}, t)$ as

$$\frac{\partial}{\partial t}\underline{\beta}(\vec{k}, t) = \underline{K}\ \underline{\beta}(\vec{k}, t), \tag{7}$$

where the elements of the column vector $\underline{\beta}$ satisfy

$$\langle \beta_j(\vec{k}, t)\, \beta_l^*(\vec{k}, t)\rangle = \delta_{jl}. \tag{8}$$

Since the $\beta_j(\vec{k}, t)$ are related to the $\alpha_j(\vec{k}, t)$ by

$$\underline{\beta}(\vec{k}, t) = \underline{U}\underline{\chi}^{-1/2}\ \underline{\alpha}(\vec{k}, t),$$

where $\underline{U}$ is an arbitrary unitary matrix and $\underline{\chi}^{-1/2}$ is given by the positive definite variance matrix $\underline{\chi}$ defined by Eq. (6), it is easy to show that

$$\underline{K} = \underline{U}\underline{\chi}^{-1/2}\underline{M}\chi^{1/2}\underline{U}^{\dagger}. \tag{9}$$

The transformed hydrodynamic matrix $\underline{K}$, thus obtained can be shown, on invoking the principle of microscopic reversibility, to have the symmetry

$$\underline{K}^{\dagger} = \underline{E}\underline{K}\underline{E}. \tag{10}$$

Here, $\underline{E}$, the signature matrix for time reversal, is diagonal with n ordered entries of plus 1 for the even thermodynamic variables and m, minus 1 entries, for odd variables arising from, say, the velocity field.

If we restrict ourselves to the case where $m = 1$, we may, without loss of generality, choose the unitary matrix $\underline{U}$ to be such that $\underline{K}$ has the form

$$\underline{K} = \begin{bmatrix} a_1 & & 0 & b_1 \\ & \ddots & & \\ 0 & & a_n & b_n \\ -b_1 & & -b_n & a_{n+1} \end{bmatrix}, \tag{11}$$

where the elements of $\underline{K}$ are real. A matrix which has been transformed to the structure displayed in Eq. (11) we shall refer to as the bordered diagonal form (BDF) of $\underline{K}$ denoted by $\underline{K}^{\mathrm{BDF}}$.

Given Eq. (11), it can be readily seen that the characteristic polynomial of $\underline{K}^{\mathrm{BDF}}$, i.e., of $\underline{K}$, can be written as

$$P(\lambda) = |\underline{K} - \lambda\underline{I}| = \prod_{i=1}^{n+1}(a_i - \lambda) + \sum_{j=1}^{n} b_j^2 \prod_{i\neq j}^{n}(a_i - \lambda), \tag{12}$$

from which it is easy to establish (see Ref. 4):

Lemma 1: For a matrix $\underline{K}$ of dimension $n+1$ with symmetry $\underline{K}^{\dagger} = \underline{E}\underline{K}\underline{E}$, where $\underline{E}$ is diagonal with the first n entries unity and the last minus one, there is a minimum of $n-1$ real roots, and these $n-1$ real roots $\lambda_1 \cdots \lambda_{n-1}$ are distributed as $a_i < \lambda_i < a_{i+1}$ for all $1 \leq i \leq n-1$, where the a_i are the elements of $\underline{K}^{\mathrm{BDF}}$.

3. DIAGONALIZABILITY

The hydrodynamic matrix $\underline{K}$ with symmetry as given by Eq. (10) can readily be shown to be nonnormal. To see this, we write, from Eq. (10),

$$\underline{K}\underline{K}^{\dagger} = \underline{E}\underline{K}^{\dagger}\underline{K}\underline{E},$$

where we have used the fact that $\underline{E}\underline{E} = \underline{I}$. Thus $(\underline{K}\underline{K}^{\dagger})_{ij} = E_{ii}E_{jj}(\underline{K}^{\dagger}\underline{K})_{ij}$ so that in general $\underline{K}\underline{K}^{\dagger} \neq \underline{K}^{\dagger}\underline{K}$. Hence the matrix $\underline{K}$ cannot be diagonalized by a unitary transformation, it can only be brought to the nearly diagonal form as displayed in Eq. (11).

When all eigenvalues of $\underline{K}$ are distinct, one can, however, diagonalize $\underline{K}$ by a *similarity* transformation[6]

$$\underline{W}^{-1}\underline{K}\underline{W} = \underline{\Lambda}, \tag{13}$$

and as was shown in Ref. 4 the diagonalizing matrix $\underline{W}$ has the symmetry

$$\underline{W}^{\dagger} = \underline{W}^{-1}\underline{E}. \tag{14}$$

However, suppose not all eigenvalues are distinct. It is easy to show that in such cases not all $\underline{K}$ matrices can be brought to diagonal form by a similarity transformation. For example consider the real matrix of Eq. (15),

$$\underline{K} = \begin{bmatrix} a_1 & b \\ -b & a_2 \end{bmatrix}, \tag{15}$$

which has the symmetry required by Eq. (10) for $\underline{E} = \mathrm{diag}\{1, -1\}$. The eigenvalues of this matrix are degenerate when

$$a_2 = a_1 \pm 2b, \tag{16}$$

and one finds that under these conditions that $\underline{K}$ cannot be brought to diagonal form by a similarity transformation. [One might remark here that the condition of Eq. (16) corresponds to the point of crossover from two complex roots $\lambda_1 = \lambda_2^*$ to the real domain at $\lambda_1 = \lambda_2$.] Since $\underline{K}$ is clearly not, in general, diagonalizable by a similarity transformation, we turn to the problem of investigating in a general way the situations where $\underline{K}$ is nondiagonlizable.

Although not all matrices can be brought to diagonal form as in Eq. (4), all matrices can, by an appropriate similarity transformation, $\underline{Y}$, be brought to a form where the right-hand side of Eq. (17) is in a lower triangular form with the eigenvalues of $\underline{K}$ along the diagonal:

$$\underline{Y}\underline{K}\underline{Y}^{-1} = \underline{T}. \tag{17}$$

Without loss of generality we can require that $\underline{Y}$ be such that $\underline{T} = \Lambda_{\mathrm{JCF}}$, the Jordan canonical form[7] (JCF), where $\underline{\Lambda}_{\mathrm{JCF}}$ is in block diagonal form as

$$\underline{\Lambda}_{\mathrm{JCF}} = \begin{bmatrix} \underline{\Lambda}_1 & & 0 \\ & \underline{\Lambda}_2 & \\ & & \ddots \\ 0 & & \underline{\Lambda}_s \end{bmatrix}. \tag{18}$$

The $\underline{\Lambda}_i$ are elementary Jordan λ_i-blocks. If $\underline{K}$ is diagonalizable, all these blocks are 1×1, the entry being λ_f, but if $\underline{K}$ is not diagonalizable, one or more of the $\underline{\Lambda}_i$ are of the form

$$\Lambda_i = \begin{bmatrix} \lambda_i & & & 0 \\ 1 & \ddots & & \\ 0 & \ddots & \ddots & \\ \vdots & & \ddots & \\ 0 & 0 \cdots & 1 & \lambda_i \end{bmatrix}. \tag{19}$$

Since an arbitrary matrix can be brought to diagonal form by a similarity transformation iff its JCF is diagonal,[8] the question of diagonalizability can be answered by examining the JCF.

4. DEGENERACY AND NONDIAGONALIZABILITY

We now proceed to discover precisely those cases in which the JCF of the $\underline{K}$ matrix of Eq. (11) is not diagonal. If all the eigenvalues of $\underline{K}$ are distinct, then, as indicated earlier, the matrix is diagonalizable, and therefore the nondiagonalizability problem arises only when a degeneracy occurs in the roots of $\underline{K}$. If any of the b_i are zero in the BDF of $\underline{K}$, then clearly the corresponding a_i is an eigenvalue and the ith basis vector an eigenvector. Thus degeneracies in roots which occur in this manner will not prevent diagonalization. For this reason we assume that all the b_i are nonzero (this is equivalent to reordering the basis vectors so that, with respect to the reordered basis, $\underline{K}$ becomes the matrix direct sum of a diagonal matrix and a matrix of the same symmetry as $\underline{K}$ with all b's nonzero). We shall henceforth concern ourselves only with that partition of the hydrodynamic matrix which, when unitarily transformed as in Eq. (9), assumes the bordered diagonal form where all $b_i \neq 0$, i.e., the $\underline{K}$ matrix is the *fully* coupled partition (FCP). We will suppress the notation FCP except where confusion could result (in which case we will use $\underline{K}^{\mathrm{FCP}}$) and will normally use just the notation $\underline{K}$ for these fully coupled matrices.

A. All a_i distinct

Lemma 2: A $\underline{K}$ matrix of dimension ≤ 4 for which all the a_i $(i=1, \cdots, n)$ of $\underline{K}^{\mathrm{BDF}}$ are distinct is diagonalizable iff all its eigenvalues are distinct.

The proof is rather lengthy, involving tedious but straightforward manipulations, and hence is relegated to the Appendix.

Lemma 2 allows us to attack the case in which all a_i $(i=1, \ldots, n)$ are distinct and the dimension of the $\underline{K}$ matrix is arbitrary. The reason is that from Lemma 1 we know that there are at least $n-1$ real eigenvalues and that if the dimension of the $\underline{K}$ matrix, $(n+1)$, is ≥ 5, there is at least one eigenvalue of multiplicity one and hence that there is at least one eigenspace of dimension equal to the multiplicity of the eigenvalue. Utilizing these facts, we can prove (see Appendix) the following theorem.

Theorem 1: A $\underline{K}$ matrix in which the a_i of $\underline{K}^{\mathrm{BDF}}$ are distinct $(i=1, \ldots, n)$ is diagonalizable iff all its eigenvalues are distinct.

The matrix defined by Eqs. (15) and (16) provides a ready illustration of a case in which the *eigenvalues* are not all distinct and hence the K matrix is not diagonalizable. For K matrices of higher dimension, degeneracy and nondiagonalizability can arise in more ways than that indicated by this simple example, and we shall return to this point in subsection C to follow.

B. Not all a_i distinct

In general it is possible that not all of the a_i $(i=1, \ldots n)$ in $\underline{K}^{\mathrm{BDF}}$ are distinct. In this case it is possible to reduce the problem to one very similar to that treated in Theorem 1 by using the following lemma.

Lemma 3: If there are p distinct a_i $(i=1, \ldots, n)$ in $\underline{K}^{\mathrm{BDF}}$, each occurring n_i times, then a_i is an eigenvalue of $\underline{K}$ of order precisely $n_i - 1$ and there exist exactly $n_i - 1$ linearly independent eigenvectors in its eigenspace.

Since the proof of this lemma introduces a useful factorization of the characteristic polynomial, we give it in detail at this point.

Proof: From Eq. (12)

$$\mathrm{ch}(\underline{K}) = P(\lambda) = \prod_{i=1}^{n+1} (a_i - \lambda) + \sum_{j=1} b_j^2 \prod_{i \neq j}^{n} (a_i - \lambda).$$

Thus if

$$a_1 = \cdots = a_{1+n_1-1} = a^1, \quad a_{n+1} = a^{p+1},$$

then the factor $(a^i - \lambda)$ occurs $n_i - 1$ times in $P(\lambda)$;

$$\therefore \mathrm{ch}(\underline{K}) = \left[\prod_{i=1}^{p} (a^i - \lambda)^{n_i - 1}\right] \cdot \left[\prod_{i=1}^{p+1} (a^i - \lambda) + \sum_{j=1}^{p} c_j^2 \prod_{i \neq j}^{p} (a^i - \lambda)\right], \tag{20}$$

where $c_j^2 = \sum_{i=n_{j-1}+1}^{n_j} b_i^2$. We denote the last factor in Eq. (20) by $Q(\lambda)$, i.e.,

$$Q(\lambda) = \prod_{i=1}^{p+1} (a^i - \lambda) + \sum_{j=1}^{p} c_j^2 \prod_{i \neq j}^{p} (a^i - \lambda).$$

[We note, that for cases where all the a_i $(i=1, \ldots, n)$ of $\underline{K}^{\mathrm{BDF}}$ are distinct, $Q(\lambda)$ is in fact the characteristic polynomial $P(\lambda)$ of $\underline{K}$.] Since $c_j^2 \neq 0$, it is easy to see that no a^i is a root of $Q(\lambda)$. Thus $(a^i - \lambda)$ occurs precisely $n_i - 1$ times as a factor of $\mathrm{ch}(\underline{K})$.

Now let $\{e_i\}_{i=1, \ldots, n+1}$ be the basis with respect to which the hydrodynamic matrix assumes the BDF. Then the set of $n_i - 1$ vectors

$$\{e_{l_i} - b_{l_i} b_{l_i+j}^{-1} e_{l_i+j}\}_{j=1, \ldots, n_i-1} = \mathbb{C}^i$$

is easily seen to consist of eigenvectors of $\underline{K}$ of eigenvalue a^i. The set $\{e_{l_i}\} \cup \mathbb{C}_i$ is, of course, linearly independent. QED

It is now possible to classify the roots of $\mathrm{ch}(\underline{K})$ as follows.

Definition: A root of $\underline{K}$ will be classified as a type I root λ_i^{I} where it is a root of $Q(\lambda)$ and will be called a type II root, λ_i^{II}, otherwise.

It will be recalled that in the proof of Lemma 3 we established that the sets $\{\lambda_i^{\mathrm{I}}\}$ and $\{\lambda_i^{\mathrm{II}}\}$ were disjoint. One can prove (see the Appendix) the following theorem.

Theorem 2: The hydrodynamic matrix is diagonable iff the type I roots of $\underline{K}$ are distinct.

C. Dimension of the elementary Jordan blocks

One can now delineate precisely the possible forms for the JCF of $\underline{K}$. From Theorem 2 (and Theorem 1 which is just a special case of Theorem 2) we know that the hydrodynamic matrix is nondiagonalizable only when there is a degeneracy in the type I roots. The obvious question is thus in what manner can such degeneracies

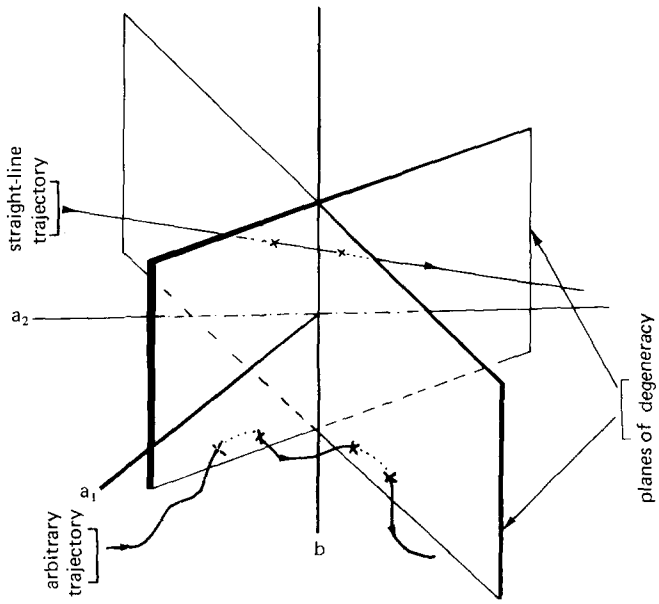

FIG. 1. Trajectories in parameter space of a 2-dimensional K matrix.

arise? The analysis of this question is carried out in the course of the proof of Theorem 2 [see Eq. (A4)] and the results are as follows:

(i) For certain regions of the parameter space defining $\underline{K}$, two of the roots of $\underline{K}$ are complex. For points in this region there are no degeneracies in type I roots.

(ii) In the remaining region of parameter space all the roots of $Q(\lambda)$ are real and there are $p+1$ such roots. Degeneracy in type I roots and hence nondiagonalizability of the hydrodynamic matrix will occur iff there are less than $p+1$ of them which are distinct. The combinations are limited to p distinct roots with one twofold degeneracy, $p-1$ distinct roots with two twofold degeneracies, and $p-1$ distinct roots with one threefold degeneracy.

The implications of these results in terms of the JCF can be stated as a corollary to Theorem 2.

Corollary: The JCF of a nondiagonalizable $\underline{K}$ matrix may contain: one 2×2 Jordan block, two 2×2 Jordan blocks, or one 3×3 Jordan block, depending on whether there is one double degeneracy in the roots of $Q(\lambda)$, two double degeneracies in the roots of $Q(\lambda)$, or one triple degeneracy in the roots of $Q(\lambda)$.

D. Hypersurface of nondiagonalizability

The preceeding section has specified the cases in which the hydrodynamic matrix is not diagonalizable. Although there are only three such cases, they may arise in a number of ways. To illustrate, let us consider the two-dimensional matrix of Eq. (15). We may completely specify a given matrix of this form by a point in $\mathbb{R}^3$ (see Fig. 1) where the coordinates will refer to the values of a_1, a_2, and b respectively. The two conditions of Eq. (16) then determine two intersecting planes in $\mathbb{R}^3$, such that any point on either of these planes corresponds to a nondiagonalizable matrix. Apart from those which lie in one of the planes or those which pass through the origin, all straight lines in $\mathbb{R}^3$ will intersect the surface of nondiagonalizability only twice. However, the variation of some physical parameter is unlikely to lead to a straight line trajectory in $\mathbb{R}^3$, rather one might expect some more complicated trajectory such as that shown in Fig. 1. In such a case one cannot state, *a priori*, how many times nondiagonalizability will arise.

Let us now consider a matrix of arbitrary dimension. For simplicity we will assume that all the a_i $(i=1,\ldots,n)$ are distinct as the more general case can be reduced to one akin to it. We may suppose that we have $n+1$ expressions for the eigenvalues in terms of the $2n+1$ parameters $a_1,\ldots,a_{n+1}$, $b_1,\ldots,b_n$ as:

$$\lambda_i=\lambda_i(a_i,\ldots,b_n).$$

The conditions $\lambda_i=\lambda_j$, $i\neq j$, define occurrences of degeneracies in $Q(\lambda)$ and hence occurrences of nondiagonalizability. The constraint

$$\lambda_i-\lambda_j=0 \tag{21}$$

always has a solution in terms of the parameters, namely all parameters zero. This is, however, incompatible with the restriction that all the a_i are distinct. Nontrivial solutions for (21) will be on a hypersurface of dimension $2n$ in the parameter space and the union of all these hypersurfaces defines the region of nondiagonalizability in parameter space. Clearly the number of such points is continuously infinite. It appears that we cannot really say anything more about the shape of the surface without knowledge of the functions λ_i. The intersection of part of an arbitrary trajectory with this hypersurface is illustrated in Fig. 2.

5. CONSEQUENCES OF NONDIAGONALIZABILITY

We have established that the elementary Jordan blocks for the hydrodynamic matrix in Eq. (11) can be either 1×1, 2×2, or 3×3. With this knowledge it is possible to determine the effect of nondiagonalizability on the mode analysis and on the spectral density matrix elements. We shall begin the analysis in terms of the Fourier components $\alpha_j(\vec{k},t)$ of an arbitrary set of state variables $\alpha_j(\vec{r},t)$ since the JCF is independent of the representation.

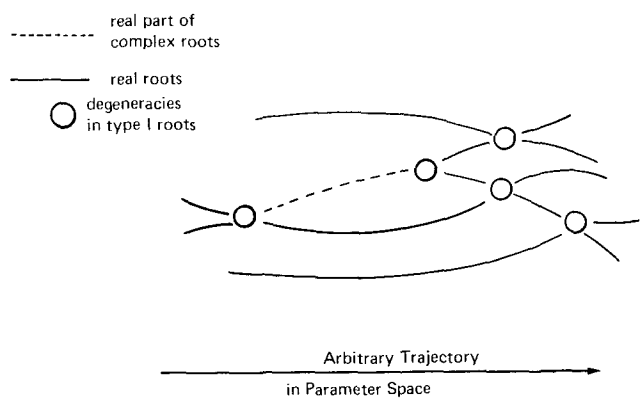

FIG. 2. Degeneracies in type I roots for an arbitrary trajectory in $n+1$-dimensional parameter space.

A. Mode analysis

When the hydrodynamic matrix is diagonalizable, we can write the $\alpha_i(\vec{k}, t)$ in terms of the normal modes,

$$\gamma_j(\vec{k}, t) = \exp(\lambda_j t)\gamma_j(\vec{k}) \tag{22}$$

as

$$\alpha_i(\vec{k}, t) = \sum_{j=1}^{n+1} V_{ij}\gamma_j(\vec{k})\exp(\lambda_j t). \tag{23}$$

The set of variables, $\gamma_f(\vec{k}, t)$, in terms of which the representation of the hydrodynamic matrix is diagonal, are related to the variables $\alpha_j(\vec{k}, t)$ by

$$\underline{\gamma} = \underline{V}^{-1}\,\underline{\alpha}, \tag{24}$$

where $\underline{V}^{-1}$ is defined by Eq. (4).

We will follow a similar procedure for the case in which hydrodynamic matrix is not diagonalizable. In these cases we have, rather than Eq. (4), that

$$\underline{V}^{-1}\underline{M}\,\underline{V} = \underline{\Lambda}_{\mathrm{JCF}} \tag{25}$$

where Λ_{JCF} is the JCF of $\underline{M}$. We will develop the analog of Eqs. (22) and (23) for the case in which $\underline{\Lambda}_{\mathrm{JCF}}$ has just one 2×2 elementary Jordan block. Let $\underline{\gamma}$ be the set of variables with respect to which $\underline{M}$ assumes this Λ_{JCF}. Then $(\partial/\partial t)\underline{\gamma} = \Lambda_{\mathrm{JCF}}\underline{\gamma}$. Let us also suppose that the 2×2 Jordan block occurs at the lower end of the diagonal. Then the first n "modes" are obviously just

$$\gamma_i(\vec{k}, t) = \exp(\lambda_i t)\gamma_i(\vec{k}), \quad 1 \leq i \leq n. \tag{26}$$

However, since there are two entries in the last row of $\underline{\Lambda}_{\mathrm{JCF}}$, we have

$$\frac{\partial}{\partial t}\gamma_{n+1} = \lambda_{n+1}\gamma_{n+1} + \gamma_n = \lambda_n\gamma_{n+1} + \gamma_n,$$

which gives

$$\gamma_{n+1}(\vec{k}, t) = [\gamma_n(\vec{k})t + \gamma_{n+1}(\vec{k})]\exp(\lambda_n t). \tag{27}$$

Or, in terms of the $\{\alpha_i(\vec{k}, t)\}$, we have

$$\alpha_i(\vec{k}, t) = \sum_{j=1}^{n} V_{ij}\gamma_j(\vec{k})\exp(\lambda_j t) + C_i(\vec{k}, t)\exp(\lambda_n t) \tag{28}$$

with $C_i(\vec{k}, t)$ of degree one in t, where

$$C_i(\vec{k}, t) = V_{i,n+1}[\gamma_n(\vec{k})t + \gamma_{n+1}(\vec{k})]. \tag{29}$$

The only difference in Eqs. (26) and (27) from the usual normal modes, e.g., Eq. (22), is the presence, in the "Jordan mode" of Eq. (27), of a polynomial in t. In the case that the JCF of $\underline{M}$ contains a 3×3 block, the three associated γ's will be respectively: an exponential in t; a product of a first degree polynomial in t times an exponential in t; and a product of a second degree polynomial in t times an exponential in t.

B. Spectral density elements

The spectral density matrix elements $S_{jl}(k, \omega)$ are defined by the Fourier transform of the correlation matrix elements $R_{jl}(k, t)$, as

$$S_{jl}(k, \omega) = \frac{\mathrm{Re}}{\pi}\int^{\infty} R_{jl}(k, t)\exp(i\omega t)\,dt, \tag{30}$$

where

$$R_{jl}(k, t) = \begin{cases} [\underline{\chi}(k, 0)\exp(-\underline{M}^T t)]_{jl}, & t < 0, \\ [\exp(\underline{M}t)\,\underline{\chi}(k, 0)]_{jl}, & t > 0. \end{cases} \tag{31}$$

When $\underline{M}$ is diagonalizable [Eq. (4)] one can, following Eq. (5), write the integrated form of Eq. (30) as

$$S_{jl}(k, \omega) = \frac{1}{\Pi}\sum_q [\underline{\chi}(k)]_{jq} V_{lf} V^{-1}_{fq}\left(\frac{\lambda_f}{\lambda_f^2 + \omega^2}\right). \tag{32}$$

When $\underline{M}$ is not diagonalizable, we have, rather than Eq. (4), the relation of Eq. (25), where $\underline{\Lambda}_{\mathrm{JFC}}$ is not diagonal and the utilization of Eqs. (30) and (31) is less straightforward. One begins by rewriting $\exp(-\underline{M}^T t)$ as

$$\exp(-\underline{M}^T t) = (\underline{V}^T)^{-1}\exp(-\underline{\Lambda}^T_{\mathrm{JCF}} t)\,\underline{V}^T. \tag{33}$$

Since

$$\exp(\underline{\Lambda}_{\mathrm{JFC}}\, t) = \exp\left(\bigoplus_{f=1}^{g}\underline{\Lambda}_f t\right) = \bigoplus_{f=1}^{g}\exp(\underline{\Lambda}_f t),$$

where the $\underline{\Lambda}_f$ are elementary Jordan blocks and $\oplus$ means direct sum. Since a maximum dimension of an elementary Jordan block is three, we need only the results that

$$\exp\left\{-\begin{bmatrix}\lambda & 1\\ 0 & \lambda\end{bmatrix} t\right\} = \begin{bmatrix}\exp(-\lambda t) & -a t\exp(-\lambda t)\\ 0 & \exp(-\lambda t)\end{bmatrix}$$

and

$$\exp\left\{-\begin{bmatrix}\lambda & 1 & 0\\ 0 & \lambda & 1\\ 0 & 0 & \lambda\end{bmatrix} t\right\}$$

$$= \begin{bmatrix}\exp(-\lambda t) & -a t\exp(-\lambda t) & \tfrac{1}{2}a^2 t^2\exp(-\lambda t)\\ 0 & \exp(-\lambda t) & -a t\exp(-\lambda t)\\ 0 & 0 & \exp(-\lambda t)\end{bmatrix},$$

where $\mathbf{a}$ is a constant of unit magnitude having units of time^{-1}. The elements $S_{jl}(k, \omega)$ for the case in which $\underline{\Lambda}_{\mathrm{JCF}}$ contains a 2×2 Jordan block and a 3×3 Jordan block respectively, (the case of the occurrence of two 2×2 blocks is not fundamentally different from that in which only one occurs and so has been omitted) can then be written as in (i) and (ii) below.

(i) If $\underline{\Lambda}_{\mathrm{JCF}}$ has a 2×2 block: then

$$S_{ij}(k, \omega) = \frac{1}{\pi}\sum_l \chi(k, 0)_{il}\left[\sum_f V_{jf}V^{-1}_{fl}\left(\frac{\lambda_f}{\lambda_f^2 + \omega^2}\right) + \mathbf{a}\left(\frac{\omega^2 - \lambda^2}{(\lambda^2 + \omega^2)^2}\right)V_{j,n+1}V^{-1}_{n,l}\right],$$

where $\lambda = \lambda_n = \lambda_{n+1}$ is the degenerate root.

(ii) If Λ_{JCF} has a 3×3 block: then

$$S_{ij}(k, \omega) = \frac{1}{\pi}\sum_l \chi(k, 0)_{il}$$

$$\times \sum_f \left(\frac{V_{jf} V_{fl}^{-1} \lambda_f}{\lambda_f^2 + \omega^2} + \frac{a(\omega^2 - \lambda^2)}{(\omega^2 + \lambda^2)^2} \times (V_{jn} V_{n-1,l}^{-1} + V_{j,n+1} V_{nl}^{-1}) + \frac{a^2(\lambda^3 - 3\omega^2\lambda)}{(\omega^2 + \lambda^2)^3} V_{j,n+1} V_{n-1,l}^{-1} \right),$$

where $\lambda = \lambda_{n-1} = \lambda_n = \lambda_{n+1}$ is the triply degenerate root.

We note that the central maximum, at $\omega = 0$, is the same, in both cases, as that for the case in which $\underline{M}$ is diagonalizable. The additional contributions, at their maximum are of order $(1/\lambda)^2$ or $(1/\lambda)^3$ as opposed to the central one which is of order $(1/\lambda)$. Thus for values of $\lambda \gg 1$ sec^{-1} these subsidiary contributions are negligible. However, for matrices for which $\lambda \sim 1$, these contributions could be significant.

CONCLUDING REMARKS

In the normal mode analysis of linearized hydrodynamic equations the problem of nondiagonability of the fourier transformed hydrodynamic matrix has frequently been set aside.[5] However, for the case where only one of the variables in the coupled hydrodynamic equations is odd under time reversal,[9] one may make the following statements: If two of the roots are complex, then the hydrodynamic matrix is certainly diagonable; if there are no complex roots, then only three types of degeneracy can bring about nondiagonalizability, although these degeneracies can be encountered for many different parameterizations of the hydrodynamic matrix. As an illustration of one of the latter situations one may cite the case where all three roots[9] of the Fourier transformed hydrodynamic matrix of a simple fluid are real, i.e., one considers a case where a particular Fourier component of the sound mode is overdamped. If there are degenerate roots, then the hydrodynamic matrix will not be diagonalizable. Indeed at the point of crossover from the propagating to the nonpropagating components of the sound mode the hydrodynamic matrix is certainly nondiagonalizable [see, for example, Eq. (16)]. Another example is the case of chemical relaxation in the presence of a radiation field,[10] where, since the hydrodynamic matrix is non-Hermitian, both real and complex roots must be considered—again at the point of crossover from real to complex roots the matrix will not be diagonalizable. Yet another instance is in the normal mode analysis of the classical Bénard problem,[11,12] where, for certain values of the parameters, two real roots may become degenerate as one passes to the overstable region.

The time dependence of the "normal modes" in the case of nondiagonalizability is no longer a simple exponential but has an additional factor, a polynomial of order one or two (depending on the order of the degeneracy). The implications of this for the spectral density matrix elements have been considered here and indicate that there would be structure in the unshifted line which would not be present if the normal modes had their usual exponential time dependence. This structure may be pronounced when the magnitude of the degenerate eigenvalue is of order unity or smaller and certainly this will be realized for soft degenerate modes.[13]

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APPENDIX

A simple and elegant method of arriving at the JCF of a matrix is provided by the theory of finitely generated (FG) modules over a principal ideal domain (PID). For a reasonably elementary and very readable account of rings, modules, and their application to the computation of canonical forms, the reader is referred to Ref. 14. The basis of the present treatment is that we can regard the $\underline{K}$ matrix of Eq. (11) as a linear transformation, α, over the vector space $\mathbb{C}_{n+1}$ of complex $(n+1)$-tuples in the standard manner. We then make the underlying group of complex $(n \pm 1)$-tuples into a module over the ring $\mathbb{C}(\lambda)$ (the ring of polynomials with complex coefficients) using α in the usual manner.[14] $\mathbb{C}(\lambda)$ is a PID, and hence we know that this module can be decomposed into a sum of cyclic submodules whose orders are polynomials in λ and which can be arranged such that the order of the ith submodule in the sum is divided by that of the $(i-1)$th. [The order of a cyclic submodule is the unique monic polynomial which generates the order ideal of the submodule in $\mathbb{C}(\lambda)$.] These polynomials, called the torsion invariants of the module, are unique up to multiplication by constants. Suppose that the torsion invariants of the module we have constructed are d_i $(i = 1, \ldots, s)$

$$d_i = \prod_{j=1}^{n_i} (\lambda - \lambda_{ij})^{P_{ij}}, \quad P_{ij} \in \mathbb{Z}, \quad \lambda_{ij} \in \mathbb{C}. \tag{A1}$$

Then one can show that the JCF of $\underline{K}$ has a Jordan λ_{ij}-block of size precisely P_{ij}.[15] Thus, if one can obtain enough information about the torsion invariants of the module constructed, one can obtain the JCF of $\underline{K}$. In the proof of the theorems we will need only one additional fact about the d_i, namely

$$\prod_{i=1}^{s} d_i = \mathrm{ch}(\underline{K}).^{16} \tag{A2}$$

Before we proceed with the proof of Lemma 2, we need to know how, in practice, one goes about obtaining the d_i. We state without proof that:

If, given a matrix $\underline{K}$ of dimension $n+1$, one can, by a sequence of elementary row and column operations, reduce the matrix $(\lambda I_{n+1} - K)$ to $\mathrm{diag}(d_1, \ldots, d_{n+1})$ with $d_1 | d_2 | \cdots | d_{n+1}$, then the nonconstant elements of the set $\{d_i\}$ are the torsion invariants of the module constructed using $\underline{K}$ in the procedure indicated above.[17]

Proof of Lemma 2

What we actually will prove here is that the module constructed using a $\underline{K}^{\mathrm{BDF}}$ with a_i $(i = 1, \ldots, n)$ distinct has only one torsion invariant which is, therefore, by Eq. (A2), the characteristic polynomial of $\underline{K}$. In view of the preceding discussion this is clearly equivalent to the statement of the lemma in the body of the text. We

already know that the statement is true for the 2×2 case so that we proceed to calculate the torsion invariants in the 3×3 and 4×4 cases. Let R_i stand for row i, C_i for column i, and $\longleftrightarrow$ for transposition.

(i) 3×3 matrix:

$$\begin{bmatrix} \lambda-a_1 & 0 & -b_1 \\ 0 & \lambda-a_2 & -b_2 \\ b_1 & b_2 & \lambda-a_3 \end{bmatrix}$$

$$\xrightarrow{R_3 \leftrightarrow R_1} \begin{bmatrix} b_1 & b_2 & \lambda-a_3 \\ 0 & \lambda-a_2 & -b_2 \\ \lambda-a_1 & 0 & -b_1 \end{bmatrix}$$

$$\xrightarrow[\substack{C_2 \to -(b_2/b_1)C_1 \\ C_3 \to -[(\lambda-a_3)/b_1]C_1}]{R_3 \to -[(\lambda-a_1)/b_1]R_1} \begin{bmatrix} b_1 & 0 & 0 \\ 0 & \lambda-a_2 & -b_2 \\ 0 & -(b_2/b_1)(\lambda-a_1) & f(\lambda) \end{bmatrix},$$

where

$$f(\lambda) = -b_1 - (1/b_1)(\lambda-a_3)(\lambda-a_1)$$

$$\xrightarrow{C_3 \leftrightarrow C_2} \begin{bmatrix} b_1 & 0 & 0 \\ 0 & -b_2 & \lambda-a_2 \\ 0 & f(\lambda) & -(b_2/b_1)(\lambda-a_1) \end{bmatrix}$$

$$\xrightarrow[R_3 \to -[f(\lambda)/b_1]R_2]{C_3 \to (1/b_2)(\lambda-a_2)C_2} \begin{bmatrix} b_1 & 0 & 0 \\ 0 & -b_2 & 0 \\ 0 & 0 & -(b_2/b_1)(\lambda-a_1)+g(\lambda) \end{bmatrix},$$

where $g(\lambda) = f(\lambda)(\lambda-a_2)/b_2$. QED

(ii) 4×4 matrix: Following a similar procedure, one may show that

$$\begin{bmatrix} \lambda-a_1 & 0 & 0 & -b_1 \\ 0 & \lambda-a_2 & 0 & -b_2 \\ 0 & 0 & \lambda-a_3 & -b_3 \\ b_1 & b_2 & b_3 & \lambda-a_4 \end{bmatrix}$$

$$\to \begin{bmatrix} b_1 & 0 & 0 & 0 \\ 0 & -b_2 & 0 & 0 \\ 0 & 0 & (a_1-a_3) & 0 \\ 0 & 0 & 0 & h(\lambda) \end{bmatrix},$$

where

$$h(\lambda) = \frac{b_2}{b_1}(\lambda-a_1) - \frac{b_1}{b_2}(\lambda-a_2) - \frac{1}{b_1 b_2}(\lambda-a_1)(\lambda-a_2)(\lambda-a_4) - \frac{b_3^2(\lambda-a_1)(\lambda-a_2)}{b_1 b_2(a_1-a_3)}.$$ QED

As indicated in the text, we can now use the result of this lemma to prove Theorem 1. We will proceed to do so in the same way in which we proved the lemma, namely by showing that ch($\underline{K}$) is the only torsion invariant of the module we have constructed.

Proof of Theorem 1

Lemma 2 tells us that for the lowest possible dimensions of $\underline{K}^{BDF}$ the theorem is true. We proceed by induction. Suppose $n+1 \geq 5$.

Then by Lemma 1 $\exists$ at least one root, λ_0, of $\underline{K}^{BDF}$ with multiplicity $1 \Rightarrow \exists\ v \ni \mathbb{C}_{n+1}$ $\alpha(v) = \lambda_0 v$.

The $n+2$ vectors $B = \{v, e_{n+1}, e_1, \ldots, e_n\}$ are linearly dependent where $\{e_1, \ldots, e_{n+1}\}$ is the basis for $\mathbb{C}_{n+1}$ with respect to which $\underline{K}$ assumes the form $\underline{K}^{BDF}$.

$\therefore$ $\exists$ a first e_i which is a linear combination of the preceeding vectors. It is clearly not e_{n+1}.

The set $B - \{e_i\}$ is then a new basis for $\mathbb{C}_{n+1}$.

Let $\langle v \rangle$ be the subspace generated by v.

Then $\mathbb{C}_{n+1} \tilde{=} [\mathbb{C}_{n+1}/\langle v \rangle] \oplus \langle v \rangle$

If $\bar{\alpha}$ is the map induced on $\mathbb{C}_{n+1}/\langle v \rangle$ by α, then the module structure on $\mathbb{C}_{n+1}/\langle v \rangle$ via $\bar{\alpha}$ is the same as that on $\mathbb{C}_{n+1}/\langle v \rangle$ via α. Consider the following basis for $\mathbb{C}_{n+1}/\langle v \rangle$: $\{[e_1], \ldots, [e_{i-1}], [e_{i+1}], \ldots, [e_{n+1}]\}$, where $[e_j]$ is the equivalence class of e_j. The matrix $\underline{\bar{K}}$ of $\bar{\alpha}$ with respect to this basis is just $\underline{K}$ with the ith column and row removed. By hypothesis, therefore $\mathbb{C}_{n+1}/\langle v \rangle$ has only one torsion invariant, ch($\underline{\bar{K}}$).

By our choice of λ_0, ch($\underline{\bar{K}}$) and $(\lambda - \lambda_0)$ are relatively prime. It is known that the direct sum of two cyclic modules whose orders are relatively prime is also a cyclic module of order the product of the orders of the summands.[18]

Therefore, $\mathbb{C}_{n+1}$ is a cyclic module of order $(\lambda - \lambda_0)\,\mathrm{ch}(\underline{\bar{K}}) = \mathrm{ch}(\underline{K})$. This implies that ch($\underline{K}$) is the only torsion invariant of $\mathbb{C}_{n+1}$. QED

We are now prepared to prove Theorem 2, our main result. Lemma 3 and a modified form of Theorem 1 are the tools required. The idea behind the proof is very similar to that of Theorem 1. We decompose $\mathbb{C}_{n+1}$ into cyclic modules of relatively prime order in order to calculate the torsion invariants of the module we have constructed.

Proof of Theorem 2

Referring to Lemma 3, we call $e_{l_i} = e^i$. It is clear that

$$\bigcup_{i=1}^{p} \mathbb{C}_i \bigcup_{i=1}^{p+1} \{e^i\}$$

is a basis for $\mathbb{C}_{n+1}$. Let $\mathbb{C}_{n+1}^{\mathrm{red}} = \langle \cup_{i=1}^{p} \mathbb{C}^i \rangle$ the subspace generated by the union of the $\mathbb{C}^i$. Then $\mathbb{C}_{n+1} \cong \mathbb{C}_{n+1}^{\mathrm{red}} \oplus \mathbb{C}_{n+1}/\mathbb{C}_{n+1}^{\mathrm{red}}$.

A basis for the second summand is $B = \{[e^i], \ldots, [e^{p+1}]\}$.

Proceeding as in the proof of Theorem 1, we see that $\mathbb{C}_{n+1}/\mathbb{C}_{n+1}^{\text{red}}$ made into a module via α has the same structure as $\mathbb{C}_{n+1}/\mathbb{C}_{n+1}^{\text{red}}$ made into a module via the induced map $\bar{\alpha}$. Thus we can use the matrix of $\bar{\alpha}$ with respect to B to investigate the torsion invariants of this summand. One can easily show that $\underline{\bar{K}}$, the matrix of $\bar{\alpha}$ with respect to B, has the following form:

$$\underline{\bar{K}} = \begin{bmatrix} a^1 & & & & c_1^2/b_1 \\ & & 0 & & \vdots \\ & a^2 & & & \vdots \\ & \ddots & \ddots & & \vdots \\ 0 & & \ddots & & \vdots \\ & & & a^p & c_p^2/b_p \\ -b_1 & -b_2 & \cdots\cdots & -b_p & a^{p+1} \end{bmatrix}$$

This is not exactly in the same form as that of Theorem 1. However, using exactly the same procedure as before, one can easily show that the results of Theorem 1 hold equally well for this matrix. Thus the only torsion invariant for $\mathbb{C}_{n+1}/\mathbb{C}_{n+1}^{\text{red}}$ is $\text{ch}(\underline{\bar{K}}) = q(\lambda)$.

Now the restriction of α to $\mathbb{C}_{n+1}^{\text{red}}$ has $n-p$ eigenvectors while $\mathbb{C}_{n+1}^{\text{red}}$ has dimension $n-p$. Thus, the restriction is diagonalizable and therefore $\mathbb{C}_{n+1}^{\text{red}}$ has as many torsion invariants as the largest integer in the set $\{n_i - 1\}$, call it κ. Each of the last $n_i - 1$ torsion invariants has $(\lambda - a_i)$ occurring as a linear factor. The last torsion invariant is just $\Pi_{i=1}^{p}(\lambda - a_i)$. Thus $\mathbb{C}_{n+1}^{\text{red}} = \mathbb{C}_{n+1}^{\text{red},1} \oplus \cdots \oplus \mathbb{C}_{n+1}^{\text{red},\kappa}$, where $\mathbb{C}_{n+1}^{\text{red},\kappa}$ has the order $\Pi_{i=1}^{p}(\lambda - a_i) = r(\lambda)$.

Lemma 3 tells us that a_i is not a root of $Q(\lambda)$ and hence $r(\lambda)$, $Q(\lambda)$ are relatively prime. Therefore,

$$\mathbb{C}_{n+1}^{\text{red},\kappa'} = \frac{\mathbb{C}_{n+1}}{\mathbb{C}_{n+1}^{\text{red}}} \oplus \mathbb{C}_{n+1}^{\text{red},\kappa}$$

is cyclic of order $r(\lambda)Q(\lambda)$. Since the lower order torsion invariants of $\mathbb{C}_{n+1}^{\text{red}}$ divide $r(\lambda)$, they also divide $r(\lambda)q(\lambda)$. Therefore, the decomposition

$$\mathbb{C}_{n+1} \cong \mathbb{C}_{n+1}^{\text{red},1} \oplus \cdots \oplus \mathbb{C}_{n+1}^{\text{red},\kappa-1} \oplus \mathbb{C}_{n+1}^{\text{red},\kappa'} \tag{A3}$$

provides a torsion invariant decomposition of $\mathbb{C}_{n+1}$. Proceeding to the JCF of α, since the orders of the first $\kappa - 1$ summands in Eq. (A3) have only linear factors the Jordan blocks arising from them are 1×1. The only Jordan blocks of dimension greater than one thus arise from the order of $\mathbb{C}_{n+1}^{\text{red},\kappa'}$. It is clear that this will occur only for a degeneracy in the roots of $Q(\lambda)$. Since the a^i in $(\underline{\bar{K}})$ are distinct $\text{ch}(\underline{\bar{K}})$ has $p-1$ distinct real roots, $\lambda_1, \ldots, \lambda_{p-1}$ such that $a_1 < \lambda_1 < a_2 < \cdots < \lambda_{p-1} < a_p$. Since there are no equivalent restrictions on the remaining two type I roots, λ_p, λ_{p+1}, the following cases of degeneracy may arise.

(i) $\lambda_{p+1} = \lambda_p \neq \lambda_i, \quad i = 1, \ldots, p-1,$

(ii) $\lambda_{p+1} = \lambda_i$ or $\lambda_p = \lambda_i, \quad \lambda_p \neq \lambda_{p+1}, \quad i = 1, \ldots, p-1,$

(iii) $\lambda_{p+1} = \lambda_i, \quad \lambda_p = \lambda_j, \quad \lambda_p \neq \lambda_{p+1}, \quad i, j = 1, \ldots, p-1,$

(iv) $\lambda_p = \lambda_{p+1} = \lambda_i, \quad i = 1, \ldots, p-1.$

These are the only situations in which non-unit-sized Jordan blocks will arise.

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On the density of the Breit-Wigner functions

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It is shown, for certain sequences $\{\lambda_i\}$ in the complex plane, that linear combinations of the Breit-Wigner functions $\{B_i\}$ approximate, in the mean square, any function in $L^2(0,\infty)$. Implications and numerical use of this result are discussed.

I. INTRODUCTION

As W. Klink[1] has noted, it has been useful in certain problems of physics to approximate a function $f:(0,\infty)\to C$ by a superposition of Breit—Wigner (hereafter abbreviated B—W) functions B_i defined by

$$B_i(x)=1/(x+\lambda_i)\quad i=1,2,\cdots, \tag{1}$$

where $x\in R^+=(0,\infty)$, $\lambda_i\in C-R^-$, $R^-=(-\infty,0]$.

Each of the functions B_i is in $L^2(R^+)$, the Hilbert space of Lebesgue square integrable functions with norm induced by the inner product

$$(f,g)=\int_0^\infty f(x)\overline{g(x)}\,dx,\quad f,g\in L^2(R^+). \tag{2}$$

In this paper, we consider the problem of approximating functions $f\in L^2(R^+)$ by linear combinations of B—W functions. Straightforward calculations show that if $\{\lambda_i\}$, $i=1,2,\cdots$, is a set of distinct scalars (as we will assume in the remainder of the paper) the corresponding set $\{B_i\}$ of B—W functions is a linearly independent set. However, $\{B_i\}$ is not an orthogonal set.[1]

If one considers a finite set of B—W functions $\{B_1,\cdots,B_N\}$ and if $f\in \text{span}\{B_1,\cdots,B_N\}$, then there are unique scalars $c_1,\cdots,c_N$ such that

$$f=\sum_{i=1}^N c_iB_i. \tag{3}$$

The coefficients $\{c_1,\cdots,c_N\}$ are given by

$$c_i=(f,\phi_i),\quad i=1,\cdots,N, \tag{4}$$

where $\{\phi_1,\cdots,\phi_N\}$ is a set of functions biorthogonal to $\{B_1,\cdots,B_N\}$; that is, $(B_i,\phi_j)=\delta_{ij}$. For this case Klink[1] constructs functions, call them $y_1,\ldots,y_N$ such that

$$c_i=\int_0^\infty f(x)\overline{y_i(x)}\,dx,\quad i=1,\cdots,N. \tag{5}$$

If, however, we consider arbitrary functions f in $L^2(R^+)$ and infinite sets of B—W functions $\{B_i\,;i=1,2,\cdots\}$ the above procedure breaks down. We note, first of all, that the functions y_i constructed by Klink are not in $L^2(R^+)$ and thus the integral

$$\int_0^\infty f(x)\overline{y_i(x)}\,dx \tag{6}$$

will not exist for all functions f in $L^2(R^+)$. In Sec. II we show that for certain sequences $\{\lambda_1,\lambda_2,\cdots\}$, $\text{span}\{B_1,B_2,\cdots\}$ is dense in $L^2(R^+)$ and thus any function $f\in L^2(R^+)$ can be arbitrarily well approximated by linear combinations of B—W functions. However, for these same sequences, we show that there is not a set $\{\phi_i\}$ of functions biorthogonal to $\{B_i\}$ and thus $\{B_i\}$ cannot be a Schauder basis for $L^2(R^+)$; that is, not every f in $L^2(R^+)$ can be represented

$$f=\sum_i c_iB_i \tag{7}$$

where the c_i's are unique.

In Sec. III we consider best approximations of functions $f\in L^2(R^+)$ by finite linear combinations of B—W functions. We show that for a given set of B—W functions $\{B_1,\cdots,B_N\}$ there are infinitely many sets of functions $\{\phi_1,\cdots,\phi_N\}$ biorthogonal to $\{B_1,\cdots,B_N\}$. However, there is a unique set $\{\phi_1,\cdots,\phi_N\}$ such that for every $f\in L^2(R^+)$ the function

$$f_N=\sum_{i=1}^N(f,\phi_i)B_i$$

is the best $L^2(R^+)$ approximation to f by linear combinations of $\{B_1,\cdots,B_N\}$. Since Klink's biorthogonal functions are not in $L^2(R^+)$,[2] they cannot coincide with this set $\{\phi_i\}_1^N$ of functions biorthogonal to the $\{B_i\}_1^N$ that give the best $L^2(R^+)$ approximation to f.

Section IV and V concern, respectively, possible effects of error on the approximations and the problem of approximating functions of polynomial growth as $x\to+\infty$. These latter results are applicable to cases where scattering amplitudes grow like x^2 in the energy.

II. DENSITY OF THE BREIT-WIGNER FUNCTIONS

The main result of this section may be stated as follows: If (a) the $\{\lambda_i\}$ accumulate at a finite point in $C-R^-$, or (b) $\lambda_i=s+rp_i$ where $r>0$, $\text{Re}(s)>0$, $p_1=0$, $p_i>0$ for $i=2,3,\cdots$, $\lim_{i\to\infty}p_i=\infty$, and

$$\sum_{i=2}^\infty\frac{1}{p_i}=\infty,$$

then $\text{span}\{B_i\}$ is dense in $L^2(R^+)$.

We remark that the conclusion follows in case (a) from a result of Ribaric[3] and in case (b) from theorems of Lerch and Muntz.[4,5] Adaptation of these results to our problem is straightforward but the proof is included for completeness.

Proof Case (a): Let $F(\lambda)$ be the Stieltjes transform of $f\in L^2(R^+)$, defined

$$F(\lambda)\equiv\int_0^\infty\frac{f(x)}{x+\lambda}\,dx \tag{8}$$

which is analytic in $C-R^-$. Since f is known, F is also known. Note that $F(\bar\lambda_i)=(f,B_i)$. Let $\{\psi_i\}$ be an orthonor-

mal sequence obtained from $\{B_i\}$ (by the Gram–Schmidt process, say)

$$\psi_i = c_{i1}B_1 + c_{i2}B_2 + \cdots + c_{ii}B_i, \quad i = 1, 2, \cdots. \tag{9}$$

Hence,

$$(f, \psi_i) = \sum_{k=1}^{i} c_{ik} F(\lambda_k). \tag{10}$$

Now consider the sum

$$\sum_{i=1}^{\infty} (f, \psi_i)\psi_i. \tag{11}$$

By (9) each ψ_i is a linear combination of B_i's. Since f is in $L^2(R^+)$, Bessel's inequality assures that the series in (11) converges to some function in $L^2(R^+)$. Call this function g. We now need to show that $f = g$.

Let $G(\lambda)$ be the Stieltjes transform of g. $G(\bar{\lambda}_i) = F(\bar{\lambda}_i)$, $i = 1, 2, \cdots$, since g and f have the same Fourier coefficients. Indeed, making use of (10) we obtain

$$c_{11}F(\bar{\lambda}_1) = (f, \psi_i) = (g, \psi_1) = c_{11}\int_0^{\infty} \frac{g(x)}{x + \lambda_1}\, dx = c_{11}G(\bar{\lambda}_1)$$

and inductively, having $F(\bar{\lambda}_i) = G(\bar{\lambda}_i)$, $i = 1, 2, \cdots, n-1$, we obtain

$$c_{11}F(\bar{\lambda}_1) + \cdots + c_{n-1,n}F(\bar{\lambda}_{n-1}) + c_{nn}F(\bar{\lambda}_n) = c_{11}G(\bar{\lambda}_1) + \cdots + c_{n-1,n}G(\bar{\lambda}_{n-1}) + c_{nn}G(\bar{\lambda}_n)$$

and hence

$$F(\bar{\lambda}_n) = G(\bar{\lambda}_n).$$

Since the λ_i accumulate at a finite point in the region of analyticity of F and G, the identity theorem gives $F \equiv G$ in $C - R^-$ and by the uniqueness of the Stieltjes transform, $f = g$ a. e.

Proof Case (b): The proof is exactly the same up to the point of application of the identity theorem, which cannot be used since the λ_i's no longer must accumulate at a finite point.

Let $h = f - g$. We must show $h = 0$ a. e. Since f and g have the same Fourier coefficients, $H(\lambda)$, the Stieltjes transform of h, has the property that $H(\lambda_i) = 0$, $i = 1, 2, \cdots$. Moreover, since the Stieltjes transform is just an iterated Laplace transform, [6] we have

$$\int_0^{\infty} \exp(-\lambda_i t)(\mathcal{L}h)(t)\, dt = 0, \quad i = 1, 2, \cdots, \tag{12}$$

where $\mathcal{L}h$ is the Laplace transform of h. Since $h \in L^2(R^+)$, $\mathcal{L}h \in L^2(R^+)$, [7] and so $\mathcal{L}h$ is in $L(0, T)$ for all finite T. The result follows by applying Muntz's generalization of Lerch's theorem.

Klink[1] asks under what conditions it is possible to write

$$f = \sum_{i=1}^{\infty} c_i B_i \tag{13}$$

for $f \in L^2(R^+)$. A set of functions $\{\alpha_k\}$ is said to be a Schauder basis in a normed vector space S with norm $\|\cdot\|$ if for every element $\psi \in S$ there is a unique sequence of scalars $\{c_k\}$ such that

$$\lim_{N \to \infty} \|\psi - \sum_{k=1}^{N} c_k \alpha_k\| = 0. \tag{14}$$

Although $\text{span}\{B_i\}$ is dense in $L^2(R^+)$ for cases (a) and (b), we can show that the $\{B_i\}$ do not form a Schauder basis in $L^2(R^+)$. The reason the B_i's fail to be a Schauder basis is that in the construction of partial sums, everytime another term of the series is added on, the preceding coefficients in the sum change.

Theorem: If $\{\lambda_i\}$ is as in case (a) or (b), then a sequence $\{\phi_i\}$ biorthogonal to $\{B_i\}$ does not exist in $L^2(R^+)$.

Proof: The proof is by contradiction. Suppose $\{\phi_i\}$ is a sequence in $L^2(R^+)$ biorthogonal to $\{B_i\}$. Since $(\phi_1, B_k) = 0$ for all $k \geq 2$,

$$\phi_1 \in (\text{span}\{B_k : k \geq 2\})^{\perp}$$

($\perp$ denotes the orthogonal complement in Hilbert space) and obviously

$$\phi_1 \notin \overline{\text{span}}\{B_k : k \geq 2\}.$$

However, $\text{span}\{B_k : k \geq 2\}$ is dense in $L^2(R^+)$ since the sequence $\mu_n = \lambda_{n+1}$, $n = 1, 2, \cdots$, satisfies the conditions in case (a) or, respectively, case (b). This means $\phi_1 \in \overline{\text{span}}\{B_k : k \geq 2\}$ a contradiction.

Corollary: If $\{\lambda_i\}$ is as in case (a) or (b) then $\{B_i\}$ is not a Schauder basis.

Proof: The proof is by contradiction. Suppose $\{B_i\}$ is a Schauder basis. If

$$f = \sum_{i=1}^{\infty} c_i(f) B_i, \tag{15}$$

then each mapping $f \to c_i(f)$ is a continuous linear functional on $L^2(R^+)$. [8] Thus, for every i there is a unique $\phi_i \in L^2(R^+)$ such that

$$(f, \phi_i) = c_i(f). \tag{16}$$

By uniqueness of the expansion (15)

$$(B_k, \phi_i) = \delta_{k,i} \tag{17}$$

as is easily seen by choosing $f = B_k$. Thus $\{\phi_i\}$ is a sequence biorthogonal to $\{B_i\}$, an impossibility due to the result of the last theorem.

III. FINITE EXPANSIONS

If a function $f \in L^2(R^+)$ is to be approximated by a superposition of a finite number of B–W functions $B_i = 1/(x + \lambda_i)$, $i = 1, \cdots, N$, then of course f_N, the best approximation of f with respect to the $L^2(R^+)$ norm, is the orthogonal projection of f onto $\text{span}\{B_1, \cdots, B_N\}$. In order to find a formula for f_N, we recall that if $\lambda_1, \cdots, \lambda_N$ are distinct, then the set of functions $\{B_i : i = 1, \cdots, N\}$ is a linearly independent set. Thus the functions f_N can be obtained by using the Gram–Schmidt orthonormalization procedure to find an orthonormal basis $\{\psi_1, \cdots, \psi_N\}$ for $\text{span}\{B_1, \cdots, B_N\}$

$$f_N = \sum_{i=1}^{N} (f, \psi_i)\psi_i. \tag{18}$$

As Klink[1] indicates, it is sometimes desirable to write f_N in terms of the functions $\{B_i\}$ instead of the orthonormalized functions $\{\psi_i\}$. That is we would like to write

$$f_N=\sum_{i=1}^{N} c_iB_i. \tag{19}$$

It follows from the Gram–Schmidt orthonormalization procedure that

$$\psi_i=c_{i1}B_1+\cdots+c_{ii}B_i, \quad i=1,\cdots,N, \tag{20}$$

substituting this expansion for ψ_i into Eq. (18) and recombining the coefficients will give Eq. (19).

However, as Klink[1] observes, if $f\in \text{span}\{B_1,\cdots,B_N\}$ and if $\{\phi_1,\cdots,\phi_N\}$ is a set of functions biorthogonal to $\{B_1,\cdots,B_N\}$, then

$$f=\sum_{i=1}^{N}(f,\phi_i)B_i. \tag{21}$$

There are infinitely many different sets of functions $\{\phi_1,\cdots,\phi_N\}$ biorthogonal to $\{B_1,\cdots,B_N\}$. In fact, since $\dim[\text{span}\{B_i: i=1,\cdots,N\}]=N$ and $\dim[\text{span}\{B_i: i=1,\cdots,N, i\neq j\}]=N-1$, for the function ϕ_j we can take any function, appropriately normalized, in the orthogonal complement of $\text{span}\{B_i: i=1,\cdots,N, i\neq j\}$ with a component in the B_j direction.

Proposition 1: Given the set of distinct B–W functions $\{B_1,\cdots,B_N\}$, then there is a unique[9] set of $L^2(R^+)$ functions $\{\phi_1,\cdots,\phi_N\}$ biorthogonal to $\{B_1,\cdots,B_N\}$ such that for every $f\in L^2(R^+)$

$$f_N=\sum_{i=1}^{N}(f,\phi_i)B_i. \tag{22}$$

Proof: Let $H_N=\text{span}\{B_n: n=1,\cdots,N\}$ and for each $j=1,\cdots,N$ let $H_{N,j}=\text{span}\{B_n: n=1,\cdots,N, n\neq j\}$. Since $\dim H_N=N$ and $\dim H_{N,j}=N-1$, there is a unique function $\phi_j\in H_N$ such that $(B_k,\phi_j)=\delta_{k,j}$, $k=1,\cdots,N$. For this set of functions $\{\phi_1,\cdots,\phi_N\}$ and for any $f\in L^2(R^+)$ we have Eq. (22). The uniqueness follows from the fact that the coefficients c_n in Eq. (19) are unique and that if $\phi_j\neq\hat{\phi}_j$ then there is at least one function $f\in L^2(R^+)$ such that $(f,\phi_j)\neq(f,\hat{\phi}_j)$.

Given a set of B–W functions $\{B_1,\cdots,B_N\}$ we now give two ways of determining the unique biorthogonal set of Proposition 1.

Method 1: Consider the matrix $(M_{i,j})$ where $M_{i,j}=(B_i,B_j)$. As Klink[1] observes

$$\phi_j=\sum_{i=1}^{N}N_{i,j}B_i,$$

where the matrix $(N_{i,j})=(M_{i,j})^{-1}$. Even though $(M_{i,j})^{-1}$ exists, the matrix $(M_{i,j})$ may be ill-conditioned, especially if the λ_j are close together. Thus if $(M_{i,j})^{-1}$ is found numerically, a very significant error can be introduced into the coefficients $N_{i,j}$.

Method 2: Take the ordered set $B_1,\cdots,B_N$ and perform the Gram–Schmidt orthogonalization procedure: Letting $\psi_1=B_1$ and assuming $\psi_1,\cdots,\psi_{i-1}$ are calculated, let

$$\psi_i=B_i-\sum_{k=1}^{i-1}\frac{(B_k,\psi_k)}{(\psi_k,\psi_k)}\psi_k;$$

then the last function ψ_N is such that $(B_i,\psi_N)=0$, $i=1,\cdots,N-1$, and $(B_N,\psi_N)\neq 0$. Thus $\phi_N=\psi_N/(B_N,\psi_N)$. To find the function ϕ_j we reorder the functions $\{B_n\}$ so that B_j is last and then proceed as above. Of course, by judicious reordering, the amount of work involved can be greatly reduced.

IV. EFFECT OF ERROR

It was shown in Sec. II that for any f in $L^2(R^+)$, the series

$$\sum_{i=1}^{\infty}(f,\psi_i)\psi_i,$$

where $\{\psi_i\}$ is an orthonormal sequence obtained from $\{B_i\}$, converges in $L^2(R^+)$ to f. The construction was based upon the Stieltjes transform of f.

Let us suppose that the Stieltjes transform of f is known with error $\epsilon(\lambda)$. Call it $F(\lambda)+\epsilon(\lambda)$. Further, let $\{B_n\}$, $n=1,2,\cdots,N$, be the finite set of B–W functions with which we plan to approximate f in the best $L^2(R^+)$ fashion. Using the main result, we have

$$f\approx\sum_{i=1}^{N}\left(\sum_{j=1}^{N}c_{ij}[F(\lambda_j)+\epsilon(\lambda_j)]\right)\psi_i \tag{23}$$

where the c_{ij} and ψ_i are defined as in (9). So we have

$$f\approx\sum_{i=1}^{N}\left(\sum_{j=1}^{N}c_{ij}F(\lambda_j)\right)\psi_i+\sum_{i=1}^{N}\left(\sum_{j=1}^{N}[c_{ij}\epsilon(\lambda_j)]\right)\psi_i \tag{24}$$

and it is clear that determination of the behavior of the c_{ij}'s shows how the error ϵ is magnified in the approximation to f.

To this end, recall that the Gram matrix[10]

$$G=\begin{pmatrix}(B_1,B_1)&\cdots&(B_1,B_N)\\ \vdots&&\vdots\\ (B_N,B_1)&\cdots&(B_N,B_N)\end{pmatrix} \tag{25}$$

has a minimum eigenvalue $m\geq 0$, and this number is called the measure of independence of $B_1,\cdots,B_N$. Thus the vanishing of the Gramian $[\equiv\det(G)]$ is necessary and sufficient for the linear dependence of the B_i's. The result of interest here is that if $m\geq\mu$ and the B_i's are orthogonalized as in (9), then

$$|c_{ij}|\leq 1/\sqrt{\mu}$$

for all i and j. The consequences of this result are given below.

Note that the entries of G are given by

$$(B_i,B_j)=\frac{1}{\lambda_i-\lambda_j}\log\frac{\lambda_i}{(\lambda_j)}, \quad i\neq j,$$

$$=\arg(\lambda_i)/\text{Im}(\lambda_i), \quad i=j,\ \lambda_i\notin R,$$

$$=1/\lambda_i, \quad i=j,\ \lambda_i\in R.$$

Let $\hat{\lambda}_i=k\lambda_i$, $i=1,2,\cdots,N$, $k>0$, and $\hat{B}_i$ be defined (26)

$$\hat{B}_i(x)=1/(x+\hat{\lambda}_i), \quad x\in R^+.$$

Then $(\hat{B}_i,\hat{B}_j)=k^{-1}(B_i,B_j)$, the measure of independence of $\hat{B}_1,\cdots,\hat{B}_N$ is m/k and the orthogonalization coefficients $\hat{c}_{ij}$ associated with the $\{\hat{B}_i\}$ are bounded:

$$|\hat{c}_{ij}|\leq\sqrt{k/\mu}. \tag{27}$$

This shows that the closer a set of λ_i's is pushed toward the origin (i.e., choosing k small) the smaller the orthogonalization coefficients. A numerical example with $N=3$ is listed in Table I. (Calculations done on Hewlett Packard HP9830). Note the $\sqrt{k}$ dependence in the $c_{i,j}$'s.

At first glance, it appears that to minimize error in the approximation in (24) one needs to merely push the λ_i's closer to the origin. However, $\epsilon(\lambda_i)$ will, in general, increase as $\lambda_i \to 0$, since

$$F(\lambda_i) + \epsilon(\lambda_i) = \int_0^\infty \frac{f(x)}{x+\lambda_i}\,dx. \tag{28}$$

Since $f(x)$ is only assumed to be in $L^2(R^+)$, when λ_i is near zero the integrand in (28) can be nearly singular at the origin. Therefore, for a given f the best choice of $\{\lambda_i\}$, $i=1, 2, \cdots, N$, will most likely be close to the origin, but not so close that $\epsilon(\lambda_i)$ increase faster than the $|c_{ij}|$ decrease. The choice is problem dependent and no general choice criterion can be given.

V. WEIGHT FUNCTIONS

Since scattering amplitudes may not be square integrable functions, but may grow at infinity like x^2, we consider for each real number k the Hilbert space

$$H_k = \{f : \int_0^\infty (x+1)^k |f(x)|^2\,dx < \infty\},$$

with inner product

$$(f, g)_k = \int_0^\infty (x+1)^k f(x)\overline{g(x)}\,dx.$$

$L^2(R^+)$ is then H_0.

A B—W function $B(x) = 1/(x+\lambda)$ is then in every space H_k for $k < 1$.

If $k_1 < k_2$, then clearly $H_{k_2} \subset H_{k_1}$ both algebraically and topologically. Moreover, since the functions of compact support are dense in every space H_k, we have as a vector space, H_{k_2} is dense in H_{k_1}.

The work of the preceeding sections can be adapted to any of the spaces H_k, $k<1$, by merely changing the inner product from $\int_0^\infty f(x)\overline{g(x)}\,dx$ to $\int_0^\infty (x+1)^k f(x)\overline{g(x)}\,dx$ this allows us to approximate scattering amplitudes with polynomial growth by B—W functions.

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A nonlinear system of Euler–Lagrange equations. Reduction to the Korteweg–de Vries equation and periodic solutions

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The Euler–Lagrange equations, which correspond to a variational principle with a Lagrange function depending on arbitrary functions and their first order derivatives, are shown to be reducible to the Korteweg–de Vries equation under a small—but finite—amplitude approximation. Closed form periodic solutions to the Euler–Lagrange equations are found for a particular case, and the modulational stability of these solutions is discussed. Equations for waves in cold plasma are discussed as examples.

1. INTRODUCTION

A wide class of nonlinear partial differential equations of mathematical physics can be derived from a variational principle with a Lagrangian of the following type type[1]:

$$L(n_1, \circ\circ\circ, n_k; \varphi_1, \cdots, \varphi_l; \varphi_{1x}, \cdots, \varphi_{lx}; \varphi_{1t}, \circ\cdots, \varphi_{lt}; \alpha_{1x}, \cdots, \alpha_{mx}; \alpha_{1t}, \circ\cdots, \alpha_{mt}) \tag{1}$$

where $\varphi_{lx}, \varphi_{lt}$ are space and time derivatives, respec-respectively.

If we consider stationary solutions, i.e., ones depending only on a variable $\Theta = kx - \omega t$ ($k = \text{const}$, $\omega = \text{const}$) we can obtain from (1) an equivalent Hamilton system, which is autonomous and conservative as the independent variables x, t or their combination Θ do not appear explicitly. Thus the existence of an energy in0 integral is assured and we would not expect to find any damped solutions. The most interesting features of autonomous, conservative systems are periodic solutions, the trajectories of which usually fill up a subspace in a corresponding phase space whereas nonconservative systems have at most isolated periodic trajectories—limit cycles.

These properties of stationary solutions of the variational equations originating from (1) show that we are considering a nonlinear dispersive system. It is the dispersion that balances the nonlinearity effects resulting in formation of periodic solutions. In nonlinear dissipative systems the nonlinear steepening of waves is balanced by dissipative effects leading to shock waves and with both the dispersion and dissipation present we can expect stationary solutions in a form of shocks of an oscillating structure.[2]

It has been shown,[3,4] that certain classes of nonlinear equations, under the weak nonlinearity and long wavelength approximations can be reduced to either the Korteweg–de Vries equation

$$n_\tau + nn_\xi + \delta n_{\xi\xi\xi} = 0$$

or the Burgers equation

$$n_\tau + nn_\xi - \nu n_{\xi\xi} = 0$$

depending on whether the system is dispersion or dissipation dominated. It is shown in the present paper that, under similar assumptions, the system of equations originating from (1) can be reduced to the Korteweg–de Vries (KdV) equation. By way of example, equations for waves in cold plasma are considered, which, in a different form, have been already reduced to the KdV equation.[3] This reduction is particularily relevant as the KdV equation has been solved.[5]

Some fairly general theorems concerning the existence of periodic solutions of conservative dynamic systems have been proved,[6] but, for practical reasons, it is useful to look for periodic solutions in a closed form. Although the last problem has also been studied extensively in classical mechanics,[7] it seems that there remain some important cases to be solved. Here stationary periodic solutions of equations originating from (1) are found for the case of only one φ function and an arbitrary number of parameter functions n_i, which appear in (1) only by themselves and without derivatives, and potentials α_i, the last appearing in (1) only through their derivatives. It is also assumed that the dependence of the Lagrangian (1) on all the derivatives $\varphi_i, \varphi_t, \alpha_{ix}, \alpha_{it}$ is quadratic. Again the equations for waves in cold plasma are discussed as example but it is worth noting that all the equations considered by Whitham[8] in his study of dispersive waves fall within this clase.

The modulational stability of nonlinear dispersive waves, the theory of which in the Lagrangian formalism has been formulated by Whitham,[8] is also discussed here. The theory is specified for the case of a "quadratic" Lagrangian so that the existence of periodic stationary solutions in closed form is assured.

Finally, a nondispersive case is discussed and a condition for the equations to be hyperbolic is obtained. The condition might prove relevant for the stability theory of Ref. 8.

2. REDUCTION TO THE KORTEWEG-DE VRIES (KdV) EQUATION

A. Waves in cold plasma

Let us first consider a Lagrangian

$$L = n(\alpha_t + \tfrac{1}{2}\alpha_x^2) + G(n; \varphi, \varphi_x, \varphi_t) \tag{2}$$

and the variational principle

$$\delta \int \int L\, dx\, dt = 0.$$

The corresponding Euler-Lagrangian (E—L) equations are

$$\delta\alpha:\ n_t+(n\alpha_x)_x=0, \tag{3}$$

$$\delta n:\ \alpha_t+\tfrac{1}{2}\alpha_x^2+G_n=0, \tag{4}$$

$$\delta\varphi:\ G_{\varphi_t t}+G_{\varphi_x x}-G_\varphi=0, \tag{5}$$

where

$$G_{\varphi_t t}=\left(\frac{\partial}{\partial t}\frac{\partial G}{\partial \varphi_t}\right), \text{ etc.}$$

If we take n for density and α for a velocity potential $u=\alpha_x$, then (3) is the continuity equation and (4), after differentiation with respect to x, yields the equation of motion.

For ion–acoustic waves in cold collisionless plasma we set $G=-\frac{1}{2}\varphi_x^2+n\varphi-e^\varphi$ where φ denotes now the electrostatic potential, and the variational equations become[2]

$$n_t+(nu)_x=0,\quad u_t+uu_x+\varphi_x=0,\quad \varphi_{xx}-e^\varphi+n=0.$$

With $\varphi\equiv B$ (magnetic field intensity) and

$$G=-\frac{1}{2n}B_x^2-\tfrac{1}{2}B^2+nB \tag{6}$$

we obtain from (3)–(5) equations for hydromagnetic waves in cold plasma propagating across the magnetic field[2]:

$$n_t+(nu)_x=0,\quad u_t+nu_x+\frac{B}{n}B_x=0,\quad (B_x/n)_x=n-B. \tag{7}$$

Su and Gardner[3] considered these equations as special cases of a different (in general) class of equations and they did not derive the equations from any variational principle.

Assume first, that $G=G(n,\varphi)$, i.e., we drop the dependence of G on the derivatives φ_x,φ_t. Equation (5) yields now

$$G_\varphi(n,\varphi)=0. \tag{8}$$

Differentiating Eqs. (4) and (5) and replacing φ_x in (4) by the corresponding expression calculated by differentiation of (8), we get

$$n_t+(nu)_x=0,\quad u_t+nu_x+\frac{a^2}{n}n_x=0 \tag{9}$$

where $u=\alpha_x$, $a^2/n=G_{nn}-G_{n\varphi}^2/G_{\varphi\varphi}$. We assume that $a^2>0$. The set of Eqs. (9) is hyperbolic and its characteristic roots are $\lambda=n\pm a$. This set is also homogeneous in derivatives and thus it can have stationary solutions in a form of steady states and jump discontinuities only. The set (9) is thus dissipation–and dispersion free and we can see that it is the derivatives φ_x,φ_t in (2) that are responsible for the dispersion. If we linearize Eqs. (9) around a uniform state $n=n_0$, $u=0$, $\varphi=\varphi_0$, we obtain a wave equation

$$u_{tt}-a_0^2u_{xx}=0 \tag{10}$$

with $a_0^2=a^2(n_0,\varphi_0,0)$.

The main step toward reduction to the Korteweg–de Vries equation is to introduce (after Gardner & Morikawa[3]) the transformation

$$\xi=\epsilon^\alpha(x-a_0t),\quad \tau=\epsilon^{\alpha+1}t \tag{11}$$

where ϵ denotes the amplitude of the initial disturbance and is assumed to be small compared with unity. The transformation (11) includes coordinate contraction and transformation to a waveframe so that the final equation shall describe slow changes of one of the waves governed by the wave equation (10). The exponent $\alpha>0$ is to be determined so that there be no dependence on ϵ in the final equation.

We assume, that the function $G(n,\varphi,\varphi_x,\varphi_t)$ and its derivatives $G_n,G_\varphi,G_{\varphi x},G_{\varphi t}$ can be Taylor-expanded around the uniform state $n=n_0$, $\varphi=\varphi_0$. After the transformation (11) has been applied to Eqs. (3) and (4), the following equations are obtained:

$$\epsilon n_\tau+(u-a_0)n_\xi+nu_\xi=0, \tag{12}$$

$$\epsilon u_\tau+(u-a_0)u_\xi+G_{n\xi}=0. \tag{13}$$

Equation (13) shall yield the KdV equation, and Eq. (12) together with (5) will be used for elimination of u and φ.

We also assume that the functions n, u, and φ have an asymptotic representation:

$$\begin{aligned} n&=n_0+\epsilon n^{(1)}+\epsilon^2n^{(2)}+\cdots,\\ u&=\epsilon u^{(1)}+\epsilon^2u^{(2)}+\cdots,\\ \varphi&=\varphi_0+\epsilon\varphi^{(1)}+\epsilon^2\varphi^{(2)}+\cdots. \end{aligned} \tag{14}$$

Inserting the representation (14) into (12), we obtain

$$\begin{aligned} &\epsilon\frac{\partial}{\partial\tau}(\epsilon n^{(1)}+\epsilon^2n^{(2)}+\cdots)+[(\epsilon u^{(1)}+\epsilon^2u^{(2)}+\cdots)-a_0]\\ &\times\frac{\partial}{\partial\xi}(\epsilon n^{(1)}+\epsilon^2n^{(2)}+\cdots)+(n_0+\epsilon n^{(1)}+\epsilon^2n^{(2)}+\cdots)\\ &\times\frac{\partial}{\partial\xi}(\epsilon u^{(1)}+\epsilon^2u^{(2)}+\cdots)=0 \end{aligned}$$

involving a sequence of equations

$$(\epsilon^1)\quad n_0u_\xi^{(1)}-a_0n_\xi^{(1)}=0, \tag{15}$$

$$(\epsilon^2)\quad n_\tau^{(1)}+u^{(1)}n_\xi^{(1)}-a_0n_\xi^{(2)}+n_0u_\xi^{(2)}+n^{(1)}u_\xi^{(1)}=0 \tag{16}$$

Equation (5) can be written as

$$\epsilon^{\alpha+1}\frac{\partial}{\partial\tau}G_{\varphi t}-a_0\epsilon^\alpha\frac{\partial}{\partial\xi}G_{\varphi t}+\epsilon^\alpha\frac{\partial}{\partial\xi}G_{\varphi x}-G_\varphi=0. \tag{17}$$

Next, the functions $G_{\varphi t}$, $G_{\varphi x}$, and G_φ can be expanded. For $G_{\varphi x}$, e.g., we have

$$\begin{aligned} G_{\varphi x}=&G_{\varphi_x n0}\Delta n+\tfrac{1}{2}G_{\varphi_x nn0}(\Delta n)^2+\cdots\\ &+G_{\varphi_x\varphi0}\Delta\varphi+\tfrac{1}{2}G_{\varphi_x\varphi\varphi0}(\Delta\varphi)^2+\cdots\\ &+G_{\varphi_x\varphi_x0}\Delta\varphi_x+\tfrac{1}{2}G_{\varphi_x\varphi_x\varphi_x0}(\Delta\varphi_x)^2+\cdots\\ &+G_{\varphi_x\varphi_t0}\Delta\varphi\ +\tfrac{1}{2}G_{\varphi_x\varphi_t\varphi_t0}(\Delta\varphi_t)^2+\cdots, \end{aligned}$$

where $\Delta n=n-n_0=\epsilon n^{(1)}+\epsilon^2n^{(2)}+\cdots$,

$$G_{\varphi_x n0}=(\partial^2G/\partial\varphi_x\partial n)\Big|_{n=n_0,\ \varphi=\varphi_0}, \text{ etc.}$$

Equation (17) yields now a recurrent set of equations

$$\begin{aligned} &(\epsilon^0)\quad G_{\varphi0}=0,\\ &(\epsilon^1)\quad G_{\varphi n0}n^{(1)}+G_{\varphi\varphi0}\varphi^{(1)}=0,\\ &(\epsilon^2)\quad -[G_{\varphi n0}n^{(2)}+G_{\varphi\varphi0}\varphi^{(2)}+\tfrac{1}{2}G_{\varphi nn0}(n^{(1)})^2+\tfrac{1}{2}G_{\varphi\varphi\varphi0}(\varphi^{(1)})^2]\\ &\quad+\epsilon^{\alpha-1}[n_\xi^{(1)}(G_{\varphi_x n0}-G_{\varphi_t n0})] \end{aligned} \tag{18}$$

$$+\epsilon^{2\alpha-1}[\varphi_{\xi\xi}^{(1)}(G_{\varphi_x\varphi_x 0}-2a_0G_{\varphi_x\varphi_t 0}+a_0^2G_{\varphi_t\varphi_t 0})]=0 \quad (19)$$

The term of the order of $\epsilon^{2\alpha-1}$ has been left in (19) because the coefficient at $\epsilon^{\alpha-1}$ will ultimatily disappear so that with $\alpha=\frac{1}{2}$ we shall obtain $\epsilon^{2\alpha-1}=1$.

A similar sequence of equations originates from (12):

$$(\epsilon^1)\quad -a_0u_\xi^{(1)}+G_{nn0}n_\xi^{(1)}+G_{n\varphi 0}\varphi_\xi^{(1)}=0, \quad (20)$$

$$(\epsilon^2)\quad u^{(1)}+u^{(1)}u_\xi^{(1)}-a_0u_\xi^{(2)}G_{nn0}n_\xi^{(2)}+G_{nnn0}n_\xi^{(1)}n^{(1)}+G_{n\varphi 0}\varphi_\xi^{(2)}$$
$$+G_{n\varphi\varphi 0}\varphi_\xi^{(1)}\varphi^{(1)}+\epsilon^{\alpha-1}[G_{n\varphi_x 0}-a_0G_{n\varphi_t 0}]\varphi_{\xi\xi}^{(1)}=0, \quad (21)$$

Equation (20) coincides with (15) [if we take account of (18)] to yield

$$n_0u^{(1)}=a_0n^{(1)}$$

with proper boundary conditions assumed, e.g., $u^{(1)}=0$ and $n^{(1)}=0$ for $\xi\to\infty$.

The equations formed of terms of the order of ϵ^2, i.e., (16), (19), and (21), result now in a single equation

$$2\frac{a_0}{n_0}n^{(1)}+\left(2\frac{a_0^2}{n_0^2}+An^{(1)}\right)n_\xi^{(1)}+\epsilon^{2\alpha-1}Bn_{\xi\xi\xi}^{(1)}=0, \quad (22)$$

where A and B are constant coefficients

$$A=\frac{a_0^2}{n_0^2}+\left(G_{nnn0}-G_{\varphi nn0}\frac{G_{n\varphi 0}}{G_{\varphi\varphi 0}}\right)+\frac{G_{n\varphi 0}^2}{G_{\varphi\varphi 0}^2}\left(G_{n\varphi\varphi 0}-G_{\varphi\varphi\varphi 0}\frac{G_{n\varphi 0}}{G_{\varphi\varphi 0}}\right),$$

$$B=-\frac{G_{\varphi n0}^2}{G_{\varphi\varphi 0}^2}(G_{\varphi_x\varphi_x 0}-2a_0G_{\varphi_x\varphi_t 0}+a_0^2G_{\varphi_t\varphi_t 0}).$$

Taking $\alpha=\frac{1}{2}$ and performing a linear transformation in (22)

$$n=\frac{a_0}{n_0}+\frac{An_0}{2a_0}n^{(1)},$$

we arrive at the normal form of the Korteweg–de Vries equation

$$n_\tau+nn_\xi+Cn_{\xi\xi\xi}=0,$$

where $C=Bn_0/2a_0$.

B. Equations originating from $L=L(n;\varphi,\varphi_x,\varphi_t;\alpha_x,\alpha_t)$

In this more general case, the E–L equations are

$$\begin{aligned}&\delta n:\quad n_\xi^{(1)}+L_n=0,\\ &\delta\varphi:\quad L_{\varphi_t t}+L_{\varphi_x x}=L_\varphi,\\ &\delta\alpha:\quad L_{\alpha_t t}+L_{\alpha_x x}=0.\end{aligned} \quad (23)$$

First, we introduce new variables

$$\alpha_x=u,\quad \alpha_t=v,$$

so that

$$u_t=v_x. \quad (24)$$

Now, we can apply the transformation (11) and use the representation (14), the expression for v being similar to that of u, although we have no simple interpretation for a as in the former case. Here, the parameter a_0 shall be determined from an algebraic equation obtained in the first order of approximation.

To lowest order we get

$$(\epsilon^0)\quad L_{n0}=0,\quad L_{\varphi 0}=0,$$

which is equivalent to the condition that there exist constant state solutions.

The "first order" equations are

$$(\epsilon^1)\quad L_{nn0}n^{(1)}+L_{n\varphi 0}\varphi^{(1)}+L_{n\alpha_x 0}u^{(1)}+L_{n\alpha_t 0}v^{(1)}=0, \quad (25)$$

$$L_{\varphi n0}n^{(1)}+L_{\varphi\varphi 0}\varphi^{(1)}+L_{\varphi\alpha_x 0}u^{(1)}+L_{\varphi\alpha_t 0}v^{(1)}=0, \quad (26)$$

$$(L_{\alpha_x n0}-a_0L_{\alpha_t n0})n_\xi^{(1)}+(L_{\alpha_x\varphi 0}-a_0L_{\alpha_t\varphi 0})\varphi_\xi^{(1)}$$
$$+(L_{\alpha_x\alpha_x 0}-a_0L_{\alpha_t\alpha_x 0})u_\xi^{(1)}+(L_{\alpha_x\alpha_t 0}-a_0L_{\alpha_t\alpha_t 0})v_\xi^{(1)}=0, \quad (27)$$

$$a_0u_\xi^{(1)}+v_\xi^{(1)}=0. \quad (28)$$

From these equations, differentiating (25) and (26) with respect to ξ and using (28) to eliminate $u^{(1)}$ in favor of we get a linear system of algebraic equations for

$$Az_\xi^{(1)}=0, \quad (29)$$

with a symmetric matrix

$$A=\begin{pmatrix}p_1 & s_1 & s_2\\ s_1 & p_2 & s_3\\ s_2 & s_3 & p_3\end{pmatrix}\equiv\begin{pmatrix}L_{nn0} & L_{n\varphi 0} & L_{n\alpha_x 0}-a_0L_{n\alpha_t 0}\\ L_{\varphi n0} & L_{\varphi\varphi 0} & L_{\varphi\alpha_x 0}-a_0L_{\varphi\alpha_t 0}\\ L_{\alpha_x n0}-a_0L_{\alpha_t n0} & L_{\alpha_x\varphi 0}-a_0L_{\alpha_t\varphi 0} & L_{\alpha_x\alpha_x 0}-2a_0L_{\alpha_t\alpha_x 0}+a_0^2L_{\alpha_t\alpha_t 0}\end{pmatrix}. \quad (30)$$

The compatibility condition for (29)

$$\det A=0 \quad (31)$$

is a second-degree algebraic equation for a_0, so that we can assume that a_0 is known. The condition, in turn, that a_0 be real is a certain limitation on the class of possible constant states $n=n_0$, $\varphi=\varphi_0$.

The element of A depends only on constant parameters n_0, φ_0, so that basing on (29) we can write

$$z^{(1)}=n^{(1)}r_0\quad (\text{if } z^{(1)}\to 0 \text{ for } \xi\to-\infty), \quad (32)$$

where r_0 is an eigenvector of A with the component corresponding to $n^{(1)}$ normalized to unity. There exist three linearily independent eigenvectors of A:

$$r_0^{(1)}=\left(1,\frac{s_2s_3-s_1p_3}{p_2p_3-s_3^2},\frac{s_1s_3-s_2p_2}{p_2p_3-s_3^2}\right)\equiv(r_{0n}^{(1)},r_{0\varphi}^{(1)},r_{0u}^{(1)}),$$

$$r_0^{(2)}=\left(1,\frac{s_2^2-p_1p_3}{s_1p_3-s_2s_3},\frac{p_1s_3-s_1s_2}{s_1p_3-s_2s_3}\right),$$

$$r_0^{(3)}=\left(1,\frac{s_1s_2-p_1s_3}{s_1s_3-p_2s_2},\frac{p_1p_2-s_1^2}{s_1s_3-p_2p_2}\right),$$

but we have no need to use any particular one so we shall write $r_0=(r_{0n},r_{0\varphi},r_{0u})$.

The "second order" equations, in turn, have the form

$$(\epsilon^2)\quad Az_\xi^{(2)} + Bfn^{(1)}n_\xi^{(1)} + gn_\tau^{(1)} + \epsilon^{\alpha-1}hn_{\xi\xi}^{(1)} - \epsilon^{2\alpha-1}jn_{\xi\xi\xi}^{(1)} = 0. \tag{33}$$

$$B = \begin{pmatrix} L_{nnn0} & L_{n\varphi\varphi0} & L_{n\alpha_x\alpha_x} + a_0^2 L_{n\alpha_t\alpha_t0} \\ L_{\varphi nn0} & L_{\varphi\varphi\varphi0} & L_{\varphi\alpha_x\alpha_x0} + a_0^2 L_{\varphi\alpha_t\alpha_t0} \\ & & L_{\alpha_x\alpha_x\alpha_x} - a_0 L_{\alpha_t\alpha_x\alpha_x0} \\ L_{\alpha_x nn0} - a_0 L_{\alpha_t nn0} & L_{\alpha_x\varphi\varphi0} - a_0 L_{\alpha_t\varphi\varphi0} & + a_0^2(L_{\alpha_x\alpha_t\alpha_t} - a_0 L_{\alpha_t\alpha_t\alpha_t}) \end{pmatrix}$$

and the column vectors f, g, j, and h are

$$f = \begin{pmatrix} r_{0n}^2 \\ r_{0\varphi}^2 \\ r_{0u}^2 \end{pmatrix},\quad g = \begin{pmatrix} L_{n\alpha_t0}r_{0n} \\ L_{\varphi\alpha_t0}r_{0\varphi} \\ L_{\alpha_t n0}r_{0n} + L_{\alpha_t\varphi0}r_{0\varphi} + 2(L_{\alpha_x\alpha_t} - a_0 L_{\alpha_t\alpha_t0})r_{0u} \end{pmatrix}$$

$$j = \begin{pmatrix} 0 \\ a_0^2 L_{\varphi_t\varphi_t} - 2a_0 L_{\varphi_x\varphi_t0} + L_{\varphi_x\varphi_x} \\ 0 \end{pmatrix},\quad h = \begin{pmatrix} pr_{0\varphi} \\ -pr_{0n} - qr_{0u} \\ qr_{0\varphi} \end{pmatrix},$$

with $p = L_{n\varphi_x0} - a_0 L_{n\varphi_t0}$, $q = L_{\varphi_x\alpha_x0} - a_0(L_{\varphi_t\alpha_x0} + L_{\varphi_x\alpha_t0}) + a_0^2 L_{\varphi_t\alpha_t}$.

At this point, it is enough to multiply (33) by an eigenvector of A (left and right eigenvector are the same because A is symmetric) to eliminate $z_\xi^{(2)}$ and obtain a single equation for $n^{(1)}$:

$$r_0 Bfn^{(1)}n_\xi^{(1)} + r_0 gn_\tau^{(1)} + \epsilon^{\alpha-1}r_0 hn_{\xi\xi}^{(1)} - \epsilon^{2\alpha-1}r_0 jn_{\xi\xi\xi}^{(1)} = 0. \tag{34}$$

A crucial point here is that

$$r_0 h = pr_{0n}r_{0\varphi} - pr_{0\varphi}r_{0n} - qr_{0\varphi}r_{0u} + qr_{0u}r_{0\varphi} = 0, \tag{35}$$

so that there is no "dissipative" term $n_{\xi\xi}^{(1)}$ and, by taking $\alpha = \frac{1}{2}$ in (34), we get the Korteweg–de Vries equation

$$r_0 gn_\tau^{(1)} + r_0 Bfn^{(1)}n_\xi^{(1)} - r_0 jn_{\xi\xi\xi}^{(1)} = 0,$$

and the (constant) coefficients can be easily scaled out. It seems that it would not have been possible to obtain this result if the matrix A had not been symmetric.

C. General case of $L = L(n_1, \ldots, n_k; \varphi_1, \ldots, \varphi_l, \varphi_{1x}, \ldots, \varphi_{lx}, \varphi_{1t}, \ldots, \varphi_{lt}, \alpha_{1x}, \ldots, \alpha_{mx}, \alpha_{1t}, \ldots, \alpha_{mt})$

The extension of the argument in Sec. 2b to cover this general case can be obtained automatically so that there is no need to discuss it in detail.

The E–L equations are now

$$\begin{aligned} &\delta n_p\colon && L_{n_p} = 0, && p = 1, \ldots, k, \\ &\delta\varphi_r\colon && L_{\varphi_r t} + L_{\varphi_r x} - L_{\varphi_r} = 0, && r = 1, \ldots, l, \\ &\delta\alpha_s\colon && L_{\alpha_s t} + L_{\alpha_s x} = 0, && s = 1, \ldots, m, \end{aligned}$$

and we again introduce

$$\alpha_{s_x} = u_s,\quad \alpha_{s_t} = v_s,\quad s = 1, \ldots, m.$$

It can be easily verified that the matrix analogous to A of Eq. (30) is again symmetric, but the equation $\det A = 0$ is now of higher degree.

Some idea of the changes the equations of Sec. 2b must undergo to hold for this case can be obtained from the form of an element of A; instead of L_{nn0} in (30), we have

Here $z^{(2)} = (n^{(2)}, \varphi^{(2)}, u^{(2)})$, $v^{(2)}$ has been eliminated in favor of $u^{(2)}$, the matrix A multiplying $z_\xi^{(2)}$ is simply (30), the matrix B is

now

$$\begin{pmatrix} L_{n_1n_10} & L_{n_1n_20} & \cdots & L_{n_1n_k0} \\ L_{n_2n_10} & L_{n_2n_20} & \cdots & L_{n_2n_k0} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ L_{n_kn_10} & L_{n_kn_20} & \cdots & L_{n_kn_k0} \end{pmatrix}.$$

3. PERIODIC SOLUTIONS

A. Waves in cold plasma

We consider again a Lagrangian similar to (2),

$$L = n(\alpha_t + \tfrac{1}{2}\alpha_x^2) + G,$$

but now we require that G be a second degree polynomial with respect to φ_x, φ_t, i.e.,

$$G = a\varphi_x^2 + b\varphi_x\varphi_t + c\varphi_t^2 + d\varphi_x + e\varphi_x + f,$$

with a, b, c, d, e, and f depending on n and φ.

The cold plasma equations of Sec. 2 are certainly of the form discussed here but formerly we had no reason to restrict that much the class of equations under consideration.

We look for stationary solutions, i.e., solutions depending only on

$$\theta = kx - \omega t,\quad k = \text{const},\quad \omega = \text{const},$$

and we shall use a notation $du/d\theta = \dot{u}$, etc. It can be easily verified, that the form of variational equations (3)–(5) should be the same after the θ variable has been introduced as if we introduced this variable directly in the Lagrangian L. Thus we now consider a variational principle

$$\delta \int L\, d\theta = 0,$$

with

$$L = \tfrac{1}{2}k^2 n\dot{\alpha}^2 - n\omega\dot{\alpha} + \lambda\dot{\varphi}^2 + H\dot{\varphi} + f$$

and

$$\lambda = ak^2 - bk\omega + c\omega^2,\quad H = dk - e\omega.$$

The function α appears in the Lagrangian only through its derivatives, so

$$\frac{\partial L}{\partial\dot{\alpha}} = n(k^2\dot{\alpha} - \omega) \equiv p = \text{const}.$$

This equation is analogous to the continuity equation (3). We can use it to eliminate $\dot{\alpha}$ and consider, instead of L, a function

$$R \equiv p\dot{\alpha} - L = g + \lambda\dot{\varphi}^2 + H\dot{\varphi} + f = R(n, \varphi; p),$$

where

$$g=\frac{p^2}{2nk^2}+\frac{p\omega}{k^2}+\frac{n\omega^2}{k^2}.$$

We are left now with two equations

$$\frac{d}{d\theta}\left(\frac{\partial R}{\partial \dot\varphi}\right)-\frac{\partial R}{\partial \varphi}=0,$$
$$\frac{\partial R}{\partial n}=0. \tag{36}$$

These equations imply that

$$A\equiv \dot\varphi\frac{\partial R}{\partial \dot\varphi}-R=\text{const}$$

and after the definition of the R function has been taken into account we get

$$\dot\varphi^2=\frac{g+f+A}{\lambda}=r(n,\varphi). \tag{37}$$

The second equation of Eqs. (36) can be used to calculate n in terms of φ

$$0=\frac{\partial R}{\partial n}=\frac{\partial \lambda}{\partial n}\dot\varphi^2+\frac{\partial H}{\partial n}\dot\varphi+\frac{\partial (f+g)}{\partial n}=\frac{\partial \lambda}{\partial n}r+\frac{\partial H}{\partial n}\sqrt{r}+\frac{\partial (f+g)}{\partial n},$$

and this is enough to write an implicit form of the solution of (37).

$$\theta+\theta_0=\int\frac{d\varphi}{\sqrt{r(\varphi)}}$$

Two simple zeros φ_1 and φ_2 of the function $r(\varphi)$ are required for the solution being periodic

$$r=0,\quad \frac{\partial r}{\partial \varphi}\neq 0. \tag{38}$$

B. Equations originating from a Lagrangian with quadratic dependence on derivatives

We consider now E-L equation for a Lagrange function depending on an arbitrary number of functions, similarily to (1), but now we assume a specific form of dependence of the Lagrangian on the derivatives

$$\begin{aligned}L=&a_{ij}\alpha_{ix}\alpha_{jx}+b_i\alpha_{ix}\varphi_x+c\varphi_x^2\\&+d_{ij}\alpha_{it}\alpha_{jt}+e_i\alpha_{it}\varphi_t+f\varphi_t^2\\&+g_i\alpha_{ix}\varphi_t+h_i\alpha_{it}\varphi_x+i_{ij}\alpha_{it}\alpha_{jx}\\&+j_i\alpha_{ix}+k_i\alpha_{it}+l\varphi_x+m\varphi_t+n.\end{aligned} \tag{39}$$

A summation convention has been assumed here, $\alpha_{ij}\alpha_{ix}\times\alpha_{jx}\equiv\sum_{i,j=1}^{m}\alpha_{ij}\alpha_{ix}\alpha_{jx}$, etc., and all the coefficients $\alpha_{ij}, b_i, c, \cdots$ are functions of n_i and φ.

An additional simplification introduced in (39), as compared with (1), is that there is only one φ function left. This is to assure that all but one of the Lagrange equations can be eliminated. Then periodic solutions, in a closed form, to the single second order equation left (that corresponding to variations of φ) shall be obtained taking advantage of the quadratic dependence of the Lagrangian on the derivatives.

It is easy to verify that correct "stationary" equations can be obtained by applying a substitution

$$\theta=kx-\omega t$$

directly to the Lagrangian (39) and writing the E–L equations for the variational principle

$$\delta\int L(n_i,\varphi,\dot\varphi,\dot\alpha_j)\,d\theta=0. \tag{40}$$

The Lagrangian in (40) is a quadratic form in $\dot\varphi$ and $\dot\alpha_j$

$$L=A_{ij}\dot\alpha_i\dot\alpha_j+B_i\dot\alpha_i\dot\varphi+C_i\dot\alpha_i+D\dot\varphi^2+E\dot\varphi+n, \tag{41}$$

where

$$\tfrac{1}{2}A_{ij}=k^2a_{ij}-k\omega i_{ij}+\omega^2 d_{ij},$$
$$B_i=k^2b_i+\omega^2e_i-k\omega(g_i+h_i),\quad C_i=kj_i-\omega k_i,$$
$$D=ck^2+A\omega^2,\quad E=kl-\omega m.$$

The "stationary" E–L equations are

$$\delta\varphi:\ \frac{d}{d\theta}\frac{\partial L}{\partial\dot\varphi}-\frac{\partial L}{\partial\varphi}=0, \tag{42}$$

$$\delta\alpha_r:\ \frac{d}{d\theta}\frac{\partial L}{\partial\dot\alpha_r}=0,\quad r=1,\ldots,m \tag{43}$$

$$\delta n_s:\ \frac{\partial L}{\partial n_s}=0,\qquad s=1,\ldots,k. \tag{44}$$

Now we are going to get rid of the potential functions α_r going over to a new set of variables by means of a transformation

$$p_r=\frac{\partial L}{\partial\dot\alpha_r},\quad r=1,\ldots,m.$$

This last transformation can be reversed to calculate the $\dot\alpha_r$ in terms of p_r

$$\dot\alpha_r=\frac{\partial R}{\partial p_r},\quad r=1,\ldots,m,$$

with

$$R=R(\theta,n_i,\varphi,\dot\varphi,p_r)=p_s\hat{\dot\alpha}_s-\hat L,$$

provided that

$$\det\left(\frac{\partial^2 L}{\partial\dot\alpha_i\dot\alpha_j}\right)_{i,j=1,\ldots,m}=\det A_{ij}\neq 0.$$

We write $\hat{\dot\alpha}_s,\hat L$ instead of $\dot\alpha_s, L$ to indicate that all the $\dot\alpha_s$ have been expressed here by the new variables p_s.

Equation (43) integrates simply to give

$$p_r=A_{rs}\dot\alpha_s+B_r\dot\varphi+C_r=p_{r0}=\text{const},\quad r=1,\ldots,m, \tag{45}$$

and Eqs. (42) and (44) are now

$$\frac{d}{d\theta}\left(\frac{\partial R}{\partial\dot\varphi}\right)-\frac{\partial R}{\partial\varphi}=0, \tag{46}$$

$$\frac{\partial R}{\partial n_s}=0,\quad s=1,\ldots,k. \tag{47}$$

The function R is a quadratic form in $\dot\varphi$:

$$R=X\dot\varphi^2+Y\dot\varphi+Z,$$

where

$$X=\tfrac{1}{4}A_{rs}A^{-1}_{rj}A^{-1}_{is}B_jB_i-D,\quad Y=-\tfrac{1}{4}A_{rs}A^{-1}_{rj}A^{-1}_{is}[(p_j+C_j)B_i+(p_i+C_i)B_j]-E$$

and

$$Z=p_j(p_i+C_i)+p_i(p_j+C_j)-m,\ i,j,r,s=1,\ldots,m.$$

Eq. (46) has an integral

$$\dot\varphi\frac{\partial R}{\partial\dot\varphi}-R=X\dot\varphi^2-Z\equiv A=\text{const},$$

so that

$$\dot\varphi^2=\frac{A+Z}{X}=r(n_s,\varphi),\quad s=1,\ldots,k. \tag{48}$$

This formula together with Eq. (47) yields an equation for eliminating n_s:

$$\frac{\partial X}{\partial n_s}r(n_s,\varphi)\pm\frac{\partial Y}{\partial n_s}\sqrt{r(n_s,\varphi)}+\frac{\partial Z}{\partial n_s}=0,\quad s=1,\ldots,k. \tag{49}$$

Once the n_s are eliminated, Eq. (48) can be integrated to give a periodic solution

$$\theta+\theta_0=\int^{\varphi}\frac{d\varphi}{\sqrt{r(\varphi)}}, \tag{50}$$

oscillating between two simple zeros of $r(\varphi)$.

All the functions $n_s=n_s\varphi(\theta)$ are determined by Eq. (49) together with (50) and the α_r can be readily calculated from Eq. (45):

$$\alpha_r=\int t_r[\varphi(\theta)]\,d\theta+\alpha_{r0},\quad r=1,\ldots,m,$$

where

$$t_r=A^{-1}_{rs}(p_{r0}-B_r\sqrt{r(\varphi)}-C_r).$$

4. QUASIPERIODIC SOLUTIONS AND MODULATIONAL STABILITY

Whitham[8] presented a method for describing slow variations of nonlinear dispersive waves and studying their stability. The method relied on a Lagrangian being known for the studied equations to be derived from a corresponding variational principle and the existence of a stationary periodic solution was also assumed. Here we are going to specify the Whitham's theory for the "quadratic" Lagrangian (39), of which we know that it gives origin to equations having periodic stationary solutions in a closed form.

Let us consider E–L equations of a three function (n,φ,α) variational principle

$$\delta\int\int L(n,\varphi,\varphi_x,\varphi_t,\alpha_x,\alpha_t)\,dx\,dt=0. \tag{51}$$

It is assumed that there exists a stationary solution of the E–L equations of (51) depending only on

$$\theta=kx-\omega t,\quad k,\omega=\text{const}, \tag{52}$$

and we look for a more general solution resulting from slow variations of this uniform wavetrain solution. The first step is to represent the solution in the form, e.g., for φ

$$\varphi(x,t)=\Phi(\Theta,X,T,\epsilon), \tag{53}$$

with

$$X=\epsilon x,\quad T=\epsilon t,\quad \theta=\epsilon^{-1}\Theta(X,T),$$

$$\omega(X,T)=-\theta_t=-\Theta_t,\quad k(X,T)=\theta_x=\Theta_x.$$

The phase function $\theta=\theta(x,t)$ is introduced as a generalization of (52) and ϵ is a parameter, which, at a later step, shall be taken small and an expansion shall be used:

$$\Phi=\Phi_0+\epsilon\Phi^{(1)}+\epsilon^2\Phi^{(2)}+\cdots. \tag{54}$$

Equations describing the more general "quasiperiodic," solutions sought can be obtained by introducing (53) directly to the Lagrangian of (51) and writing a three variable variational principle

$$\delta\int\int\int_0^{2\pi}L(N,\Phi,k\Phi_\theta+\epsilon\Phi_x,-\omega\Phi_\theta+\epsilon\Phi_T,kA_\theta+\epsilon A_x+\beta,-\omega A_\theta+\epsilon A_T-\gamma)\,dX\,dT\,d\theta=0, \tag{55}$$

where, instead of α and n, we used

$$\alpha=A(\theta,X,T,\epsilon)+\psi(X,T),\quad n=N(\theta,X,T,\epsilon), \tag{56}$$

together with

$$\psi=\epsilon^{-1}\Psi(X,T),\quad \beta=\Psi_x,\quad \gamma=-\Psi_T.$$

The "pseudofrequencies" β,γ appeared here because we included ψ in (56) to obtain a more general solution as α is only a potential and we expect only its derivatives to be periodic in θ to lowest order in ϵ. The period has been taken to be 2π for the analogy to the sinusoidal waves of linear theory be preserved.

If we define an average Lagrangian $\bar L$ as the inner integral of (55) and use expansions of the type of (54), then, to lowest order, we have

$$\delta\int\int\bar L(N_0,\Phi_0,k\Phi_{0\theta},-\omega\Phi_{0\theta},kA_{0\theta}+\beta,-\omega A_{0\theta}-\gamma)\,dX\,dT=0. \tag{57}$$

The variation of (55) with respect to N,Φ, and A results in E–L equations, which, to lowest order, have solutions periodic in θ, characterized by amplitudes $N^0(X,T)$, $\Phi^0(X,T)$, $A^0(X,T)$, frequency $\omega(X,T)$, wavevector $k(X,T)$ and pseudofrequencies $\beta(X,T)$ and $\gamma(X,T)$. With these solutions substituted into (57) we can calculate $\bar L=\mathcal{L}(\Phi^0,A^0,\omega,k,\beta,\gamma)$. Then, taking variations in (57) with respect to $N^0,\Phi^0,A^0,\Theta(X,T)$, and $\Psi(C,T)$, we obtain equations

$$\mathcal{L}_{\Phi^0}=0,\quad \mathcal{L}_{A^0}=0, \tag{58}$$

$$\frac{\partial}{\partial T}\mathcal{L}_\omega-\frac{\partial}{\partial X}\mathcal{L}_\kappa=0,\quad \frac{\partial}{\partial T}\mathcal{L}_\gamma-\frac{\partial}{\partial X}\mathcal{L}_\beta=0, \tag{59}$$

together with equations arising from the definitions of ω, k, β, γ

$$k_T+\omega_x=0\ \text{ and }\ \beta_T+\gamma_x=0. \tag{60}$$

The set of Eqs. (58)–(60) describes slow changes in the parameters of the lowest-order periodic solution of the original equations and if this is a hyperbolic set then any changes in these parameters can propagate and we expect the periodic solution to be stable. The term "modulational stability" is sometimes used for this type of stability.

The averaged Lagrangian has a simple form if the transformation to Hamilton variables is used

$$\Pi_1=\frac{\partial L}{\partial\Phi_{\theta0}},\quad \Pi_2=\frac{\partial L}{\partial A_{\theta0}}$$

and

$$H(\Pi_1,\Pi_2,\Phi_0;\Theta,\Psi)=\Pi_1\Phi_{\theta0}+\Pi_2A_{\theta0}-L.$$

As Π_2 does not depend on θ, A_θ is periodic and H is an energy integral, we have

$$\Pi_2 = p_{r0}(X,T), \quad H = A(X,T),$$

$$\mathcal{L} = \frac{1}{2\pi}\oint \Pi_1 d\Phi_0 - H, \tag{61}$$

where $\oint \cdots d\Phi_0$ denotes integration over one complete cycle of Φ_0.

The Lagrangian discussed in Sec. 3b depends on a number of potentials α_j, $j=1,\ldots,m$, and on more than one n function, so we shall have now a larger number of equations:

$$\mathcal{L}_A = 0; \quad \mathcal{L}_{p_{r0}} = 0,$$

$$\frac{\partial}{\partial T}\mathcal{L}_\omega - \frac{\partial}{\partial X}\mathcal{L}_\kappa = 0, \tag{62}$$

$$\frac{\partial}{\partial T}\mathcal{L}_{\gamma_{r0}} - \frac{\partial}{\partial X}\mathcal{L}_{\beta_r} = 0,$$

and

$$k_T + \omega_x = 0, \quad \beta_{r_T} + \gamma_{r_x} = 0,$$

with r running over $1,\ldots,m$.

In order to calculate the averaged Lagrangian $\mathcal{L}$ we repeat the entire procedure of Sec. 3b with a slight change involved by the pseudofrequencies β_r and γ_r. It is understood, moreover, that all the "constant" are now functions of X and T and vary according to (62). For Π_1 of (61) we have then

$$\Pi_1 = B_i t_i + 2D\sqrt{r} + E,$$

where only E is now different from the one in Sec. 3b, and

$$E = lk - \omega m + k^2\beta_i b_i - \omega^2\gamma_i e_i + \omega k(h_i\gamma_i - \beta_i g_i).$$

It is clear that this change in the definition of E involves also (slight) changes in the expression for r.

The ultimate effectiveness of the method depends on the possibility of calculation of the integral (61) and this might be quite complicated in practical cases.

5. THE NONDISPERSIVE CASE

We obtained a dispersion-free system by omitting the φ_x and φ_t derivatives in the corresponding Lagrangian (see Ref. 8). Now, let us discuss a more general case of a Lagrangian (which is similar to the one discussed in Ref. 9)

$$L(n_1,\ldots,n_k;\alpha_{1x},\ldots,\alpha_{mx};\alpha_{1t},\ldots,\alpha_{mt})$$

involving the following Euler–Lagrange equations:

$$\delta n_p\colon \; L_{n_p} = 0, \quad p = 1,\ldots,k$$

$$\delta\alpha_s\colon \; L_{\alpha_{st}t} + L_{\alpha_{sx}x} = 0, \quad s = 1,\ldots,m.$$

Introducing new variables

$$q_{2i} = \alpha_{it}, \quad q_{2i-1} = -L_{\alpha_{ix}}$$

and using the (δn_p) equations to find $n_p = n_p(q_i)$, we can write for the E–L equations

$$L^{(0)}_{q_i t} + L^{(1)}_{q_i x} = 0, \quad l = 1,\ldots,2m,$$

where

$$L^{(0)}(q_i) \equiv L(n_p(q_i); \alpha_{ix}(q_i), q_{2i}) - \alpha_{ix}(q_i)L_{\alpha_{ix}} = L + \alpha_{ix}q_{2i-1},$$

$$L^{(1)}(q_i) \equiv -q_{2i}q_{2i-1}.$$

An alternative form of the last equation is

$$L^{(0)}_{q_l q_n} q_{nt} + L^{(1)}_{q_l q_n} q_{nx} = 0, \quad n = 1,\ldots,2m,$$

and, as the matrix $L^{(1)}_{q_l q_n}$ is symmetric, the system is symmetric-hyperbolic, if the matrix $L^{(0)}_{q_l q_n}$ is positive defined. This last result might be of use in the stability investigations described in Sec. 4.

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A general setting for Casimir invariants*

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This paper contains a general description of the theory of invariants under the adjoint action of a given finite-dimensional complex Lie algebra G, with special emphasis on polynomial and rational invariants. The familiar "Casimir" invariants are identified with the polynomial invariants in the enveloping algebra $\mathfrak{A}(G)$. More general structures (quotient fields) are required in order to investigate rational invariants. Some useful criteria for G having only polynomial or rational invariants are given. Moreover, in most of the physically relevant Lie algebras the exact computation of the maximal number of algebraically independent invariants turns out to be very easy. It reduces to finding the rank of a finite matrix. We apply the general method to some typical examples.

1. INTRODUCTION

The subject of polynomial invariants (for a given Lie algebra G) is strongly related to physics. As a matter of fact it was under the efforts of some relevant physicists (H. B. G. Casimir, G. Racah, ···) that this subject began to grow up. H. B. G. Casimir in collaboration with B. L. van der Waerden first introduced the quadratic invariant for semisimple Lie groups. Surprisingly enough, G. Racah[1] was able in the 1950's to give an explicit construction for the polynomial invariants in the case G semisimple. What are now called "Casimir invariants" originated in their work.

While physicists[2] own interest was centered in the semisimple case, because of the crucial role played by semisimple Lie groups in modern physics, the first general rigorous results obtained by the mathematicians (the name of C. Chevalley is particularly relevant here) also refered to the invariant elements in the enveloping algebra of semisimple Lie algebras.

It is perhaps because of this coincidence that a groundless belief has developed in physical literature (in a more or less explicit form) in the sense that the only possible invariants for a general Lie algebra are of polynomial type. Sometimes the contrary is true, and such general operators as exponentials[2] and so on are called "Casimir invariants" without an explicit definition of the meaning of this term.

In this paper we propose to identify the Casimir invariants as the polynomial invariants of G. Then we give simple examples showing the need for more general invariants. Thus, more general structures than the enveloping algebra are required. To our knowledge, the only well-defined structures of this type are the quotient fields. Section 3 is devoted to the description of rational invariants, and gives sufficient conditions for a given G having only polynomial and/or rational invariants. A simple formula is given which permits the exact computation of the number of algebraically independent polynomial and/or rational invariants. This formula reduces the problem to computing a matrix rank. We apply the general method to some physically relevant Lie algebras in Sec. 5.

2. POLYNOMIAL INVARIANTS

Henceforth G will denote any finite-dimensional Lie algebra over the field $\mathbb{C}$ (complex numbers), with commutation relations $[A_i, A_j] = \sum_k C_{ij}^k A_k$ $(i, j, k = 1, 2, \ldots, n)$ in a given basis $\{A_j\}_1^n$. In Sec. 4, G will be assumed to be algebraic.

A. The enveloping algebra[3]

We denote by S the symmetric algebra of G. It is isomorphic to $\mathbb{C}[a_1, a_2, \ldots, a_n]$, the usual polynomial ring in n commutative variables $a_1, \ldots, a_n$. The set of all homogeneous polynomials in S of degree m will be denoted $S^{(m)}$.

On the other hand we will consider $\mathfrak{A}$, the enveloping algebra of G, consisting of all (noncommutative, in general) polynomials in $A_1, \ldots, A_n$. The linear subspace of $\mathfrak{A}$ generated by the monomials $A_1^{r_1} A_2^{r_2} \cdots A_n^{r} n$ $(r_1 + r_2 + \cdots + r_n \leq m)$ will be denoted by $\mathfrak{A}_{(m)}$. Given $u \in \mathfrak{A}$, we will refer to the integer $d(u) \equiv \inf\{p \mid u \in \mathfrak{A}_{(p)}\}$ as the degree of u in $\mathfrak{A}$. One obviously has

$$\mathbb{C} = \mathfrak{A}_{(0)} \subset \mathfrak{A}_{(1)} \subset \cdots \subset \mathfrak{A}_{(m)} \subset \cdots,$$

$$\bigcup_{m \geq 0} \mathfrak{A}_{(m)} = \mathfrak{A}, \qquad \mathfrak{A}_{(m)}\, \mathfrak{A}_{(p)} \subset \mathfrak{A}_{(m+p)}.$$

B. The adjoint action

This is defined to be the action of G on itself by the following derivations $\mathrm{ad}A: A' \in G \to [A, A'] \in G$. In this paper, however, we are going to consider also the adjoint action of G on S and $\mathfrak{A}$, as given by the following formulae for a basis $\{A_j\}_1^n$ of G:

$$p = p(a) \equiv p(a_1, \ldots, a_n) \in S \xrightarrow{\mathrm{Ad}A_j} \hat{A}_j(p) \equiv \sum_{k,l} C_{jl}^k a_k \frac{\partial_p}{\partial a_l} \in S, \tag{1}$$

$$u \in \mathfrak{A} \xrightarrow{\mathrm{Ad}A_j} [A_j, u] \equiv A_j u - u A_j \in \mathfrak{A}, \tag{2}$$

and by linearity for any $A \in G$.

C. Polynomial invariants. Definition

Because of its key role in that follows, we isolate the subsets:

$$\mathfrak{A}^I \equiv \{u \in \mathfrak{A} \mid [A_j, u] = 0, \forall j\} \subset \mathfrak{A},$$

$$S^I \equiv \{p \in S \mid \hat{A}_j(p) = 0, \forall j\} \subset S.$$

They are the invariants in $\mathfrak{A}$, S, respectively, under the adjoint action of G.

Definition 1: The elements in $\mathfrak{A}^I$ are called *polynomial (or Casimir) invariants* of G.

Definition 2: Given a weight function (≡ one-dimensional representation) $\lambda: G \to \mathbb{C}$, we say $u \in \mathfrak{A}$ is a λ-semi-invariant in if $[A,u]=\lambda(A)u$, $\forall\ A \in G$. We denote by $\mathfrak{A}_\lambda^{I/2}$ the set of all λ-semi-invariants in $\mathfrak{A}$.

Definition 2′: $p \in S$ is said to be a λ-semi-invariant in S if $\hat{A}(p)=\lambda(A)p$, $\forall\ A \in G$. Let us write $S_\lambda^{I/2}$ for the set of all λ-semi-invariants in S.

D. The canonical isomorphism $\phi: S \to \mathfrak{A}$

Let us consider the linear map $\phi: S \to \mathfrak{A}$ defined by symmetrization as follows:

$$\phi(a_{\alpha_1}a_{\alpha_2}\cdots a_{\alpha_r})=\frac{1}{r!}\sum_{\sigma\in\Pi_r} A_{\alpha_{\sigma(1)}}A_{\alpha_{\sigma(2)}}\cdots A_{\alpha_{\sigma(r)}}$$

where Π_r stands for the permutation group of r objects.

Lemma 1[3]: (i) ϕ is a linear isomorphism.

(ii) ϕ commutes with the adjoint action, i.e., $\phi(\hat{A}(p))=[A,\phi(p)]$, $\forall\ p \in S$.

(iii) Let $\mathfrak{A}^{(j)} \equiv \phi(S^{(j)})$. Then $\mathfrak{A}_{(m)}=\oplus_0^m \mathfrak{A}^{(j)}$.

(iv) $p_1 \in S^{(m_1)}$, $p_2 \in S^{(m_2)} \Rightarrow d(\phi(p_1p_2))=m_1+m_2$. Moreover, $\phi(p_1p_2)-\phi(p_1)\phi(p_2) \in \mathfrak{A}_{(m_1+m_2-1)}$.

It follows that the Abelian algebras S^I, $\mathfrak{A}^I$ are linearly isomorphic. This can be strengthened[4] to read:

Lemma 2: S^I and $\mathfrak{A}^I$ are algebraically isomorphic.[5]

Thus the transcendence degrees of S^I, $\mathfrak{A}^I$ over $\mathbb{C}$ are identical. In other words, the cardinal, τ of a maximal set of algebraically independent elements in S^I is the same as for $\mathfrak{A}^I$. Moreover, since the adjoint action on S takes $S^{(m)}$ into $S^{(m)}$, the elements in the maximal set can be chosen to be homogeneous.

Lemma 3: Let $\{p_j\}_1^r$ homogeneous algebraically independent in S^I. Then $\{\phi(p_j)\}_1^r$ are algebraically independent in $\mathfrak{A}^I$.

Proof: Suppose that there exists a finite set $I \subset \mathbb{N}^r$, ($\mathbb{N}$, natural numbers) and nonzero complex numbers $\lambda_{s_1,\ldots,s_r}\ |(s_1,\ldots,s_r) \in I$, such that

$$\sum_I \lambda_{s_1,\ldots,s_r}\phi(p_1)^{s_1}\cdots\phi(p_r)^{s_r}=0.$$

Let $d_i (i=1,\ldots,r)$ the degrees of the homogeneous polynomials $p_i (i=1,\ldots,r)$. Let $I_{\max}$ be the subset of I constituted by the elements $(s_1,\ldots,s_r)$ such that $\sum_{i=1}^r s_i d_i$ is maximal in I. Then, by making use of Lemma 1 (iv), we have

$$\sum_{I_{\max}} \lambda_{s_1,\ldots,s_r}\phi(p_1^{s_1}\cdots p_r^{s_r})=0$$

and, according to Lemma 1 (i),

$$\sum_{I_{\max}} \lambda_{s_1,\ldots,s_r}\, p_1^{s_1}\cdots p_r^{s_r}=0,$$

which is a contradiction. QED

We close this section with a crucial result relating τ (the maximal number of algebraically independent Casimir invariants) to the rank of the antisymmetric matrix $M_G=((M_G)_{ij})$ with $(M_G)_{ij} \equiv \sum_k C_{ij}^k a_k$. We write

$$r(G) \equiv \sup_{(a_1,\ldots,a_n)} \operatorname{rank} M_G.$$

Then we have the following upper bound for τ:

Theorem 1: With the above notations $\tau \leq \dim G - r(G)$ (3)

Proof: Follows from Lemma 2 and a classical theorem[6] stating that the system of differential equations,

$$\sum_{j,k} C_{ij}^k a_k \frac{\partial f}{\partial a_j}=0 \quad (i=1,\ldots,n), \tag{4}$$

has exactly $n-r(G)$ functionally independent solutions. The polynomial solutions can be identified with elements in S^I. QED

Remark: Let $\{p_j\}_1^\tau$ a maximal set of homogeneous algebraically independent elements in S^I (see Lemma 3). Then $\{\phi(p_j)\}_1^\tau$ is a maximal set of algebraically independent Casimir invariants.

E. Examples

The essential feature we want to emphasize is the fact that, generally speaking, equality will not be accessible in (3), because of the existence of nonpolynomial solutions. It is this simple remark[7] that invalidates the conclusion in Ref. 8. This is best understood by looking at some low-dimensional examples.

Example 1: Let G be the Lie algebra of $GL(2)$, $\dim G=4$.

$$[A_1,A_2]=[A_2,A_4]=A_2, \quad [A_3,A_1]=[A_4,A_3]=A_3,$$
$$[A_2,A_3]=A_1-A_4, \quad [A_1,A_4]=0,$$

$$r(G)=\text{generic rank}\begin{pmatrix} 0 & a_2 & -a_3 & 0 \\ -a_2 & 0 & a_1-a_4 & a_2 \\ a_3 & a_4-a_1 & 0 & -a_3 \\ 0 & -a_2 & a_3 & 0 \end{pmatrix}=2$$

Two independent (polynomial) solutions of the system (4) are

$$p_1(a)=a_1+a_4, \quad p_2(a)=a_1^2+a_4^2+2a_2a_3.$$

With the aid of the canonical isomorphism ϕ we obtain the maximal set of algebraically independent polynomial invariants:

$$C_1=A_1+A_4, \quad C_2=A_1^2+A_4^2+A_2A_3+A_3A_2.$$

In this case, equality is satisfied in (3).

Example 2: (Dilatations and translations in the plane)

$$[A_3,A_1]=A_1, \quad [A_3,A_2]=A_2, \quad [A_1,A_2]=0.$$

Now $r(G)=2$, and there is no polynomial solutions of system (4). However, there is a rational solution $f(a)=a_1/a_2$.

Example 3: Let us consider now the three-dimensional Lie algebra:

$$[A_1,A_2]=0, \quad [A_1,A_3]=A_1+A_2, \quad [A_2,A_3]=A_2.$$

We find $r(G)=2$, and there is no rational solutions. The system (4) admits the solution $f(a)=a_1/a_2-\ln a_2$.

Summarizing, we conclude that polynomial solutions of (4) (hence polynomial invariants in $\mathfrak{A}$) do not generally exhaust all possible solutions of that system. This suggests the following definition.

Definition 3: We call f a *formal invariant* of G if it is a solution of (4). It seems to us that such definition is, from the point of view of the adjoint action, the most general definition of an invariant object. In the case f is a rational function of $a_1,\ldots,a_n$, we are going to see that f gives rise to an associated "rational" invariant (Sec. 3). Until now one has not been able to do so for general formal invariants.

We note also that the exponential invariant proposed in Ref. 2 is not a formal invariant, in the sense of our definition 3.

3. RATIONAL INVARIANTS

A. The quotient field[9]

It is a well known fact that $\mathfrak{A}$ is a Noetherian ring without zero divisors. Thus, one can construct its quotient field, denoted $D(\mathfrak{A})$, the elements of which are of the form uv^{-1} with $u,v\in\mathfrak{A}$ and $v\neq 0$. Given $r=uv^{-1}\in D(\mathfrak{A})$, it can be decomposed as $r=u'^{-1}v'$ with $u',v'\in\mathfrak{A}$ and $u'\neq 0$. Any pair of fractions $r_1,r_2\in D(\mathfrak{A})$ can be reduced to common denominator, so that one can define on $D(\mathfrak{A})$ all required operations to make $D(\mathfrak{A})$ a noncommutative field.

Similarly the quotient field of S will be denoted by $D(S)$. It is isomorphic to the field $\mathbb{C}(a_1,\ldots,a_n)$ of rational functions in n commuting variables.

B. The extended ajoint action

For every $r_1,r_2\in D(\mathfrak{A})$ we write $[r_1,r_2]\equiv r_1r_2-r_2r_1$. For instance, if $u,v\in\mathfrak{A}$ and $v\neq 0$, we get $[u,v^{-1}]=-v^{-1}[u,v]v^{-1}$. Therefore, we are able to extend the adjoint action of G to the quotient fields $D(\mathfrak{A})$, $D(S)$ as follows:

$$h=h(a)\in D(S)\xrightarrow{\mathrm{ad}A_j}\hat{A}_j(h)=\sum_{k,l}c_{jl}^{k}a_k\frac{\partial h}{\partial a_l}\in D(S), \tag{1'}$$

$$r\in D(\mathfrak{A})\xrightarrow{\mathrm{ad}A_j}[A_j,r]\equiv A_jr-rA_j\in D(\mathfrak{A}). \tag{2'}$$

Let us write $D(S)^I\equiv\{h\in D(S)\mid\hat{A}_j(h)=0,\ \forall\, j\}$, $D(\mathfrak{A})^I\equiv\{r\in D(\mathfrak{A})\mid[A_j,r]=0,\ \forall\, j\}$

Definition 4: The elements in $D(\mathfrak{A})^I$ will be called the *rational invariants* of G. We notice that $D(\mathfrak{A})^I$ contains $D(\mathfrak{A}^I)$, the quotient field of $\mathfrak{A}^I$. Consequently, all polynomial invariants are included in $D(\mathfrak{A})^I$. Another useful remark is that given $u,v\in\mathfrak{A}(v\neq 0)$, a necessary condition for $uv^{-1}\in D(\mathfrak{A})^I$ is $[u,v]=0$.

The next two propositions are concerned with the structure of $D(S)^I$, $D(\mathfrak{A})^I$.

Proposition 1: With the above conventions:

(i) $h\in D(S)^I\Longleftrightarrow h=p_1/p_2$, where $p_1,p_2\in S_\lambda^{I/2}$ for some weight λ.

(ii) There exists a maximal algebraically independent set $\{h_1,\ldots,h_r\}$ in $D(S)^I$ such that $h_i=p_i/q_i$, with homogeneous $p_i,q_i\in S_i^{I/2}$, for some λ_i $(i=1,2,\ldots,r)$.

Proof: (i) Let $p_1,p_2\in\mathbb{C}[a_1,\ldots,a_n]$ relatively prime polynomials such that $h=p_1/p_2$. If $h\in D(S)^I$, then

$$0=\hat{A}_j(h)=[\hat{A}_j(p_1)p_2-p_1\hat{A}_j(p_2)]/p_2^2,\qquad\forall_j.$$

Therefore,

$$\hat{A}_j(p_1)/p_1=\hat{A}_j(p_2)/p_2\in\mathbb{C}.$$

On the other hand, if $p_1,p_2\in S_\lambda^{I/2}$, then obviously $h\equiv p_1/p_2\in D(S)^I$.

(ii) Let $g_1,\ldots,g_r$ a maximal algebraically independent set in $D(S)^I$. We write $g_i=p_i/q_i$ with p_i,q_i λ_i-semi-invariants in S $(i=1,\ldots,r)$. Let $p_i=\sum_{k=0}^{d_i}p_i^{(k)}$ and let $q_i=\sum_{l=0}^{c_i}q_i^{(l)}$ the decomposition in homogeneous terms. The adjoint action on S takes $S^{(m)}$ into itself. Therefore, $p_i^{(k)}$ and $q_i^{(l)}$ $(k=0,\ldots,d_i,\ l=0,\ldots,c_i)$ are λ_i-semi-invariants (λ_i the weight of p_i and q_i) $(i=1,\ldots,r)$. The elements $h_i^{(l,k)}=q_i^{(l)}/p_i^{(k)}$ $(i=1,\ldots,r,\ l=0,\ldots,c_i;\ k=0,\ldots,d_i)$ are in $D(S)^I$. Moreover,

$$g_i=\frac{p_i}{q_i}=\frac{1}{\sum_{l=0}^{c_i}h_i^{(l,0)}}+\frac{1}{\sum_{l=0}^{c_i}h_i^{(l,1)}}+\cdots+\frac{1}{\sum_{l=0}^{c_i}h_i^{(l,d_i)}}.$$

Then $g_i,\ldots,g_r$ are algebraically dependent on $h_i^{(c,k)}$, $i=1,\ldots,r$, $l=0,\ldots,c_i$, $k=0,\ldots,d_i$, and we can choose a maximal algebraically independent set among the $h_i^{(l,k)}$.

Proposition 2: (i) $p\in S_\lambda^{I/2}\Longleftrightarrow\phi(p)\in\mathfrak{A}_\lambda^{I/2}$.

(ii) $u.\ v\in\mathfrak{A}_\lambda^{I/2}(v\neq 0)\Rightarrow uv^{-1}\in D(\mathfrak{A})^I$.

(iii) The set $\mathfrak{A}^{I/2}\equiv\cup_\lambda\mathfrak{A}_\lambda^{I/2}$ is Abelian.

(iv) Let $\{h_i=p_i/q_i\}_1^r$ be an algebraically independent set in $D(S)^I$, with homogeneous $p_i,q_i\in S_{\lambda_i}^{I/2}$, for some λ_i $(i=1,\ldots,r)$. Then $\{\phi(p_i)\phi(q_i)^{-1}\}_1^r$ are also algebraically independent in $D(\mathfrak{A})^I$.

Proof: (i) Follows from Lemma 1, part (ii).

(ii) $A\in G\Rightarrow[A,uv^{-1}]=[A,u]v^{-1}-uv^{-1}[A,v]v^{-1}=\lambda uv^{-1}-uv^{-1}\lambda vv^{-1}=0$.

(iii) See, for instance, Ref. 2.

(iv) Suppose that there exists a finite set $I\subset\mathbb{N}^r$ and complex numbers $\lambda_{s_1,\ldots,s_r}\neq 0$ $[(s_1,\ldots,s_r)\in I]$ such that

$$\sum_I\lambda_{s_1,\ldots,s_r}(\phi(p_i)\phi(q_i)^{-1})^{s_1}\cdots(\phi(p_r)\phi(q_r)^{-1})^{s_r}=0.$$

In view of part (iii) this implies

$$\sum_I\lambda_{s_1,\ldots,s_r}\phi(p_i)^{s_1}\cdots\phi(p_r)^{s_r}[\phi(q_1)^{s_1}\cdots\phi(q_r)^{s_r}]^{-1}=0. \tag{5}$$

Let $\lambda_{(s)}\equiv\lambda_{s_1,\ldots,s_r}$, $\phi(p)^{(s)}\equiv\phi(p_1)^{s_1}\cdots\phi(p_r)^{s_r}$, $\phi(q)^{(s)}\equiv\phi(q_1)^{s_1}\cdots\phi(q_r)^{s_r}$, and $\prod_I\phi(q)^{(s)}$ be the product of all $\phi(q)^{(s)}$. By multiplying by $\prod_I\phi(q)^{(s)}$ Eq. (5) becomes

$$\sum_I\lambda_{(s)}\phi(p)^{(s)}\prod_{I-(s)}\phi(q)^{(t)}=0.$$

Let d_i, e_i be respectively the degrees of the homogeneous polynomials p_i, q_i $(i=1,2,\ldots,r)$. Let us write $I_{\max}$ for the subset of I consisting of those elements $(s)=(s_1,\ldots,s_r)$ such that $\sum_{i=1}^r s_id_i+\sum_{i=1}^r\sum_{(t)\neq(s)}l_ie_i$ is maximal in I. Then Lemma 1, part (iv) yields

$$\sum_{I_{\max}} \lambda_{(s)} \phi\left(p^{(s)} \prod_{I=(s)} q^{(t)}\right) = 0 \Rightarrow \sum_{I_{\max}} \lambda_{(s)} p^{(s)} \prod_{I=(s)} q^{(t)} = 0. \tag{6}$$

Now let us multiply (6) by $\Pi_I q^{(s)}$ to conclude

$$\sum_{I_{\max}} \lambda_{s_1,\ldots,s_r} h_1^{s_1} \cdots h_r^{s_r} = 0.$$

Thereby contradicting the hypothesis. QED

The result of Lemma 2 admits a direct generalization to the quotient fields[10]:

Lemma 2′: The fields $D(S)^I$ and $D(\mathfrak{A})^I$ are isomorphic.

An important consequence is the equality between the maximal number of algebraically independent elements (transcendence degree) of $D(S)^I$ and of $D(\mathfrak{A})^I$. Let us call τ' this number. By the same argument already used in Theorem 1, we obtain

Theorem 1′:

$$\tau' \leq \dim G - r(G). \tag{3′}$$

Remark: Let $\{h_i\}_1^{\tau'}$ be a maximal set in $D(S)^I$ of the type indicated in Proposition 2 (iv). Then $\{\phi(p_i)\phi(q_i)^{-1}\}_1^{\tau'}$ is a maximal algebraically independent set in $D(\mathfrak{A})^I$.

The preceding Example 3 shows that equality is not always reached in (3′). It would be helpful to know of as many Lie algebras as possible having only rational invariants. In other words, we are interested in those G such that $\tau' = \dim G - r(G)$. We now undertake this problem.

4. THE CASE G ALGEBRAIC[11]

One sufficient condition for the nonexistence of irrational formal invariants for G can be deduced from a result of J. Dixmier.[12]

Theorem 2: Let G a finite-dimensional algebraic Lie algebra over a commutative field of characteristic zero. Then the maximal number of algebraically independent elements in $D(S)^I$ equals $\dim G - r(G)$.

Corollary 1:

$$G \text{ algebraic} \Rightarrow \tau' = \dim G - r(G). \tag{3″}$$

Another important problem is to characterize the class of all Lie algebras G such that the number of algebraically independent Casimir invariants τ equals $\dim G - r(G)$.

If we restrict our attention to algebraic Lie algebras, then a simple sufficient condition is $D(\mathfrak{A})^I = D(\mathfrak{A}^I)$ (in this case every rational invariant is a quotient of Casimir invariants). This sufficient condition holds for any nilpotent[13] or semisimple[14] Lie algebra.

The case G semisimple is the best known.[15] Since G is automatically algebraic,[11] we conclude $\tau = \dim G - r(G)$ In other words, the number of algebraically independent Casimir invariants equals the rank[16] of G.

Now we generalize the semisimple result to a larger class of Lie algebras, including many other Lie algebras of frequent use in physics.

Theorem 3: $[G, G] = G \Longrightarrow D(\mathfrak{A})^I = D(\mathfrak{A}^I)$.

Proof: The only admissible weight for such Lie algebra is $\lambda \equiv 0$. From Proposition 1 part (i) we see that $D(S)^I = D(S^I)$. Furthermore, Lemmas 2 and 2′ imply $D(\mathfrak{A})^I = D(\mathfrak{A}^I)$. QED

Since $[G, G] = G$ forces G to be algebraic,[11] we obtain the following important result:

Corollary 2: $[G, G] = G \Rightarrow \tau = \dim G - r(G)$.

In such cases Casimir invariants are all we need in order to describe the set of formal invariants of G.

5. APPLICATIONS

While it is not generally true that $\tau' = \dim G - r(G)$, there are many physically relevant Lie algebras having only rational invariants. We quote a few typical examples. According to what has been said, we are provided with two quantitative statements (Corollary 1 and Corollary 2 above) concerning the number of algebraically independent invariants. Finding the explicit form of the invariants is a quite different problem. In the following examples it has been solved in a straightforward way.

(a) $G = \{J_i, P_i\}_{i=1}^3$ with commutation relations

$$[J_i, J_j] = i\epsilon_{ijk} J_k, \quad [J_i, P_j] = i\epsilon_{ijk} P_k, \tag{7a}$$

$$[P_i, P_j] = 0 \quad (i, j, k = 1, 2, 3). \tag{7b}$$

It is the Lie algebra of $E(3)$, the Euclidean group in three dimensions. It satisfies $[G, G] = G$. An easy calculation shows $r(G) = 4$. A maximal set of (polynomial) invariants is given by

$$C_1 = \mathbf{P}^2, \quad C_2 = \mathbf{JP}.$$

(a′) If we add dilatations to $E(3)$, we obtain $G' = \{J_i, P_i, D\}_{i=1}^3$. The only new (nonzero) commutators are

$$[D, P_j] = iP_j, \quad (j = 1, 2, 3). \tag{8}$$

One finds $r(G') = 6$, $\tau = 0$, $\tau' = 1$. There is a rational invariant $(\mathbf{JP})^2(\mathbf{P}^2)^{-1}$.

(b) Let G be the Lie algebra of the Galilei group $G = \{J_i, K_i, P_i, H\}_{i=1}^3$. The commutation relations are in addition to (7)

$$[J_i, K_j] = i\epsilon_{ijk} K_k, \quad [K_j, H] = iP_j \quad (i, j, k = 1, 2, 3); \tag{9}$$

one easily verified $r(G) = 8$, $\tau = \tau' = 2$. A maximal set of invariants is given by

$$C_1 = \mathbf{P}^2, \quad C_2 = (\mathbf{K} \times \mathbf{P})^2.$$

(b′) Let $G' = \{J_i, K_i, P_i, H, M\}_{i=1}^3$ be the Lie algebra of the central extension of Galilei group, with modified commutation relations:

$$[K_i, P_j] = i\delta_{ij} M \tag{10}$$

In this case $r(G') = 8$, $\tau = \tau' = 3$, with a maximal set

$$C_1 = M, \quad C_2 = MH - \tfrac{1}{2}\mathbf{P}^2, \quad C_3 = (M\mathbf{J} - \mathbf{K} \times \mathbf{P})^2.$$

(b″) Now let $G'' = \{J_i, K_i, P_i, H, M, D\}_{i=1}^3$, $D \equiv$ dilatations. This is a 12-dimensional Lie algebra with added relations:

$$[D, P_j] = -iP_j, \quad [D, K_j] = iK_j, \tag{11a}$$

$$[D, H] = -2iH \quad (j = 1, 2, 3). \tag{11b}$$

We get this time $r(G'')=10$, $\tau=\tau'=2$, with maximal set

$$C_1=M, \quad C_2=(M\mathbf{J}-\mathbf{K}\times\mathbf{P})^2$$

Remark: The Lie algebras in (b), (b'), (b'') do not satisfy the hypothes is in Corollary 2.

(c) Let us consider now the Poincaré group. Its Lie algebra G admits the usual basis $\{J_{\mu\nu}, P_\mu\}$ $(\mu, \nu = 0, 1, 2, 3)$, $J_{\mu\nu}=-J_{\nu\mu}$. The commutation relations are

$$[J_{\mu\nu}, J_{\rho\sigma}]=i(g_{\nu\rho}J_{\mu\sigma}-g_{\mu\rho}J_{\nu\sigma}-g_{\mu\sigma}J_{\rho\nu}+g_{\nu\sigma}J_{\rho\mu}), \tag{12a}$$

$$[J_{\rho\sigma}, P_\mu]=i(g_{\mu\sigma}P_\rho-g_{\mu\rho}P_\sigma). \tag{12b}$$

As we see $[G, G]=G$. In fact $\tau=\tau'=2$, with the well-known (Casimir) invariants:

$$C_1=P^2, \quad C_2=W^2,$$

where $W^\mu=\frac{1}{2}\epsilon^{\mu\nu\lambda\rho}J_{\nu\lambda}P_\rho$.

(c') By adding dilatations to G, we go into the so-called Weyl group, with Lie algebra

$$G'=\{J_{\mu\nu}, P_\mu, D\} \text{ and } [D, P_\mu]=-iP_\mu. \tag{13}$$

An easy calculation shows $r(G')=10$. This time there is no polynomial invariants. It is straightforward to verify that $P^2(W^2)^{-1}$ is a (rational) invariant for G'.

(d) In a series of articles[17] P. Roman *et al.* have investigated some Lie groups containing the Poincaré group. We proceed to compute the number of their independent invariants in the light of the general results stated in Sec. 4.

Let us begin with[17] $SO(3,1)\times(T_4^P\times T_4^\pi)$. Its Lie algebra admits a basis $\{J_{\mu\nu}, P_\mu, \Pi_\mu\}$ such that both sets $\{J_{\mu\nu}, P_\mu\}$ and $\{J_{\mu\nu}, \Pi_\mu\}$ satisfy the Poincaré commutation relations. Moreover,

$$[P_\mu, \Pi_\nu]=0 \quad (\mu, \nu=0, 1, 2, 3). \tag{14}$$

Hence $\dim G=14$, and we find $r(G)=10$. Since $[G, G]=G$, we conclude that $\tau=\tau'=4$. By letting $W^\mu=\frac{1}{2}\epsilon^{\mu\nu\rho\sigma}J_{\nu\rho}P_\sigma$ and $V^\mu=\frac{1}{2}\epsilon^{\mu\nu\rho\sigma}J_{\nu\rho}\Pi_\sigma$, a maximal set of invariants is given by

$$C_1=P^2, \quad C_2=\Pi^2, \quad C_3=P\Pi, \quad C_4=W\Pi=-VP.$$

This is to be compared with Ref. 17 where neither the number nor the explicit form of its six (!) independent polynomial invariants are correctly stated.

(d') By addition of a new generator S to (d), we obtain a Lie algebra called G_5 in Ref. 17. This generator verifies

$$[S, P_\mu]=0, \quad [S, \Pi_\mu]=iP_\mu \quad (\mu=0, 1, 2, 3). \tag{15}$$

We find $\dim G=15$, $r(G)=12$. Furthermore, $\tau=\tau'=3$, with Casimir invariants:

$$C_1=P^2, \quad C_2=(P\Pi)^2-P^2\Pi^2, \quad C_3=W\Pi,$$

once again in contradiction with Ref. 17.

(d'') Finally let us consider the Lie algebra of the group[17] H_5 which admits for its Lie algebra a basis $\{J_{\mu\nu}, P_\mu, \Pi_\mu, S, C, D\}$. The only new nonzero commutators are

$$[C, P_\mu]=-i\Pi_\mu, \quad [D, P_\mu]=-iP_\mu, \tag{16a}$$

$$[D, \Pi_\mu]=i\Pi_\mu, \quad [D, C]=2iC, \tag{16b}$$

$$[S, C]=iD, \quad [S, D]=2iS. \tag{16c}$$

In this case we find $\dim G=17$, $[G, G]=G$, $r(G)=14$. Therefore, $\tau=\tau'=3$. A maximal algebraically independent set of polynomial invariants is the following:

$$C_1=(P\Pi)^2-P^2\Pi^2,$$

$$C_2=\tfrac{1}{2}J_\mu\,(P^\mu\Pi^\nu-P^\nu\Pi^\mu)+S\Pi^2+CP^2-DP\Pi,$$

$$C_3=W\Pi.$$

The last one was not considered in Ref. 17.

Remark: By its very definition $r(G)$ is always an even integer (rank of an antisymmetric matrix M_G). In consequence, as can be verified in all preceding examples, the number of formal invariants has the same parity as $\dim G$ does. In particular, G algebraic $\Rightarrow \tau'=\dim G$ (mod 2).

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One-dimensional excited state reduced Coulomb Green's function

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The nth excited state reduced Coulomb Green's function in coordinate space for the one-dimensional Kepler problem is investigated, and a closed expression for this function is obtained.

I. INTRODUCTION

Reduced Green's functions defined by

$$K(\mathbf{r}_2, \mathbf{r}_1, E_n) \equiv -\frac{\hbar^2}{2m} \sum_{k\neq n} \sum_l \frac{\varphi_{kl}(\mathbf{r}_2)\varphi_{kl}^*(\mathbf{r}_1)}{E_k - E_n} \tag{1.1}$$

are basic structures occurring in Rayleigh–Schrödinger bound state perturbation theory for a quantum mechanical particle moving in a potential field $V(\mathbf{r})$. Here the E_k denote the distinct energy eigenvalues of the unperturbed Hamiltonian

$$H_0 = -(\hbar^2/2m)\nabla^2 + V(\mathbf{r}) \tag{1.2}$$

including continuum eigenvalues, if they occur.[1] The φ_{kl} are the corresponding eigenfunctions of H_0, l being a degeneracy quantum number. The energy E_n is one of the bound state eigenvalues of H_0. The reduced Green's function (1.1) is just the coordinate space representative of the familar sum over intermediate states encountered in the Rayleigh–Schrödinger bound state perturbation theory. As such the reduced Green's function enters in the calculation of the first order corrections to the bound state wavefunctions belonging to the eigenvalue E_n, and also in the second order corrections to the energies of these states, when the Hamiltonian H_0 is modified by the addition of a perturbation term. An important part of the work of any bound state perturbation calculation is thus summarized in the function $K(\mathbf{r}_2, \mathbf{r}_1, E_n)$. Since this function is independent of the particular perturbation problem; in principle it could be calculated once and for all and then used as a tool in the investigation of various physical effects.

The reduced Green's function is related to the Green's function

$$G(\mathbf{r}_2, \mathbf{r}_1, E) \equiv -\frac{\hbar^2}{2m} \sum_k \sum_l \frac{\varphi_{kl}(\mathbf{r}_2)\varphi_{kl}^*(\mathbf{r}_1)}{E_k - E} \tag{1.3}$$

of the Hamiltonian H_0, in that $K(\mathbf{r}_2, \mathbf{r}_1, E_n)$ is obtained from $G(\mathbf{r}_2, \mathbf{r}_1, E)$ by removing the nth pole term

$$-\frac{\hbar^2}{2m} \sum_l \frac{\varphi_{nl}(\mathbf{r}_2)\varphi_{nl}^*(\mathbf{r}_1)}{E_n - E} \tag{1.4}$$

and evaluating the other terms at $E = E_n$. In Eq. (1.3) E takes on arbitrary complex values not in the eigenvalue spectrum, discrete and continuous, of H_0. We refer to $K(\mathbf{r}_2, \mathbf{r}_1, E_n)$ as the "nth excited state reduced Green's function" and (when necessary to avoid ambiguity) to $G(\mathbf{r}_2, \mathbf{r}_1, E)$ as the "full Green's function."

Reduced *Coulomb* Green's functions, for which H_0 is the Coulomb Hamiltonian, are of interest for example as a possible tool for use in atomic and molecular calculations, and have been the subject of a number of previous investigations. Hameka[2] has derived a relatively simple closed form expression for the S-wave component of the ground state reduced Coulomb Green's function in three-dimensional space; and subsequently Hostler[3] expressed the complete ground state reduced Coulomb Green's function, including all partial wave contributions, in closed form. More recently, Swierkowski and Suffczynski,[4] investigated the excited state three-dimensional reduced Coulomb Green's function.

We will here obtain a closed expression, Eq. (2.28), for the excited state reduced Green's function of the one-dimensional Kepler problem. The one-dimensional Kepler problem is of special interest because of its rellative simplicity and because of a result of Hostler[5] that the one-dimensional Coulomb Green's function and related structures serve as generating functions for the corresponding objects in spaces of any higher odd dimensionality. Because of this relation between Coulomb Green's functions in spaces of different dimensionality, the results to be presented here for the one-dimensional Kepler problem are significant also for the three-dimensional problem.

Our plan of attack is to obtain the one-dimensional reduced Green's function from the known one dimensional Coulomb Green's function of Meixner[6,7]

$$\begin{aligned} &G_{1D}(r_2, r_1; E) \\ &\quad = -\tfrac{1}{2}a_1 i\nu\Gamma(1-i\nu)W_{i\nu;1/2}(2r_>/a_1 i\nu)M_{i\nu;1/2}(2r_</a_1 i\nu), \\ &\quad E = -\hbar^2/2ma_1^2(i\nu)^2, \quad \mathrm{Re}(i\nu) > 0, \quad a_1 = 4\pi\hbar^2/mZe^2, \end{aligned} \tag{1.5}$$

by exploiting the relation between the reduced Green's function and the full Green's function. This is made possible by the formula

$$K_{1D}(u, v; E_n) = \frac{\partial}{\partial E}\left[(E - E_n)G_{1D}(r_2, r_1; E)\right]\Big|_{E=E_n}, \tag{1.6}$$

$$u \equiv 2r_>/na_1, \quad v \equiv 2r_</na_1,$$

which expresses the relation between the two functions analytically.[8,9]

Equation (1.6) is readily verified by use of the eigenfunction expansion (1.3). Let O denote the operation performed on the full Green's function in Eq. (1.6). Then for any function $f(E)$

$$Of(E) = \partial[(E - E_n)f(E)]/\partial E\,|_{E=E_n}.$$

Let O be applied term by term to the eigenfunction expansion (1.3). When O acts on the terms regular at $E=E_n$ it simply evaluates them at $E=E_n$. However, when O acts on the pole term (1.4) it removes the (simple) pole and gives the derivative of a constant, which is zero. As a result the eigenfunction expansion (1.3) is converted into precisely the sum of terms (1.1), i.e., into the reduced Green's function. According to Eq. (1.6) in order to calculate the reduced Green's function one merely has to differentiate an appropriate expression involving the full Green's function with respect to energy, and substitute $E=E_n$. The expression being differentiated is analytic at E_n since the pole of the full Green's function is removed by the factor $E-E_n$.

By Eq. (1.5) the Coulomb parameter $i\nu$ is a function of energy determined through the conditions $E=-\hbar^2/2ma_1^2(i\nu)^2$ and $\mathrm{Re}\,i\nu>0$. The latter condition $\mathrm{Re}(i\nu)>0$ renders $i\nu$ a unique function of E, for E values not in the eigenvalue spectrum of the Coulomb Hamiltonian. The bound state eigenvalues of the Coulomb Hamiltonian (Bohr energy levels) correspond to the values $i\nu=n=1,2,3,\cdots$ of the Coulomb parameter: $E_n=-\hbar^2/2ma_1^2n^2$. Before proceeding with the differentiation in Eq. (1.6) it is convenient to make a change of independent variables from E to the Coulomb parameter $i\nu$. In terms of $i\nu$ as independent variable the effect of the operator O is

$$Of(i\nu)=\tfrac{1}{2}n\left[\frac{\partial}{\partial i\nu}\left((i\nu-n)\,\frac{(i\nu+n)}{(i\nu)^2}f(i\nu)\right)\right]\Bigg|_{i\nu=n}. \tag{1.7}$$

The pole of the full Green's function occurs at the point $i\nu=n$ in the complex $i\nu$ plane and is removed by the factor $(i\nu-n)$ in Eq. (1.7) when $f(i\nu)$ is taken to be the full Green's function.

Section IIA begins with the result of substituting the expression (1.5) for the full Green's function into Eq. (1.7) to give the reduced Green's function in the form (2.1). Since the Whittaker functions $W_{i\nu;1/2}$ and $\mathcal{M}_{i\nu;1/2}$ appearing in Meixner's Green's function have variable order; differentiation of the Green's function with respect to $i\nu$ will entail differentiation of the Whittaker functions with respect to their order. This differentiation of the Whittaker functions with respect to order is the principal difficulty in the calculation of the reduced Green's function. This problem has been dealt with before within the context of the earlier calculation of the ground state reduced Coulomb Green's function. There relatively simple expressions

$$[\partial W_{k;1/2}/\partial k]\big|_{k=1}=e^{-z/2}[z\ln z-1], \tag{1.8}$$

$$[\partial \mathcal{M}_{k;1/2}/\partial k]\big|_{k=1}=e^{-z/2}-e^{-z/2}\left(z+1+z\int_0^z dt\,\frac{(e^t-1)}{t}\right) \tag{1.9}$$

for the derivatives with respect to order $[\partial W_{k;1/2}/\partial k]|_{k=1}$ and $[\partial \mathcal{M}_{k;1/2}/\partial k]|_{k=1}$ were obtained by term by term differentiation of appropriate infinite series representations of the Whittaker functions.[2,3] It has been found that the straightforward application of this same method to the derivatives with respect to order

$$[\partial W_{k;n/2}/\partial k]\big|_{k=(n+1)/2} \quad \text{and} \quad \partial \mathcal{M}_{k;n/2}/\partial k]\big|_{k=(n+1)/2}$$

provides the natural generalization of Eqs. (1.8) and (1.9) to Whittaker functions of higher order. The appropriate infinite series representations of the Whittaker functions required for this are[10,11]

$$\mathcal{M}_{k;n/2}=\frac{z^{(1+n)/2}e^{-z/2}}{n!}+\frac{z^{(1+n)/2}}{n!}e^{-z/2}\sum_{\lambda=1}^{\infty}\frac{[\tfrac{1}{2}(1+n)-k]_\lambda z^\lambda}{[1+n]_\lambda\lambda!} \tag{1.10}$$

and

$$\begin{aligned}W_{k;n/2}=&\frac{\sin\pi[\frac{1}{2}(1+n)-k]}{\pi[\frac{1}{2}(1+n)-k]}\,\Gamma[\tfrac{1}{2}(1+n)+k]\,\frac{z^{(1+n)/2}e^{-z/2}}{n!}\\&-\frac{\sin\pi[\frac{1}{2}(1+n)-k]}{\pi}\,\Gamma[\tfrac{1}{2}(1+n)+k]\,\mathcal{M}_{k;n/2}\ln z\\&-\frac{\sin\pi[\frac{1}{2}(1+n)-k]}{\pi}\,\Gamma[\tfrac{1}{2}(1+n)+k]\,\frac{z^{(1+n)/2}e^{-z/2}}{n!}\\&\times\{\Psi[\tfrac{1}{2}(1+n)-k+1]-\Psi[1]-\Psi[1+n]\}\\&+[\tfrac{1}{2}(1+n)-k]\,\frac{\Gamma[\frac{1}{2}(1+n)+k]}{\Gamma[\frac{1}{2}(1+n)-k+1]}\,z^{(1+n)/2}e^{-z/2}\\&\times\sum_{\lambda=1}^{n}\frac{(\lambda-1)!}{(n-\lambda)!z^\lambda}\,\frac{1}{\Gamma[\frac{1}{2}(1-n)+k+\lambda]}\\&-\frac{\sin\pi[\frac{1}{2}(1+n)-k]}{\pi}\,\Gamma[\tfrac{1}{2}(1+n)+k]\,z^{(1+n)/2}e^{-z/2}\\&\times\sum_{\lambda=1}^{\infty}\frac{[\frac{1}{2}(1+n)-k]_\lambda}{(n+\lambda)!}\{\Psi[\tfrac{1}{2}(1+n)-k+\lambda]\\&-\Psi[1+\lambda]-\Psi[1+\lambda+n]\}\frac{z^\lambda}{\lambda!}.\end{aligned} \tag{1.11}$$

Here the notation $[\alpha]_\lambda\equiv\alpha(\alpha+1)(\alpha+2)\cdots(\alpha+\lambda-1)$, $\lambda=1,2,3,\cdots$, $[\alpha]_0\equiv1$ is used. Note that for $\lambda=1,2,3,\cdots$, $[\frac{1}{2}(1+n)-k]_\lambda$ contains a factor $[\frac{1}{2}(1+n)-k]$ having a zero at $k=\frac{1}{2}(1+n)$. In each equation all except the first term has a zero at $k=\frac{1}{2}(n+1)$. The occurrence of these zeros gives rise to considerable simplification in the derivatives with respect to order when k is set equal to $\frac{1}{2}(n+1)$, and this is the feature which makes the calculation of

$$[\partial W_{k;n/2}/\partial k]\big|_{k=(n+1)/2} \quad \text{and} \quad [\partial \mathcal{M}_{k;1/2}/\partial k]\big|_{k=(n+1)/2}$$

go entirely parallel to the earlier ground state calculation. Because of the occurrence of the zeros; relatively few terms generated by the term by term differentiation of Eqs. (1.10) and (1.11) with respect to k actually contribute after setting $k=\frac{1}{2}(n+1)$, and relatively simple expressions, Eqs. (2.5) and (2.6), are obtained for the more general derivatives with respect to order.

Equations (2.5) and (2.6) still do not provide the derivatives with respect to order

$$[\partial W_{k;1/2}/\partial k]\big|_{k=n} \quad \text{and} \quad [\partial \mathcal{M}_{k;1/2}/\partial k]\big|_{k=n}$$

needed for the calculation of the reduced Green's function, but in Sec. IIA it is shown that the latter derivatives can be related to the derivatives of Eqs. (2.5) and (2.6) by use of appropriate identities for the Whittaker functions. However, in the explicit evaluation of the

derivatives $[\partial W_{k;1/2}/\partial k]_{k=n}$ and $[\partial \mathcal{M}_{k;1/2}/\partial k]|_{k=n}$ a considerable proliferation of terms is encountered. Sections IIB and IIC are devoted to organizing and simplifying these terms for $[\partial W_{k;1/2}/\partial k]|_{k=n}$ and $[\partial \mathcal{M}_{k;1/2}/\partial k]|_{k=n}$, respectively. In these reductions we are guided by the possibility of writing the new derivatives with respect to order without the introduction of new hypergeometric functions not already appearing in the ground state reduced Coulomb Green's function. Also as far as possible all polynomials encountered are written in terms of the same orthogonal set of Laguerre polynomials, $L_p^1(z)$, $p=0,1,2,3,\cdots$. Our final result, Eq. (2.28), is a rather symmetric and relatively compact expression for the one-dimensional excited state reduced Coulomb Green's function. This result is presented and discussed in Sec. IID.

Finally, in Sec. IIE we investigate the differential equation and orthogonality condition which determine $K_{1D}(u,v,E_n)$ uniquely. This leads to an interesting alternate derivation of Eq. (2.28).

II. DERIVATION OF EXCITED STATE GREEN'S FUNCTION

A. Further development of equations for $K_{1D}(u, v, E_n)$

When Eqs. (1.5) and (1.6) are combined and the result expressed in terms of $i\nu$ as independent variable instead of E, we obtain [see Eq. (1.7) for the form of the operator O in Eq. (1.6) when $i\nu$ is the independent variable]

$$K_{1D}(u,v,E_n) = \tfrac{1}{4}na_1\frac{\partial}{\partial i\nu}\left(\frac{\pi(i\nu-n)}{\sin\pi(i\nu-n)}\frac{(-1)^{(n-1)}}{\Gamma(1+i\nu)}(n+i\nu)\times W_{i\nu;1/2}(2r_>/a_1 i\nu)\mathcal{M}_{i\nu;1/2}(2r_</a_1 i\nu)\right)\Big|_{i\nu=n}. \quad (2.1)$$

The removal of the pole at $i\nu=n$ of the full Green's function is reflected in the structure of Eq. (2.1) in which the combination $\pi(i\nu-n)/\sin\pi(i\nu-n)$ is analytic near $i\nu=n$. The terms generated in the differentiation in Eq. (2.1) can be simplified as in Ref. 3 by use of the identities[12]

$$\mathcal{M}_{n+(1+\mu)/2}(z) = n!\,z^{(1+\mu)/2}e^{-z/2}L_n^\mu(z)/\Gamma(1+n+\mu) \quad (2.2a)$$

$$W_{n+(1+\mu)/2}(z) = (-1)^n n!\,z^{(1+\mu)/2}e^{-z/2}L_n^\mu(z), \quad (2.2b)$$

and[13]

$$(\partial/\partial z)\Gamma(z) = \Gamma(z)\Psi(z), \quad (2.3)$$

$$\Psi(1+n) = \Psi(1) + \sum_{\lambda=1}^{n}\frac{1}{\lambda}, \quad \Psi(1) = -\gamma. \quad (2.4)$$

Here γ is the Euler–Mascheroni constant. As discussed in the introduction the calculation of the derivatives with respect to order $[\partial W_{k;1/2}/\partial k]|_{k=n}$ and $[\partial \mathcal{M}_{k;1/2}/\partial k]|_{k=n}$ needed in Eq. (2.1) proceeds in two steps. We first obtain the generalization

$$[\partial \mathcal{M}_{k;n/2}(z)/\partial k]|_{k=(n+1)/2} = -z^{(n+1)/2}e^{-z/2}\int_0^z dt\,t^{-n-1}\left(e^t - \sum_{\lambda=0}^{n}\frac{t^\lambda}{\lambda!}\right) \quad (2.5)$$

and

$$[\partial W_{k;n/2}(z)/\partial k]|_{k=(n+1)/2} \quad (2.6)$$

$$= n!\,\mathcal{M}_{(n+1)/2;n/2}(z)\ln z - z^{(n+1)/2}e^{-z/2}\sum_{\lambda=1}^{n}\frac{n!}{(n-\lambda)!\lambda z^\lambda},$$

to Whittaker functions of higher order of the earlier ground state results of Eqs. (1.8) and (1.9). This is accomplished by term-by-term differentiation of Eqs. (1.10) and (1.11), followed by substitution of $k=\frac{1}{2}(n+1)$. Then we seek to relate these derivatives with respect to order to the derivatives with respect to order needed in Eq. (2.1). The equations bridging the gap between the derivatives of Eqs. (2.5) and (2.6) and the derivatives with respect to order needed in Eq. (2.1) are found to be the special cases of[14]

$$\frac{d^p}{dz^p}\left(e^{-z/2}z^{(n-1)/2}\mathcal{M}_{k;n/2}(z)\right) = e^{-z/2}z^{(n-1-p)/2}\mathcal{M}_{k+p/2;(n-p)/2}(z) \quad (2.7)$$

and

$$\frac{d^p}{dz^p}\left(e^{-z/2}z^{(n-1)/2}W_{k;n/2}(z)\right) = (-1)^p e^{-z/2}z^{(n-1-p)/2}W_{k+p/2;(n-p)/2}(z), \quad (2.8)$$

for which $p=n-1$. If both sides of Eqs. (2.7) and (2.8) with $p=n-1$ are differentiated with respect to k and evaluated at $k=\frac{1}{2}(n+1)$, then on the right-hand sides the desired quantities $[\partial \mathcal{M}_{k;1/2}(z)/\partial k]|_{k=n}$ and $[\partial W_{k;1/2}(z)/\partial k]|_{k=n}$ appear. These quantities are thus expressed in terms of derivatives which can be evaluated in terms of Eqs. (2.5) and (2.6). In the following, some further reductions are used to simplify the derivatives with respect to order, before substituting in Eq. (2.1).

B. Further reduction of the expression for $[\partial W_{k;\frac{1}{2}}(z)/\partial k]|_{k=n}$

Use of Eq. (2.6) in conjunction with the derivative with respect to k, evaluated at $k=\frac{1}{2}(n+1)$, of Eq. (2.8) with $p=n-1$ leads to the expression

$$(-1)^{n-1}n!\,e^{z/2}\frac{d^{n-1}}{dz^{n-1}}\left(e^{-z/2}z^{(n-1)/2}\mathcal{M}_{(n+1)/2;n/2}\ln z\right) - (-1)^{n-1}n!\,e^{z/2}\frac{d^{n-1}}{dz^{n-1}}\left(\sum_{\lambda=1}^{n}\frac{e^{-z}z^{n-\lambda}}{(n-\lambda)!\lambda}\right)$$

for $[\partial W_{k;1/2}/\partial k]|_{k=n}$. This expression is further reduced as[15]

$$(-1)^{n-1}n!\,e^{z/2}\sum_{\lambda=0}^{n-1}\binom{n-1}{\lambda}\frac{d^{n-1-\lambda}}{dz^{n-1-\lambda}}\left[e^{-z/2}z^{(n-1)/2}\mathcal{M}_{(n+1)/2;n/2}\right]\times\frac{d^\lambda}{dz^\lambda}(\ln z) - (-1)^{n-1}n!\,e^{z/2}\sum_{\lambda=1}^{n}\frac{(n-1)!\,z^{-\lambda+1}e^{-z}L_{n-1}^{-\lambda+1}}{(n-\lambda)!\lambda}$$

$$= (-1)^{n-1}n!\,e^{z/2}\sum_{\lambda=0}^{n-1}\binom{n-1}{\lambda}\frac{(n-1-\lambda)!}{n!}e^{-z}z^{\lambda+1}L_{n-1-\lambda}^{\lambda+1}\cdot\frac{d^\lambda}{dz^\lambda}(\ln z) - (-1)^{n-1}n!\,e^{z/2}\sum_{\lambda=1}^{n}\frac{e^{-z}}{\lambda}(-1)^{\lambda-1}L_{n-\lambda}^{\lambda-1},$$

by use of Eq. (2.7) with $p=n-1-\lambda$, Eq. (2.2a), and the two identities[16]

$$L_n^\mu(z) = \frac{e^z z^{-\mu}}{n!}\frac{d^n}{dz^n}(e^{-z}z^{\mu+n}), \quad \mu \text{ arbitrary}, \quad (2.9)$$

and[17]

$$\frac{(-z)^m}{m!}L_n^{m-n}(z)=\frac{(-z)^n}{n!}L_m^{n-m}(z),\quad n,m=0,1,2,\cdots. \tag{2.10}$$

The $\lambda=0$ part of the first λ-sum above is written separately. After working out the derivatives of the logarithm, the remaining part of the first λ-sum is combined with the second λ-sum to give

$$\begin{aligned}[\partial W_{k;1/2}/\partial k]\big|_{k=n}&=(-1)^{n-1}(n-1)!\,e^{-z/2}zL_{n-1}^1\ln z\\&\quad+(-1)^{n-1}(n-1)!\,e^{-z/2}\sum_{\lambda>0}\frac{(-1)^{\lambda-1}}{\lambda}(zL_{n-1-\lambda}^{\lambda+1}-nL_{n-\lambda}^{\lambda-1}).\end{aligned} \tag{2.11}$$

The identities[18]

$$\frac{d^p}{dz^p}L_n^\mu(z)=(-1)^pL_{n-p}^{\mu+p}(z) \tag{2.12}$$

and[19]

$$z\frac{d}{dz}L_n^\mu=-\mu L_n^\mu+(\mu+n)L_n^{\mu-1} \tag{2.13}$$

allow the combination of Laguerre polynomials in Eq. (2.11) to be rewritten as

$$zL_{n-1-\lambda}^{\lambda+1}-nL_{n-\lambda}^{\lambda-1}=\lambda L_{n-\lambda}^\lambda-2nL_{n-\lambda}^{\lambda-1}.$$

After this rearrangement, one of the two terms of the λ-sum becomes[20]

$$\sum_{\lambda=1}^{n}(-1)^{\lambda-1}L_{n-\lambda}^\lambda=L_{n-1}^0. \tag{2.14}$$

At this point we have the formula

$$\begin{aligned}[\partial W_{k;1/2}/\partial k]\big|_{k=n}&=(-1)^{n-1}(n-1)!\,e^{-z/2}zL_{n-1}^1\ln z\\&\quad+(-1)^{n-1}(n-1)!\,e^{-z/2}L_{n-1}^0\\&\quad-(-1)^{n-1}(n-1)!\,2ne^{-z/2}\sum_{\lambda>0}\frac{(-1)^{\lambda-1}}{\lambda}L_{n-\lambda}^{\lambda-1}.\end{aligned} \tag{2.15}$$

This remaining λ-sum is investigated in Appendix B where it is shown that

$$\sum_{\lambda>0}\frac{(-1)^{\lambda-1}}{\lambda}L_{n-\lambda}^{\lambda-1}(z)=\frac{\partial L_n^\mu(z)}{\partial\mu}\bigg|_{\mu=-1} \tag{2.16}$$

and that the derivative with respect to μ can be re-expanded as

$$\frac{\partial L_n^\mu(z)}{\partial\mu}\bigg|_{\mu=-1}=\frac{1}{n}-z\sum_{0<\lambda<n}\frac{L_{n-1-\lambda}^1}{\lambda(n-\lambda)} \tag{2.17}$$

in which only the lower index of the Laguerre polynomial varies with the summation variable λ. The final result of the reductions of this subsection is the formula

$$\begin{aligned}&\frac{\partial}{\partial k}\left(\frac{(-1)^{n-1}}{(n-1)!}W_{k;1/2}\right)\bigg|_{k=n}\\&\quad=e^{-z/2}\left(zL_{n-1}^1\ln z+L_{n-1}^0-2+2nz\sum_{0<\lambda<n}\frac{L_{n-1-\lambda}^1}{\lambda(n-\lambda)}\right),\end{aligned} \tag{2.18}$$

and this is the form which will be used with Eq. (2.1) for the reduced Green's function.

C. Further reduction of the expression for $[\partial W_{k;1/2}/\partial k]\,|_{k=n}$

In the integral of Eq. (2.5) the substitution

$$\frac{1}{t^{n+1}}=\frac{(-1)^n}{n!}\frac{d^{n+1}}{dt^{n+1}}\ln t$$

is made and $n+1$ integrations by parts are performed giving

$$\begin{aligned}&\int_0^z dtt^{-n-1}\left(e^t-\sum_{\lambda=0}^{n}\frac{t^\lambda}{\lambda!}\right)\\&\quad=-\frac{1}{n!}\int_0^z dte^t\ln t+\frac{1}{n!}(e^z-1)\ln z\\&\qquad-\frac{1}{n!}\sum_{p=0}^{n-1}\frac{(n-p-1)!}{z^{n-p}}\left(e^z-\sum_{\alpha=0}^{n-p}\frac{z^\alpha}{\alpha!}\right),\end{aligned}$$

which is transformed into

$$\begin{aligned}&\int_0^z dtt^{-n-1}\left(e^t-\sum_{\lambda=0}^{n}\frac{t^\lambda}{\lambda!}\right)\\&\quad=\frac{g(z)}{n!}-\sum_{p=0}^{n-1}\frac{(n-1-p)!}{n!z^{n-p}}\left(e^z-\sum_{\alpha=0}^{n-p}\frac{z^\alpha}{\alpha!}\right),\end{aligned} \tag{2.19}$$

$$g(z)\equiv\int_0^z dt\,\frac{e^t-1}{t}=-ze^z\int_0^1 dte^{-tz}\ln(1-t), \tag{2.20}$$

by changing the integration variable in $\int_0^z dte^t\ln t$ to ξ where $t=(1-\xi)z$ and performing another integration by parts. The function $g(z)$ occurred before in connection with the ground state reduced Green's function. It has the simple differentiation property

$$dg(z)/dz=(e^z-1)/z \tag{2.21}$$

which is needed occasionally. Our task is now to substitute the right-hand side of Eq. (2.19) into Eq. (2.5), substitute that into Eq. (2.7) with $p=n-1$, differentiate, and simplify. Some of the initial steps in this reduction are

$$\begin{aligned}&[\partial W_{k;1/2}/\partial k]\big|_{k=n}\\&\quad=-\frac{e^{z/2}}{n!}\sum_{\lambda=0}^{n-1}\binom{n-1}{\lambda}\frac{d^{n-1-\lambda}}{dz^{n-1-\lambda}}[z^ne^{-z}]\frac{d^\lambda}{dz^\lambda}g(z)+\frac{e^{z/2}}{n}\\&\qquad-e^{z/2}\sum_{p=0}^{n-1}\sum_{\alpha=0}^{n-p}\frac{(n-1-p)!}{n!\alpha!}(n-1)!\,z^{\alpha+p-(n-1)}e^{-z}L_{n-1}^{\alpha+p-(n-1)}\\&\quad=-\frac{e^{-z/2}}{n}zL_{n-1}^1g(z)\\&\qquad-\frac{e^{-z/2}}{n!}\sum_{0<\lambda\le n-1}\binom{n-1}{\lambda}(n-1-\lambda)!\,z^{\lambda+1}L_{n-1-\lambda}^{1+\lambda}\frac{d^{\lambda-1}}{dz^{\lambda-1}}\left[\frac{e^z-1}{z}\right]\\&\qquad+\frac{e^{z/2}}{n}\\&\qquad-e^{-z/2}\sum_{p=0}^{n-1}\sum_{\alpha=0}^{n-p}\frac{(n-1-p)!(\alpha+p)!}{n!\alpha!}(-1)^{\alpha+p+n-1}L_{\alpha+p}^{n-1-(\alpha+p)}\\&\quad=-\frac{e^{-z/2}}{n}zL_{n-1}^1g(z)\\&\qquad-\frac{e^{z/2}}{n}\sum_{0<\lambda\le n-1}\frac{z^{\lambda+1}}{\lambda!}L_{n-1-\lambda}^{1+\lambda}\sum_{\rho=0}^{\lambda-1}\binom{\lambda-1}{\rho}\frac{d^\rho}{dz^\rho}\frac{1}{z}\end{aligned}$$

$$+\frac{e^{-z/2}}{n}\sum_{0<\lambda\le n-1}\frac{z^{\lambda+1}}{\lambda!}\,L^{1+\lambda}_{n-1-\lambda}\,\frac{d^{\lambda-1}}{dz^{\lambda-1}}\,\frac{1}{z}$$

$$+\frac{e^{z/2}}{n}$$

$$+e^{-z/2}L^{-1}_{n}\sum_{p=0}^{n-1}\frac{1}{n-p}$$

$$-e^{-z/2}\sum_{\lambda=1}^{n}\frac{(n-\lambda)!}{n!}(-1)^{\lambda-1}L^{\lambda-1}_{n-\lambda}\sum_{p=0}^{n-\lambda}\frac{(n-1-p)!}{(n-\lambda-p)!}$$

$$=-\frac{e^{-z/2}}{n}\,zL^{1}_{n-1}g(z)$$

$$-\frac{e^{z/2}}{n}\sum_{0<\lambda\le n-1}\frac{(-1)^{\lambda-1}}{\lambda}\,zL^{1+\lambda}_{n-1-\lambda}\sum_{\sigma=0}^{\lambda-1}\frac{(-z)^{\sigma}}{\sigma!}$$

$$+\frac{e^{-z/2}}{n}\sum_{0<\lambda\le n}\frac{(-1)^{\lambda-1}}{\lambda}\,[\lambda L^{\lambda}_{n-\lambda}-nL^{\lambda-1}_{n-\lambda}]$$

$$+\frac{e^{z/2}}{n}-\frac{e^{-z/2}}{n}\,zL^{1}_{n-1}\sum_{\lambda=1}^{n}\frac{1}{\lambda}$$

$$-e^{-z/2}\sum_{0<\lambda\le n}\frac{(-1)^{\lambda-1}}{\lambda}\,L^{\lambda-1}_{n-\lambda}.$$

To obtain the expression to the right of the first equal sign here Eq. (2.9) was used. The next step in the reduction follows from Eqs. (2.21) and (2.10). In the next to the last step in the reduction the $\lambda-1$ derivatives of $z^{-1}\exp z$ are worked out, and the double sum involving $L^{n-1-(\alpha+p)}_{\alpha+p}$ is rearranged by taking $\lambda=n-(\alpha+p)$ as new summation variable, with the $\lambda=0$ term split off as a separate term. The last expression was obtained by using Eqs. (2.12) and (2.13) as in Sec. IIB, to reduce $zL^{1+\lambda}_{n-1-\lambda}=-(zd/dz)L^{\lambda}_{n-\lambda}$, and also by using a form of Lerch's theorem[21]

$$\sum_{p=0}^{n-\lambda}\binom{n-1-p}{\lambda-1}=\binom{n}{\lambda}.$$

Use of Eqs. (2.14), (2.16), (2.17), now gives the final result of the reductions of this section:

$$[\partial\mathcal{H}_{k;1/2}/\partial k]\big|_{k=n}$$

$$=\frac{e^{-z/2}}{n}\left[-zL^{1}_{n-1}g(z)+L^{0}_{n-1}-2\right.$$

$$\left.+2nz\sum_{0<\lambda<n}\frac{L^{1}_{n-1-\lambda}}{\lambda(n-\lambda)}-zL^{1}_{n-1}\sum_{\lambda=1}^{n}\frac{1}{\lambda}\right]$$

$$+\frac{e^{z/2}}{n}\mathcal{O}(z). \tag{2.22}$$

The polynomial

$$\mathcal{O}(z)\equiv 1-z\sum_{0<\lambda<n}\frac{(-1)^{\lambda}}{\lambda}\,L^{1+\lambda}_{n-1-\lambda}\sum_{\sigma=0}^{\lambda-1}\frac{(-z)^{\sigma}}{\sigma!} \tag{2.23}$$

is studied in Appendix C, where it is shown to have the simple integral representation

$$\mathcal{O}(z)=\int_0^{\infty}ds\,e^{-s}\,\frac{sL^{1}_{n-1}(s)-zL^{1}_{n-1}(z)}{s-z}\quad. \tag{2.24}$$

From this integral representation other forms of $\mathcal{O}(z)$ can be derived.[22] Two of these are

$$\mathcal{O}(z)=1+\sum_{0<\lambda<n}\frac{(\lambda-1)!}{z^{\lambda-1}}\left[L^{1}_{n-1}-\sum_{\rho=0}^{\lambda-1}\binom{n}{n-1-\rho}\frac{(-z)^{\rho}}{\rho!}\right] \tag{2.25}$$

in which $\mathcal{O}(z)$ is exhibited as a sum of $z^{-(\lambda-1)}$ times truncated forms of $L^{1}_{n-1}(z)$, and

$$\mathcal{O}(z)=1-z\sum_{0<\lambda<n}\int_0^1 d\xi\,\xi^{n-1-\lambda}L^{1}_{\lambda-1}(\xi z), \tag{2.26}$$

which is free of indeterminate forms. The expression (2.18) for $[\partial W_{k;1/2}/\partial k]\big|_{k=n}$ and (2.22) for $[\partial\mathcal{H}_{k;1/2}/\partial k]\big|_{k=n}$ have each been checked by direct substitution into their respective differential equations (2.36 a,b) to be derived in Sec. IIE. In checking the expression (2.22) the differential equation

$$z\frac{d^2\mathcal{O}}{dz^2}+z\frac{d\mathcal{O}}{dz}+n\mathcal{O}=L^{1}_{n-1}-2zL^{2}_{n-2} \tag{2.27}$$

for $\mathcal{O}$ was encountered. The check of Eq. (2.27) is included in Appendix C.

D. Closed form for excited state reduced Coulomb Green's functions

The necessary ingredients needed for the evaluation of $K_{1D}(u,v;E_n)$ using Eq. (2.1) have now been assembled. Basic among these ingredients are the two new results expressed in Eqs. (2.18) and (2.22). By working out the derivative in Eq. (2.1) the following expression for $K_{1D}(u,v;E_n)$ is obtained[23]:

$$K_{1D}(u,v;E_n)$$

$$=\tfrac{1}{2}a_1e^{-(u+v)/2}uvL^{1}_{n-1}(u)L^{1}_{n-1}(v)\left(\ln u-g(v)\right.$$

$$\left.+\frac{u+v}{2n}+\frac{1}{2n}-2\sum_{\lambda=1}^{n}\frac{1}{\lambda}-2+\gamma\right)$$

$$+\tfrac{1}{2}a_1e^{-(u+v)/2}vL^{1}_{n-1}(v)\mathcal{L}(u)+\tfrac{1}{2}a_1e^{-(u+v)/2}uL^{1}_{n-1}(u)\mathcal{L}(v)$$

$$+\tfrac{1}{2}a_1e^{-(u-v)/2}uL^{1}_{n-1}(u)\mathcal{O}(v), \tag{2.28}$$

$$\mathcal{L}(z)\equiv L^{1}_{n-1}-2+2nz\sum_{0<\lambda<n}\frac{L^{1}_{n-1-\lambda}}{\lambda(n-\lambda)}+(z-1)L^{1}_{n-2}. \tag{2.29}$$

This is the excited state reduced Coulomb Green's function for the one-dimensional Kepler problem. The similarity in form between Eq. (2.28) and the earlier ground state result[24] in one dimension is quite remarkable. In the ground state case ($n=1$), the factors L^{1}_{n-1}, $\mathcal{O}$, and $\mathcal{L}$ become just factors of $\pm1(L^{1}_{0}=\mathcal{O}\big|_{n=1}=1$, $\mathcal{L}\big|_{n=1}=-1)$. The expression (2.28) consists essentially of terms of the ground state result which have picked up additional "form factors" made up of the polynomials L^{1}_{n-1}, $\mathcal{O}$, and $\mathcal{L}$. For example, the same $\ln u$ and $g(v)$ terms of the ground state result appear again in the excited state Green's function except that they pick up the additional form factor $L^{1}_{n-1}(u)L^{1}_{n-1}(v)$. No new hypergeometric functions appear in the excited state Green's function.

As pointed out in the introduction, our expression (2.28) can be used to generate excited state reduced Coulomb Green's functions in spaces of higher odd dimensionality. In particular, the three-dimensional reduced Green's function can be calculated as[5]

$$K_{3D}(\mathbf{r}_2,\mathbf{r}_1,E_n)=-\frac{1}{2\pi na_1|\mathbf{r}_2-\mathbf{r}_1|}\left(\frac{\partial}{\partial u}-\frac{\partial}{\partial v}\right)K_{1D}(u,v,E_n)$$

in which $K_{1D}(u,v,E_n)$ is the expression (2.28). What is essentially the result of Swierkowski and Suffczynski[4]

for the three-dimensional reduced Green's function is thereby obtained by a straightforward differentiation of the simpler one-dimensional function.

In view of the relation

$$g_{l=0}(r_2, r_1; E) = (r_2 r_1)^{-1} G_{1D}(r_2, r_1; E) \tag{2.30}$$

between the S-wave component[25] of the full three-dimensional Coulomb Green's function and the Coulomb Green's function in one-dimensional space, and the fact that this relation will be preserved by the operations of Eq. (1.6) generating the reduced Green's functions, it is apparent that the expression (2.28) doubles as essentially [i.e., aside from the factor $(r_2 r_1)^{-1}$], the s-wave component of the three-dimensional excited state reduced Coulomb Green's function. Thus Eq. (2.28) is essentially the excited state generalization of Hameka's original result.[26]

E. Differential equation and orthogonality condition

The differential equation of the reduced Coulomb Green's function is derived by investigating the effect of the differential operator $H-E_n$, where H is the Hamiltonian, on the eigenfunction expansion (1.1) defining $K(\mathbf{r}_2, \mathbf{r}_1; E_n)$. For the one-dimensional Kepler problem this differential equation is

$$\left(\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2 a_1} - \frac{1}{n^2 a_1^2}\right) K_{1D}(r_2, r_1; E_n)$$

$$= \delta(r_2 - r_1) - e^{-(r_2+r_1)/na_1} \frac{4 r_2 r_1}{n^5 a_1^3} L_{n-1}^1(2r_2/na_1) L_{n-1}^1(2r_1/na_1). \tag{2.31}$$

As shown in Ref. 3, the differential equation together with suitable regularity conditions at the origin and at infinity uniquely determine the reduced Green's function, except as regards its component in the sense of Hilbert space along the energy eigensubspace of H to energy E_n. Thus the solution of Eq. (2.31) becomes unique when the magnitude of the projection of $K_{1D}(r_2, r_1; E_n)$ along the energy eigensubspace to energy E_n is prescribed. A look at the eigenfunction expansion (1.1) shows that this projection is zero.

$$\int_0^\infty dr_2 \phi_n^*(r_2) K_{1D}(r_2, r_1; E_n) = 0, \tag{2.32}$$

where

$$\phi_n(r_2) = \frac{e^{-r_2/na_1}(2r_2/na_1) L_{n-1}^1(2r_2/na_1)}{n^{3/2} a_1^{1/2}} \tag{2.33}$$

is the nth state energy eigenfunction. The orthogonality condition (2.32) together with the differential equation (2.31) and boundary conditions serve to uniquely characterize the reduced Green's function. A remarkable simplification of the differential equation for K_{1D} occurs if one expresses K_{1D} as a function of the two variables $u = 2r_>/na_1$ and $v = 2r_</na_1$, instead of r_2 and r_1. By use of the equations

$$\partial u/\partial r_2 = 2\theta(r_2 - r_1)/na_1, \quad \partial v/\partial r_2 = 2\theta(r_1 - r_2)/na_1 \tag{2.34}$$

in which $\theta(x)$ is the unit step function, with $d\theta(x)/dx = \delta(x)$, one finds that the differential equation (2.31) splits into three relations[27]

$$\left(\frac{\partial^2}{\partial u^2} - \frac{1}{4} + \frac{n}{u}\right) K_{1D}(u, v; E_n) = -\frac{a_1(-1)^{n-1}}{4(n-1)!} W_{n;1/2}(u) \mathcal{M}_{n;1/2}(v), \tag{2.35a}$$

$$\left(\frac{\partial^2}{\partial v^2} - \frac{1}{4} + \frac{n}{v}\right) K_{1D}(u, v; E_n) = -\frac{a_1(-1)^{n-1}}{4(n-1)!} W_{n;1/2}(u) \mathcal{M}_{n;1/2}(v), \tag{2.35b}$$

$$\left(\frac{\partial}{\partial u} - \frac{\partial}{\partial v}\right) K_{1D}(u, v; E_n)\Big|_{u=v} = na_1/2. \tag{2.35c}$$

The two differential equations (2.35a,b) have the advantage that separable solutions can be found. The condition (2.35c) ensures that the delta function singularity of $\partial^2 K_{1D}/\partial r_2^2$ has unit magnitude as required by Eq. (2.31). It should be emphasized that Eqs. (2.35a,b,c) and boundary conditions must be supplemented by the orthogonality relation (2.32) in order to provide a unique characterization of K_{1D}. In the following we indicate briefly how the closed expression for K_{1D} can be rederived from the stand point of the differential equation.

Inhomogeneous terms of the form occurring in Eqs. (2.35 a,b,c) can be generated by differentiation of the homogeneous Whittaker's equation for $W_{k;1/2}(nu/k)$ and $\mathcal{M}_{k;1/2}(nv/k)$ with respect to the order k, followed by substitution of $k = n$. Thus

$$[\partial W_{k;1/2}(nu/k)/\partial k]\big|_{k=n}$$

$$= [\partial W_{k;1/2}(u)/\partial k]\big|_{k=n} - (u/n)\dot{W}_{n;1/2}(u)$$

and

$$[\partial \mathcal{M}_{k;1/2}(nv/k)/\partial k]\big|_{k=n}$$

$$= [\partial \mathcal{M}_{k;1/2}(v)/\partial k]\big|_{k=n} - (v/n)\dot{\mathcal{M}}_{n;1/2}(v)$$

obey the inhomogeneous equations

$$\left(\frac{\partial^2}{\partial u^2} - \frac{1}{4} + \frac{n}{u}\right)\left(\frac{\partial W_{k;1/2}}{\partial k}\Big|_{k=n} - \frac{u}{n}\dot{W}_{n;1/2}\right) = -\frac{1}{2n} W_{n;1/2} \tag{2.36a}$$

and

$$\left(\frac{\partial^2}{\partial v^2} - \frac{1}{4} + \frac{n}{v}\right)\left(\frac{\partial \mathcal{M}_{k;1/2}}{\partial k}\Big|_{k=n} - \frac{v}{n}\dot{\mathcal{M}}_{n;1/2}\right) = -\frac{1}{2n}\mathcal{M}_{n;1/2}. \tag{2.36b}$$

Comparison of Eqs. (2.36a,b) and Eqs. (2.35a,b) shows that the function

$$\frac{na_1}{2}\frac{(-1)^{n-1}}{(n-1)!}\frac{\partial W_{k;1/2}(nu/k)}{\partial k}\Big|_{k=n} \mathcal{M}_{n;1/2}(v)$$

obeys the inhomogeneous Eq. (2.35a) and the homogeneous form of Eq. (2.35b), while the function

$$\frac{na_1}{2}\frac{(-1)^{n-1}}{(n-1)!} W_{n;1/2}(u)\frac{\partial \mathcal{M}_{k;1/2}(nv/k)}{\partial k}\Big|_{k=n}$$

obeys the inhomogeneous Eq. (2.35b) and the homogeneous form of Eq. (2.35a). Addition of these two functions therefore produces a simultaneous solution of both inhomogeneous Eqs. (2.35a,b). But the sum of these functions is just

$$\frac{na_1}{2}\frac{(-1)^{n-1}}{(n-1)!}\frac{\partial}{\partial k}[W_{k;1/2}(nu/k)\mathcal{M}_{k;1/2}(nv/k)]\big|_{k=n} \tag{2.37}$$

a particular integral of Eqs. (2.35a,b). The most general solution of Eqs. (2.35a,b) is then

$$K_{1D}=\frac{na_1}{2}\frac{(-1)^{n-1}}{(n-1)!}\frac{\partial}{\partial k}\left[W_{k;1/2}(nu/k)/\mathcal{N}_{k;1/2}(nv/k)\right]\Big|_{k=n}$$

$$+C\frac{na_1}{2}\frac{(-1)^{n-1}}{(n-1)!}W_{n;1/2}(u)/\mathcal{N}_{n;1/2}(v), \qquad (2.38)$$

which is just (2.37) plus a general solution of the homogeneous Eqs. (2.35a,b) obeying appropriate boundary conditions. It is evident that the differential equation has lead back to the original representation (2.1) of K_{1D} modulo a solution of the homogeneous equation—additional terms in Eq. (2.1) generated by the action of $\partial/\partial iv$ on factors outside both Whittaker functions are proportional to $W_{n;1/2}(u)/\mathcal{N}_{n;1/2}(v)$ and are homogeneous solutions as demanded by Eq. (2.38).

When we investigate the effect of imposing the further condition (2.35c) on our solution (2.38) we find that the constant C drops out, and we encounter the relation

$$u\det\begin{bmatrix} L^1_{n-1}(u) & O(u) \\ L^1_{n-1}(u) & O(u)\end{bmatrix}$$

$$=-n+u[L^1_{n-1}(u)]^2+(1-u)L^1_{n-1}(u)O(u)$$

which can be shown to be an identity by showing that the derivatives of both sides are equal, and that both sides agree for $u=0$. In order to show that the derivates are equal, the differential equation (2.27) for O and the differential equation of the Laguerre polynomials is required. Our general solution (2.38) therefore obeys condition (2.35c), for any value of C.[28]

The orthogonality relation (2.32) will now be used to fix the value of the constant C, whereby complete agreement between Eqs. (2.38) and (2.1) including the magnitude of the homogeneous solution is achieved. The integration region in Eq. (2.32) is split up into two parts $0\le r_2\le r_1$ and $r_1\le r_2\le+\infty$:

$$\int_0^{r_1}dr_2\varphi_n^*(r_2)K_{1D}(2r_1/na_1,\,2r_2/na_1;E_n)$$

$$+\int_{r_1}^{\infty}dr_2\varphi_n^*(r_2)K_{1D}(2r_2/na_1,\,2r_1/na_1;E_n)=0.$$

The function $K_{1D}(u,v;E_n)$ is understood here, and the relations $u=2r_>/na_1$, $v=2r_</na_1$ have been taken into account in arriving at this expression. For convenience, we denote $2r_2/na_1$ by u and $2r_1/na_1$ by v in both integrals obtaining

$$\int_0^v du e^{-u/2}uL^1_{n-1}(u)K_{1D}(v,u;E_n)$$

$$+\int_v^{\infty}du e^{-u/2}uL^1_{n-1}(u)K_{1D}(u,v;E_n)=0$$

which is then rearranged in the form

$$\Lambda(v)=0, \qquad (2.39)$$

where

$$\Lambda(v)\equiv\int_0^{\infty}du e^{-u/2}uL^1_{n-1}(u)K_{1D}(u,v;E_n)$$

$$-\int_0^v du e^{-u/2}uL^1_{n-1}(u)[K_{1D}(u,v;E_n)-K_{1D}(v,u;E_n)].$$

Equation (2.39), which must hold identically in the variable v, provides in alternate expression of the orthogonality relation in terms of the variables u and v. The function $\Lambda(v)$ is here understood to be constructed with the general solution (2.38) of Eqs. (2.35a,b,c). It will be shown that this function $\Lambda(v)$ obeys the homogeneous Whittaker's equation $(\partial^2/\partial v^2-\frac{1}{4}+n/v)\Lambda(v)=0$, for any value of C. Thus

$$\frac{\partial\Lambda(v)}{\partial v}=\int_0^{\infty}du e^{-u/2}uL^1_{n-1}(u)\frac{\partial K_{1D}(u,v,E_n)}{\partial v}$$

$$-\int_0^v du e^{-u/2}uL^1_{n-1}(u)\left[\frac{\partial K_{1D}(u,v,E_n)}{\partial v}-\frac{\partial K_{1D}(v,u,E_n)}{\partial v}\right],$$

$$\frac{\partial^2\Lambda(v)}{\partial v^2}=\int_0^{\infty}du e^{-u/2}uL^1_{n-1}(u)\frac{\partial^2 K_{1D}(u,v,E_n)}{\partial v^2}$$

$$-\int_0^v du e^{-u/2}uL^1_{n-1}(u)\left(\frac{\partial^2K_{1D}(u,v,E_n)}{\partial v^2}-\frac{\partial^2K_{1D}(v,u,E_n)}{\partial v^2}\right)$$

$$-e^{-v/2}vL^1_{n-1}(v)\left(\frac{\partial K_{1D}(u,v,E_n)}{\partial v}-\frac{\partial K_{1D}(v,u,E_n)}{\partial v}\right)\Big|_{u=v}$$

and

$$\left(\frac{\partial^2}{\partial v^2}-\frac{1}{4}+\frac{n}{v}\right)\Lambda(v)$$

$$=\int_0^{\infty}du e^{-u/2}uL^1_{n-1}(u)\left(\frac{\partial^2}{\partial v^2}-\frac{1}{4}+\frac{n}{v}\right)K_{1D}(u,v,E_n)$$

$$-\int_0^v du e^{-u/2}uL^1_{n-1}(u)\left[\left(\frac{\partial^2}{\partial v^2}-\frac{1}{4}+\frac{n}{v}\right)K_{1D}(u,v,E_n)\right.$$

$$\left.-\left(\frac{\partial^2}{\partial v^2}-\frac{1}{4}+\frac{n}{v}\right)K_{1D}(v,u,E_n)\right]$$

$$-e^{-v/2}vL^1_{n-1}(v)\left(\frac{\partial K_{1D}(u,v,E_n)}{\partial v}-\frac{\partial K_{1D}(v,u,E_n)}{\partial v}\right)\Big|_{u=v}.$$

When this relation is simplified by use of Eqs. (2.35a, b, c) [and Eqs. (2.2a, b)]; the integral with variable limit drops out due to a vanishing integrand and the other terms simplify to

$$\left(\frac{\partial^2}{\partial v^2}-\frac{1}{4}+\frac{n}{v}\right)\Lambda(v)$$

$$=-\frac{a_1}{4n}\int_0^{\infty}du e^{-u}u^2[L^1_{n-1}(u)]^2e^{-v/2}vL^1_{n-1}(v)$$

$$+\frac{na_1}{2}e^{-v/2}vL^1_{n-1}(v)$$

which vanishes identically, by virtue of the integral

$$\int_0^{\infty}du e^{-u/2}u^2[L^1_{n-1}(u)]^2=2n^2.$$

It can be shown that in addition to the homogeneous Whittaker's equation the boundary condition $\Lambda(0)=0$ is obeyed by $\Lambda(v)$, again for any C. Now we wish to choose C to make $\Lambda(v)$ vanish identically. This can be achieved by imposing the further boundary condition $[\partial\Lambda(v)/\partial v]|_{v=0}=0$; since the trivial null solution is the only solution of the homogeneous Whittaker's equation obeying both boundary conditions $\Lambda(0)=0$ and $[\partial\Lambda(v)/\partial v]|_{v=0}=0$. The problem of exploiting the orthogonality relation (2.39) is thus reduced to the problem of exploiting

the addition boundary condition $[\partial\Lambda(v)/\partial v]|_{v=0}=0$. More explicity, this boundary condition reads

$$\int_0^\infty du e^{-u/2} u L_{n-1}^1(u) \left.\frac{\partial K_{1D}(u,v,E_n)}{\partial v}\right|_{v=0} = 0 \tag{2.40}$$

which proves to be adequate for the unique determination of C, as required by the arguments above. When the derivatives in Eq. (2.38) are worked out using Eqs. (2.18) and (2.22) then Eq. (2.38) goes over essentially into the closed expression (2.28) for K_{1D} except for the coefficient of the term

$$\tfrac{1}{2}a_1 e^{-(u+v)/2} uv L_{n-1}^1(u) L_{n-1}^1(v).$$

If one further applies Eq. (2.40), the equation

$$\begin{aligned} & n\int_0^\infty du e^{-u} u^2 [L_{n-1}^1(u)]^2 \left(\ln u + \frac{u}{2n} - 2 - \sum_{\lambda=1}^n \frac{1}{\lambda} + C\right) \\ & + n\int_0^\infty du e^{-u} u L_{n-1}^1(u) \mathcal{L}(u) \\ & + \int_0^\infty du e^{-u} u^2 [L_{n-1}^1(u)]^2 [-\tfrac{1}{2}\mathcal{L}(0) + \dot{\mathcal{L}}(0) + \tfrac{1}{2}\mathcal{O}(0) + \dot{\mathcal{O}}(0)] \\ & = 0 \end{aligned} \tag{2.41}$$

results. The calculation is completed by use of the relations

$$\mathcal{L}(0) = -1, \quad \mathcal{O}(0) = 1,$$

$$\frac{\dot{\mathcal{L}}(0)}{n} = \frac{-2}{n} + 2\sum_{\lambda=1}^n \frac{1}{\lambda}, \tag{2.42}$$

$$\frac{\dot{\mathcal{O}}(0)}{n} = 1 - \sum_{\lambda=1}^n \frac{1}{\lambda}, \tag{2.43}$$

$$\int_0^\infty du e^{-u} u^2 \ln u [L_{n-1}^1(u)]^2 = 2n^2 - n + 2n^2 \sum_{\lambda=1}^n \frac{1}{\lambda} - 2n^2 \tag{2.44}$$

and standard integrals involving Laguerre polynomials. Equations (2.42), (2.43), and (2.44) are derived in Appendix D. In order to evaluate the integral involving $\mathcal{L}(u)$ it was necessary to rewrite the series (2.29) introduced earlier for $\mathcal{L}(u)$ as[29]

$$\begin{aligned} \mathcal{L}(u) = 2n \sum_{\lambda=1}^n & \frac{-L_{n-\lambda}^1 + 2L_{n-\lambda-1}^1 - L_{n-\lambda-2}^1}{\lambda} \\ & - (n-2)L_{n-1}^1 + (2n-3)L_{n-2}^1 - (n-1)L_{n-3}^1. \end{aligned} \tag{2.45}$$

The integral involving $\mathcal{L}(u)$ can now be evaluated with the use of the standard orthogonality and normalization integrals[30]

$$\int_0^\infty du e^{-u} u^\mu L_n^\mu(u) L_m^\mu(u) = \delta_{n,m} \frac{\Gamma(n+\mu+1)}{n!}. \tag{2.46}$$

This result of this calculation is

$$C = \frac{1}{2n} - \sum_{\lambda=1}^n \frac{1}{\lambda} + \gamma.$$

As mentioned earlier, this brings Eq. (2.38) into complete agreement with our earlier derivation.

APPENDIX A

Equation (2.14) follows quite simply from the integral representation[31]

$$L_n^\mu(z) = \frac{1}{2\pi i}\oint_{(0+)} dt e^{-tz} \frac{(1+t)^{n+\mu}}{t^{n+1}}. \tag{A1}$$

Thus

$$L_{n-\lambda}^\lambda = \frac{1}{2\pi i}\oint dt e^{-tz} \frac{(1+t)^n}{t^{n+1}} t^\lambda,$$

$$\sum_{\lambda=1}^n (-1)^{\lambda-1} L_{n-\lambda}^\lambda = -\frac{1}{2\pi i}\oint dt e^{-tz} \frac{(1+t)^n}{t^{n+1}} \sum_{\lambda=1}^n (-t)^\lambda.$$

Here $\Sigma_{\lambda=1}^n$ can be replaced by $\Sigma_{\lambda=1}^\infty$ since the high powers of t in the additional terms remove the pole of the integrand and give zero contribution after integration. Thus

$$\sum_{\lambda=1}^n (-1)^{\lambda-1} L_{n-\lambda}^\lambda = -\frac{1}{2\pi i}\oint dt e^{-tz} \frac{(1+t)^n}{t^{n+1}} \left(\frac{1}{1+t} - 1\right)$$

$$\sum_{\lambda=1}^n (-1)^{\lambda-1} L_{n-\lambda}^\lambda = \frac{1}{2\pi i}\oint dt e^{-tz} \frac{(1+t)^{n-1}}{t^n}$$

$$\sum_{\lambda=1}^n (-1)^{\lambda-1} L_{n-\lambda}^\lambda = L_{n-1}^0. \qquad \text{QED}$$

APPENDIX B

Equations (2.16) and (2.17) will be derived here. The integral representation (A1) is differentiated with respect to μ to give

$$\frac{\partial L_n^\mu}{\partial \mu} = \frac{1}{2\pi i}\oint_{(0+)} dt e^{-tz} \frac{(1+t)^{n+\mu}}{t^{n+1}} \ln(1+t) \tag{B1}$$

Equations (2.16) or (2.17) are obtained from Eq. (B1) according as $\ln(1+t)$ is expanded as

$$\ln(1+t) = -\sum_{\lambda=1}^\infty \frac{(-t)^\lambda}{\lambda} \tag{B2}$$

or as

$$\ln(1+t) = \sum_{\lambda=1}^\infty \left(\frac{t}{1+t}\right)^\lambda \Big/ \lambda. \tag{B3}$$

As in Appendix A only the first n terms of either sum (B2) or (B3) contribute to the contour integral (B1). If the truncated series are substituted into Eq. (B1) and Eq. (A1) is used to identify the resulting integrals, the following expansions of $\partial L_n^\mu/\partial\mu$ are obtained:

$$\frac{\partial L_n^\mu}{\partial \mu} = \sum_{\lambda=1}^n \frac{(-1)^{\lambda-1}}{\lambda} L_{n-\lambda}^{\lambda+\mu} \tag{B4}$$

and

$$\frac{\partial L_n^\mu}{\partial \mu} = \sum_{\lambda=1}^n \frac{1}{\lambda} L_{n-\lambda}^\mu. \tag{B5}$$

Here Eqs. (B4) and (B5) arise from the use of the series (B2) and (B3), respectively. Equation (B4) implies Eq. (2.16) as a special case obtained for $\mu=-1$. Substitution of $\mu=-1$ in Eq. (B5) gives

$$\left.\frac{\partial L_n^\mu}{\partial \mu}\right|_{\mu=-1} = \sum_{\lambda=1}^n \frac{1}{\lambda} L_{n-\lambda}^{-1}. \tag{B6}$$

This expression is further transformed by use of the identity

$$L_p^{-1} = -\frac{z}{p} L_{p-1}^1, \tag{B7}$$

$$p \geq 1,$$

which is a special case of Eq. (2.10). Care must be exercised in this use of Eq. (B7) since the $\lambda = n$ term of Eq. (B6) does not obey the $p \geq 1$ condition. Separation

of the $\lambda = n$ term and use of Eq. (B7) then converts Eq. (B6) into Eq. (2.17). QED

APPENDIX C

The representations (2.24), (2.25), and (2.26) of $O(z)$ will be derived in this appendix, and the differential equation (2.27) will be verified. We begin with the representations of $O(z)$. These representations are transformed by introducing a new polynomial $O(z)$ through

$$O = 1 + zO. \tag{C1}$$

The integral representation

$$O(z) = \int_0^\infty ds e^{-s} \frac{L^1_{n-1}(s) - L^1_{n-1}(z)}{s - z} \tag{C2}$$

follows from Eq. (2.24) if one replaces the coefficient of $L^1_{n-1}(s)$ in the numerator by $s = (s-z) + z$ and splits the integral into a sum of two parts.[32] The desired representations of $O(z)$ will be established if it can be shown that the integral (C2) for $O(z)$ can be expanded in the forms

$$O(z) = -\sum_{0<\lambda<n} \frac{(-1)^{\lambda-1}}{\lambda} L^{1+\lambda}_{n-1-\lambda} \sum_{\sigma=0}^{\lambda-1} \frac{(-z)^\sigma}{\sigma!} \tag{C3}$$

$$O(z) = \sum_{0<\lambda<n} \frac{(\lambda-1)!}{z^\lambda} \left[L^1_{n-1} - \sum_{\rho=0}^{\lambda-1} \binom{n}{n-1-\rho} \frac{(-z)^\rho}{\rho!} \right], \tag{C4}$$

and

$$O(z) = -\sum_{0<\lambda<n} \int_0^1 d\xi \xi^{n-1-\lambda} L^1_{\lambda-1}(\xi z), \tag{C5}$$

corresponding respectively to Eqs. (2.23), (2.25) and (2.26).

To transform the integral (C2) into the form (C3) we begin by Taylor expanding the difference $L^1_{n-1}(s) - L^1_{n-1}(z)$ in the integrand in ascending powers of $s-z$

$$L^1_{n-1}(s) - L^1_{n-1}(z) = \sum_{\lambda=1}^{n-1} \frac{(s-z)^\lambda}{\lambda!} \frac{d^\lambda}{dz^\lambda} L^1_{n-1}(z) \tag{C6}$$

or

$$L^1_{n-1}(s) - L^1_{n-1}(z) = \sum_{\lambda=1}^{n-1} (s-z)^\lambda \frac{(-1)^\lambda}{\lambda!} L^{1+\lambda}_{n-1-\lambda}(z),$$

by Eq. (2.12). Each term of Eq. (C6) contains a factor $s-z$, since $\lambda \geq 1$. Therefore, when Eq. (C6) is substituted into Eq. (C2) one obtains simply

$$\begin{aligned} O &= \int_0^\infty ds e^{-s} \sum_{\lambda=1}^{n-1} (s-z)^{\lambda-1} \frac{(-1)^\lambda}{\lambda} L^{1+\lambda}_{n-1-\lambda}(z) \\ &= \sum_{\lambda=1}^{n-1} \frac{(-1)^\lambda}{\lambda!} L^{1+\lambda}_{n-1-\lambda}(z) \int_0^\infty ds e^{-s} \sum_{\sigma=0}^{\lambda-1} \binom{\lambda-1}{\sigma} (-z)^\sigma s^{\lambda-1-\sigma} \\ &= \sum_{\lambda=1}^{n-1} \frac{(-1)^\lambda}{\lambda!} L^{1+\lambda}_{n-1-\lambda}(z) \sum_{\sigma=0}^{\lambda-1} \frac{(\lambda-1)!}{\sigma!(\lambda-1-\sigma)!} (-z)^\sigma (\lambda-1-\sigma)!, \end{aligned}$$

or

$$O = -\sum_{0<\lambda<n} \frac{(-1)^{\lambda-1}}{\lambda} L^{1+\lambda}_{n-1-\lambda}(z) \sum_{\sigma=0}^{\lambda-1} \frac{(-z)^\sigma}{\sigma!},$$

which is just Eq. (C3). Thus, Eqs. (C2) and (C3) are equivalent.

To obtain the representation (C4) from the integral (C2) we begin by expanding the Laguerre polynomials in the integrand using[33]

$$L^\mu_n = \sum_{\rho=0}^{n} \binom{n+\mu}{n-\rho} \frac{(-z)^\rho}{\rho!} \tag{C7}$$

and reducing the ratios $(s^\rho - z^\rho)/(s-z)$ according to

$$\frac{s^\rho - z^\rho}{s - z} = \sum_{\sigma=0}^{\rho-1} z^\sigma s^{\rho-1-\sigma}, \tag{C8}$$

$$\rho = 1, 2, 3, \cdots.$$

Making these expansions and integrating term by term gives the double series representation

$$O = \sum_{\rho=1}^{n-1} \binom{n}{n-1-\rho} \frac{(-1)^\rho}{\rho!} \sum_{\sigma=0}^{\rho-1} z^\sigma (\rho-1-\sigma)!$$

which can be written

$$O = \sum_{0<\lambda<n} \frac{(\lambda-1)!}{z^\lambda} \sum_{\rho=\lambda}^{n-1} \binom{n}{n-1-\rho} \frac{(-z)^\rho}{\rho!} \tag{C9}$$

by a change of summation indices from

$$\rho \text{ and } \sigma \text{ to } \rho \text{ and } \lambda = \rho - \sigma.$$

The ρ-sum in Eq. (C9) will be recognized as just the truncated form of L^1_{n-1} which appears in Eq. (C4). This establishes the equivalence of Eqs. (C2) and (C4).

In order to obtain the representation (C5) we extract a factor $s-z$ from the numerator $L^1_{n-1}(s) - L^1_{n-1}(z)$ of the integrand of Eq. (C2) by means of the device

$$\begin{aligned} L^1_{n-1}(s) - L^1_{n-1}(z) &= -L^1_{n-1}((1-\xi)s + \xi z) \Big|_{\xi=0}^{\xi=1} \\ &= -\int_0^1 d\xi \frac{\partial}{\partial \xi} L^1_{n-1}((1-\xi)s + \xi z) \\ &= -(s-z) \int_0^1 d\xi L^2_{n-1}((1-\xi)s + \xi z). \end{aligned}$$

Thus

$$O = -\int_0^\infty ds e^{-s} \int_0^1 d\xi L^2_{n-2}((1-\xi)s + \xi z). \tag{C10}$$

The identity[34]

$$L^{\mu_1+\mu_2+1}_n(x+y) = \sum_{\lambda=0}^{n} L^{\mu_1}_\lambda(x) L^{\mu_2}_{n-\lambda}(y) \tag{C11}$$

is used to split up the Laguerre polynomial in Eq. (C10) into a sum of separable functions of s and z

$$O = -\int_0^\infty ds e^{-s} \int_0^1 d\xi \sum_{\lambda=0}^{n-2} L^0_{n-2-\lambda}((1-\xi)s) L^1_\lambda(\xi z).$$

Now by Eq. (C7)

$$\begin{aligned} &\int_0^\infty ds e^{-s} L^0_{n-2-\lambda}((1-\xi)s) \\ &= \int_0^\infty ds e^{-s} \sum_{\rho=0}^{n-2-\lambda} \binom{n-2-\lambda}{n-2-\lambda-\rho} \frac{[-(1-\xi)]^\rho}{\rho!} s^\rho \\ &= \sum_{\rho=0}^{n-2-\lambda} \binom{n-2-\lambda}{n-2-\lambda-\rho} [-(1-\xi)]^\rho \\ &= [1-(1-\xi)]^{n-2-\lambda} \\ &= \xi^{n-2-\lambda}. \end{aligned}$$

Substitution of this value of the s integral into Eq. (C12) and changing the summation index to $\lambda' = \lambda + 1$ gives Eq. (C5). QED

As the final result of this appendix it will be verified that $O(z)$ obeys the differential equation (2.27). In order to do this, we first convert Eq. (2.27) into the equivalent relation

$$z\frac{d^2}{dz^2}O+(2+z)\frac{d}{dz}O+(n+1)O = \frac{L^1_{n-1}-n}{z}-2L^2_{n-2} \tag{C13}$$

for $O(z)$. It will be sufficient to show that $O(z)$ obeys Eq. (C13). This will be done by use of the integral representation (C2) of $O(z)$. The derivative dO/dz is computed by differentiating Eq. (C2) under the integral sign. One of the terms of the intergrand produced by this differentiation contains the factor $\partial/\partial z(s-z)^{-1}$. This factor is converted into a factor $(-\partial/\partial s)(s-z)^{-1}$ and then the derivative $\partial/\partial s$ is removed from the denominator $(s-z)^{-1}$ by an integration by parts. This technique leads to the relation

$$\frac{dO}{dz}=-\int_0^\infty ds e^{-s}\frac{L^2_{n-1}(s)-L^2_{n-1}(z)}{s-z}+\frac{L^1_{n-1}(z)-n}{z}, \tag{C14}$$

the last terms $(L^1_{n-1}(z)-n)/z$ being "surface" terms from the integration by parts. Also, the identities (2.12) and[35]

$$L^\mu_n=L^{\mu+1}_n-L^{\mu+1}_{n-1} \tag{C15}$$

were required. Applying this same technique to Eq. (C14) leads to

$$\frac{d^2O}{dz^2}=\int_0^\infty ds e^{-s}\frac{L^3_{n-1}(s)-L^3_{n-1}(z)}{s-z} + \frac{\frac{1}{2}n(n+1)-L^2_{n-1}(z)}{z}-\frac{L^1_{n-1}(z)-n}{z^2}-\frac{L^2_{n-2}(z)}{z}. \tag{C16}$$

For the differential equation $z\,dO/dz$ and $z\,d^2O/dz^2$ are required. In computing these quantities using Eqs. (C14) and (C16) the nonsymmetric combinations $zL^{2,3}_{n-1}(s)-zL^{2,3}_{n-1}(z)$ under the integral signs are encountered. These are reduced by writing the coefficient of $L^{2,3}_{n-1}(s)$ as $z=(z-s)+s$ and then splitting off the symmetric parts $sL^{2,3}_{n-1}(s)-zL^{2,3}_{n-1}(z)$. One then encounters the integrals[36]

$$\int_0^\infty ds e^{-s}L^2_{n-1}(s)=n \quad\text{and}\quad \int_0^\infty ds e^{-s}L^3_{n-1}(s)=\tfrac{1}{2}n(n+1).$$

The results of these reductions are

$$z\frac{dO}{dz}=-\int_0^\infty ds e^{-s}\frac{sL^2_{n-1}(s)-zL^2_{n-1}(z)}{s-z}+L^1_{n-1}(z) \tag{C17}$$

and

$$z\frac{d^2O}{dz^2}=\int_0^\infty ds e^{-s}\frac{sL^3_{n-1}(s)-zL^3_{n-1}(z)}{s-z} - L^2_{n-1}(z)-L^2_{n-2}(z)-\frac{L^1_{n-1}(z)-n}{z}. \tag{C18}$$

The representations (C18), (two times) (C14), (C17), and $(n+1$ times) (C2) are now combined to produce the representation

$$z\frac{d^2O}{dz^2}+(2+z)\frac{dO}{dz}+(n+1)O = \int_0^\infty ds e^{-s}\frac{e^{-s}}{s-z}\{[sL^3_{n-1}(s)-(2+s)L^2_{n-1}(s)+(n+1)L^1_{n-1}(s)] - [zL^3_{n-1}(z)-(2+z)L^2_{n-1}(z)+(n+1)L^1_{n-1}(z)]\} - 2L^2_{n-2}(z)+\frac{L^1_{n-1}(z)-n}{z} \tag{C19}$$

of the left hand side of the differential equation (C13). But the integral in Eq. (C19) vanishes by virtue of the identity[37]

$$zL^{\mu+1}_n-(\mu+z)L^\mu_n+(n+\mu)L^{\mu-1}_n=0 \tag{C20}$$

and consequently Eq. (C19) goes over into the required differential Eq. (C13).

APPENDIX D

Here Eqs. (2.42), (2.43), and (2.44) will be derived. Equation (2.42) follows from the representation (2.29)

$$\mathcal{L}(z)=L^1_{n-1}(z)-2+2nz\sum_{0<\lambda<n}\frac{L^1_{n-1-\lambda}(z)}{\lambda(n-\lambda)}+(z-1)L^1_{n-2}(z)$$

of $\mathcal{L}(z)$. Thus

$$\dot{\mathcal{L}}(0)=\dot{L}^1_{n-1}(0)+2n\sum_{0<\lambda<n}\frac{L^1_{n-1-\lambda}(0)}{\lambda(n-\lambda)}+L^1_{n+2}(0)-\dot{L}^1_{n-3}(0).$$

But by Eq. (2.12) $\dot{L}^1_{n-1}=-L^2_{n-2}$ and $\dot{L}^1_{n-2}=-L^2_{n-3}$. Also, by Eq. (C7)

$$L^2_{n-2}(0)=\binom{n}{n-2}=\frac{n(n-1)}{2},\quad L^1_{n-1-\lambda}(0)=\binom{n-\lambda}{n-\lambda-1}=(n-\lambda),$$
$$L^2_{n-3}(0)=\frac{(n-1)(n-2)}{2}.$$

This gives $\dot{\mathcal{L}}(0)=2n\Sigma_{\lambda=1}^n 1/\lambda-2$ which implies Eq. (2.42) when divided by n.

In order to obtain Eq. (2.43), we first note that $O(0)=O(0)$, because of Eq. (C1). The representation (C5) of O gives for $O(0)$ the value

$$\begin{aligned}O(0)&=-\sum_{\lambda=1}^{n-1}\int_0^1 d\xi\,\xi^{n-1-\lambda}L^1_{\lambda-1}(0)\\&=-\sum_{\lambda=1}^{n-1}\frac{1}{n-\lambda}\binom{\lambda}{\lambda-1}\\&=-\sum_{\lambda=1}^{n-1}\frac{\lambda}{n-\lambda}\\&=\sum_{\lambda=1}^{n-1}\frac{(n-\lambda)-n}{n-\lambda}\\&=n-1-n\sum_{\lambda=1}^{n-1}\frac{1}{\lambda}\\&=n-n\sum_{\lambda=1}^{n}\frac{1}{\lambda},\end{aligned}$$

and this implies Eq. (2.43) when divided by n.

As the final result of this appendix, we obtain Eq. (2.44). This is obtained from the standard integral[38]

$$\int_0^\infty du e^{-u}u^{\mu+1}[L_n^\mu(u)]^2 = (2n+\mu+1)\frac{\Gamma(n+\mu+1)}{n!} \qquad \text{(D1)}$$

by differentiation with respect to μ. This differentiation produces

$$\int_0^\infty du e^{-u}u^{\mu+1}\ln u[L_n^\mu(u)]^2 + \int_0^\infty du e^{-u}u^{\mu+1}2L_n^\mu(u)\frac{\partial L_n^\mu(u)}{\partial\mu}$$

$$= \frac{\Gamma(n+\mu+1)}{n!} + (2n+\mu+1)\frac{\Gamma(n+\mu+1)}{n!}\Psi(n+\mu+1) \qquad \text{(D2)}$$

in which the desired integral having the factor $\ln u$ in the integrand appears. In the second integral of Eq. (D2) the factor $\partial L_n^\mu/\partial\mu$ is expanded using Eq. (B5) and the factor uL_n^μ is expanded as[39]

$$uL_n^\mu = (2n+\mu+1)L_n^\mu - (n+\mu)L_{n-1}^\mu - (n+1)L_{n+1}^\mu \qquad \text{(D3)}$$

giving

$$\int_0^\infty du e^{-u}u^{\mu+1}2L_n^\mu(u)\frac{\partial L_n^\mu(u)}{\partial\mu}$$

$$= \sum_{\lambda=1}^{n}\frac{2}{\lambda}(2n+\mu+1)\int_0^\infty du e^{-u}u^\mu L_{n-\lambda}^\mu(u)L_n^\mu(u)$$

$$-\sum_{\lambda=1}^{n}\frac{2}{\lambda}(n+\mu)\int_0^\infty du e^{-u}u^\mu L_{n-\lambda}^\mu(u)L_{n-1}^\mu(u)$$

$$-\sum_{\lambda=1}^{n}\frac{2}{\lambda}(n+1)\int_0^\infty du e^{-u}u^\mu L_{n-\lambda}^\mu(u)L_{n+1}^\mu(u) \qquad \text{(D4)}$$

in which orthogonality of the Laguerre polynomials eliminates all terms except the $\lambda=1$ term of the second sum. This surviving term is evaluated with the help of Eq. (2.46). Thus

$$\int_0^\infty du e^{-u}u^{\mu+1}2L_n^\mu(u)\frac{\partial L_n^\mu(u)}{\partial\mu} = -2n\frac{\Gamma(n+\mu+1)}{n!}. \qquad \text{(D5)}$$

Equations (D2) and (D5) imply

$$\int_0^\infty du e^{-u}u^{\mu+1}\ln u[L_n^\mu(u)]^2$$

$$= (2n+1)\frac{\Gamma(n+\mu+1)}{n!} + (2n+\mu+1)\frac{\Gamma(n+\mu+1)}{n!}\Psi(n+\mu+1). \qquad \text{(D6)}$$

The desired integral (2.44) now follows as a special case of Eq. (D6) obtained by setting $\mu=1$ and changing n into $n-1$.

[1]Quantization in a large sphere would be required to give the sum in Eq. (1.1) a meaning for the continuum states.
[2]H. F. Hameka, J. Chem. Phys. 47, 2728 (1967); and erratum in J. Chem. Phys. 48, 4810 (1968).
[3]L. Hostler, Phys. Rev. 178, 126 (1969).
[4]Swierkowski and Suffczynski, Bull. Acad. Polon. Sci. **XXI**, 285 (1973).
[5]L. Hostler, J. Math. Phys. 11, 2966 (1970), Eq. (9).
[6]J. Meixner, Math. Z. 36, 677 (1933).
[7]The functions $W_{i\nu;1/2}$ and $M_{i\nu;1/2}$ are Whittaker functions as defined in Herbert Bucholz, *Die Konfluente Hypergeometrische Function* (Springer-Verlag, Berlin, 1953).
[8]Reference 3, Eq. (2.4).
[9]The function $K_{1D}(u,v;E_n)$ in Eq. (1.6) is obtained by expressing $K_{1D}(r_>,r_<;E_n)$ as a function of the two variables $u\equiv 2r_>/na_1$ and $v\equiv 2r_>/na_1$ instead of $r_>$ and $r_<$.
[10]Reference 7, p. 12, Eq. (7); and p. 22, Eq. (25a) together with p. 21, Eq. (24a).
[11]The identities $z\Gamma(z)=\Gamma(1+z)$, $\Gamma(z)\Gamma(1-z)=\pi/\sin\pi z$ [Whittaker and Watson, *A Course of Modern Analysis* (Cambridge U. P., Cambridge, 1927), 4th. ed., pp. 237 and 239] have been used to write Eq. (1.11) in such a way as to resolve all ambiguities due to expressions which assumed an indeterminate form for $k=\frac{1}{2}(n+1)$. Another identity, $(1/z)+\psi(z)=\psi(1+z)$, needed in this connection is obtained by differentiating both sides of the equation $z\Gamma(z)=\Gamma(1+z)$ and using the defining equation $\Gamma(z)\psi(z)\equiv d\Gamma(z)/dz$ (Whittaker and Watson, p. 236).
[12]Reference 7, p. 13, Eq. (10) (with the upper sign), and p. 23, Eq. (28a).
[13]See Ref. 11.
[14]Reference 7, p. 46, Eq. (41b), and p. 47, (43b).
[15]Multiple derivatives of a product of two factors are expanded by use of the identity

$$\frac{d^n}{dz^n}(fg) = \sum_{\rho=0}^{n}\binom{n}{\rho}\frac{d^\rho f}{dz^\rho}\frac{d^{n-\rho}g}{dz^{n-\rho}}$$

in which $\binom{n}{\rho}$ is the binomial coefficient.
[16]Reference 7, p. 135, Eq. (2).
[17]Reference 7, p. 136, Eq. (6e).
[18]Reference 7, p. 136, Eq. (8).
[19]Reference 7, p. 137, Eq. (10g).
[20]Equation (2.14) is derived in Appendix A.
[21]Bateman, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953), Vol. 1, p. 86, Eq. (16), with $m=n+1-\lambda$, $u\to n-\lambda$, $v\to n-1$.
[22]Derivations will be found in Appendix C.
[23]To obtain this form a term zL_{n-2}^2 was reduced using Eq. (2.12) and Ref. 7, p. 137, Eq. (10g) to give $zL_{n-2}^2 = -z(d/dz)L_{n-1}^1(z) = -(n-1)L_{n-1}^1(z)+nL_{n-2}^1(z)$.
[24]Reference 5, Eq. (17).
[25]The partial wave components $g_l(r_2,r_1;E)$, $l=0,1,2,\ldots$, of the three-dimensional Green's function are defined through the partial wave expansion

$$G_{3D}(\mathbf{r}_2\mathbf{r}_1;E) = \sum_{l=0}^{\infty}\frac{2l+1}{4\pi}P_l(\cos\theta)g_l(r_2,r_1;E).$$

For the Coulomb Green's function

$$g_l(r_2,r_1;E) = -\tfrac{1}{2}i\nu a_1(r_2r_1)^{-1}\Gamma(1+l-i\nu)W_{i\nu;1/2+l}(2r_>/i\nu a_1) \times M_{i\nu;1/2+l}(2r_</i\nu a_1).$$

For $l=0$, the S-wave component, this is seen to agree with Eq. (1.5), aside from the factor $(r_2r_1)^{-1}$.
[26]Reference 2, Eqs. (97) of the erratum.
[27]The right-hand sides of Eqs. (2.35a,b) have been rewritten using

$$\exp[-(r_2+r_1)/na_1](2r_2/na_1)(2r_1/na_1)n^{-1}L_{n-1}^1(2r_2/na_1)L_{n-1}^1(2r_1/na_1)$$
$$= \exp[-(r_>+r_<)/na_1](2r_>/na_1)(2r_>/na_1)n^{-1}L_{n-1}^1(2r_>/na_1) \times L_{n-1}^1(2r_</na_1),$$

which follows from the symmetry of the expression on the left hand side under interchange of r_2 and r_1, and Eqs. (2.2a,b).
[28]Therefore, the differential Eqs. (2.35a,b) together with appropriate boundary conditions and the orthogonality relations already uniquely determine $K_{1D}(u,v;E_n)$.
[29]Equation (2.10) was used to rewrite $\mathcal{L}$ as

$$\mathcal{L} = L_{n-1}^1 - 2 + 2n\sum_{0\le\lambda<n}\frac{-L_{n-\lambda}^{-1}}{\lambda} - (n-1)L_{n-1}^{-1} - L_{n-2}^1.$$

Equation (2.45) was obtained from this expression by repeated use of the identity $L_n^\mu = L_n^{\mu+1} - L_{n-1}^{\mu+1}$ [Ref. 7, p. 136, Eq. (8) combined with p. 137, Eq. (10d)].
[30]Reference 7, p. 136, Eq. (9).
[31]Reference 7, p. 135, Eq. (2).
[32]The integral $\int_0^\infty ds e^{-s}L_{n-1}^1(s)=1$, $n=1,2,3,\ldots$, is required.

This integral may be established for example, by writing it as

$$-\int_0^\infty ds e^{-s}\frac{dL_n^0(s)}{ds} = -e^{-s}L_n^0(s)\Big|_0^\infty - \int_0^\infty ds e^{-s}L_n^0(s)L_0^0(s)$$

and using Eq. (2.46).

[33]Reference 7, p. 135, Eq. (1).

[34]Reference 7, p. 142, Eq. (17).

[35]See Ref. 29.

[36]A special case of Eq. (C11) gives

$$L_n^m(s) = \sum_{\lambda=0}^{n} L_\lambda^0(s)L_{n-\lambda}^{m-1}(0) = \sum_{\lambda=0}^{n}\binom{n-\lambda+m-1}{n-\lambda} L_\lambda^0(s);$$

the integral

$$\int_0^\infty ds e^{-s}L_n^m(s) = \sum_{\lambda=0}^{n}\binom{n-\lambda+m-1}{n-\lambda}\int_0^\infty ds e^{-s}L_\lambda^0(s)L_0^0(s)$$

$$= \binom{n+m-1}{n}$$

now follows from Eq. (2.46). Substitution of $m=2$ or 3 and $n \to n-1$ gives the special cases of this integral cited in the text.

[37]Reference 7, p. 137, Eq. (10a).

[38]Equation (D1) is obtained by splitting the integrand into the product $e^{-u}u^\mu L_n^\mu$ times uL_n^μ. The second factor is expanded as [Ref. 7, p. 137, Eq. (10b)]

$$uL_n^\mu = (2n+\mu+1)L_n^\mu - (n+\mu)L_{n-1}^\mu - (n+1)L_{n+1}^\mu$$

and then Eq. (2.46) is used.

[39]See Ref. 38.

Continuous subgroups of the fundamental groups of physics. I. General method and the Poincaré group*

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We present a general method for reducing the problem of finding all continuous subgroups of a given Lie group G with a nontrivial invariant subgroup N, to that of classifying the subgroups of N and the subgroups of the factor group G/N. The method is applied to classify all continuous subgroups of the Poincaré group (PG) and of the Lorentz group extended by dilatations [the homogeneous similitude group (HSG)]. Lists of representatives of each conjugacy class of subalgebras of the Lie algebras of the groups PG and HSG are given in the form of tables.

I. INTRODUCTION

The present article is the first in a series devoted to a study of the subgroup structure of the fundamental groups of physics. In this first installment we present a general method for classifying all continuous subgroups of any Lie group that has a nontrivial continuous invariant subgroup. We then apply the method to find all classes of continuous subgroups of the Poincaré group PG (the inhomogeneous Lorentz group) with respect to conjugation under the Poincaré group itself (i. e., with respect to inner automorphisms of the Poincaré group).

Part 2 of this series is appearing simultaneously and is devoted to a classification of all continuous subgroups of the similitude group of space–time, i. e., the Poincaré group extended by dilatations.[1] Articles in preparation will deal with the de Sitter groups, the conformal group of space–time and other groups of interest. This series was preceded by two related articles. In the first[2] we developed a method for constructing all maximal solvable subgroups of an arbitrary semisimple Lie group and applied it to construct all maximal solvable subgroups of $SU(p,q)$. In the same paper we found all continuous subgroups of $SU(2,1)$. All maximal solvable subgroups for the groups $SO(p,q)$ were obtained in a separate article.[3]

The importance of studying the subgroup structure of a given group has been discussed previously.[2,3] Let us just mention several points here.

1. There exists a direct connection between group representation theory for a given group and its subgroup structure. On one hand, this connection is provided by the theory of induced representations, where different subgroups can be used to induce representations of a group.[4] On the other hand, chains of subgroups will provide us with bases for group representations. Indeed, each chain of continuous subgroups provides us with a chain of subalgebras of the corresponding Lie algebra. Let us restrict ourselves to algebras whose enveloping algebras have nontrivial centers, i. e., to algebras that have Casimir operators. We can then define bases for representations of the group as the common eigenfunctions of a complete set of commuting operators, consisting of the Casimir operators of all the algebras in a definite chain of subalgebras (which we may have to supplement by some further operators). Each nonconjugate chain of subgroups thus provides us with a different basis. For physical applications one usually needs a definite and specific basis, rather than just an abstract one. Different bases will in general lead to quite different applications, in particular, to different expansions of physical quantities, like scattering amplitudes and form factors. Indeed, when the basis functions are realized in definite representation spaces we find that different bases correspond to different special functions. Let us mention that discrete subgroups of Lie groups are also of very definite interest in this connection. Indeed, bases for the representations of Lie groups, previously called "nonsubgroup bases," have numerous applications.[5] The basis functions in this case are eigenfunctions of certain operators, not related to any Lie subgroup, which may however be invariants of certain discrete subgroups. For a discussion of expansions of scattering amplitudes in terms of representations of the Lorentz and Galilei groups and in particular of the role of different subgroup and nonsubgroup bases we refer to a recent review.[6]

2. Most symmetries of interest in physics are broken, e.g., by the presence of symmetry breaking interactions or boundary conditions. The symmetry breaking often reduces the symmetry group to one of its subgroups. A classification of subgroups thus provides a classification of possible symmetry breakings.

3. Different subgroups of a given group correspond to different Lie subalgebras whose generators can be identified with certain physical observables. A classification of the Lie subalgebras thus provides us with a list of different possible sets of observables for a given system. Different observables clearly correspond to different possible physical situations, e.g., to different possible measurements performed on the system (e.g., angular momentum versus linear momentum).

The above considerations are valid for any group figuring in physics (or elsewhere) but are particularly true for any group reflecting the fundamental properties of space–time. Such are the Galilei group for nonrelativistic physics, the Poincaré group in the relativistic case, the de Sitter groups for curved universes and also the similitude group and conformal group of space–time.

The present article is devoted to the Poincaré group, all other groups mentioned above will be the subject of subsequent publications. The importance of the Poincaré group, underlying the whole kinematics of any relativistic theory, is obvious.

In addition to the points listed above for arbitrary Lie groups, the subgroups of the Poincaré group are of interest for further reasons. Thus:

1. An elementary physical system is conventionally defined to be a system whose state vector transforms according to an irreducible unitary representation of the Poincaré group.[7] This refers to an isolated system in vacuum. If we wish to discuss elementary systems (particles) in external fields that break the homogeneity and isotropy of space–time, then it seems natural to consider the largest subgroup of the Poincaré group that leaves the external field invariant and use its unitary irreducible representations to define elementary particles.

2. A related problem arises when formulating relativistic equations for particles in external fields (e.g., generalizations of the Bargmann–Wigner[8] equations). The equations involving the fields will no longer be Poincaré invariant, they may however be invariant with respect to various subgroups of the Poincaré group. The use of the corresponding integrals of motion will simplify the treatment of these equations and the representation theory of the corresponding group will provide properties of their solutions.

3. When developing elementary particle dynamics, e.g., two particle interactions, it sometimes proves to be fruitful to give up relativistic covariance (i.e., an over-all Minkowski space–time viewpoint) and to proceed in specific frames of reference. This in turn may lead to the use of different subgroups of the Poincaré group. In particular, the infinite momentum frame[9,10] or Dirac's "front form" of dynamics[11] lead to an eight-parameter subgroup of the Poincaré group and to "Galilean subdynamics."[12,13]

4. The subgroups of the Poincaré group will have applications even in classical physics. Indeed, the Maxwell equations of classical electrodynamics are Poincaré invariant (in vacuum) and as a matter of fact they are even conformally invariant. A classification of subgroups again provides us with a classification of external fields (classical electromagnetic fields) that can be introduced into the Maxwell equations to describe various physical situations.

In Sec. 2 of this paper we present a general algorithm for classifying the subalgebras of a Lie algebra L with a nontrivial ideal N into conjugacy classes with respect to a group of automorphisms A. Two interesting special cases are treated separately in greater detail. One is the case when the ideal N is Abelian and the algebra L splits over N, the second is that when L is the algebraic sum of two Lie algebras $L = L_1 \oplus L_2$. The results of Sec. 2 are applied in Sec. 3 to obtain all conjugacy classes of subalgebras of P, the Lie algebra of the Poincaré group, with respect to transformations of the Poincaré group itself. In Sec. 4 we provide another application of the results of Sec. 2, namely we use the Lie–Goursat method to classify all subalgebras of $D \oplus LSL(2, C)$, i.e., the Lie algebra of the homogeneous Lorentz group, extended by dilatations.

Section 5 contains our conclusions and future outlook, as well as some comments on related papers that recently came to our attention.[14,15]

2. GENERAL METHOD FOR CLASSIFYING THE SUBALGEBRAS OF LIE ALGEBRAS WITH NONTRIVIAL IDEALS

A. Introductory comments

In this section we develop a general method for classifying the subalgebras of a Lie algebra L of finite dimension $d(L) = \dim_k L$ over a field k. We consider the case when L has a nontrivial ideal N of dimension $d(N) = \dim_k N$ $[0 < d(N) < d(L)]$. Our aim is to reduce the problem of finding all conjugacy classes of subalgebras of L (conjugacy under some group of automorphisms A) to that of classifying the subalgebras of the ideal N and of the factor algebra $F = L/N$ under related groups of automorphisms.

The task can be conveniently linearized if the ideal N is Abelian. It becomes particularly simple if L splits over N, that is there exists a representative subalgebra $\bar{F}$ such that $\bar{F} \cap N = 0$ and $\bar{F} + N = L$. Note that this is precisely the case which we encounter when considering the algebra of the Poincaré group, since it is the semidirect product of the homogeneous Lorentz group $O(3,1)$ [locally isomorphic to $SL(2, C)$] and the four-dimensional Abelian group of translations T_4. Thus in this case N is the algebra LT_4 of translations, $\bar{F}$ is the algebra $LO(3,1)$, and A is the inner automorphism group of P. The required list of conjugacy classes of subalgebras of $LO(3,1)$ under transformations by $O(3,1)$ is known[16,17] and we shall make full use of it in the next section. The conjugacy classes of subalgebras of LT_4 under PG are easy to find, hence an algorithm reducing the problem for the Poincaré algebra P to that of $LO(3,1)$ and LT_4 would clearly be of use.

In part B of this section we present an algorithm solving our classification problem in the simplest case, i.e., when N is Abelian and $\bar{F} \cap N = 0$ (up to conjugacy under A). We also restrict ourselves to the case when A is the group of inner automorphisms of the considered algebra L, i.e., $A = G = \exp L$ is the Lie group generated by the algebra L. The algorithm makes use of cohomology theory but is presented in a directly usable manner, i.e., as a "kitchen recipe," operative for physicists interested in the subalgebra structure of a specific algebra.

In part C we formulate the algorithm more generally, considering the ideal N to be not necessarily Abelian and the algebra L not necessarily splitting over N, and prove that the algorithm does actually provide us with a complete list of representatives of all mutually nonconjugate classes of subalgebras of L. The important special case of invariant algebraic sums of Lie algebras is treated in part D and leads to a Lie–Goursat type[18–20] classification method.

B. Algorithm for classifying the subalgebras of a Lie algebra with an Abelian ideal

Consider a Lie algebra L of finite dimension $d(L)$ over a field k with an Abelian ideal N of dimension $d(N)$ satisfying $0 < d(N) < d(L)$. Consider the factor algebra $F = L/N$ and assume that a representative subalgebra $\bar{F}$ of L exists such that

$$\bar{F} \cap N = 0, \quad L = \bar{F} + N. \tag{1}$$

Consider also a group A of automorphisms of L over k leaving N invariant and containing all automorphisms of the form

$$\begin{aligned} &\exp[\mathrm{ad}(n)] : L \to L, \ (n \in N), \\ &\exp[\mathrm{ad}(n)](X) = X + [n, X], \ (X \in L). \end{aligned} \tag{2}$$

Note that the set $\exp[\mathrm{ad}(N)]$ of all special automorphisms $\exp[\mathrm{ad}(n)]$ with n in N is an Abelian normal subgroup of A. If k is the real number field then those automorphisms are the traditional inner automorphisms associated with the elements of N.

We wish to provide a representative list $S(L, N, A)$ of A-conjugacy classes of k-subalgebras of L. Since all automorphisms in A leave N invariant the action of A induces an automorphism group $\bar{A} = \omega A$ of F according to the homorphism

$$\begin{aligned} &\omega : A \to \mathrm{Aut}_k(F) \\ &\omega\alpha(x/N) = \alpha(x)/N \quad (\alpha \in A, x \in L) \end{aligned} \tag{3}$$

of A into the automorphism group of F over k.

Step 1: Find all conjugacy classes of subalgebras of the algebra F under conjugation by the group $\bar{A}$ and choose a representative algebra of each class. Label these subalgebras F_i $(i = 0, 1, \ldots, p)$ with $F_0 = F$ and $F_p = 0$. Further consider each algebra F_i separately. For each F_i find $\bar{F}_i$, the representative subalgebra contained in $\bar{F}$, and its normalizer in the group A, i.e., the subgroup $\mathrm{Nor}_A F_i$ of A leaving F_i invariant. If k is the real field the Lie algebra $L\mathrm{Nor}_A F_i$ of $\mathrm{Nor}_A F_i$ satisfies

$$[L\mathrm{Nor}_A F_i, F_i] \subseteq F_i; \tag{4a}$$

in fact,

$$L\mathrm{Nor}_A F_i = \mathrm{Nor}_L F_i = \{x \mid x \in L, [x, F_i] \subseteq F_i\}. \tag{4b}$$

It must however be remembered that the normalizer of F_i in A may also contain additional discrete elements not obtained by exponentiating $L\mathrm{Nor}_A F_i$.

Any k-subalgebra S of L determines the subalgebra $(S+N)/N$ of F. There exists an element α of A such that $\omega\alpha[(S+N)/N] = \bar{F}_i$ is a member of the representative lists $S(\bar{F}, 0, \bar{A})$ uniquely determined by S.

Before describing the remaining steps of the recipe it is necessary to point out that our problem leads to the execution of a number of computational cycles.

We want to find a list of A-conjugacy classes of the k-subalgebras S of L for which it was already stipulated that $(S+N)/N$ is one of the F_i's. We observe that $S \cap N$ is an Abelian ideal of S, invariant under the action of $\bar{F}_i$, which under the action of $\mathrm{Nor}_A F_i$ may be transformed into a privileged position without changing the previous stipulation (Step 2 below).

Having fixed $S \cap N$, it is now clear that S will be found as a subalgebra of $\bar{F}_i + N$ and that the remaining task is to pick out a representative set of conjugacy classes under the group $A^* = \mathrm{Nor}_A(F_i) \cap \mathrm{Nor}_A(S \cap N)$ acting on $\bar{F}_i + N$. It is to our advantage, computationally, to take factor algebras over $S \cap N$.

Thus the scene of action became

$$\tilde{L} = (\bar{F}_i + N)/S \cap N \tag{5a}$$

with the Abelian ideal

$$\tilde{N} = N/S \cap N \tag{5b}$$

and the representative subalgebra

$$\tilde{F}_i = (\bar{F}_i + S \cap N)/S \cap N, \tag{5c}$$

isomorphic to F_i.

The group under consideration is the group $\tilde{A}$ of all automorphisms $\tilde{\alpha}$ of $\tilde{L}$ that are induced by the action of the elements α of $\mathrm{Nor}_A(F_i) \cap \mathrm{Nor}_A(S \cap N)$. The task is to determine a representative set $R(\tilde{L}, \tilde{N}, \tilde{A})$ of the $\tilde{A}$-conjugacy classes of k-subalgebras

$$\tilde{S} = S/S \cap N \tag{6}$$

of $\tilde{L}$ representing $\tilde{L}/\tilde{N} \approx F_i$. Note that $\tilde{A}$ contains all automorphisms of the form $\exp[\mathrm{ad}(\tilde{n})]$ with $\tilde{n}$ in $\tilde{N}$.

At this point it is clear that this task has to be performed many times over ("there are many algorithmic cycles to go through"), depending on the choice of F_i and the fixation of $S \cap N$. However, in explaining the individual task we avail ourselves of the initial notation of Sec. 2. Thus we change $\tilde{L}$ to L, $\tilde{N}$ to N, $\tilde{A}$ to A.

Step 2: For each subalgebra F_i find all invariant subspaces in N, i.e., all subspaces N_{ia} satisfying

$$[F_i, N_{ia}] \subseteq N_{ia}. \tag{7}$$

Classify all N_{ia} into conjugacy classes under $\mathrm{Nor}_A F_i$ and choose one representative $\bar{N}_{ia}$ of each conjugacy class. Each such representative provides us with a subalgebra of L that is a "split extension" of N_{ia} by F_i:

$$F_i + N_{ia}, \quad F_i \subseteq F, \quad N_{ia} \subseteq N. \tag{8}$$

In this manner we obtain a representative set of all split extensions for all F_i under A-conjugacy, i.e., all subalgebras of L that can be written in the form (8).

Step 3 will consist of finding all nontrivial splits of L, i.e., algebras for which a basis can be chosen in the form

$$B_k + \sum_i c_{ki} X_i, \quad \sum_j d_{rj} X_j, \tag{9}$$

where $c_{ki} \in k$ and $d_{rj} \in k$ are fixed constants (not all zeros) which cannot be transformed simultaneously into zero by an element of A. To ensure that the generators (9) form a Lie algebra the additional terms $\sum c_{ki} X_i$ must form 1-cocycles of cohomology theory. Among these there are certain trivial cocycles, called *coboundaries* which are the ones that can be transformed away by the group $\exp(\mathrm{ad}N)$. These should be

used to simplify (9). To do that one proceeds as follows.

Step 3: Represent the algebra F on the space N by the matrices (β^i_{ab}) defined by

$$[B_i, X_a] = \sum_b \beta^i_{ab} X_b, \tag{10}$$

where

$$\{B_1, B_2, \ldots, B_{d(F)}\} \tag{11}$$

is a basis chosen in F and

$$\{X_1, X_2, \ldots, X_{d(N)}\} \tag{12}$$

is a basis chosen in N. Obviously one has

$$[\beta^i, \beta^k] = \sum_j f^j_{ik} \beta^j, \tag{13}$$

where f^j_{ik} are the structure constants of $\bar{F}$, i. e., $[B_i, B_k] = \sum_j f^j_{ik} B_j$

For each B_i define a 1-cocycle as a vector in N with components c_{ij} in the chosen basis

$$\gamma(B_i) = \sum_j c_{ij} X_j. \tag{14}$$

The components c_{ij} must satisfy a set of linear homogeneous equations obtained from the conditions

$$\gamma([B_i, B_k]) = \beta^i \gamma(B_k) - \beta^k \gamma(B_i) = \sum_j f^j_{ik} \gamma(B_j). \tag{15}$$

Find first the coboundaries $\partial(B_i) = [B_i, X]$ for some X of N which happen to solve (15) in a trivial manner. We use the following equation for the components d_{ik} of the basic coboundaries:

$$\partial^{(k)}(B_i) = [B_i, X_k] = \sum_j \beta^i_{kj} X_j = \sum_j d^k_{ij} X_j \quad [k = 1, 2, \ldots, d(N)]. \tag{16}$$

Forming linear combinations $X = \sum_k x_k X_k$, we find the components of the vector $\partial(B_i)$ [for each $i = 1, 2, \ldots, d(F)$] from

$$\partial(B_i) = \sum_j d_{ij} X_j = \sum_k x_k \sum_j d^k_{ij} X_j. \tag{17}$$

Since Eqs. (15) for c_{ik} are linear homogeneous and since also d_{ij} are solutions of (15), the numbers

$$c_{ij} + \sum_k x_k d^k_{ij} \tag{18}$$

will *also* be solutions for arbitrary choice of x_k in (18). We use this freedom to simplify Eqs. (15), e. g., by requiring that as few as possible of the basic solutions of (15) together with the 1-coboundaries span all cocycles over k.

This is done, e. g., by producing an adapted k-basis $Y_1, Y_2, \ldots, Y_{d(N)}$ of N as follows.

Seek out the first nonzero 1-coboundary among the $\partial^{(k)}$'s, say $\partial Y_1 = \partial^{(k_1)}$ with

$$Y_1 = X_i, \quad Y_k = X_{k-1}, \quad \partial Y_k = 0 \quad (1 < k \leq i_1). \tag{19}$$

Thus $\partial Y_1(B_j) \neq 0$, say $d^{I_1}_{ji} \neq 0$. Replace the subsequent 1-coboundaries $\partial^{(k)}$ by ∂Y_k, where

$$Y_k = X_k - \frac{d^{I_1}_{kk_1}}{d^{I_1}_{jk_1}} X_k \quad [i < k \leq d(N)]. \tag{20}$$

For the new k-basis $Y_1, Y_2, \ldots, Y_{d(N)}$ of N we have new commutation rules

$$[B_i, Y_k] = \sum d^{I_1}_{ik} Y_{l_1}, \tag{21}$$

such that we have the zero components

$$d^{I_1}_{kk_1} = 0 \quad \text{if } 1 < k \leq d(N),$$

but

$$d^{I_1}_{j_1 k_1} \neq 0, \quad j_1 = 1.$$

Now continue if possible in the same manner to simplify $Y_2, \ldots, Y_{d(N)}$.

In the end we will find a new k-basis $Y_1, \ldots, Y_{d(N)}$ of N such that the structure constants of (21) satisfy

$$d^{I_j}_{ki_j} \neq 0, \; d^{I_j}_{ii_j} = 0 \quad \text{if } k < i \leq d(N), \qquad 1 \leq j \leq r,$$

$$d^j_{ik} = 0 \quad \text{if } r < j \leq d(N) \quad [i = 1, 2, \ldots, d(N)]. \tag{22}$$

Then $\partial Y_1, \ldots, \partial Y_r$ form a k-basis of 1-coboundary space. With this simplification of the 1-coboundaries we obtain the required additional solution basis of (15) by imposing the condition

$$c_{l_j i_j} = 0 \quad (1 \leq j \leq r) \tag{23}$$

in addition to (15) on the c_{ij}. Examples are shown in Sec. 3.

Thus, Step 3 consists of finding a k-basis of the 1-cocycles $\gamma(B_k)$, $B_k \in F$ modulo the linear space of the 1-coboundaries of $\bar{F}$ acting on N. So far we took into consideration only the transformation action by the elements of $\exp(\mathrm{ad}N)$.

Step 4: If the algebra F_i has any outer automorphisms (i. e., $\mathrm{Nor}_A F_i$ properly contains $\exp F_i$) use them to further simplify the generators (9).

In the case of the real number field $k = R$ the group A has a natural topology so that the component of 1_A forms a normal subgroup A_1 of A. In the applications we are confined to the case that A is a closed subgroup of the full group of automorphisms of L over R. In that case A_1 happens to be a continuous Lie group with infinitesimal ring LA_1 and the transformation effect of A_1 on the 1-cocycles can be described totally by the action of LA_1. Even though in the Poincaré group case the ensuing linearization of the search for the A-equivalence classes was never used it should be pointed out for further applications.

Firstly, let us observe that LA_1 is a subalgebra of the R-derivation algebra $\mathrm{Der}_R L$ of L. Then for every element D of LA_1 we have

$$\begin{aligned} &D(x+y) = D(x) + D(y), \\ &D(\lambda x) = \lambda D(x), \\ &D([x, y]) = [D(x), y] + [x, D(y)], \end{aligned} \tag{24}$$

where $x, y \in L$, $\lambda \in R$. Also, $D(N) \subseteq N$ because of the invariance of N under A.

We associate with D the 1-cocycle D_γ of $\bar{F}_i$ acting on N defined by

$$D_\gamma(B) = \gamma(D(B)) - D(\gamma(B)). \tag{25}$$

The 1-cocycle properties of D_γ can be directly verified by lengthy computations. The mapping γ on D_γ defines a linear transformation ΔD of the linear space $C'(F, N)$ of all 1-cocycles of F_i acting on N. It leaves invariant the linear subspace $B'(F_i, N) = \partial N$ of all 1-coboundaries of F_i acting on N. The mapping Δ of LA_1 into $\mathrm{End}_R[C'(F_i, N)]$ is a representation in the Lie theoretical sense.

Using the exponential function we obtain a representation ψ of A_1 acting on $C'(F_i, N)$ via the rule

$$\psi(\exp D)(\gamma) = \exp(\Delta D)(\gamma)$$

which, due to the fact that

$$A_1 = \langle \exp(LA_1) \rangle,$$

permits an accounting for the transformation effect of A_1 on the factor algebra

$$H'(F_i, N) = C'(F_i, N)/B'(F_i, N)$$

completely in terms of the representation Δ of LA_1, with $C'(F_i, N)$ as representation space. It is now only a question of forming the orbits of A_1 acting on $H'(F_i, N)$ and representing each orbit by a single element.

In the applications the discrete factor groups A/A_1 will always be finite and one gauges the effect of this factor group by a careful case for case discussion.

C. The classification of subalgebras of Lie algebras with proper nonzero ideals

Consider the following situation. Let a Lie algebra L of finite dimension $d(L)$ over a field k, an ideal N of L such that N is a linear space of dimension $d(N)$ over k satisfying the inequalities $0 < d(N) < d(L)$ and a group A of automorphisms of L over k that leave N invariant be given. It is clear that also in this case there is the homomorphism

$$\omega : A \to \mathrm{Aut}_k(F),$$

$$\omega\alpha(x/N) = \alpha(x)/N$$

of A into the automorphism group of the factor algebra

$$F = L/N$$

over k.

Speaking in more general terms than we did in part B we ask which advantage we can draw from the knowledge of the behavior of F under $\omega G = \bar{G}$ and from N under G/N for the task of establishing a representative list $S(L, N, G)$ of the G-equivalence classes of k-subalgebras of L.

Initially we apply the same 3 steps as in part B.

Step 1: Find a list $S(F, 0, \bar{G})$ of the $\bar{G}$-equivalence classes of k-subalgebras of F. For each member F_i of $S(F, 0, \bar{G})$ find the normalizer

$$\mathrm{Nor}_A(F_i) = \{\alpha \mid \alpha \in A \ \& \ \omega\alpha(F_i) = F_i\}$$

of F_i in A.

Step 2: For each member F_i of $S(F, 0, \bar{G})$ find a representative set $S(N, 0, \mathrm{Nor}_A(F_i)/N)$ of the $\mathrm{Nor}_A(F_i)$-equivalence classes of k-subalgebras of N. Delete from the list all those members for which the normalizer in L does not cover F_i. This is safe because the deleted members could not serve as $S \cap N$ in the case $S/N = F_i$. There remains the sublist $S(N, 0, \mathrm{Nor}_A(F_i)/N, F_i)$ of all members X of $S(N, 0, \mathrm{Nor}_A(F_i)/N)$ with the property that the normalizer

$$\mathrm{Nor}_L(X) = \{x \mid x \in L \ \& \ [x, S] \subseteq S\}$$

covers F_i so that

$$(X + N)/N \supseteq F_i.$$

Hence the k-subalgebra

$$\mathrm{Nor}_{F_i}(X) = \{x \mid x \in \mathrm{Nor}_L(X) \ \& \ x/N \in F_i\}$$

of $\mathrm{Nor}_L(X)$ satisfies the condition that

$$[\mathrm{Nor}_{F_i}(X) + N]/N = F_i.$$

It follows that $\mathrm{Nor}_{F_i}(X) \cap N$ is a k-ideal of $\mathrm{Nor}_{F_i}(X)$ with factor algebra isomorphic to F_i.

Delete from the list $S(N, 0, \mathrm{Nor}_A(F_i)/N, F_i)$ all members X for which the Lie algebra $\mathrm{Nor}_{F_i}(X)$ does not split over the ideal $\mathrm{Nor}_{F_i}(X) \cap N$. This is safe because the deleted members could not serve as $S \cap N$ such that $S/N = F_i$. There remains the sublist $R(N, 0, \mathrm{Nor}_A(F_i)/N, F_i)$, consisting of representatives X of those $\mathrm{Nor}_A(F_i)$-equivalence classes of k-subalgebras of N for which

(a) $(\mathrm{Nor}_L(X) + N)/N \supseteq F_i$,

(b) $\mathrm{Nor}_{F_i}(X)$ contains a k-subalgebra $R(X, N, F_i)$

satisfying the conditions

$$R(X, N, F_i) \cap N = 0,$$

$$R(X, N, F_i) + (\mathrm{Nor}_{F_i}(X) \cap N) = \mathrm{Nor}_{F_i}(X).$$

Step 3: For each member X of $R(N, 0, \mathrm{Nor}_A(F_i)/N, F_i)$ form the Lie algebras

$$\tilde{L} = \mathrm{Nor}_{F_i}(X)/X,$$

$$\tilde{N} = \tilde{L} \cap N/X,$$

$$\tilde{F} = \tilde{L}/\tilde{N},$$

$$\bar{F} = [R(X, N, F_i) + X]/X$$

and the group $\tilde{A}$ of all automorphisms $\tilde{\alpha}$ of $\tilde{L}$ of the form

$$\tilde{\alpha}(y/X) = \alpha(y)/X,$$

$$[y \in \tilde{L}, \alpha \in \mathrm{Nor}_A(X) \cap \mathrm{Nor}_{F_i}(X)].$$

We observe that each member of $\tilde{A}$ is a k-linear automorphism of $\tilde{L}$ leaving invariant the k-ideal $\tilde{N}$ of $\tilde{L}$ and that $\bar{F}$ is a representative subalgebra of $\tilde{L}$ modulo $\tilde{N}$ so that the splitting conditions are satisfied

$$\tilde{F} \cap \tilde{N} = 0, \quad \tilde{F} + \tilde{N} = \tilde{L}.$$

There remains the task of establishing a representative list $R(\tilde{L}, \tilde{N}, \tilde{A})$ of the $\tilde{A}$-conjugacy classes of k-subalgebras of $\tilde{L}$ that form a representative subalgebra of $\tilde{L}$ modulo $\tilde{N}$. If that task is solved then to each member $\tilde{S}$ of $R(\tilde{L}, \tilde{N}, \tilde{A})$ there corresponds in one-to-one fashion the k-subalgebra

$$S = \{x \mid x \in L \ \& \ x/X \in \tilde{S}\}$$

such that the S's for all X's and all F_i's together are compiled into the desired list $S(L, N, A)$.

Changing notations as previously from $\tilde{L}$ to L, $\tilde{N}$ to N, $\tilde{F}$ to F, $\tilde{A}$ to A we have the initial situation of this section with the additional information that L is a splitting extension of N so that there is given a k-subalgebra $\bar{F}$ of L for which

$$\bar{F} \cap N = 0, \quad \bar{F} + N = L.$$

The initial task is reduced to the less demanding task of establishing a representative list $R(L, N, A)$ of the A-equivalence classes of all k-subalgebras S of L for which

$$S \cap N = 0, \quad S + N = L.$$

Again as in part B, we observe that the elements of S are of the form

$$B + \gamma(B) \quad (B \in \bar{F})$$

such that γ is characterized as a k-linear mapping γ of B in N subject to the additional conditions

$$\gamma([B, B']) = [B, \gamma(B')] - [B', \gamma(B)] + [\gamma(B), \gamma(B')] \quad (B, B' \in \bar{F}). \tag{26}$$

Again, a k-linear mapping γ of B in N satisfying (26) may be called a 1-cocycle of $\bar{F}$ acting on the k-ideal N of L via Lie multiplication. However, due to the additional term $[\gamma(B), \gamma(B')]$ on the right-hand side of (26) the system of equations (26) for the 1-cocycle is not necessarily linear homogeneous so that the set $C^1(\bar{F}, N)$ of all 1-cocycles of $\bar{F}$ acting on N may not be a linear space over k. Also, in general, we will not have a nicely behaved linear subspace of 1-coboundaries so that the discussion of $C^1(\bar{F}, N)$ and the orbits of A acting on $C^1(\bar{F}, N)$ requires new tools (e.g., of algebraic geometry in case A is an algebraic group) for its successful treatment.

We abandon the discussion of the most general problem and ask instead the obvious question: Which further advantage can we draw from the existence of a nonzero ideal N_1 of L that is properly contained in N and invariant under A, for the purpose of establishing the list $S(L, N, A)$, provided we have all the required information for L/N_1.

It is clear that $S(L, N_1, A)$ serves in the capacity of $S(L, N, A)$, since in fact the only connection of N with the problem of finding $S(L, N, A)$ is the condition that N be invariant under A.

In order to carry out Step 1 for the task $S(L, N_1, A)$ we need to establish

$$S(L/N, N/N_1, \omega_1 A),$$

where ω_1 is the homomorphism

$$\omega_1 : A \to \mathrm{Aut}_k(L/N_1)$$

$$\omega_1 \alpha(x/N_1) = \alpha(x)/N_1 \quad (\alpha \in A, x \in L).$$

For example, in the case that $N_1 = [N, N] = DN$, the task of establishing $S(L/N_1, N/N_1, \omega_1 A)$ essentially is solved by the methods explained in part B where a small modification will be needed only in case $\omega_1 A$ would not contain all automorphisms of L/N_1 of the type $\exp[\mathrm{ad}(n)]$ with n in N/N_1.

Similarly, in the case that

$$[N_1, N_1] = 0,$$

i.e., that N_1 is a nonzero Abelian A-invariant ideal of L properly contained in N, the task of establishing $S(L, N_1, A)$ is solved by the methods of part B provided we can carry out Step 1 which is tantamount to establishing $S(L/N_1, N/N_1, N, A)$.

There remains the discussion of the case that N is a perfect ideal of L which does not contain any nonzero Abelian ideal of L.

Over fields of reference of characteristic 0 it is known that the radical ideal $R(N)$ of an ideal N of a finite-dimensional Lie algebra L always is again an ideal. In other words there only remains to discuss the case that

$$0 = R(N) \subset N = [N, N] < L,$$

i.e., N is a semisimple ideal of L. It is known that in this case (for characteristic 0) there holds the decomposition

$$L = N \dot{+} Z_L(N)$$

of L into the direct sum of N and the centralizer

$$Z_L(N) = \{x \mid x \in L \ \& \ [x, N] = 0\}.$$

Clearly, both N and $Z_L(N)$ are invariant under A. Then we have a special case of the Lie—Goursat problem which we deal with in its general form below in part D.

D. The Lie-Goursat classification method for the subalgebras of albegraic sums of Lie algebras

The Goursat problem[18] is that of establishing a list of representatives $S(G_1, G_2, A)$ of the classes of A-conjugate subgroups of the direct product $G_1 \otimes G_2$ of two groups. The conjugacy is considered with respect to a given group A of automorphisms of $G_1 \otimes G_2$, leaving each factor G_1 and G_2 in the direct product invariant. It is assumed that the corresponding subgroup classification problem has already been solved for the groups G_1 and G_2.

Correspondingly, the Lie—Goursat problem is that of establishing a representative list $S(L_1, L_2, A)$ of the classes of A-conjugate k-subalgebras of the algebraic sum $L = L_1 \oplus L_2$ of two Lie algebras L_1 and L_2 over the field k. Here A is a group of automorphisms of L over k, leaving L_1 and L_2 invariant. We wish to reduce the problem to well-defined classification problems for subalgebras of L_1 and L_2 and their factor algebras.

We use the Goursat lemma for quasirings. We recall that a quasiring is a system with two binary operations, addition and multiplication, such that the system is a module under addition and the multiplication is distributive on both sides. If L_1 and L_2 are both quasirings then $L_1 \oplus L_2$ is defined as the set of all symbols $a_1 \oplus a_2$ ($a_i \in L_i$, $i = 1, 2$) with "componentwise" operational rules:

$$a_1 \oplus a_2 = b_1 \oplus b_2 \Leftrightarrow a_i = b_i, \quad i = 1, 2,$$

$$a_1 \oplus a_2 + b_1 \oplus b_2 = (a_1 + b_1) \oplus (a_2 + b_2),$$
$$(a_1 \oplus a_2)(b_1 \oplus b_2) = a_1 b_1 \oplus a_2 b_2 \tag{27}$$
$$(a_i, b_i \in L_i,\ i = 1, 2).$$

Note that the mappings

$$\eta_i : L_i \rightarrow L_1 \oplus L_2,$$
$$\eta_1(a_1) = a_1 \oplus 0; \quad \eta_2(a_2) = 0 \oplus a_2\ , \tag{28}$$
$$(a_i \in L_i, i = 1, 2)$$

are monomorphisms with ideals as images such that $L_1 \oplus L_2 = \eta_1 L_1 + \eta_2 L_2$ and that the converse of this statement holds as well. Usually L_i and $\eta_i L_i$ are identified. We shall abbreviate the words "subquasiring" to "subring" and "factor quasiring" to "factor ring." Now let $L_1 \oplus L_2$ be the algebraic sum of two quasirings L_1 and L_2. We have:

(a) For every subring S of $L_1 \oplus L_2$ there exist the ideals $S \cap L_1$, $S \cap L_2$ and their direct sum $S \cap L_1 \oplus S \cap L_2$, which is also an ideal of S. The projection homomorphisms

$$\theta_i S \rightarrow L_i,$$
$$\theta_1 x = (x + L_2) \cap L_1, \qquad \theta_2 x = (x + L_1) \cap L_2 \tag{29}$$

of S into $L_i (i = 1, 2)$, such that $S \cap L_i$ is an ideal of $\theta_i S (i = 1, 2)$ and that we have a Goursat isomorphism of $\theta_1 S_1 / S \cap L_1$ on $\theta_2 S_2 / S \cap L_2$ $(x \in S)$.

(b) Conversely, given two subrings S_i of L_i $(i = 1, 2)$ and ideals N_i of S_i and an isomorphism σ of the factor ring S_1/N_1 onto the factor ring S_2/N_2, then there exists the subring $S = \{x_1 \oplus x_2 \,|\, x_1 \in S_1,\ x_2 \in S_2$ and $\sigma(x_1/N_1) = x_2/N_2\}$ of $L_1 \oplus L_2$, such that

$$\theta_i S = S_i, \quad S \cap L_i = N_i \quad (i = 1, 2).$$

Proof: (a) All that needs to be shown is the existence of the Goursat isomorphism (also called the Goursat twist). For this purpose we observe that the congruence

$$\theta_1 x \equiv \theta_1 y \pmod{S \cap L_1}.$$

implies an equation

$$x = y + u \quad \text{with } u \in S \cap L_1,$$

so that

$$x + L_1 = y + u + L_1 = y + L_1,$$
$$\theta_2 x = (x + L_1) \cap L_2 = (y + L_1) \cap L_2 = \theta_2 y.$$

We hence have the onto mapping

$$\sigma : \theta_1 S / S \cap L_1 \rightarrow \theta_2 S / S \cap L_2,$$
$$\sigma(\theta_1 x / S \cap L_1) = \theta_2 x / S \cap L_2 \quad (x \in S). \tag{30}$$

Since both θ_1 and θ_2 preserve addition and multiplication, the same is true for σ. The kernel of the epimorphism σ consists of all cosets $\theta_1 x / S \cap L_1$ $(x \in S)$ for which $\theta_2 x$ belongs to $S \cap L_2$. In other words

$$x = \theta_1 x + \theta_2 x,$$
$$\theta_i x \in L_i \quad (i = 1, 2),$$
$$\theta_2 x \in S \cap L_2.$$

This implies that $\theta_1 x = x - \theta_2 x$ belongs to S. Hence $\theta_1 x \in S \cap L_1$, $\theta_2 x / S \cap L_1 = 0$. Thus the isomorphism property of σ is established.

(b) For the converse we must verify the subring property of S which is straightforward because σ preserves addition and multiplication.

We thus obtain the following algorithmic solution of the Lie–Goursat problem (we use the same notations as in the beginning of this section).

Step 1: Establish a representative list $S(L_1, 0, A/L_1)$ of the A-conjugacy classes of k-subalgebras of L_1 and their normalizers in A.

Step 2: For each member S_{1i} of $S(L_1, 0, A/L_1)$ establish a representative list $S(L_2, 0, \mathrm{Nor}_A S_{1i}/L_2)$. For each S_2 of $S(L_2, 0, \mathrm{Nor}_A S_{1i}/L_2)$ find the normalizer

$$\mathrm{Nor}_A(S_{1i} \oplus S_2) = \mathrm{Nor}_A(S_{1i}) \cap \mathrm{Nor}_A(S_2).$$

Step 3: For given S_{1i} and S_2 establish a representative list $S(S_{1i}, S_2, \mathrm{Nor}_A(S_{1i} \oplus S_2)$ of the $\mathrm{Nor}_A(S_{1i} \oplus S_2)$ equivalence classes of pairs of subalgebras. Find

$$N_{1i} \lhd S_{1i}, \quad N_2 \lhd S_2$$

for which

$$S_{1i}/N_{1i} \underset{k}{\approx} S/N_2$$

and find the intersection

$$A^* = \mathrm{Nor}_A(S_{1i} \oplus S_2) \cap \mathrm{Nor}_A(N_{1i} \oplus N_2).$$

Step 4: For given S_{1i}, S_2, N_{1i}, and N_2 determine a representative list $S(S_{1i}, S_2, N_{1i}, N_2, A^*)$ of the A^*-equivalence classes of the Lie algebra isomorphisms of S_{1i}/N_{1i} and S_2/N_2.

Step 5: Form all the Goursat twisted subalgebras

$$S = \{x_1 + x_2 \,|\, x_1 \in S_{1i},\ x_2 \in S_2 \text{ and } \sigma(x_1/N_{1i}) = x_2/N_2\}$$

for σ of $S(S_{1i}, S_2, N_{1i}, N_2, A^*)$ and compile the desired list $S(L_1 \oplus L_2, 0, A)$ by gathering together, for all σ's of $S(S_{1i}, S_2, N_{1i}, N_2, A^*)$ all N_{1i}, N_2 of $S[S_{1i}, S_2, \mathrm{Nor}_A(S_{1i} \oplus S_2)]$, all S_2 of $S[L_2, 0, \mathrm{Nor}_A(S_{1i})/L_2]$ and all S_{1i} of $S(L_1, 0, A/L_1)$.

An application of the Lie–Goursat method to a classification of the subalgebras of the algebra of the homogeneous Lorentz group, extended by dilatations, follows in Sec. 4.

3. CONTINUOUS SUBGROUPS OF THE POINCARÉ GROUP

A. Subgroups of the homogeneous Lorentz group

Let us first introduce some necessary notations. The Poincaré group can be defined as the group of linear transformations

$$x'_\mu = \Lambda_{\mu\nu} x_\nu + a_\mu \tag{31}$$

of a real linear vector space with metric

$$ds^2 = dx_0^2 - dx_1^2 - dx_2^2 - dx_3^2, \tag{32}$$

leaving the distance (32) invariant.

Its Lie algebra has 10 generators. We chose a basis that is convenient for our purposes, although it differs from the one conventionally used in physics. Let us write the generators of the homogeneous Lorentz group in a four-dimensional representation as

$$B_1=\begin{pmatrix} i & 0 & 0 & 0\\ 0 & -i & 0 & 0\\ 0 & 0 & -i & 0\\ 0 & 0 & 0 & i\end{pmatrix},\quad B_2=\begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix},\quad B_3=\begin{pmatrix} 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & 0 & 0\end{pmatrix}$$

$$B_4=\begin{pmatrix} 0 & i & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & i\\ 0 & 0 & 0 & 0\end{pmatrix},\quad B_5=\begin{pmatrix} 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & -1 & 0\end{pmatrix},\quad B_6=\begin{pmatrix} 0 & 0 & 0 & 0\\ i & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & i & 0\end{pmatrix}. \tag{33}$$

The generators of translations are

$$X_1=\begin{pmatrix} 0 & 0 & 0 & i\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix},\quad X_2=\begin{pmatrix} 0 & 0 & 1 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix},\quad X_3=\begin{pmatrix} 0 & 0 & i & 0\\ 0 & 0 & 0 & i\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}$$

$$X_4=\begin{pmatrix} 0 & 0 & 0 & 0\\ 0 & 0 & i & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}. \tag{34}$$

Note that all the above matrices satisfy

$$XJ+JX^{+}=0 \tag{35}$$

with

$$J=\begin{pmatrix} 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 1 & 0 & 0 & 0\end{pmatrix}. \tag{36}$$

All complex matrices X satisfying (35) and $\det X=1$ constitute a realization of the algebra of the pseudo-unitary group $SU(2,2)$. This is convenient for our future purposes since we can in a simple manner enlarge the basis (33), (34) to that of the similitude group, by adding the element

$$D=\begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & -1 & 0\\ 0 & 0 & 0 & -1\end{pmatrix}. \tag{37}$$

The conformal group of space–time would then be obtained by adding four more generators (of special conformal transformations). We shall need the commutation relations of the Poincaré algebra; they are summarized in Table I.

The translations commute:

$$[X_\mu, X_\nu]=0,\quad \mu,\nu=0,1,2,3.$$

The relation to the usual physical operators, namely the angular momentum L_i (rotations), boosts K_i (proper Lorentz transformations), energy–momentum P_0, P_i (translations) is as follows ($i=1,2,3$):

$$B_1=2L_3,\qquad B_2=-2K_3,\qquad B_3=-L_2-K_1,$$
$$B_4=L_1-K_2,\quad B_5=L_2-K_1,\quad B_6=L_1+K_2, \tag{38}$$

and

$$X_1=\tfrac{1}{2}(P_0-P_3),\quad X_2=P_2,\qquad X_3=-P_1,\quad X_4=\tfrac{1}{2}(P_0+P_3). \tag{39}$$

The subalgebras of $F=LSL(2,C)$ are known[16,17] and we list them and some of their properties in Table II. In the first column we introduce a notation for each subalgebra, in the second we give its dimension $\dim_R F_i$ (over the field of real numbers), in the third we list the generators. In the fourth we give $\mathrm{Nor}_{LG}F_i$, i. e., the normalizer of F_i in the Lorentz group $LG\approx\exp F\approx SL(2,C)$. Relevant comments are made in the fifth column.

Notice that F_5 and F_{11} are actually infinite classes of subalgebras, depending on one real continuous parameter $0<c<\pi$, $c\neq\pi/2$. We could have combined several subalgebras together by simply letting c take all values $0\leq c<\pi$ (then F_5, F_6, F_7 and F_{11}, F_{12}, F_{13} would have been bunched together). This was actually done, e. g., in Ref. 16. However, the properties of these algebras are sufficiently specific for $c=0$ and $c=\pi/2$ to justify their separate treatment. All other entries F_j ($j\neq5$, $j\neq11$) are single algebras, not depending on any parameters.

The normalizers sometimes involve discrete elements. In particular, we have

$$Z_1=\begin{pmatrix} 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\\ 0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\end{pmatrix}=B_3-B_5,\quad Z_2=\begin{pmatrix} i & 0 & 0 & 0\\ 0 & -i & 0 & 0\\ 0 & 0 & -i & 0\\ 0 & 0 & 0 & i\end{pmatrix}=B_1, \tag{40}$$

and C_4 is a cyclic group consisting of the elements $Z_2, Z_2^2=-1, Z_2^3=-Z_2$ and $Z_2^4=1$. The symbol $\square$ indicates a semidirect product of two groups where the second group is an invariant subgroup. Note that Z_1 is a rotation through π about axis 2, Z_2 a rotation through π about axis 3.

TABLE I. Commutation relations for the Poincaré algebra.

	B_1	B_2	B_3	B_4	B_5	B_6	X_1	X_2	X_3	X_4
B_1	0	0	$2B_4$	$-2B_3$	$-2B_6$	$2B_5$	0	$2X_3$	$-2X_2$	0
B_2	0	0	$2B_3$	$2B_4$	$-2B_5$	$-2B_6$	$2X_1$	0	0	$-2X_4$
B_3	$-2B_4$	$-2B_3$	0	0	B_2	B_1	0	0	$2X_1$	X_3
B_4	$2B_3$	$-2B_4$	0	0	B_1	$-B_2$	0	$-2X_1$	0	$-X_2$
B_5	$2B_6$	$2B_5$	$-B_2$	$-B_1$	0	0	X_3	0	$2X_4$	0
B_6	$-2B_5$	$2B_6$	$-B_1$	B_2	0	0	X_2	$2X_4$	0	0

TABLE II. Representatives of conjugacy classes of subalgebras of $F=LSL(2,C)$ under $SL(2,C)$. In column 3 the generators to the right of the semicolon span the derived algebra of F_j.

Notation	$\dim_R F_i$	R-basis	$\mathrm{Nor}_{LG}F_i$	Comment on subgroup
F_1	6	$;B_1,\ldots,B_6$	Inner	$SL(2,C)$
F_2	4	$B_1,B_2;B_3,B_4$	Inner	Borel
F_3	3	$;B_1,B_3-B_5,\ B_4+B_6$	Inner	$SU(2)$
F_4	3	$;B_1,B_3+B_5,\ B_4-B_6$	$\exp F_4 \cup \exp F_4 \cdot Z_1$	$SU(1,1)$
F_5	3	$B_c=\cos c B_1+\sin c B_2;B_3,B_4$, $0<c<\pi/2,\ \pi/2<c<\pi$	$\exp F_2$	$S(3)$
F_6	3	$B_1;B_3,B_4$	$\exp F_2$	$E(2)$
F_7	3	$B_2;B_3,B_4$	$\exp F_2$	$D \square T_H$
F_8	2	$B_2;B_3$	$C_4 \square \exp F_8$	$C(1)$
F_9	2	$B_1,B_2;$	$\exp F_9 \cup \exp F_9 \cdot Z_1$	Abelian, T_C
F_{10}	2	$B_3,B_4;$	$\exp F_2$	Abelian, T_H
F_{11}	1	$B_c=\cos c B_1+\sin c B_2;$ $0<c<\pi/2,\ \pi/2<c<\pi$	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$S(1)$
F_{12}	1	$B_1;$	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(2)$
F_{13}	1	$B_2;$	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(1,1)$
F_{14}	1	$B_3;$	$C_4 \square \exp F_7$	$E(1)$
F_{15}	0	0	$\exp F_1$	1

To each subalgebra F_j of $LSL(2,C)$ there corresponds a continuous subgroup $\exp F_j$ of the Lorentz group. We do not go into the question of discrete centers, etc., for these groups and do not discuss the question of how many different locally isomorphic Lie groups correspond to each algebra.

Most of the groups are obvious (see last column in Table II). We shall call $\exp B_4 = B$ the Borel subgroup[21] since it is the maximal solvable subgroup of $SL(2,C)$. Throughout we denote

$$B_c=\cos c B_1+\sin c B_2, \quad 0<c<\pi, \quad c\neq\pi/2. \tag{41}$$

The corresponding group which we denote

$$S(1)=\exp F_{11} \tag{42}$$

corresponds to a rotation about a space axis with a simultaneous boost along the same axis (a "screw" with c the corresponding angle). Similarly, we denote

$$S(3)=\exp F_5. \tag{43}$$

This group corresponds to screw-like transformations along one axis and translations in the plane perpendicular to this axis.

The group $\exp F_8$ corresponds to transformations of a straight line, i.e., translations and dilatations:

$$x'=ax+b. \tag{44}$$

A matrix realization of $\exp F_8$ is given by

$$g=\begin{pmatrix} a & b \\ 0 & 1 \end{pmatrix}$$

acting on the vector $x=\binom{x}{1}$. We shall denote this group $C(1)$, the conformal group in one dimension.

The groups $\exp F_9$ and $\exp F_{10}$ are both Abelian and can be interpreted as translations. Since $\exp F_9$ contains a compact generator B_1 it can be identified with translations on a cylinder; $\exp F_{10}$ corresponds to translations on a plane. More precisely, if we interpret the Lorentz group as the group of motions of a real Lobachevsky space then $\exp F_{10}$ corresponds to translations on a locally Euclidean subspace—an horosphere.[22] Let us denote

$$T_C=\exp F_9, \quad T_H=\exp F_{10}. \tag{45}$$

The group $\exp F_7 \sim D \square T_H$ corresponds to dilatations and translations in a plane.

B. Splitting subalgebras of the Poincaré algebra

We now proceed to apply the algorithm of Sec. 2B, to find all subalgebras of the Poincaré algebra P. Step 1 has already been performed, i.e., we have given a list of representatives F_i of the conjugacy classes of subalgebras of the factor algebra $F=LSL(2,C)=P/N$, where $N=LT_4$ is the algebra of the translations. Conjugation was considered under the proper orthochronous Lorentz group and the normalizers $\mathrm{Nor}_{LG}F_i$ in the Lorentz group were also found. All of this is summarized in Table II.

Step 2 of the algorithm will provide us with all subalgebras $P_{j,k}$ of P that split over their intersection with the translations (are splitting extensions of $N_{j,k}\subseteq N$ by F_j, where $N_{j,k}$ is a subalgebra of N). This step must be performed separately for each subalgebra F_j, i.e., for each F_j we must find all invariant subspaces $N_{j,k}\subseteq N$. They satisfy $[F_j,N_{j,k}]\subseteq N_{j,k}$ and provide us with the requested algebras according to the prescription $P_{j,k}=F_j+N_{j,k}$. The label k simply serves to distinguish different invariant subspaces $N_{j,k}$ corresponding to the same F_j and different subalgebras $P_{j,k}$ of P.

Simultaneously, we apply Step 4, i.e., use elements of $\mathrm{Nor}_{LG}F_j/(\exp F_j)$, i.e., the outer part of the normalizer, to simplify $N_{j,k}$.

For each F_j we thus face a trivial problem of linear algebra. Let us run through the individual F_j.

F_1—The algebra F_1 is represented irreducibly on the space N. Hence the only invariant subsapces are

$$N_{1,1}=LT_4, \quad N_{1,2}=0. \tag{46}$$

F_2—The Borel subalgebra F_2 has four invariant subspaces in N, namely

$$N_{2,1}=LT_4, \quad N_{2,2}=\{X_1,X_2,X_3\}, \quad N_{2,3}=\{X_1\}, \quad N_{2,4}=0. \tag{47}$$

Obviously, we have $[F_2,N_{2,j}]\subseteq N_{2,j}$ and we check directly that there are no other invariant subspaces.

F_3—Since F_3 is the Lie algebra of $SU(2)$, it is immediately clear that the invariant subspaces are

$$N_{3,1}=LT_4,\quad N_{3,2}=\{X_1-X_4,X_2,X_3\},\quad N_{3,3}=\{X_1+X_4\},\quad N_{3,4}=0. \tag{48}$$

Here $N_{3,2}$ are the space components of linear momentum p_1,p_2,p_3 and $N_{3,3}$ is the time-component (energy) p_0 [see (39)].

F_4—Since F_4 is the Lie algebra of $SU(1,1)$, the results are equally obvious:

$$N_{4,1}=LT_4,\quad N_{4,2}=\{X_1+X_4,X_2,X_3\},\quad N_{4,3}=\{X_1-X_4\},\quad N_{4,4}=0. \tag{49}$$

F_5—Putting $[F_5,N_{5j}]\subseteq N_{5j}$, we find

$$N_{5,1}=LT_4,\quad N_{5,2}=\{X_1,X_2,X_3\},\quad N_{5,3}=\{X_1\},\quad N_{5,4}=0. \tag{50}$$

F_6—The same holds as for F_5, i. e.,

$$F_{6,1}=LT_4,\quad N_{6,2}=\{X_1,X_2,X_3\},\quad N_6=\{X_1\},\quad N_{6,4}=0. \tag{51}$$

F_7—The invariant subspaces in this case are $\{0\}$, $\{X_1\}$, $\{X_1,X_2\cos\phi+X_3\sin\phi,\ 0\le\phi<\pi\}$, $\{X_1,X_2,X_3\}$ and LT_4. However, remembering that the normalizer of F_7 is $\mathrm{Nor}_{LG}F_7=\exp F_2$ (see Table II), we can simplify the subspace: $\{X_1,X_2\cos\phi+X_3\sin\phi\}$. Indeed, we have

$$\exp(xB_1)(\cos\phi X_2+\sin\phi X_3)\exp(-xB_1)=\cos(2x+\phi)X_2+\sin(2x+\phi)X_3. \tag{52}$$

Putting $x=-\phi/2$ we transform our subspace into $\{X_1,X_2\}$. Thus we obtain

$$N_{7,1}=LT_4,\quad N_{7,2}=\{X_1,X_2,X_3\},\ N_{7,3}=\{X_1,X_2\},\quad N_{7,4}=\{X_1\},\ N_{7,5}=0. \tag{53}$$

F_8—The invariant subspaces obtained by investigating the equation $[F_8,N_{8,k}]\subseteq N_{8,k}$ are

$$N_{8,1}=LT_4,\quad N_{8,2}=\{X_1,X_2,X_3\},\quad N_{8,3}=\{X_1,X_3,X_4\},$$
$$N_{8,4}=\{X_1,X_2\},\quad N_{8,5}=\{X_1,X_3\},\quad N_{8,6}=\{X_1,X_2+bX_3,b\neq0\}.$$
$$N_{8,7}=\{X_1\},\quad N_{8,8}=\{X_2\},\quad N_{8,9}=0. \tag{54}$$

The normalizer in this case is $C_4\,\square\,\exp F_8$ and we can check that it cannot be used to simplify the invariant subspaces (e. g., the value of b in $N_{8,6}$ is invariant under $\mathrm{Nor}_{LG}F_8$).

F_9—The invariant subspaces directly obtained are LT_4, $\{X_1,X_2,X_3\}$, $\{X_2,X_3,X_4\}$, $\{X_1,X_4\}$, $\{X_2,X_3\}$, $\{X_1\}$, $\{X_4\}$, and 0. However, the transformation Z_1 of (40) in $\mathrm{Nor}F_9$ satisfies

$$Z_1X_1Z_1^{-1}=X_4,\quad Z_1X_2Z_1^{-1}=X_2,\quad Z_1X_3Z_1^{-1}=-X_3,\quad Z_1X_4Z_1^{-1}=X_1. \tag{55}$$

The subspaces X_1 and X_4 and similarly $\{X_1X_2X_3\}$ and $\{X_2,X_3,X_4\}$ are thus conjugate to each other and we obtain the following independent invariant subspaces:

$$N_{9,1}=LT_4,\quad N_{9,2}=\{X_1,X_2,X_3\},\quad N_{9,3}=\{X_2,X_3\},\quad N_{9,4}=\{X_1,X_4\},$$
$$N_{9,5}=\{X_1\},\quad N_{9,6}=0. \tag{56}$$

F_{10}—The invariant subspaces obtained for F_{10} are LT_4, $\{X_1,X_2,X_3\}$, $\{X_1,\cos\phi X_2+\sin\phi X_3,0\le\phi\le\pi\}$, and $\{X_1\}$. We can again make use of the fact that $\exp xB_1$ is in the normalizer of F_{10} and rotate $\cos\phi X_2+\sin\phi X_3$ into X_2, leaving X_1 invariant. Thus we obtain

$$N_{10,1}=LT_4,\quad N_{10,2}=\{X_1,X_2,X_3\},\quad N_{10,3}=\{X_1,X_2\},$$
$$N_{10,4}=\{X_1\},\quad N_{10,5}=0. \tag{57}$$

F_{11}—The invariant subspaces of B_c are found directly to be

$$N_{11,1}=LT_4,\quad N_{11,2}=\{X_1,X_2,X_3\},\quad N_{11,3}=\{X_2,X_3\},$$
$$N_{11,4}=\{X_1,X_4\},\quad N_{11,5}=\{X_1\},\quad N_{11,6}=0. \tag{58}$$

F_{12}—The operator B_1 leaves the space aX_1+bX_4 invariant for any a and b. However, using the fact that $\exp(xB_1+yB_2)$ and Z_1 are in the normalizer of F_{12}, we can transform aX_1+bX_4 into X_1 if $ab=0$, into X_1+X_4 if $ab>0$, or into X_1-X_4 if $ab<0$. Similarly, the three-dimensional invariant subspace $\{aX_1+bX_4,X_2,X_3\}$ can also be simplified. We obtain the following independent (nonconjugate) invariant subspaces:

$$N_{12,1}=LT_4,\ N_{12,2}=\{X_1,X_2,X_3\},\ N_{12,3}=\{X_1-X_4,X_2,X_3\},$$
$$N_{12,4}=\{X_1+X_4,X_2,X_3\},\quad N_{12,5}=\{X_1,X_4\},\quad N_{12,6}=\{X_2,X_3\},$$
$$N_{12,7}=\{X_1\},\quad N_{12,8}=\{X_1-X_4\},\quad N_{12,9}=\{X_1+X_4\},$$
$$N_{12,10}=0. \tag{59}$$

F_{13}—The operator B_2 leaves both X_1 and X_4 invariant. However, Z_1 is in the normalizer of F_{13} and transforms X_4 into X_1. Similarly, aX_2+bX_3 is invariant for any a and b but can be rotated by $\exp xB_1$ into X_2. The invariant subspaces $\{X_1,X_2\cos\phi+X_3\sin\phi,\ 0\le\phi<\pi\}$ can similarly all be rotated into $\{X_1,X_2\}$. The other invariant subspaces are obtained directly. Thus

$$N_{13,1}=LT_4,\quad N_{13,2}=\{X_1,X_2,X_3\},\quad N_{13,3}=\{X_1,X_3,X_4\},$$
$$N_{13,4}=\{X_1,X_4\},\quad N_{13,5}=\{X_1,X_2\},\quad N_{13,6}=\{X_2,X_3\},$$
$$N_{13,7}=\{X_1\},\quad N_{13,8}=\{X_2\},\quad N_{13,9}=0. \tag{60}$$

F_{14}—The operator B_3 leaves the following spaces invariant:

$$N_{14,1}=LT_4,\quad N_{14,2}=\{X_1,X_2,X_3\},\quad N_{14,3}=\{X_1,X_3,X_4\},$$
$$N_{14,4}=\{X_1,X_2\},\quad N_{14,5}=\{X_1,X_3\},\quad N_{14,6}=\{X_1,X_2+bX_3,b\neq0\},$$
$$N_{14,7}=\{X_1\},\quad N_{14,8}=\{X_2\},\quad N_{14,9}=0. \tag{61}$$

Since $\mathrm{Nor}_{LG}F_{14}$ does not contain $\exp B_1$ we cannot rotate in the $\{X_2,X_3\}$ space so each value of b in $N_{14,6}$ will correspond to a different subalgebra (mutually nonconjugate for different values of b).

F_{15}—The algebra F_{15} is empty, i. e., contains the element 0 only. The space of translations N can be split into orbits under $SL(2,C)$. We have

$$N=\begin{pmatrix}0&0&c+id&ia\\0&0&ib&-c+id\\0&0&0&0\\0&0&0&0\end{pmatrix}=aX_1+cX_2+dX_3+bX_4$$

$$=\left(\frac{a+b}{2}\right)P_0-dP_1+cP_2+\left(\frac{-a+b}{2}\right)P_3$$

[we have used (39)]. The orbits will clearly differ by their signature, i.e., by the number of mutually orthogonal timelike, spacelike and lightlike vectors contained. For $G\in SL(2,C)$ we find that the transformation

$$GNG^{-1}=N \tag{62}$$

leaves

$$\Delta=ab-c^2-d^2 \tag{63}$$

invariant. An individual vector

$$X=a_iX_i$$

will be characterized by $\Delta=a_1a_4-a_2^2-a_3^2$. We call a vector, respectively,

timelike (+) if $\Delta>0$,

spacelike (−) if $\Delta<0$,

lightlike (0) if $\Delta=0$.

The mutually nonconjugate subspaces of N and their signatures are

$$N_{15,1}=LT_4\ (+\ -\ -\ -),\quad N_{15,2}=\{X_1,X_2,X_3\}\ (0--),$$
$$N_{15,3}=\{X_1-X_4,X_2,X_3\}\ (-\ -\ -),\quad N_{15,4}=\{X_1+X_4,X_2,X_3\}\ (+--),$$
$$N_{15,5}=\{X_1,X_2\}\ (0-),\quad N_{15,6}=\{X_1,X_4\}\ (+-),$$
$$N_{15,7}=\{X_2,X_3\}\ (--),\quad N_{15,8}=\{X_1\}\ (0),\quad N_{15,9}=\{X_1+X_4\}\ (+),$$
$$N_{15,10}=\{X_1-X_4\}\ (-),\quad N_{15,11}=0, \tag{64}$$

This completes our list of invariant subspaces for all F_j. The resulting splitting subalgebras

$$P_{j,k}=F_j\overset{\circ}{+}N_{j,k}$$

are listed in Table III. The first column introduces a notation $P_{j,k}$ (k simply differentiates between different subalgebras of P obtained from the same F_j). The second lists F_j, the third gives the dimension of $P_{j,k}$ (over the field of real numbers). The generators of F_j and $N_{j,k}$ are given in columns 4 and 5. The normalizer of $P_{j,k}$ in the Lorentz group is given in the sixth column. Comments on the corresponding subgroup of the Poincaré group are given in the last column, in particular, we indicate the signature of $N_{j,k}$. Again the Borel group is the maximal solvable subgroup of $SL(2,C)$, $E(3)$ and $E(2)$ are the Euclidean groups in three and two dimensions, $E(2,1)$ and $E(1,1)$ the pseudo-Euclidean groups in three and two dimensions. $C(1)$ is the group

TABLE III. List of representatives of splitting subalgebras $P_{j,k}$ of P.

Notation $P_{j,k}$	F_j	$\dim_R P_{j,k}$	Generators of F_j	$N_{j,k}$	$\mathrm{Nor}_{LG}F_j\cap\mathrm{Nor}_{LG}N_{j,k}$	Comment on subgroup
$P_{1,1}$	F_1	10	$B_1,\dots,B_6$	X_1,X_2,X_3,X_4	Inner	$PG\simeq LG\,\square\,T_4$
$P_{1,2}$		6		0		$LG\sim SL(2,C)$
$P_{2,1}$	F_2	8	$B_1,\dots,B_4$	X_1,X_2,X_3,X_4	Inner	Borel$\,\square\,T_4$
$P_{2,2}$		7		X_1,X_2,X_3		Borel$\,\square\,(0--)$
$P_{2,3}$		5		X_1		Borel$\,\square\,(0)$
$P_{2,4}$		4		0		Borel
$P_{3,1}$	F_3	7	B_1,B_3-B_5,B_4+B_6	X_1,X_2,X_3,X_4	Inner	$SU(2)\,\square\,T_4$
$P_{3,2}$		6		X_1-X_4,X_2,X_3		$SU(2)\,\square\,(---)\sim E(3)$
$P_{3,3}$		4		X_1+X_4		$SU(2)\otimes(+)$
$P_{3,4}$		3		0		$SU(2)$
$P_{4,1}$	F_4	7	B_1,B_3+B_5,B_4-B_6	X_1,X_2,X_3,X_4	$\exp F_4\cup\exp F_4\cdot Z_1$	$SU(1,1)\,\square\,T_4$
$P_{4,2}$		6		X_1+X_4,X_2,X_3		$SU(1,1)\square(+--)\sim E(2,1)$
$P_{4,3}$		4		X_1-X_4		$SU(1,1)\otimes(-)$
$P_{4,4}$		3		0		$SU(1,1)$
$P_{5,1}$	F_5	7	B_c,B_3,B_4	X_1,X_2,X_3,X_4	$\exp F_2$	$S(3)\,\square\,T_4$
$P_{5,2}$		6		X_1,X_2,X_3		$S(3)\,\square\,(0--)$
$P_{5,3}$		4		X_1		$S(3)\,\square\,(0)$
$P_{5,4}$		3		0		$S(3)$
$P_{6,1}$	F_6	7	B_1,B_3,B_4	X_1,X_2,X_3,X_4	$\exp F_2$	$E(2)\,\square\,T_4$
$P_{6,2}$		6		X_1,X_2,X_3		$E(2)\,\square\,(0--)$
$P_{6,3}$		4		X_1		$E(2)\otimes(0)$
$P_{6,4}$		3		0		$E(2)$
$P_{7,1}$	F_7	7	B_2,B_3,B_4	X_1,X_2,X_3,X_4	$\exp F_2$	$(D\,\square\,T_H)\,\square\,T_4$
$P_{7,2}$		6		X_1,X_2,X_3	$\exp F_2$	$(D\,\square\,T_H)\,\square\,(0--)$
$P_{7,3}$		5		X_1,X_2	$C_4\,\square\exp F_7$	$(D\,\square\,T_H)\,\square\,(0-)$
$P_{7,4}$		4		X_1	$\exp F_2$	$(D\,\square\,T_H)\,\square\,(0)$
$P_{7,5}$		3		0	$\exp F_2$	$(D\,\square\,T_H)$
$P_{8,1}$	F_8	6	B_2,B_3	X_1,X_2,X_3,X_4	$C_4\,\square\exp F_8$	$C(1)\,\square\,T_4$
$P_{8,2}$		5		X_1,X_2,X_3		$C(1)\,\square\,(0--)$
$P_{8,3}$		5		X_1,X_3,X_4		$C(1)\,\square\,(+--)$
$P_{8,4}$		4		X_1,X_2		$C(1)\,\square\,(0-)$
$P_{8,5}$		4		X_1,X_3		$C(1)\,\square\,(0-)$
$P_{8,6}$		4		$X_1,X_2+bX_3,\ b\neq 0$		$C(1)\,\square\,(0-)$
$P_{8,7}$		3		X_1		$C(1)\,\square\,(0)$
$P_{8,8}$		3		X_2		$C(1)\otimes(-)$
$P_{8,9}$		2		0		$C(1)$

TABLE III *continued*

Notation $P_{j,k}$	F_j	$\dim_R P_{j,k}$	Generators of F_j	$N_{j,k}$	$\mathrm{Nor}_{LG}F_j \cap \mathrm{Nor}_{LG}N_{j,k}$	Comment on subgroup
$P_{9,1}$		6		X_1, X_2, X_3, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$T_c \square T_4$
$P_{9,2}$		5		X_1, X_2, X_3	Inner	$T_c \square (0--)$
$P_{9,3}$	F_9	4	B_1, B_2	X_2, X_3	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$T_c \square (--)$
$P_{9,4}$		4		X_1, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$T_c \square (+-)$
$P_{9,5}$		3		X_1	Inner	$T_c \square (0)$
$P_{9,6}$		2		0	$\exp F_9 \cup \exp F_9 \cdot Z_1$	T_c
$P_{10,1}$		6		X_1, X_2, X_3, X_4	$\exp F_2$	$T_H \square T_4$
$P_{10,2}$		5		X_1, X_2, X_3	$\exp F_2$	$T_H \square (0--)$
$P_{10,3}$	F_{10}	4	B_3, B_4	X_1, X_2	$C_4 \square \exp F_7$	$T_H \square (0-)$
$P_{10,4}$		3		X_1	$\exp F_2$	$T_H \otimes (0)$
$P_{10,5}$		2		0	$\exp F_2$	T_H
$P_{11,1}$		5		X_1, X_2, X_3, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$S(1) \square T_4$
$P_{11,2}$		4		X_1, X_2, X_3	$\exp F_9$	$S(1) \square (0--)$
$P_{11,3}$	F_{11}	3	B_c	X_2, X_3	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$S(1) \square (--)$
$P_{11,4}$		3		X_1, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$S(1) \square (+-)$
$P_{11,5}$		2		X_1	$\exp F_9$	$S(1) \square (0)$
$P_{11,6}$		1		0	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$S(1)$
$P_{12,1}$		5		X_1, X_2, X_3, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(2) \square T_4$
$P_{12,2}$		4		X_1, X_2, X_3	$\exp F_9$	$O(2) \square (0--)$
$P_{12,3}$		4		$X_1 - X_4, X_2, X_3$	$\exp F_{12} \cup \exp F_{12} \cdot Z_1$	$O(2) \square (---)$
$P_{12,4}$		4		$X_1 + X_4, X_2, X_3$	$\exp F_{12} \cup \exp F_{12} \cdot Z_1$	$O(2) \square (+--)$
$P_{12,5}$	F_{12}	3	B_1	X_1, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(2) \otimes (+-)$
$P_{12,6}$		3		X_2, X_3	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(2) \square (--)$
$P_{12,7}$		2		X_1	$\exp F_9$	$O(2) \otimes (0)$
$P_{12,8}$		2		$X_1 - X_4$	$\exp F_{12} \cup \exp F_{12} \cdot Z_1$	$O(2) \otimes (-)$
$P_{12,9}$		2		$X_1 + X_4$	$\exp F_{12} \cup \exp F_{12} \cdot Z_1$	$O(2) \otimes (+)$
$P_{12,10}$		1		0	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(2)$
$P_{13,1}$		5		X_1, X_2, X_3, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(1,1) \square T_4$
$P_{13,2}$		4		X_1, X_2, X_3	$\exp F_9$	$O(1,1) \square (0--)$
$P_{13,3}$		4		X_1, X_3, X_4	$C_4 \square (\exp F_{13} \cup \exp F_{13} \cdot Z_1)$	$O(1,1) \square (+--)$
$P_{13,4}$		3		X_1, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(1,1) \square (+-)$
$P_{13,5}$	F_{13}	3	B_2	X_1, X_2	$C_4 \square \exp F_{13}$	$O(1,1) \square (0-)$
$P_{13,6}$		3		X_2, X_3	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(1,1) \otimes (--)$
$P_{13,7}$		2		X_1	$\exp F_9$	$O(1,1) \square (0)$
$P_{13,8}$		2		X_2	$C_4 \square (\exp F_{13} \cup \exp F_{13} \cdot Z_1)$	$O(1,1) \otimes (-)$
$P_{13,9}$		1		0	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$O(1,1)$
$P_{14,1}$		5		X_1, X_2, X_3, X_4	$C_4 \square \exp F_7$	$E(1) \square T_4$
$P_{14,2}$		4		X_1, X_2, X_3	$C_4 \square \exp F_7$	$E(1) \square (0--)$
$P_{14,3}$		4		X_1, X_3, X_4	$C_4 \square \exp F_8$	$E(1) \square (+--)$
$P_{14,4}$		3		X_1, X_2	$C_4 \square \exp F_7$	$E(1) \otimes (0-)$
$P_{14,5}$	F_{14}	3	B_3	X_1, X_3	$C_4 \square \exp F_7$	$E(1) \square (0-)$
$P_{14,6}$		3		$X_1, X_2 + bX_3,\ b \neq 0$	$C_4 \square \exp F_7$	$E(1) \square (0-)$
$P_{14,7}$		2		X_1	$C_4 \square \exp F_7$	$E(1) \otimes (0)$
$P_{14,8}$		2		X_2	$C_4 \square \exp F_8$	$E(1) \otimes (-)$
$P_{14,9}$		1		0	$C_4 \square \exp F_7$	$E(1)$
$P_{15,1}$		4		X_1, X_2, X_3, X_4	$SL(2,C)$	T_4
$P_{15,2}$		3		X_1, X_2, X_3	$\exp F_2$	$(0--)$
$P_{15,3}$		3		$X_1 - X_4, X_2, X_3$	$\exp F_3$	$(---)$
$P_{15,4}$		3		$X_1 + X_4, X_2, X_3$	$\exp F_4 \cup \exp F_4 \cdot Z_1$	$(+--)$
$P_{15,5}$		2		X_1, X_2	$C_4 \square \exp F_7$	$(0-)$
$P_{15,6}$	F_{15}	2	0	X_1, X_4	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$(+-)$
$P_{15,7}$		2		X_2, X_3	$\exp F_9 \cup \exp F_9 \cdot Z_1$	$(--)$
$P_{15,8}$		1		X_1	$\exp F_2$	(0)
$P_{15,9}$		1		$X_1 + X_4$	$\exp F_3$	$(+)$
$P_{15,10}$		1		$X_1 - X_4$	$\exp F_4 \cup \exp F_4 \cdot Z_1$	$(-)$
$P_{15,11}$		0		0	$SL(2,C)$	

of transformations of a straight line (44); $S(3)$ and $S(1)$ are defined in (42) and (43).

The normalizers of column 6 are easy to obtain from $\mathrm{Nor}_{LG}F_j$ of Table II by inspecting its action on $N_{j,k}$. We do not present the details.

C. Nonsplitting subalgebras of the Poincaré algebra

Following the algorithm of Sec. 2B we now come to Step 3, which together with Step 4 will provide us with a list of all the remaining subalgebras of P, namely those that are nonsplit extensions of the subalgebras $N_{jk} \subset N$ by F_j.

The algebras F_1, F_3, and F_4 [corresponding to $SL(2,C)$, $SU(2)$ and $SU(1,1)$] are semisimple and hence cannot provide any nonsplit extensions. All other subalgebras F_j of F are contained in F_2 [the only maximal solvable subalgebra of $LSL(2,C)$] and we need only consider F_2 and its subalgebras in connection with Step 3.

First of all let us construct the matrix representations (10) of F_2 on N. Using the commutation relations of Table I, we find

$$\beta^1=\begin{pmatrix}0&0&0&0\\0&0&-2&0\\0&2&0&0\\0&0&0&0\end{pmatrix},\quad \beta^2=\begin{pmatrix}2&0&0&0\\0&0&0&0\\0&0&0&0\\0&0&0&-2\end{pmatrix},$$
$$\beta^3=\begin{pmatrix}0&0&2&0\\0&0&0&0\\0&0&0&1\\0&0&0&0\end{pmatrix},\quad \beta^4=\begin{pmatrix}0&-2&0&0\\0&0&0&-1\\0&0&0&0\\0&0&0&0\end{pmatrix}. \tag{65}$$

[in the basis given by (33) and (34)]. These matrices immediately provide us with the basis coboundaries of Eq. (16), (17). Indeed, we have

$$\begin{aligned}\partial B_1&=2x_3X_2-2x_2X_3,\\ \partial B_2&=-2x_1X_1+2x_4X_4,\\ \partial B_3&=-2x_3X_1-x_4X_3,\\ \partial B_4&=2x_2X_1+x_4X_2.\end{aligned} \tag{66}$$

The four arbitrary constants $x_1,\ldots,x_4$ can be used to simplify the nontrivial 1-cocycles (14). Indeed, adding combinations of the coboundaries to cocycles corresponds to simplifying possible generators of subalgebras by transformations of the type $\exp N$.

Let us now consider the individual subalgebras F_j of $LSL(2,C)$, remembering that the semisimple subalgebras F_1, F_3, and F_4 are of no interest in this connection.

F_2—The Borel subalgebra F_2 does not provide any nonsplitting extensions. Indeed the generators of a nonsplit subalgebra would be

$$\tilde{B}_k=B_k+\sum_{i=1}^{4}c_{ki}X_i,\quad k=1,\ldots,4,$$

and

$$N_{2,j},\quad j=1,\ldots,4, \tag{67}$$

where N_{2j} is one of the invariant subspaces (47). Putting $2x_3=c_{12}$, $-2x_2=c_{13}$ and subtracting ∂B_1 from $\tilde{B}_1$ we obtain $c_{12}=c_{13}=0$ in (67). Similarly, put $-2x_1=c_{21}$, $2x_4=c_{24}$ and subtracting ∂B_2 from $\tilde{B}_2$, we obtain $c_{21}=c_{24}=0$ in (67). Using relations of the type (15) or demanding directly that $\tilde{B}_1,\ldots,\tilde{B}_4$ with $N_{2,j}$ form an algebra, we find that for each of the four subspaces $N_{2,j}$ of (47) these conditions lead to the equations

$$c_{ki}=0,\quad k=1,\ldots,4,\quad i=1,\ldots,4,$$

i.e., to splitting subalgebras already listed above in Table III.

F_5—The results in this case are the same as for F_2, namely no nonsplitting algebras are obtained.

F_6—This case leads to new subalgebras, so we consider it in somewhat greater detail. The generators involving F_6 can be written as

$$\begin{aligned}\tilde{B}_1&=B_1+a_1X_1+a_4X_4,\\ \tilde{B}_3&=B_3+c_1X_1+c_2X_2+c_4X_4,\\ \tilde{B}_4&=B_4+d_1X_1+d_2X_2+d_3X_3+d_4X_4.\end{aligned} \tag{68}$$

We have already made use of the coboundaries ∂B_1, ∂B_3, and ∂B_4 to eliminate a_2, a_3, and c_3. The commutation relations are

$$\begin{aligned}[\tilde{B}_1,\tilde{B}_3]&=2B_4+(2c_2-a_4)X_3,\\ [\tilde{B}_1,\tilde{B}_4]&=-2B_3+2d_2X_3-2d_3X_2+a_4X_2,\\ [\tilde{B}_3,\tilde{B}_4]&=2d_3X_1+d_4X_3+2c_2X_1+c_4X_2.\end{aligned} \tag{69}$$

Now consider the individual invariant subspaces $N_{6,j}$ of (51). Adding $N_{6,1}=LT_4$ to (68), we obviously obtain the splitting subalgebra $P_{6,1}$. The other cases are less trivial.

Take $N_{6,2}=\{X_1,X_2,X_3\}$. We can immediately put $a_1=c_1=c_2=d_1=d_2=d_3=0$ in (68). From (69) we find $c_4=d_4=0$ and we obtain the subalgebra:

$$B_1+aX_4,B_3,B_4,X_1,X_2,X_3,\quad a\neq 0. \tag{70}$$

According to Step 4 of the algorithm we can further simplify (70) using other automorphisms of F_7. Indeed, we have

$$\exp(xB_2)(B_1+aX_4)\exp(-xB_2)=B_1+\epsilon X_4,\quad \epsilon=\pm 1, \tag{71}$$

where $\exp(2x)=a/\epsilon$ and $\epsilon=\pm 1$ for sign $a=\pm 1$. The other generators are left unchanged by $\exp xB_2$ and we obtain two new algebras:

$$\left.\begin{matrix}\tilde{P}_{6,5}\\ \tilde{P}_{6,6}\end{matrix}\right\} B_1+\epsilon X_4,B_3,B_4,X_1,X_2,X_3,\quad \epsilon=\pm 1. \tag{72}$$

Note that these algebras are new—not only are they not conjugate to any of the splitting subalgebras of Table III but they are not even isomorphic to any of them.

Now take $N_{6,3}=\{X_1\}$. We put $a_1=c_1=d_1=0$ in (68). The commutation relations (69) imply in this case $d_2=d_4=c_4=0$ and ultimately $a_4=0$, $d_3=c_2$. The subalgebra in this case is reduced to

$$B_1,B_3+cX_2,B_4+cX_3,\ X_1,\quad -\infty<c<\infty.$$

This can again be simplified using the outer automorphism $\exp xB_2$ and we again obtain two new algebras:

$$\left.\begin{matrix}\tilde{P}_{6,7}\\ \tilde{P}_{6,8}\end{matrix}\right\} B_1,B_3+\epsilon X_2,B_4+\epsilon X_3,X_1,\quad \epsilon=\pm 1. \tag{73}$$

Finally, take $N_{6,4}=0$. The commutation relations (69) now imply $d_1=d_2=d_4=c_1=c_4=a_4=c_2=d_3=0$. Thus we have

$$B_1+aX_1,B_3,B_4.$$

Again $\exp xB_2$ can be used to simplify and we obtain two algebras

$$\left.\begin{matrix}\tilde{P}_{6,9}\\ \tilde{P}_{6,10}\end{matrix}\right\} B_1+\epsilon X_1,B_3,B_4,\quad \epsilon=\pm 1. \tag{74}$$

These are both isomorphic to $P_{6,4}=F_6$ but not conjugate to this algebra under the Poincaré group.

F_7—The generators involving F_7 can, after subtracting the appropriate combinations of coboundaries (66), be written as

$$\tilde{B}_2=B_2+b_iX_i,\quad \tilde{B}_3=B_3+c_iX_i,\quad \tilde{B}_4=B_4+d_iX_i,$$
$$b_1=b_4=c_1=d_1=0. \tag{75}$$

The commutation relations are

$$[\tilde{B}_2, \tilde{B}_3] = 2B_3 - 2c_4X_4 - 2b_3X_1,$$
$$[\tilde{B}_2, \tilde{B}_4] = 2B_4 - 2d_4X_4 + 2b_2X_1, \quad (75')$$
$$[\tilde{B}_3, \tilde{B}_4] = 2d_3X_1 + d_4X_4 + 2c_2X_1.$$

Consider the invariant subspaces $N_{7,k}$ of (53). $N_{7,1}$, $N_{7,2}$, and $N_{7,5}$ lead to splitting subalgebras only (all $b_i = c_i = d_i = 0$). Consider $N_{7,3} = \{X_1, X_2\}$. We have $b_2 = c_2 = d_2 = 0$ and (75') implies $c_3 = c_4 = d_3 = d_4 = 0$. The obtained algebra is $\{B_2 + cX_3, B_3, B_4, X_1, X_2;\ x \neq 0\}$. The element Z_2 in the normalizer $\mathrm{Nor}_{LG}F_7$ [see (40)] transforms

$$Z_2(B_2 + cX_3)Z_2^{-1} = B_2 - cX_3.$$

No further simplifications are possible, and so we obtain a class of subalgebras:

$$\tilde{P}_{7,6}: \quad B_2 + cX_3, B_3, B_4, X_1, X_2; \quad 0 < c < \infty. \quad (76)$$

Taking $N_{7,4} = \{X_1\}$ as the invariant subspace, we find $c_i = d_i = 0$ $(i = 1, \ldots, 4)$, thus obtaining the algebra $\tilde{B}_2 = B_2 + b_2X_2 + b_3X_3, B_3, B_4, X_1$; $b_2^2 + b_3^2 \neq 0$. The transformation $(\exp xB_1)$ with $2x = \pi/2 - \arctan(b_3/b_2)$ simplifies this class of algebras to its final form:

$$\tilde{P}_{7,7}: \quad B_2 + cX_3, B_3, B_4, X_1; \quad 0 < c < \infty. \quad (77)$$

F_8—We take the generators as

$$\tilde{B}_2 = B_2 + b_iX_i, \quad \tilde{B}_3 = B_3 + c_iX_i. \quad (78)$$

Putting $x_1 = -b_1/2$, $x_4 = +b_4/2$, $x_3 = -c_1/2$ and replacing $\tilde{B}_2, \tilde{B}_3$ by $\tilde{B}_2 - \partial B_2$, $\tilde{B}_3 - \partial B_3$, we obtain generators in the form (78) with $b_1 = b_4 = c_1 = 0$. The commutation relation is

$$[\tilde{B}_2, \tilde{B}_3] = 2\{B_3 - b_3X_1 - c_4X_4\} \quad (79)$$

implying that $c_2 = c_3 = c_4 = 0$. The generators (78) thus reduce to

$$\tilde{B}_2 = B_2 + b_2X_2 + b_3X_3, \quad \tilde{B}_3 = B_3, \quad b_2^2 + b_3^2 \neq 0. \quad (80)$$

The only nontrivial outer element in the normalizer of F_8 is Z_2 (40) and its presence makes it possible to consider one of the coefficients b_2 or b_3 to be nonnegative. Now let us consider the individual invariant subspaces $N_{8,k}$ (54). Adding $N_{8,1}$, $N_{8,2}$, or $N_{8,8}$ to (80) leads to splitting subalgebras only $(b_i = c_i = 0,\ i = 1, \ldots, 4)$. Let us consider the other cases. Taking $N_{8,3} = \{X_1, X_3, X_4\}$, we have $b_3 = 0$ and we obtain

$$\tilde{P}_{8,10}: \quad B_2 + aX_2, B_3, X_1, X_3, X_4, \quad 0 < a < \infty. \quad (81)$$

Taking $N_{8,4} = \{X_1, X_2\}$, we have $b_2 = 0$, so that

$$\tilde{P}_{8,11}: \quad B_2 + aX_3, B_3, X_1, X_2, \quad 0 < a < \infty. \quad (82)$$

Taking $N_{8,5} = \{X_1, X_3\}$, we have $b_3 = 0$ and we obtain

$$\tilde{P}_{8,12}: \quad B_2 + aX_2, B_3, X_1, X_3, \quad 0 < a < \infty. \quad (83)$$

Taking $N_{8,6} = \{X_1, X_2 + bX_3, b \neq 0\}$, we obtain

$$\tilde{P}_{8,13}: \quad B_2 + aX_2, B_3, X_1, X_2 + bX_3, \quad a > 0, \quad b \neq 0. \quad (84)$$

For $N_{8,7} = \{X_1\}$ we distinguish three cases:

$$\tilde{P}_{8,14}: \quad B_2 + aX_3, \quad B_3, \quad X_1, \quad 0 < a < \infty,$$
$$\tilde{P}_{8,15}: \quad B_2 + aX_2, \quad B_3, \quad X_1, \quad 0 < a < \infty, \quad (85)$$
$$\tilde{P}_{8,16}: \quad B_2 + aX_2 + bX_3, \quad B_3, X_1, \quad 0 < a < \infty, \quad b \neq 0.$$

Finally, take $N_{8,9} = 0$. Relation (79) implies $b_3 = 0$ and we obtain

$$\tilde{P}_{8,17}: \quad B_2 + aX_2, B_3, \quad 0 < a < \infty. \quad (86)$$

F_9—The same procedure as above shows that the subalgebra F_9 does not yield any nonsplitting subalgebras of P.

F_{10}—Using the coboundaries (66) we can write the generators as

$$\tilde{B}_3 = B_3 + a_2X_2 + a_4X_4, \quad \tilde{B}_4 = B_4 + b_2X_2 + b_3X_3 + b_4X_4, \quad (87)$$

satisfying

$$[\tilde{B}_3, \tilde{B}_4] = 2(b_3 + a_2)X_1 + a_4X_2 + b_4X_3. \quad (88)$$

The normalizer of $(F_{10} \dotplus N_{10,k})$ always includes $G = \exp(xB_1 + yB_2)$, except for the case $N_{10,3} = \{X_1, X_2\}$ when only $\exp yB_2$ and Z_1 are available (see Table III). Let us first consider $N_{10,k}$ of (57) with $k \neq 3$. Then we can use $G = \exp(xB_1 + yB_2)$ to simplify (87). Writing

$$G = \begin{pmatrix} \alpha & 0 & 0 & 0 \\ 0 & \alpha^{-1} & 0 & 0 \\ 0 & 0 & \alpha^* & 0 \\ 0 & 0 & 0 & \alpha^{*-1} \end{pmatrix}, \quad \alpha = |\alpha| \exp(i\phi), \quad (89)$$

we can transform $\{\tilde{B}_3, \tilde{B}_4\}$ into

$$\begin{aligned}
\tilde{\tilde{B}}_3 &= G\tilde{B}_3G^{-1}\cos 2\phi - G\tilde{B}_4G^{-1}\sin 2\phi \\
&= |\alpha|^2 B_3 + (a_2\cos^2\phi + b_3\sin^2\phi - b_2\cos 2\phi \sin 2\phi)X_2 \\
&\quad + [(a_2 - b_3)\cos 2\phi \sin 2\phi - b_2\sin^2 2\phi]X_3 \\
&\quad + \frac{1}{|\alpha|^2}(a_4\cos 2\phi - b_4\sin 2\phi)X_4, \\
\tilde{\tilde{B}}_4 &= G\tilde{B}_3G^{-1}\sin 2\phi + G\tilde{B}_4G^{-1}\cos 2\phi \\
&= |\alpha|^2 B_4 + [(a_2 - b_3)\cos 2\phi \sin 2\phi + b_2\cos^2 2\phi]X_2 \\
&\quad + (a_2\sin^2 2\phi + b_3\cos^2 2\phi + b_2\sin 2\phi \cos 2\phi)X_3 \\
&\quad + \frac{1}{|\alpha|^2}(a_4\sin 2\phi + b_4\cos 2\phi)X_4.
\end{aligned} \quad (90)$$

Using the coboundaries (66), again, we simplify to

$$\begin{aligned}
B_3' &= |\alpha|^2 B_3 + (a_2\cos^2 2\phi + b_3\sin^2 2\phi - b_2\cos 2\phi \sin\phi)X_2 \\
&\quad + \frac{1}{|\alpha|^2}(a_4\cos 2\phi - b_4\sin 2\phi)X_4, \\
B_4' &= |\alpha|^2 B_4 + [(a_2 - b_3)\sin 4\phi + b_2\cos 4\phi]X_2 \\
&\quad + (a_2\sin^2 2\phi + b_3\cos^2 2\phi + b_2\sin 2\phi \cos 2\phi)X_3 \\
&\quad + \frac{1}{|\alpha|^2}(a_4\sin 2\phi + b_4\cos 2\phi)X_4.
\end{aligned} \quad (91)$$

Now consider individual cases. The subspace $N_{10,1}$ can obviously not give any nonsplitting subalgebras.

Take $N_{10,2} = \{X_1, X_2, X_3\}$. Then $a_2 = b_2 = b_3 = 0$. We put

$$\tan 2\phi = -b_4/a_4, \quad |\alpha|^4 = (a_4^2 + b_4^2)^{1/2},$$

and obtain the subalgebra

$$\tilde{P}_{10,6}: \quad B_3 + X_4, B_4, X_1, X_2, X_3. \quad (92)$$

Take $N_{10,3} = \{X_1, X_2\}$. Then B_1 is not in the normalizer and we must put $\phi = 0$ or $\pi/2$ in (89). We have $a_2 = b_2 = 0$ and from (88) also $b_4 = 0$. Taking $\phi = 0$ in (91), we have

$$B_3' = |\alpha|^2 B_3 + (a_4/|\alpha|^2)X_4, \quad B_4' = |\alpha|^2 B_4 + b_3X_3.$$

TABLE IV. List of representatives of nonsplitting subalgebras $\tilde{P}_{j,k}$ of P.

Notation $\tilde{P}_{j,k}$	F_j	$\dim_R \tilde{P}_{j,k}$	$N_{j,k}$	Generators not in $N_{j,k}$	Nor$_{PG}\tilde{P}_{j,k}$	Comment
$\tilde{P}_{6,5}$	F_6	6	X_1, X_2, X_3	B_1+X_4, B_3, B_4	$C_4 \square P_{6,1}$	
$\tilde{P}_{6,6}$		6	X_1, X_2, X_3	B_1-X_4, B_3, B_4	$C_4 \square P_{6,1}$	
$\tilde{P}_{6,7}$		4	X_1	$B_1,\ B_3+X_2, B_4+X_3$	$C_4 \square P_{6,7}$	
$\tilde{P}_{6,8}$		4	X_1	$B_1,\ B_3-X_2, B_4-X_3$	$C_4 \square \tilde{P}_{6,7}$	
$\tilde{P}_{6,9}$		3	0	B_1+X_1, B_3, B_4	$C_4 \square P_{6,3}$	$\simeq P_{6,4}$
$\tilde{P}_{6,10}$		3	0	B_1-X_1, B_3, B_4	$C_4 \square P_{6,3}$	$\simeq P_{6,4}$
$\tilde{P}_{7,6}$	F_7	5	X_1, X_2	$B_2+aX_3, B_3, B_4,\ a>0$	$P_{7,2}$	
$\tilde{P}_{7,7}$		4	X_1	$B_2+aX_3, B_3, B_4,\ a>0$	$P_{7,2}$	
$\tilde{P}_{8,10}$	F_8	5	X_1, X_3, X_4	$B_2+aX_2, B_3,\ a>0$	$P_{8,1}$	$\simeq P_{8,3}$
$\tilde{P}_{8,11}$		4	X_1, X_2	$B_2+aX_3, B_3,\ a>0$	$P_{8,2}$	
$\tilde{P}_{8,12}$		4	X_1, X_3	$B_2+aX_2, B_3,\ a>0$	$P_{8,2}$	$\simeq P_{8,5}$
$\tilde{P}_{8,13}$		4	$X_1, X_2, +bX_3,\ b\neq 0$	$B_2+aX_2, B_3,\ a>0$	$P_{8,2}$	$\simeq P_{8,6}$
$\tilde{P}_{8,14}$		3	X_1	$B_2+aX_3, B_3,\ a>0$	$P_{8,2}$	
$\tilde{P}_{8,15}$		3	X_1	$B_2+aX_2, B_3,\ a>0$	$P_{8,2}$	$\simeq P_{8,7}$
$\tilde{P}_{8,16}$		3	X_1	$B_2+aX_2+bX_3, B_3,\ a>0,\ b\neq 0$	$P_{8,2}$	
$\tilde{P}_{8,17}$		2	0	$B_2+aX_2, B_3,\ a>0$	$P_{8,8}$	$\simeq P_{8,9}$
$\tilde{P}_{10,6}$	F_{10}	5	X_1, X_2, X_3	B_3+X_4, B_4	$\tilde{P}_{10,1}$	
$\tilde{P}_{10,7}$		4	X_1, X_2	$B_3+X_4, B_4+bX_3,\ b\neq 0$	$\tilde{P}_{10,6}$	
$\tilde{P}_{10,8}$		4	X_1, X_2	B_3+X_4, B_4	$P_{10,6}$	
$\tilde{P}_{10,9}$		4	X_1, X_2	B_3, B_4+X_3	$C_4 \square P_{10,2}$	
$\tilde{P}_{10,10}$		4	X_1, X_2	B_3, B_4-X_3	$C_4 \square P_{10,2}$	
$\tilde{P}_{10,11}$		3	X_1	B_3, B_4+X_2	$C_4 \square P_{10,2}$	$\simeq P_{10,4}$
$\tilde{P}_{10,12}$		3	X_1	$B_3+X_2, B_4+aX_2+X_3,\ a>0$	$C_4 \square P_{10,2}$	
$\tilde{P}_{10,13}$		3	X_1	$B_3-X_2, B_4+aX_2-X_3,\ a>0$	$C_4 \square P_{10,2}$	
$\tilde{P}_{10,14}$		3	X_1	B_3+X_2, B_4+X_3	$C_4 \square P_{6,2}$	
$\tilde{P}_{10,15}$		3	X_1	B_3-X_2, B_4-X_3	$C_4 \square \tilde{P}_{6,2}$	
$P_{10,16}$		2	0	B_3, B_4+X_2	$C_4 \square P_{10,11}$	$\simeq P_{10,5}$
$\tilde{P}_{12,11}$	F_{12}	4	X_1, X_2, X_3	B_1+X_4	$C_4 \square P_{12,1}$	$\simeq P_{12,2}$
$\tilde{P}_{12,12}$		4	X_1, X_2, X_3	B_1-X_4	$C_4 \sqcup P_{12,1}$	$\simeq P_{12,2}$
$\tilde{P}_{12,13}$		4	X_1-X_4, X_2, X_3	$B_1+a(X_1+X_4),\ a>0$	$C_4 \square P_{12,1}$	$\simeq P_{12,3}$
$\tilde{P}_{12,14}$		4	X_1+X_4, X_2, X_3	$B_1+b(X_1-X_4),\ b\neq 0$	$C_4 \sqcup (P_{12,1} \cup P_{12,1} \cdot Z_1)$	$\simeq P_{12,4}$
$\tilde{P}_{12,15}$		3	X_2, X_3	B_1+X_4	$C_4 \square P_{12,1}$	$\simeq P_{12,6}$
$\tilde{P}_{12,16}$		3	X_2, X_3	B_1-X_4	$C_4 \sqcup P_{12,1}$	$\simeq P_{12,6}$
$\tilde{P}_{12,17}$		3	X_2, X_3	$B_1+a(X_1+X_4),\ a>0$	$C_4 \square P_{12,1}$	$\simeq P_{12,6}$
$\tilde{P}_{12,18}$		3	X_2, X_3	$B_1+b(X_1-X_4),\ b\neq 0$	$C_4 \sqcup (P_{12,1} \cup P_{12,1} \cdot Z_1)$	$\simeq P_{12,6}$
$\tilde{P}_{12,19}$		2	X_1	B_1+X_4	$C_4 \square P_{12,5}$	$\simeq P_{12,7}$
$\tilde{P}_{12,20}$		2	X_1	B_1-X_4	$C_4 \sqcup P_{12,5}$	$\simeq P_{12,7}$
$\tilde{P}_{12,21}$		2	X_1-X_4	$B_1+a(X_1+X_4),\ a>0$	$C_4 \square P_{12,5}$	$\simeq P_{12,8}$
$\tilde{P}_{12,22}$		2	X_1+X_4	$B_1+b(X_1-X_4),\ b\neq 0$	$C_4 \sqcup (P_{12,5} \cup P_{12,5} \cdot Z_1)$	$\simeq P_{12,9}$
$\tilde{P}_{12,23}$		1	0	B_1+X_4	$C_4 \square P_{12,5}$	$\simeq P_{12,10}$
$\tilde{P}_{12,24}$		1	0	B_1-X_4	$C_4 \sqcup P_{12,5}$	$\simeq P_{12,10}$
$\tilde{P}_{12,25}$		1	0	$B_1+a(X_1+X_4),\ a>0$	$C_4 \square P_{12,5}$	$\simeq P_{12,10}$
$P_{12,26}$		1	0	$B_1+b(X_1-X_4),\ b\neq 0$	$C_4 \sqcup (P_{12,5} \cup P_{12,5} \cdot Z_1)$	$\simeq P_{12,10}$
$\tilde{P}_{13,10}$	F_{13}	4	X_1, X_3, X_4	$B_2+aX_2,\ a>0$	$P_{13,1}$	$\simeq P_{13,3}$
$\tilde{P}_{13,11}$		3	X_1, X_3	$B_2+aX_2,\ a>0$	$P_{13,2}$	$\simeq P_{13,5}$
$\tilde{P}_{13,12}$		3	X_1, X_4	$B_2+aX_2,\ a>0$	$P_{13,1}$	$\simeq P_{13,4}$
$\tilde{P}_{13,13}$		2	X_1	$B_2+aX_2,\ a>0$	$P_{13,2}$	$\simeq P_{13,7}$
$\tilde{P}_{13,14}$		2	X_3	$B_2+aX_2,\ a>0$	$P_{13,6}$	$\simeq P_{13,8}$
$\tilde{P}_{13,15}$		1	0	$B_2+aX_2,\ a>0$	$P_{13,6}$	$\simeq P_{13,9}$
$\tilde{P}_{14,10}$	F_{14}	4	X_1, X_2, X_3	B_3+X_4	$P_{10,1}$	$\simeq P_{14,2}$
$\tilde{P}_{14,11}$		4	X_1, X_3, X_4	B_3+X_2	$C_4 \sqcup P_{14,1}$	$\simeq P_{14,3}$
$\tilde{P}_{14,12}$		4	X_1, X_3, X_4	B_3-X_2	$C_4 \sqcup P_{14,1}$	$\simeq P_{14,3}$
$\tilde{P}_{14,13}$		3	X_1, X_2	B_3+X_4	$P_{10,6}$	$\simeq P_{14,4}$
$\tilde{P}_{14,14}$		3	X_1, X_3	B_3+X_4	$P_{14,1}$	$\simeq P_{14,5}$
$\tilde{P}_{14,15}$		3	X_1, X_3	B_3+X_2	$C_4 \sqcup P_{10,1}$	$\simeq P_{14,5}$
$\tilde{P}_{14,16}$		3	X_1, X_3	B_3-X_2	$C_4 \sqcup P_{10,1}$	$\simeq P_{14,5}$
$\tilde{P}_{14,17}$		3	$X_1, X_2+bX_3, b\neq 0$	B_3+X_4	$P_{14,10}$	$\simeq P_{14,6}$
$\tilde{P}_{14,18}$		3	$X_1, X_2+bX_3,\ b\neq 0$	B_3+X_2	$C_4 \sqcup P_{10,2}$	$\simeq P_{14,6}$
$\tilde{P}_{14,19}$		3	$X_1, X_2+bX_3,\ b\neq 0$	B_3-X_2	$C_4 \sqcup P_{10,2}$	$\simeq P_{14,6}$
$\tilde{P}_{14,20}$		2	X_1	B_3+X_4	$P_{14,10}$	$\simeq P_{14,7}$
$\tilde{P}_{14,21}$		2	X_1	B_3+X_2	$C_4 \sqcup P_{10,2}$	$\simeq P_{14,7}$
$\tilde{P}_{14,22}$		2	X_1	B_3-X_2	$C_4 \sqcup P_{10,2}$	$\simeq P_{14,7}$
$\tilde{P}_{14,23}$		2	X_2	B_3+X_4	$\tilde{P}_{14,13}$	$\simeq P_{14,8}$
$\tilde{P}_{14,24}$		1	0	B_3+X_4	$\tilde{P}_{14,13}$	$\simeq P_{14,9}$
$\tilde{P}_{14,25}$		1	0	B_3+X_2	$C_4 \sqcup P_{14,4}$	$\simeq P_{14,9}$
$P_{14,26}$		1	0	B_3-X_2	$C_4 \sqcup P_{14,4}$	$\simeq P_{14,9}$

The presence of Z_2 in the normalizer allows us to take $a_4 \geq 0$, and then set $|\alpha|^4 = a_4$ $(a_4 \neq 0)$ or $|\alpha|^2 = \pm b_3$ $(a_4 = 0,\ b_3 \gtrless 0)$. Taking $\phi = \pi/2$ in (91) we obtain the same result. Thus, we obtain the algebras

$$\begin{aligned}
&\tilde{P}_{10,7}\colon\ B_3 + X_4,\quad B_4 + bX_3,\quad X_1, X_2,\quad b \neq 0,\\
&\tilde{P}_{10,8}\colon\ B_3 + X_4,\quad B_4,\quad X_1, X_2,\\
&\tilde{P}_{10,9}\colon\ B_3,\quad B_4 + X_3,\quad X_1, X_2,\\
&\tilde{P}_{10,10}\colon\ B_3,\quad B_4 - X_3,\quad X_1, X_2.
\end{aligned} \tag{93}$$

Taking $N_{10,4} = \{X_1\}$ we find $a_4 = b_4 = 0$ from (88). In (90) we choose $\tan 4\phi = (a_2 - b_3)/b_2$ and obtain

$$B_3' = |\alpha|^2 B_3 + \frac{a_2 + b_3}{2} X_2,$$

$$B_4' = |\alpha|^2 B_4 + [(a_2 - b_3)^2 + b_2^2]^{1/2} X_2 + \frac{a_2 + b_3}{2} X_3.$$

If $b_3 = -a_2$ we put $|\alpha|^2 = (4a_2^2 + b_2^2)^{1/2}$ and obtain

$$\tilde{P}_{10,11}\colon\ B_3, B_4 + X_2, X_1. \tag{94}$$

If $b_3 \neq -a_2$ we obtain two different subalgebras for $[(a_2 - b_3)^2 + b_2^2]$ equal or not equal to zero. Thus,

$$\begin{aligned}
&\tilde{P}_{10,12}\colon\ B_3 + X_2,\quad B_4 + aX_2 + X_3,\quad X_1,\quad 0 < a < \infty,\\
&\tilde{P}_{10,13}\colon\ B_3 - X_2,\quad B_4 + aX_2 - X_3,\quad X_1,\quad 0 < a < \infty,\\
&\tilde{P}_{10,14}\colon\ B_3 + X_2,\quad B_4 + X_3,\quad X_1,\\
&\tilde{P}_{10,15}\colon\ B_3 - X_2,\quad B_4 - X_3,\quad X_1.
\end{aligned} \tag{95}$$

Finally, take $N_{10,5} = 0$. Then $b_3 = -a_2$, $a_4 = b_4 = 0$. We choose $\tan 4\phi = 2a_2/b_2$ and $|\alpha|^2 = (4a_2^2 + b_2^2)^{1/2}$ in (91) to obtain

$$\tilde{P}_{10,16}\colon\ B_3, B_4 + X_2. \tag{96}$$

F_{11}—The algebra F_{11} does not lead to any nonsplitting subalgebras, since all 1-cocycles for $B_c = \cos cB_1 + \sin cB_2$, $0 < c < \pi$, $c \neq \pi/2$ can be cancelled by the coboundaries.

F_{12}—Putting $x_3 = a_2/2$, $x_2 = -a_3/2$ and subtracting ∂B_1 of (66) from $B_1 + a_i X_i$, we obtain

$$\tilde{B}_1 = B_1 + a_1 X_1 + a_4 X_4. \tag{97}$$

To this generator we add the invariant subspaces $N_{12,k}$ of (59) and then simplify using the outer part of $\mathrm{Nor}_{LG} F_{12}$, i. e., $\exp(xB_2)$ and Z_1, if these also leave the considered $N_{12,k}$ invariant. The procedure is absolutely straightforward and we drop it here, listing the results in Table IV as $\tilde{P}_{12,k}$.

F_{13}—Making use of the coboundary ∂B_2 in (66), we write

$$\tilde{B}_2 = B_2 + b_2 X_2 + b_3 X_3. \tag{98}$$

The external part of $\mathrm{Nor}_{LG} F_{13}$ is $\exp xB_1$ and Z_1. Using these to simplify for each $N_{13,k}$ of (60), we obtain the subalgebras $\tilde{P}_{13,k}$ of Table IV.

F_{14}—Using ∂B_3 of (66), we obtain

$$\tilde{B}_3 = B_3 + c_2 X_2 + c_4 X_4. \tag{99}$$

The outer part of the normalizer of F_{14} is $\exp xB_2$, $\exp yB_4$, and Z_2. Making use of these to simplify for each $N_{14,k}$ of (61), we obtain the subalgebras $\tilde{P}_{14,k}$ listed in Table IV.

In Table IV we give a list of representatives of all Poincaré group conjugacy classes of nonsplitting subalgebras of P. In the first row we introduce a symbol $\tilde{P}_{j,k}$ for each subalgebra [the tilde indicates a nonsplitting algebra, k enumerates all algebras, splitting and nonsplitting, obtained from the same F_j (column 2)]. Column 3 gives the dimension of $\tilde{P}_{j,k}$ and columns 4 and 5 the generators of $\tilde{P}_{j,k}$. The normalizer of $\tilde{P}_{j,k}$ in the Poincaré group is given in column 6. In the last column we indicate whether the corresponding $\tilde{P}_{j,k}$ is isomorphic to one of the nonsplitting subalgebras. The normalizers of column 6 are easy to derive—we just present the results.

4. CONTINUOUS SUBGROUPS OF THE HOMOGENEOUS LORENTZ GROUP EXTENDED BY DILATATIONS

In this section we apply the algorithm of Sec. 2D, to classify all the subalgebras of $D \oplus LSL(2, C)$, i. e., the direct sum of the dilatation algebra and that of the homogeneous Lorentz group. We use the realization of this algebra discussed in Sec. 3A.

Step 1 has already been performed, namely all subalgebras F_j of $LSL(2, C)$ and their normalizers $\mathrm{Nor}_{LG} F_j$ are given in Table II. Each F_j will in itself be a representative of a class of subalgebras of $D \oplus LSL(2, C)$. To each F_j we may add the generator D. We thus obtain all splitting subalgebras of $D \oplus LSL(2, C)$.

Now let us find all nonsplitting subalgebras, i. e., those obtained by a nontrivial Goursat twist. We let F_j run through all subalgebras of $F = LSL(2, C)$ (see Table II) and perform all the steps of the algorithm. Note that the semisimple algebras F_1, F_3, and F_4 cannot provide nontrivial twists. Indeed, for $B_i \in F_j$ we can obtain a generator of the type $B_i + aD$ with $a \neq 0$ only if $B_i \in [F_j, F_j]$, i. e., B_i is not in the derived algebra of F_j.

F_2—The derived algebra is $\{B_3, B_4\}$ so we can write a nonsplit subalgebra as

$$B_1 + aD, B_2 + bD, B_3, B_4,\quad a^2 + b^2 \neq 0. \tag{100}$$

Since F_2 does not have any outer automorphisms we cannot simplify (100). Thus, each pair of real numbers $-\infty < a < \infty$, $-\infty < b < \infty$, $a^2 + b^2 \neq 0$ determines a different conjugacy class of nonsplit subalgebras.

F_5—The derived algebra is $\{B_3, B_4\}$ and we obtain

$$\cos cB_1 + \sin cB_2 + aD, B_3, B_4;\quad a \neq 0,\quad 0 < c < \pi,\quad c \neq \pi/2. \tag{101}$$

The outer part of the normalizer of F_5 leaves a invariant so (101) cannot be simplified.

F_6—Similarly, as in F_5 we obtain

$$B_1 + aD, B_3, B_4,\quad a \neq 0. \tag{102}$$

F_7—As in case F_5 and F_6 we obtain

$$B_2 + aD, B_3, B_4,\quad a \neq 0. \tag{103}$$

TABLE V. Continuous subgroups of the homogeneous similitude group $D \otimes SL(2, C)$.

Notation $D_{j,k}$	F_j	$\dim_R D_{j,k}$	Twisted generators	Nontwisted generators	Comment on subgroup
$D_{1,1}$	F_1	7		$D, B_1, \ldots, B_6$	$D \otimes SL(2,C)$
$D_{1,2}$		6		$B_1, \ldots, B_6$	$\exp F_1 \simeq SL(2,C)$
$D_{2,1}$		5		D, B_1, B_2, B_3, B_4	$D \otimes B$
$D_{2,2}$	F_2	4		B_1, B_2, B_3, B_4	$\exp F_2 = B$
$D_{2,3}$		4	$B_1 + aD, B_2 + bD,\ a^2 + b^2 \neq 0$	B_3, B_4	$\simeq B$
$D_{3,1}$	F_3	4		$D, B_1, B_3 - B_5, B_4 + B_6$	$D \otimes SU(2)$
$D_{3,2}$		3		$B_1, B_3 - B_5, B_4 + B_6$	$\exp F_3 \simeq SU(2)$
$D_{4,1}$	F_4	4		$D, B_1, B_3 + B_5, B_4 - B_6$	$D \otimes SU(1,1)$
$D_{4,2}$		3		$B_1, B_3 + B_5, B_4 - B_6$	$\exp F_4 \simeq SU(1,1)$
$D_{5,1}$		4		D, B_c, B_3, B_4	$D \otimes S(3)$
$D_{5,2}$	F_5	3		B_c, B_3, B_4	$\exp F_5 \simeq S(3)$
$D_{5,3}$		3	$B_c + aD,\ a \neq 0$	B_3, B_4	$S(3)$
$D_{6,1}$		4		D, B_1, B_3, B_4	$D \otimes E(2)$
$D_{6,2}$	F_6	3		B_1, B_3, B_4	$\exp F_6 \simeq E(2)$
$D_{6,3}$		3	$B_1 + aD,\ a \neq 0$	B_3, B_4	$E(2)$
$D_{7,1}$		4		D, B_2, B_3, B_4	$D \otimes (D' \square T_H)$
$D_{7,2}$	F_7	3		B_2, B_3, B_4	$\exp F_7 \simeq (D' \square T_H)$
$D_{7,3}$		3	$B_2 + aD,\ a \neq 0$	B_3, B_4	$(D' \square T_H)$
$D_{8,1}$		3		D, B_2, B_3	$D \otimes C(1)$
$D_{8,2}$	F_8	2		B_2, B_3	$\exp F_8 \simeq C(1)$
$D_{8,3}$		2	$B_2 + aD,\ a \neq 0$	B_3	$\simeq C(1)$
$D_{9,1}$		3		D, B_1, B_2	$D \otimes T_c$
$D_{9,2}$	F_9	2		B_1, B_2	$\exp F_9 \simeq T_c$
$D_{9,3}$		2	$B_1 + a\,\mathrm{cosc}D, B_2 + a\,\mathrm{sinc}D,$ $a > 0,\ 0 \leq c \leq \pi$	0	$\simeq T$
$D_{10,1}$		3		D, B_3, B_4	$D \otimes T_H$
$D_{10,2}$	F_{10}	2		B_3, B_4	$\exp F_{10} \simeq T_H$
$D_{10,3}$		2	$B_4 + D$	B_3	$\simeq T_H$
$D_{10,4}$		2	$B_3 + D, B_4 + bD,\ -\infty < b < \infty$	0	$\simeq T_H$
$D_{11,1}$		2		D, B_c	$D \otimes S(1)$
$D_{11,2}$	F_{11}	1		B_c	$\exp F_{11} \simeq S(1)$
$D_{11,3}$		1	$B_c + aD,\ a > 0$	0	$\simeq S(1)$
$D_{12,1}$		2		D, B_1	$D \otimes O(2)$
$D_{12,2}$	F_{12}	1		B_1	$\exp F_{12} \simeq O(2)$
$D_{12,3}$		1	$B_1 + aD,\ a > 0$	0	
$D_{13,1}$		2		D, B_2	$D \otimes O(1,1)$
$D_{13,2}$	F_{13}	1		B_2	$\exp F_{13} \simeq O(1,1)$
$D_{13,3}$		1	$B_2 + aD,\ a > 0$	0	$O(1,1)$
$D_{14,1}$		2		D, B_3	$D \otimes E(1)$
$D_{14,2}$	F_{14}	1		B_3	$\exp F_{14} \simeq E(1)$
$D_{14,3}$		1	$B_3 + D$	0	$E(1)$
$D_{15,1}$	F_{15}	1		D	D

F_8—The derived algebra is B_3, so we have

$$B_2 + aD, B_3, \quad a \neq 0,$$

and this cannot be further simplified.

F_9—This algebra is Abelian, so we can write

$$B_1 + aD, B_2 + bD, \quad a^2 + b^2 \neq 0.$$

The element Z_1 in the normalizer will change the sign of a and b, so one of them can be constrained to be nonnegative. Thus we can put

$$B_1 + a\,\mathrm{cosc}D, B_2 + a\,\mathrm{sinc}D, \quad a > 0, \quad 0 \leq c < \pi. \tag{104}$$

F_{10}—The algebra is Abelian, so we have

$$B_3 + aD, B_4 + bD, \quad a^2 + b^2 \neq 0.$$

This algebra can however be simplified, using the outer part of $\mathrm{Nor}_{LG} F_{10}$, i.e., $\exp(xB_1 + yB_2)$. Indeed, if $a \neq 0$ we can transform this algebra into

$$B_3 + D, \quad B_4 + bD, \quad -\infty < b < \infty. \tag{105}$$

If $a = 0$ we obtain

$$B_3, B_4 + D. \tag{106}$$

F_{11}—We obtain

$$\mathrm{cosc}B_1 + \mathrm{sinc}B_2 + aD, \quad a > 0, \quad 0 < c < \pi, \quad c \neq \pi/2. \tag{107}$$

The presence of Z_1 in the normalizer of F_{11} makes it possible to take $a > 0$.

F_{12}—As in F_{11} we have

$$B_1 + aD, \quad a > 0. \tag{108}$$

F_{13}—As in F_{11} and F_{12} we have

$$B_2 + aD, \quad a > 0. \tag{109}$$

F_{14}—Making use of the transformation $\exp xB_2$ in the normalizer of F_{14}, we obtain one nonsplitting subalgebra

$$B_3 + D. \tag{110}$$

All subalgebras of the "homogeneous similitude algebra" $D \oplus LSL(2, C)$ are summarized in Table V. A notation $D_{j,k}$ for them is introduced in the first column, the second column indicates the subalgebra F_j they were obtained from and the third column gives their dimension over the field of real numbers. The generators of $D_{j,k}$ are given in the fourth and fifth columns. In the last column we show which groups the corresponding Lie subgroups are isomorphic to. The notations are the same as in Table II. In particular, $B_c = \cos cB_1 + \sin cB_2$, $0 < c < \pi$, $c \neq \pi/2$.

5. CONCLUSIONS

The main results of this paper are given below.

1. The general method of subgroup classification presented in Sec. 2, in particular, the algorithms of Secs. 2B–D.

2. The complete classification of subalgebras of the Poincaré algebra, summarized in Tables II, III, and IV of Sec. 3. Some properties of the subalgebras are also listed in the tables.

3. The complete classification of subalgebras of the "homogeneous similitude algebra" $D \oplus LSL(2, C)$, summarized in Table V of Sec. 4.

While finishing this paper we became aware of two preprints on the subgroups of the Poincaré group.[14,15] The authors use different methods than we do, but the results should be equivalent. We have actually made a comparison of the results and found some differences. Since neither of these papers has been published (as far as we know), we do not find it appropriate to publish a comparison. Obviously, we assert that, in cases when a contradiction occurs, our results are correct.

Our future plans were discussed in the Introduction. They involve a similar classification of subgroups of other relevant groups, a study of the properties of the subgroups of the Poincaré and similitude groups and their physical applications.

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Note added in proof: To our knowledge Ref. 14 is still not published; however, Ref. 15 has made its appearance [Rep. Math. Phys. 5, 145, 361 (1974)]. We have made a detailed comparison between their tables of subalgebras of the Poincaré algebra and ours. The only differences that occur concern two- and three-dimensional nonsplitting subalgebras (nonsymmorphic algebras in their terminology), obtained from the subalgebra $F_{10} = \{B_3, B_4\} = \{L_2 + K_1, L_1 - K_2\}$ of the Lorentz group Lie algebra (generators A_x and A_y in their notation). We have only one such two-dimensional algebra $\tilde{P}_{10,16}$, they have four (one of which depends on a continuous parameter) in their Table VIII.1. We have five such classes of three-dimensional algebras $\tilde{P}_{10,11} - \tilde{P}_{10,15}$; they have many more in their Table IX.2. The arguments that we give in our article between formulas (87) and (96) inclusively, prove that we are right, i.e., that the additional subalgebras of Ref. 15 are conjugate to others in their (and our) tables. Let us also note that in our article, as in Ref. 15, conjugacy is considered with respect to the proper orthochronous Poincaré group (without parity and/or time reversal).

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Continuous subgroups of the fundamental groups of physics. II. The similitude group*

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All subalgebras of the similitude algebra (the algebra of the Poincaré group extended by dilatations) are classified into conjugacy classes under transformations of the similitude group. Use is made of the classification of all subalgebras of the Poincaré algebra, carried out in a previous article. The results are presented in tables listing representatives of each class and their basic properties.

1. INTRODUCTION

This article is the second in a series of papers devoted to a study of the subgroup structure of Lie groups of fundamental importance in physics. In the first article,[1] further to be referred to as I, we presented a general method for classifying Lie subalgebras of Lie algebras with nontrivial ideals. The method, making use of cohomology theory, was then applied to classify all continuous subgroups of the Poincaré group (inhomogeneous Lorentz group) and of the homogeneous similitude group, i. e., the Lorentz group extended by dilatations.

In this paper we make use of the previous results to provide a classification of all continuous subgroups of the similitude group, i. e., the Poincaré group extended by dilatations.

Let us mention in passing that related problems were treated in two other previous articles. In one of them[2] we found all maximal solvable subgroups of the pseudounitary groups $SU(p,q)$ and all continuous subgroups of $SU(2,1)$. In the other[3] we discussed all maximal solvable subgroups of the pseudoorthogonal groups $SO(p,q)$.

The similitude group SG, also called the Weyl group,[4] is of considerable interest in elementary particle physics, the general theory of relativity and other fields of physics. Its importance in high energy physics is largely related to the phenomenon of scaling in deep inelastic scattering and thus to short distance behavior in elementary particle theory. For information on various approaches to scale invariance we refer to recent reviews and some of the original articles (some of them also treat the more general conformal group of space–time[5–10]). The similitude group also underlies Weyl's unified field theory[4] and can figure as a gauge group for field theories involving gravitation.[11,12]

The similitude group is an 11-parameter Lie group containing the Poincaré group as an invariant subgroup. In itself it is the largest nontrivial continuous subgroup of the conformal group of space–time.

The motivation for our interest in subgroups of Lie groups was given, e. g., in our previous articles.[1–3] Let us just mention several points. In a situation where the similitude group is an invariance group of a physical system a classification of its subgroups provides a classification of possible symmetry breaking interactions (or boundary conditions). If we are interested in the representation theory of the group SG, then each chain of subgroups will provide us with a different basis for the representations (at least those subgroups the algebras of which have enveloping algebras with nontrivial centers). Thus, if we wish to use the representation theory of SG to provide expansions of physical quantities like scattering amplitudes, we will find that different chains of subgroups provide us with different expansions having different possible applications. (This problem for the Lorentz and Galilei groups is treated in detail in the review.[13]) Different subgroups of the similitude group may be of special relevance for the construction of elementary particle dynamics in certain frames of reference (see the discussion of the infinite momentum frame and its relation to an 8-parameter subgroup of the Poincaré group[14]).

In Sec. 2 of this article we review some known results on the similitude group in order to establish notation (which is consistent with that used in I) and then discuss the method used to obtain all classes of subalgebras of the similitude algebra S (up to conjugation under the similitude group itself). In Sec. 3 we obtain our main results, i. e., a list of representatives of each conjugacy class of subalgebras of S, summarized in Tables. Section 4 is devoted to the conclusions and future outlook.

2. METHOD FOR CLASSIFYING THE SUBALGEBRAS OF THE SIMILITUDE ALGEBRA

A. The similitude group and its algebra

The similitude group SG can be defined as the group of Lorentz transformations, translations and dilatations of Minkowski space, i. e., the transformations

$$x'_\mu = h\Lambda_{\mu\nu}x_\nu + a_\mu, \quad \mu,\nu = 0,1,2,3, \tag{1}$$

where h is a real positive number, $\Lambda_{\mu\nu}$ are matrix elements of an $O(3,1)$ matrix and a_μ are real numbers. The vectors $x \equiv \{x_0, x_1, x_2, x_3\}$ are real vectors in the four-dimensional Minkowski space with metric $ds^2 = dx_0^2 - dx_1^2 - dx_2^2 - dx_3^2$.

We shall, however, make use of a different representation of SG, remembering that SG is a subgroup of the conformal group of space–time, i. e., the group of all transformations of x_μ, leaving the element ds^2 form-invariant: $ds^2 \to h\,ds'^2$. This group is isomorphic to $SU(2,2)$ (for reviews see, e. g., Refs. 5–7 and 10). We shall use a somewhat nonstandard realization of $SU(2,2)$, already introduced earlier,[1–3] namely the group of transformations G of a four-dimensional complex vector space satisfying

$$GJG^+ = J, \tag{2}$$

where

$$J = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{3}$$

(the cross on G implies Hermitian conjugation). Elements X of the Lie algebra of $SU(2,2)$ in this realization satisfy

$$X^+J + JX = 0 \tag{4}$$

and the general element of the algebra can be written as

$$X = \begin{pmatrix} \alpha & \beta & \epsilon & ia \\ \gamma & \delta & ib & -\epsilon^* \\ \xi & ic & -\delta^* & -\beta^* \\ id & -\xi^* & -\gamma^* & -\alpha^* \end{pmatrix}, \quad \alpha - \alpha^* + \delta - \delta^* = 0, \tag{5}$$

where Greek letters denote complex numbers, italic letters real ones, and the stars indicate complex conjugation. If we now consider the subalgebra of (5) leaving a two-dimensional vector space

$$z = \begin{pmatrix} \mu \\ \nu \\ 0 \\ 0 \end{pmatrix}$$

invariant, we obtain an 11-parameter subalgebra

$$S = \begin{pmatrix} d+c+iq & \alpha & \gamma & ia \\ \beta & d-c-iq & ib & -\gamma^* \\ 0 & 0 & -d+c-iq & -\alpha^* \\ 0 & 0 & -\beta^* & -d-c+iq \end{pmatrix}. \tag{6}$$

It is easy to verify that this algebra is isomorphic to that of the similitude algebra, i. e., its structure is

$$S = D \square (LSL(2,C) \square LT_4), \tag{7}$$

where $\square$ indicates a semidirect sum, D generates dilatations, LT_4 four-dimensional translations, and $LSL(2,C)$ is the algebra of the special linear group $SL(2,C)$.

For our purposes a convenient basis for the similitude algebra S is provided by the following matrices.

Dilatations:

$$D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{8}$$

The homogeneous Lorentz transformations ($LSL(2,C)$):

$$B_1 = \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \end{pmatrix}, \quad B_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$B_3 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad B_4 = \begin{pmatrix} 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{9}$$

$$B_5 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad B_6 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \end{pmatrix}.$$

Translations:

$$X_1 = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$X_3 = \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad X_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{10}$$

The dilatations satisfy the commutation relations

$$[D, B_i] = 0, \quad i = 1, \ldots, 6; \quad [D, X_a] = 2X_a, \quad a = 1, \ldots, 4, \tag{11}$$

and the translations commute:

$$[X_a, X_b] = 0, \quad a, b = 1, \ldots, 4. \tag{12}$$

All other commutation relations are given in Table I.

The usual physical notation is different and less convenient for our purposes. Throughout the article we shall use the generators B_i and X_a. Their relation to the usual generators of rotations L_i, proper Lorentz transformations (boosts) K_i $(i = 1, 2, 3)$ and translations P_μ $(\mu = 0, 1, 2, 3)$ is

$$\begin{aligned} &B_1 = 2L_3, \quad B_2 = -2K_3, \quad B_3 = -L_2 - K_1, \\ &B_4 = L_1 - K_2, \quad B_5 = L_2 - K_1, \quad B_6 = L_1 + K_2, \end{aligned} \tag{13}$$

$$X_1 = \tfrac{1}{2}(P_0 - P_3), \quad X_2 = P_2, \quad X_3 = -P_1, \quad X_4 = \tfrac{1}{2}(P_0 + P_3). \tag{14}$$

The commutation relations for the usual physical generators are

$$\begin{aligned} &[L_i, L_k] = \epsilon_{ikl} L_l, \quad [K_i, K_k] = -\epsilon_{ikl} L_l, \quad [L_i, K_k] = \epsilon_{ikl} K_l, \\ &[L_i, P_0] = 0, \quad [L_i, P_k] = \epsilon_{ikl} P_l, \\ &[K_i, P_0] = P_i, \quad [K_i, P_k] = \delta_{ik} P_0, \\ &\quad (i, k, l) = (1, 2, 3). \end{aligned} \tag{15}$$

An element of the similitude group itself can in the considered realization be written as $G = \exp S$, where S is given by (6), i. e.,

$$G = \begin{pmatrix} G_{11} & G_{12} \\ 0 & G_{22} \end{pmatrix} \tag{16}$$

and condition (2) implies that the 2×2 matrices G_{ik}

TABLE I. Commutation relations for the Poincaré algebra.

	B_1	B_2	B_3	B_4	B_5	B_6	X_1	X_2	X_3	X_4
B_1	0	0	$2B_4$	$-2B_3$	$-2B_6$	$2B_4$	0	$2X_3$	$-2X_2$	0
B_2	0	0	$2B_3$	$2B_4$	$-2B_5$	$-2B_6$	$2X_1$	0	0	$-2X_4$
B_3	$-2B_4$	$-2B_3$	0	0	B_2	B_1	0	0	$2X_1$	X_3
B_4	$2B_3$	$-2B_4$	0	0	B_1	$-B_2$	0	$-2X_1$	0	$-X_2$
B_5	$2B_6$	$2B_5$	$-B_2$	$-B_1$	0	0	X_3	0	$2X_4$	0
B_6	$-2B_5$	$2B_6$	$-B_1$	B_2	0	0	X_2	$2X_4$	0	0

satisfy

$$G_{22}J_1G_{11}^{\dagger}=J_1, \quad G_{12}J_1G_{11}^{\dagger}+G_{11}J_1G_{12}^{\dagger}=0, \tag{17}$$

with

$$J_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}.$$

Thus an element of the similitude group can be written as

$$g=\begin{pmatrix}\alpha & \beta & \epsilon & \xi\\ \gamma & \delta & \mu & \nu\\ 0 & 0 & \alpha^*/\Delta & -\beta^*/\Delta\\ 0 & 0 & -\gamma^*/\Delta & \delta^*/\Delta\end{pmatrix}, \quad \Delta=\alpha\delta-\beta\gamma=\Delta^*, \tag{18}$$

with G_{12} satisfying

$$\begin{aligned}&\alpha^*\xi+\alpha\xi^*+\beta^*\epsilon+\beta\epsilon^*=0,\\ &\gamma^*\xi+\delta^*\epsilon+\beta\mu^*+\alpha\nu^*=0,\\ &\gamma^*\nu+\gamma\nu^*+\delta^*\mu+\delta\mu^*=0.\end{aligned} \tag{19}$$

B. Classification of subalgebras of the similitude algebra

In paper I we have provided a list of representatives of all conjugacy classes of subalgebras of the Poincaré group Lie algebra. The results were summarized in three tables. The first of these (Table II of I) presents all subalgebras of the algebra of $SL(2,C)$ and hence all continuous subgroups of the homogeneous Lorentz group (these were known previously[15,16]). Table III of I presents all subalgebras of the Poincaré algebra P that split over their intersection with the translations LT_4 (i. e., the bases for these algebras can be written in a form containing elements of the type B_i and X_a only). Table IV of I lists representatives of all subalgebras of P that do not split over their intersections with LT_4 (i. e., their bases will always contain elements of the type $B_i+c_{ia}X_a$ where c_{ia} are real constants that are not all equal to zero and cannot be transformed into zero by an inner automorphism of the Poincaré group).

In this paper we take the results of I and build them up into a list of all subalgebras of the similitude algebra (up to conjugation under the similitude group). We use a related notation for the subalgebras of S, namely, $S_{j,k}$ where j runs from 1 to 15 and indicates the subalgebra F_j of $LSL(2,C)$ that has been extended to $S_{j,k}$ by translations and dilatations. The label k simply distinguishes different subalgebras obtained from the same F_j.

The procedure consists of several steps:

1. Find representatives of all conjugacy classes of subalgebras of the Poincaré algebra, that are not equivalent under the similitude group. To do this we must merely remember that the dilatation generator D commutes with all generators B_i of $SL(2,C)$, but multiplies translations by a constant [see formula (11)]. The transformation $\exp tD$ in the group SG will thus multiply all generators X_a by a constant, leaving B_i invariant. The matrix D itself is not of form (18), but we shall include it in our group of automorphisms, to simplify subalgebras of S. It corresponds to total inversion (parity times time-reversal) and is contained in the similitude group, but not in the component connected to identity. It follows that the extension of the Poincaré group by dilatations leads to the coalescence of certain nonsplitting subalgebras of the Poincaré algebra. Indeed, we have, e. g.,

$$D(B_1-X_1)D^{-1}=B_1+X_1, \tag{20}$$

$$e^{xD}(B_2+x^2X_3)e^{-xD}=B_2+X_3. \tag{21}$$

Thus the algebras $B_1\pm X_1$, while inequivalent under the Poincaré group, are conjugated under the similitude group. Similarly, the continuous set of Poincaré subalgebras $B_2+x^2X_3$, coalesces into one subalgebra B_2+X_3.

In Table II of the following section we list conjugacy classes of subalgebras of P (and of S) that are inequivalent with respect to the similitude group.

2. Subalgebras of the similitude algebra containing D as a generator. Any subalgebra of this type has the form

$$D\dotplus P_{j,k}, \tag{22}$$

where $P_{j,k}$ is a subalgebra of the Poincaré algebra. It follows from the above discussion that we thus obtain subalgebras of S if and only if $P_{j,k}$ is a splitting subalgebra of P (Table III of I) and that each splitting subalgebra of P provides a different subalgebra (22) of S.

3. Subalgebras of S not contained in the Poincaré algebra and not containing any conjugate of D under SG, such that the intersection with the Poincaré algebra splits over the translations. Choosing one generator of such an algebra as

$$D+\Sigma a_\mu B_\mu+\Sigma x_a X_a, \quad (1\leq\mu\leq 6,\ 1\leq a\leq 4), \tag{23}$$

there has to be at least one a_μ or x_a nonzero even after SG-conjugation. The other generators $\{B_\mu, X_a\}$ form one of the splitting subalgebras $P_{j,k}$ of the Poincaré algebra listed in Table III of I. To find all these subalgebras of S we consider each splitting subalgebra $P_{j,k}$ of P, add to it a generator (23) with a_μ and x_a so chosen that we obtain an algebra. The element (23) is then simplified using the normalizer of $P_{j,k}$ in the Poincaré group and

possibly further transformations involving D and normalizing (leaving invariant) the subalgebra $P_{j,k}$.

4. Subalgebras of S not contained in the Poincaré algebra and not containing any conjugate of D under SG, such that the intersection with the Poincaré algebra does not split over the translations. We choose one generator of each of these subalgebras in the form (23), the others $\{B_a + \Sigma x_{ak} X_k, X_i\}$ form one of the nonsplitting subalgebras $\tilde{P}_{j,k}$ of P listed in Table IV of I. To find all such subalgebras of S we consider each nonsplitting subalgebra $\tilde{P}_{j,k}$ of P separately and choose a_μ and x_a in (23) in the most general manner that forms an algebra with $\tilde{P}_{j,k}$. The element (23) is then simplified, using the normalizer of $\tilde{P}_{j,k}$ in the Poincaré group, supplemented by elements involving D and also normalizing $\tilde{P}_{j,k}$ (i.e., we use the normalizer of $\tilde{P}_{j,k}$ in the similitude group). This method provides a list of all subalgebras $S_{j,k}$ of S.

Several comments are in order.

1. The subalgebras of S obtained by applying the above steps 3 and 4 correspond to a generalization of the "Goursat twist"[17-19] method for obtaining subgroups of a group that is in itself the direct product of two subgroups [e.g., $O(4)$ as $O(3)\times O(3)$].

2. We could have applied directly the general method developed in I for classifying subalgebras of a given algebra. The Poincaré algebra would then have served as a nonabelian invariant subalgebra whose subalgebras are known. In this particular case we found the method described above to be more convenient.

3. COMPLETE LIST OF CONJUGACY CLASSES OF SUBALGEBRAS OF THE SIMILITUDE ALGEBRA

A. Subalgebras of the Poincaré algebra P as subalgebras of the similitude algebra

All subalgebras $P_{j,k}$ listed in Table III of I split over their intersection with the translations. These subalgebras are not affected by dilations. Hence Table II of I also provides a list of representatives of conjugacy classes of subalgebras of the similitude algebra S and no two entries are conjugate to each other under the similitude group. We shall not reproduce the table here but only refer to I. For the purposes of this article all subalgebras $P_{j,k}$ of Table III of I will be denoted $S_{j,k}$ (same value of j and k).

Table IV of I, listing all nonsplitting subalgebras $\tilde{P}_{j,k}$ of P is modified when conjugacy is considered under the similitude group. In view of formulas of the type (20) and (21) many classes coalesce. Thus Table IV of part I is replaced by the following Table II.

The first column in Table II introduces a notation for the subalgebra, the second tells us from which subalgebra of $LSL(2,C)$ it was obtained, the third lists the subalgebras $P_{j,k}$ of P that coalesce to form the same subalgebra of S up to SG conjugacy. The fourth column gives the generators of $S_{j,k}$ and the last one its dimension (over the real numbers).

B. Subalgebras of the similitude algebra containing D as a generator

A complete list of such algebras is obtained by taking each splitting subalgebra of the Poincaré group and adding D to the basis. Thus, we take all algebras listed in Table III of I and add D to them. No other subalgebras of S, containing D as a basis element exist. Again, we shall not reproduce this table and refer the reader to I. We thus obtain subalgebras which we denote

$$S_{1,3}, S_{1,4};\ S_{2,5}, -, S_{2,8};\ S_{3,5}, -, S_{3,8};\ S_{4,5}, -, S_{4,8};$$
$$S_{5,5} - S_{5,8};\ S_{6,8} - S_{6,11};\ S_{7,8} - S_{7,12};\ S_{8,18} - S_{8,27};$$

TABLE II. List of subalgebras $S_{j,k}$ that are nonsplitting subalgebras of the Poincaré algebra and that are nonconjugate under the similitude group.

Notation	F_j	$\tilde{P}_{j,k}$	Generators of $S_{j,k}$	$\dim_R S_{j,k}$
$S_{6,5}$	F_6	$\tilde{P}_{6,5}, \tilde{P}_{6,6}$	$B_1+X_4, B_3, B_4, X_1, X_2, X_3$	6
$S_{6,6}$		$\tilde{P}_{6,7}, \tilde{P}_{6,8}$	$B_1, B_3+X_2, B_4+X_3, X_1$	4
$S_{6,7}$		$\tilde{P}_{6,9}, \tilde{P}_{6,10}$	B_1+X_1, B_3, B_4	3
$S_{7,6}$	F_7	$\tilde{P}_{7,6}$	$B_2+X_3, B_3, B_4, X_1, X_2$	5
$S_{7,7}$		$\tilde{P}_{7,7}$	B_2+X_3, B_3, B_4, X_1	4
$S_{8,10}$	F_8	$\tilde{P}_{8,10}$	$B_2+X_2, B_3, X_1, X_3, X_4$	5
$S_{8,11}$		$\tilde{P}_{8,11}$	B_2+X_3, B_3, X_1, X_2	4
$S_{8,12}$		$\tilde{P}_{8,12}$	B_2+X_2, B_3, X_1, X_3	4
$S_{8,13}$		$\tilde{P}_{8,13}$	$B_2+X_2, B_3, X_1, X_2+bX_3, b\neq 0$	4
$S_{8,14}$		$\tilde{P}_{8,14}$	B_2+X_3, B_3, X_1	3
$S_{8,15}$		$\tilde{P}_{8,15}$	B_2+X_2, B_3, X_1	3
$S_{8,16}$		$\tilde{P}_{8,16}$	$B_2+X_2+bX_3, B_3, X_1, b\neq 0$	3
$S_{8,17}$		$\tilde{P}_{8,17}$	B_2+X_2, B_3	2
$S_{10,6}$	F_{10}	$\tilde{P}_{10,6}$	$B_3+X_4, B_4, X_1, X_2, X_3$	5
$S_{10,7}$		$\tilde{P}_{10,7}$	$B_3+X_4, B_4+X_3, X_1, X_2$	4
$S_{10,8}$		$\tilde{P}_{10,8}$	B_3+X_4, B_4, X_1, X_2	4
$S_{10,9}$		$\tilde{P}_{10,9}, \tilde{P}_{10,10}$	B_3, B_4+X_3, X_1, X_2	4
$S_{10,10}$		$\tilde{P}_{10,11}$	B_3, B_4+X_2, X_1	3
$S_{10,11}$		$\tilde{P}_{10,12}, \tilde{P}_{10,13}$	$B_3+X_2, B_4+bX_2+X_3, X_1, b\neq 0$	3
$S_{10,12}$		$\tilde{P}_{10,14}, \tilde{P}_{10,15}$	B_3+X_2, B_4+X_3, X_1	3
$S_{10,13}$		$\tilde{P}_{10,16}$	B_3, B_4+X_2	2
$S_{12,11}$	F_{12}	$\tilde{P}_{12,11}, \tilde{P}_{12,12}$	B_1+X_4, X_1, X_2, X_3	4
$S_{12,12}$		$\tilde{P}_{12,13}$	$B_1+X_1+X_4, X_1-X_4, X_2, X_3$	4
$S_{12,13}$		$\tilde{P}_{12,14}$	$B_1+X_1-X_4, X_1+X_4, X_2, X_3$	4
$S_{12,14}$		$\tilde{P}_{12,15}, \tilde{P}_{12,16}$	B_1+X_4, X_2, X_3	3
$S_{12,15}$		$\tilde{P}_{12,17}$	$B_1+X_1+X_4, X_2, X_3$	3
$S_{12,16}$		$\tilde{P}_{12,18}$	$B_1+X_1-X_4, X_2, X_3$	3
$S_{12,17}$		$\tilde{P}_{12,19}, \tilde{P}_{12,20}$	B_1+X_4, X_1	2
$S_{12,18}$		$\tilde{P}_{12,21}$	$B_1+X_1+X_4, X_1-X_4$	2
$S_{12,19}$		$\tilde{P}_{12,22}$	$B_1+X_1-X_4, X_1+X_4$	2
$S_{12,20}$		$\tilde{P}_{12,23}, \tilde{P}_{12,24}$	B_1+X_4	1
$S_{12,21}$		$\tilde{P}_{12,25}$	$B_1+X_1+X_4$	1
$S_{12,22}$		$\tilde{P}_{12,26}$	$B_1+X_1-X_4$	1
$S_{13,10}$	F_{13}	$\tilde{P}_{13,10}$	B_2+X_2, X_1, X_3, X_4	4
$S_{13,11}$		$\tilde{P}_{13,11}$	B_2+X_2, X_1, X_3	3
$S_{13,12}$		$\tilde{P}_{13,12}$	B_2+X_2, X_1, X_4	3
$S_{13,13}$		$\tilde{P}_{13,13}$	B_2+X_2, X_1	2
$S_{13,14}$		$\tilde{P}_{13,14}$	B_2+X_2, X_3	2
$S_{13,15}$		$\tilde{P}_{13,15}$	B_2+X_2	1
$S_{14,10}$	F_{14}	$\tilde{P}_{14,10}$	B_3+X_4, X_1, X_2, X_3	4
$S_{14,11}$		$\tilde{P}_{14,11}, \tilde{P}_{14,12}$	B_3+X_2, X_1, X_3, X_4	4
$S_{14,12}$		$\tilde{P}_{14,13}$	B_3+X_4, X_1, X_2	3
$S_{14,13}$		$\tilde{P}_{14,14}$	B_3+X_4, X_1, X_3	3
$S_{14,14}$		$\tilde{P}_{14,15}, \tilde{P}_{14,16}$	B_3+X_2, X_1, X_3	3
$S_{14,15}$		$\tilde{P}_{14,17}$	$B_3+X_4, X_1, X_2+bX_3, b\neq 0$	3
$S_{14,16}$		$\tilde{P}_{14,18}, \tilde{P}_{14,19}$	$B_3+X_2, X_1, X_2+bX_3, b\neq 0$	3
$S_{14,17}$		$\tilde{P}_{14,20}$	B_3+X_4, X_1	2
$S_{14,18}$		$\tilde{P}_{14,21}, \tilde{P}_{14,22}$	B_3+X_2, X_1	2
$S_{14,19}$		$\tilde{P}_{14,23}$	B_3+X_4, X_2	2
$S_{14,20}$		$\tilde{P}_{14,24}$	B_3+X_4	1
$S_{14,21}$		$\tilde{P}_{14,25}, \tilde{P}_{14,26}$	B_3+X_2	1

$$S_{9,7}-S_{9,12};\quad S_{10,14}-S_{10,18};\quad S_{11,7}-S_{11,12};$$
$$S_{12,23}-S_{12,32};\quad S_{13,16}-S_{13,24};\quad S_{14,22}-S_{14,30};\quad S_{15,12}-S_{15,22}. \tag{24}$$

Note that algebra $S_{15,22}$ is generated by D alone.

C. Subalgebras of S that are not contained in the Poincaré algebra do not contain any SG-conjugate of D and are such that the intersection with the Poincaré algebra splits over the translations

We consider each subalgebra $P_{j,k}$ of Table III of I, add the generator $\tilde{D}=D+a_\mu B_\mu+x_a X_a$ to it and find a_μ and x_a in such a manner as to obtain an algebra. We put $a_\mu=x_a=0$ for those generators B_μ and X_a, that are contained in $P_{j,k}$. This algebra must then be simplified using transformations contained in $\mathrm{Nor}_{SG}P_{j,k}$ (normalizer of $P_{j,k}$ in the similitude group).

In view of the fact that transformations of D by translations produce all expressions

$$\tilde{D}=D+\Sigma_a x_a X_a \tag{25}$$

it follows that for no SG-conjugate of $\tilde{D}\neq D$ can we have $a_\mu=0$, $\mu=1,\ldots,6$.

We consider several examples to illustrate our method and then list all subalgebras of this type in Table III.

The algebras $P_{1,k}$ and $P_{2,k}$ (derived from F_1 and F_2) of Table III in I cannot be extended in this way (i. e., $a_\mu=x_a=0$). Consider those derived from F_3. The generators of the homogeneous part of $P_{3,j}$ are B_1, B_3-B_5, B_4+B_6. Hence we could have

$$\tilde{D}=D+aB_2+b(B_3+B_5)+c(B_4-B_6)+x_a X_a.$$

Commuting $\tilde{D}$ with B_1, we obtain $b=c=0$, commuting with B_3-B_5, we find $a=0$. Now consider, e.g., $P_{3,4}$, not containing any translations. Commuting $\tilde{D}$ with B_1, B_3-B_5 and B_4+B_6, we find $x_2=x_3=0$, $x_1=x_4$, i. e.,

$$D+x(X_1+X_4),\quad B_1,\quad B_3-B_5,\quad B_4+B_6 \tag{26}$$

form an algebra. However, the transformation $\exp[-\frac{1}{2}x(X_1+X_4)]$ is in the normalizer of $P_{3,4}$ and we have

$$\exp[-\tfrac{1}{2}x(X_1+X_4)][D+x(X_1+X_4)]\exp[\tfrac{1}{2}x(X_1+X_4)]=D,$$

so that the algebra (26) is conjugate to one of the splitting subalgebras of (24) (and will hence not figure in Table III).

As a further example, consider the algebras $P_{10,k}$ of Table III of paper I, derived from F_{10}. The generators of the homogeneous part of $P_{10,k}$ (i. e., of F_{10}) are B_3 and B_4. Putting $\tilde{D}=D+a_1B_1+a_2B_2+a_5B_5+a_6B_6+x_aX_a$ and commuting with B_3 and B_4, we find $a_5=a_6=0$. Algebra $P_{10,1}$ is thus extended to

$$\tilde{D}=D+aB_1+bB_2, B_3, B_4, X_1, X_2, X_3, X_4,$$
$$-\infty<a<\infty,\quad -\infty<b<\infty,\quad a^2+b^2\neq 0.$$

The algebra $P_{10,2}$, on the other hand, leads to

$$\tilde{D}=D+aB_1+bB_2+xX_4, B_3, B_4, X_1, X_2, X_3.$$

The transformation $\exp yX_4$ leaves $P_{10,2}$ invariant but takes x into zero in $\tilde{D}$, if we put $y=x/2(1-b)$ for $b\neq 1$. For $b=1$, on the other hand, the transformation $\exp yD$ with $e^y=x^{-1/2}$ for $x>0$ or $D\exp yD$ with $e^y=(-x)^{-1/2}$ for $x<0$ will take x into 1. We thus obtain from $P_{10,2}$ two types of subalgebras of S:

$$D+aB_1+bB_2, B_3, B_4, X_1, X_2, X_3, \tag{27}$$
$$-\infty<a<\infty,\quad -\infty<b<\infty,\quad a^2+b^2\neq 0,$$

and

$$D+aB_1+B_2+X_4, B_3, B_4, X_1, X_2, X_3,\quad -\infty<a<\infty. \tag{28}$$

We proceed quite analogously with all subalgebras of Table III of I. The results are summarized in Table III.

TABLE III. Subalgebras of S that are not contained in P, do not contain any SG-conjugate of D and are such that their intersection with P splits over the translations.

Notations	F_j	$P_{j,k}$	$\tilde{D}$	Generators of $P_{j,k}$	$\dim_R S_{j,k}$
$S_{5,9}$	F_5	$P_{5,1}$	$D+aB_2,\ a\neq 0$	$\cos cB_1+\sin cB_2, B_3, B_4, X_1, X_2, X_3, X_4,\ 0<c<\pi,\ c\neq\pi/2$	8
$S_{5,10}$		$P_{5,2}$	$D+aB_2,\ a\neq 0$	$\cos cB_1+\sin cB_2, B_3, B_4, X_1, X_2, X_3,\ 0<c<\pi,\ c\neq\pi/2$	7
$S_{5,11}$		$P_{5,3}$	$D+aB_2,\ a\neq 0$	$\cos cB_1+\sin cB_2, B_3, B_4, X_1,\ 0<c<\pi,\ c\neq\pi/2$	5
$S_{5,12}$		$P_{5,4}$	$D+aB_2,\ a\neq 0$	$\cos cB_1+\sin cB_2, B_3, B_4,\ 0<c<\pi,\ c\neq\pi/2$	4
$S_{6,12}$	F_6	$P_{6,1}$	$D+aB_2,\ a\neq 0$	$B_1, B_3, B_4, X_1, X_2, X_3,$	8
$S_{6,13}$		$P_{6,2}$	$D+aB_2,\ a\neq 0$	$B_1, B_3, B_4, X_1, X_2, X_3,$	7
$S_{6,14}$		$P_{6,2}$	$D+B_2+X_4$	$B_1, B_3, B_4, X_1, X_2, X_3$	7
$S_{6,15}$		$P_{6,3}$	$D+aB_2,\ a\neq 0$	B_1, B_3, B_4, X_4	5
$S_{6,16}$		$P_{6,4}$	$D+aB_2,\ a\neq 0$	B_1, B_3, B_4	4
$S_{6,17}$		$P_{6,4}$	$D-B_2+X_1$	B_1, B_3, B_4	4
$S_{7,13}$	F_7	$P_{7,1}$	$D+aB_1,\ a\neq 0$	$B_2, B_3, B_4, X_1, X_2, X_3, X_4$	8
$S_{7,14}$		$P_{7,2}$	$D+aB_1,\ a\neq 0$	$B_2, B_3, B_4, X_1, X_2, X_3$	7
$S_{7,15}$		$P_{7,4}$	$D+aB_1,\ a\neq 0$	B_2, B_3, B_4, X_1	5
$S_{7,16}$		$P_{7,5}$	$D+aB_1,\ a\neq 0$	B_2, B_3, B_4	4
$S_{10,19}$	F_{10}	$P_{10,1}$	$D+aB_1+bB_2,\ a^2+b^2\neq 0$	$B_3, B_4, X_1, X_2, X_3, X_4$	7
$S_{10,20}$		$P_{10,2}$	$D+aB_1+bB_2,\ a^2+b^2\neq 0$	$B_3, B_4, X_1, X_2, X_3,$	6
$S_{10,21}$		$P_{10,2}$	$D+aB_1+B_2+X_4, -\infty<a<\infty$	B_3, B_4, X_1, X_2, X_3	6
$S_{10,22}$		$P_{10,3}$	$D+aB_2,\ a\neq 0$	B_3, B_4, X_1, X_2	5
$S_{10,23}$		$P_{10,4}$	$D+aB_1+bB_2,\ a^2+b^2\neq 0$	B_3, B_4, X_1	4
$S_{10,24}$		$P_{10,5}$	$D+aB_1+bB_2,\ a^2+b^2\neq 0$	B_3, B_4	3
$S_{10,25}$		$P_{10,5}$	$D+aB_1-B_2+X_1, -\infty<a<\infty$	B_3, B_4	3

TABLE III. (*Continued*)

$S_{11,13}$	F_{11}	$P_{11,1}$	$D+aB_1,\ a>0$	$\operatorname{cosc}B_1+\operatorname{sinc}B_2, X_1, X_2, X_3, X_4,$	$0<c<\pi,\ c\neq\pi/2$	6
$S_{11,14}$		$P_{11,2}$	$D+aB_1,\ a\neq 0$	$\operatorname{cosc}B_1+\operatorname{sinc}B_2, X_1, X_2, X_3,$	$0<c<\pi,\ c\neq\pi/2$	5
$S_{11,15}$		$P_{11,3}$	$D+aB_1,\ a>0$	$\operatorname{cosc}B_1+\operatorname{sinc}B_2, X_2, X_3,$	$0<c<\pi,\ c\neq\pi/2$	4
$S_{11,16}$		$P_{11,4}$	$D+aB_1,\ a>0$	$\operatorname{cosc}B_1+\operatorname{sinc}B_2, X_1, X_4,$	$0<c<\pi,\ c\neq\pi/2$	4
$S_{11,17}$		$P_{11,5}$	$D+aB_1,\ a\neq 0$	$\operatorname{cosc}B_1+\operatorname{sinc}B_2, X_1,$	$0<c<\pi,\ c\neq\pi/2$	3
$S_{11,18}$		$P_{11,6}$	$D+aB_1,\ a>0$	$\operatorname{cosc}B_1+\operatorname{sinc}B_2,$	$0<c<\pi,\ c\neq\pi/2$	2
$S_{12,33}$	F_{12}	$P_{12,1}$	$D+aB_2,\ a>0$	B_1, X_1, X_2, X_3, X_4		6
$S_{12,34}$		$P_{12,2}$	$D+aB_2,\ a\neq 0$	B_1, X_1, X_2, X_3		5
$S_{12,35}$		$P_{12,2}$	$D+B_2+X_4$	B_1, X_1, X_2, X_3		5
$S_{12,36}$		$P_{12,5}$	$D+aB_2, a>0$	B_1, X_1, X_4		4
$S_{12,37}$		$P_{12,6}$	$D+aB_2,\ a>0$	B_1, X_2, X_3		4
$S_{12,38}$		$P_{12,6}$	$D+B_2+X_4$	B_1, X_2, X_3		4
$S_{12,39}$		$P_{12,7}$	$D+aB_2,\ a\neq 0$	B_1, X_1		3
$S_{12,40}$		$P_{12,7}$	$D+B_2+X_4$	B_1, X_1		3
$S_{12,41}$		$P_{12,10}$	$D+aB_2,\ a>0$	B_1		2
$S_{12,42}$		$P_{12,10}$	$D+B_2+X_4$	B_1		2
$S_{13,25}$	F_{13}	$P_{13,1}$	$D+aB_1,\ a>0$	B_2, X_1, X_2, X_3, X_4		6
$S_{13,26}$		$P_{13,2}$	$D+aB_1,\ a\neq 0$	B_2, X_1, X_2, X_3		5
$S_{13,27}$		$P_{13,4}$	$D+aB_1,\ a>0$	B_2, X_1, X_4		4
$S_{13,28}$		$P_{13,6}$	$D+aB_1,\ a>0$	B_2, X_2, X_3		4
$S_{13,29}$		$P_{13,7}$	$D+aB_1,\ a\neq 0$	B_2, X_1		3
$S_{13,30}$		$P_{13,9}$	$D+aB_1,\ a>0$	B_2		2
$S_{14,31}$	F_{14}	$P_{14,1}$	$D+aB_2,\ a\neq 0$	B_3, X_1, X_2, X_3, X_4		6
$S_{14,32}$		$P_{14,1}$	$D+B_4$	B_3, X_1, X_2, X_3, X_4		6
$S_{14,33}$		$P_{14,2}$	$D+aB_2,\ a\neq 0$	B_3, X_1, X_2, X_3		5
$S_{14,34}$		$P_{14,2}$	$D+B_2+X_4$	B_3, X_1, X_2, X_3		5
$S_{14,35}$		$P_{14,2}$	$D+B_4$	B_3, X_1, X_2, X_3		5
$S_{14,36}$		$P_{14,3}$	$D+aB_2, a\neq 0$	B_3, X_1, X_3, X_4		5
$S_{14,37}$		$P_{14,4}$	$D+aB_2,\ a\neq 0$	B_3, X_1, X_2		4
$S_{14,38}$		$P_{14,4}$	$D+B_4$	B_3, X_1, X_2		4
$S_{14,39}$		$P_{14,5}$	$D+aB_2, a\neq 0$	B_3, X_1, X_3		4
$S_{14,40}$		$P_{14,5}$	$D+B_2+X_4$	B_3, X_1, X_3		4
$S_{14,41}$		$P_{14,5}$	$D+B_4$	B_3, X_1, X_3		4
$S_{14,42}$		$P_{14,6}$	$D+aB_2,\ a\neq 0$	$B_3, X_1, X_2+cX_3,\ c\neq 0$		4
$S_{14,43}$		$P_{14,6}$	$D+B_4$	$B_3, X_1, X_2+cX_3,\ c\neq 0$		4
$S_{14,44}$		$P_{14,7}$	$D+aB_2,\ a\neq 0$	B_3, X_1		3
$S_{14,45}$		$P_{14,7}$	$D+B_4$	B_3, X_1		3
$S_{14,46}$		$P_{14,8}$	$D+aB_2,\ a\neq 0$	B_3, X_2		3
$S_{14,47}$		$P_{14,8}$	$D-B_2+X_1$	B_3, X_2		3
$S_{14,48}$		$P_{14,9}$	$D+aB_2,\ a\neq 0$	B_3		2
$S_{14,49}$		$P_{14,9}$	$D-B_2+X_1$	B_3		2
$S_{14,50}$		$P_{14,9}$	$D+B_4$	B_3		2
$S_{15,23}$	F_{15}	$P_{15,1}$	$D+a(\operatorname{cosc}B_1+\operatorname{sinc}B_2),\ a>0,\ 0\leq c<\pi$	X_1, X_2, X_3, X_4		5
$S_{15,24}$		$P_{15,1}$	$D+B_3$	X_1, X_2, X_3, X_4		5
$S_{15,25}$		$P_{15,2}$	$D+a(\operatorname{cosc}B_1+\operatorname{sinc}B_2),\ a>0,\ 0\leq c<2\pi$	X_1, X_2, X_3		4
$S_{15,26}$		$P_{15,2}$	$D+B_3$	X_1, X_2, X_3		4
$S_{15,27}$		$P_{15,3}$	$D+aB_1,\ a>0$	X_1-X_4, X_2, X_3		4
$S_{15,28}$		$P_{15,4}$	$D+aB_1,\ a>0$	X_1+X_4, X_2, X_3		4
$S_{15,29}$		$P_{15,4}$	$D+a(B_4-B_6),\ a>0$	X_1+X_4, X_2, X_3		4
$S_{15,30}$		$P_{15,4}$	$D+B_1+B_3+B_5$	X_1+X_4, X_2, X_3		4
$S_{15,31}$		$P_{15,5}$	$D+aB_2,\ a\neq 0$	X_1, X_2		3
$S_{15,32}$		$P_{15,5}$	$D+(\operatorname{cosc}B_3+\operatorname{sinc}B_4),\quad 0\leq c<\pi$	X_1, X_2		3
$S_{15,33}$		$P_{15,6}$	$D+a(\operatorname{cosc}B_1+\operatorname{sinc}B_2),\quad 0\leq c<\pi$	X_1, X_4		3
$S_{15,34}$		$P_{15,7}$	$D+a(\operatorname{cosc}B_1+\operatorname{sinc}B_2),\quad 0\leq c<\pi$	X_2, X_3		3
$S_{15,35}$		$P_{15,8}$	$D+a(\operatorname{cosc}B_1+\operatorname{sinc}B_2)\quad 0\leq c<2\pi$	X_1		2
$S_{15,36}$		$P_{15,8}$	$D+B_3$	X_1		2
$S_{15,37}$		$P_{15,9}$	$D+aB_1,\ a>0$	X_1+X_4		2
$S_{15,38}$		$P_{15,10}$	$D+aB_1,\ a>0$	X_1-X_4		2
$S_{15,39}$		$P_{15,10}$	$D+a(B_3+B_5),\ a>0$	X_1-X_4		2
$S_{15,40}$		$P_{15,10}$	$D+B_1-B_3-B_5$	X_1-X_4		2
$S_{15,41}$		$P_{15,11}$	$D+a(\operatorname{cosc}B_1+\operatorname{sinc}B_2), a>0,\ 0\leq c<\pi$	0		1
$S_{15,42}$		$P_{15,11}$	$D+B_3$	0		1

In the first column the symbol $S_{j,k}$ indicates that this is the kth algebra obtained as an extension of F_j by dilations and translations. The second column lists the subalgebras F_j and the third column gives $P_{j,k'}$, i. e., the subalgebra of the Poincaré algebra that we are adding the generator $\tilde{D}$ to. All generators of $S_{j,k}$ are in columns 4 and 5. The dimension $\dim_R S_{j,k}$ of $S_{j,k}$ over the field of real numbers is given in column 6.

TABLE IV. Subalgebras of S that are not contained in P, do not contain an SG-Conjugate of D and are such that their intersection with P does not split over the translations.

Notation	F_j	$\tilde{P}_{j,k}$	$\tilde{D}$	Generators of $\tilde{P}_{j,k}$	$\dim_R S_{j,k}$
$S_{6,18}$	F_6	$S_{6,5}$	$D+B_2+xX_4, -\infty<x<\infty$	$B_1+X_4, B_3, B_4, X_1, X_2, X_3$	7
$S_{6,19}$		$S_{6,6}$	$D+B_2$	$B_1, B_3+X_2, B_4+X_3, X_1$	5
$S_{6,20}$		$S_{6,7}$	$D-B_2+xX_1, -\infty<x<\infty$	B_1+X_1, B_3, B_4	4
$S_{10,26}$	F_{10}	$S_{10,6}$	$D+\frac{1}{2}B_2$	$B_3+X_4, B_4, X_1, X_2, X_3$	6
$S_{10,27}$		$S_{10,8}$	$D+\frac{1}{2}B_2$	B_3+X_4, B_4, X_1, X_2	5
$S_{10,28}$		$S_{10,9}$	$D+B_2$	B_3, B_4+X_3, X_1, X_2	5
$S_{10,29}$		$S_{10,10}$	$D+B_2$	B_3, B_4+X_2, X_1	4
$S_{10,30}$		$S_{10,11}$	$D+B_2$	$B_3+X_2, B_4+bX_2+X_3, X_1,\ b\neq 0$	4
$S_{10,31}$		$S_{10,12}$	$D+aB_1+B_2, -\infty<a<\infty$	B_3+X_2, B_4+X_3, X_1	4
$S_{10,32}$		$S_{10,13}$	$D+B_2$	$B_3, B_4+X_2,$	3
$S_{12,43}$	F_{12}	$S_{12,11}$	$D+B_2+xX_4, -\infty<x<\infty$	B_1+X_4, X_1, X_2, X_3	5
$S_{12,44}$		$S_{12,14}$	$D+B_2+xX_4, -\infty<x<\infty$	B_1+X_4, X_2, X_3	4
$S_{12,45}$		$S_{12,17}$	$D+B_2+xX_4, -\infty<x<\infty$	B_1+X_4, X_1	3
$S_{12,46}$		$S_{12,20}$	$D+B_2+xX_4, -\infty<x<\infty$	B_1+X_4	2
$S_{14,51}$	F_{14}	$S_{14,10}$	$D+\frac{1}{2}B_2$	B_3+X_4, X_1, X_2, X_3	5
$S_{14,52}$		$S_{14,11}$	$D+B_2$	B_3+X_2, X_1, X_3, X_4	5
$S_{14,53}$		$S_{14,12}$	$D+\frac{1}{2}B_2$	B_3+X_4, X_1, X_2	4
$S_{14,54}$		$S_{14,13}$	$D+\frac{1}{2}B_2$	B_3+X_4, X_1, X_3	4
$S_{14,55}$		$S_{14,14}$	$D+B_2+xX_4, -\infty<x<\infty$	B_3+X_2, X_1, X_3	4
$S_{14,56}$		$S_{14,15}$	$D+\frac{1}{2}B_2+b(B_4+aX_4), -\infty<b<\infty$	$B_3+X_4, X_1, X_2+aX_3, a\neq 0$	4
$S_{14,57}$		$S_{14,16}$	$D+bB_2+2a(b-1)X_4, -\infty<b<\infty$	$B_3+X_2, X_1, X_2+aX_3, a\neq 0$	4
$S_{14,58}$		$S_{14,17}$	$D+\frac{1}{2}B_2$	B_3+X_4, X_1	3
$S_{14,59}$		$S_{14,18}$	$D+B_2$	B_3+X_2, X_1	3
$S_{14,60}$		$S_{14,19}$	$D+\frac{1}{2}B_2$	B_3+X_4, X_2	3
$S_{14,61}$		$S_{14,20}$	$D+\frac{1}{2}B_2$	B_3+X_4	2
$S_{14,62}$		$S_{14,21}$	$D+B_2+b(B_4-X_3),\ b\geq 0$	B_3+X_2	2

D. Subalgebras of S that are not contained in the Poincaré algebra, do not contain any SG-conjugate of D and are such that the intersection with the Poincaré algebra does not split over the translations

We consider individually each subalgebra $S_{j,k}\equiv\tilde{P}_{j,k}$ of Table II of the present article, i. e., the algebras obtained from Table IV of I by using dilatations to make certain classes of subalgebras of P coalesce. To the generators of $S_{j,k}$ we again add a further operator $\tilde{D}=D+a_\mu B_\mu+x_a X_a$, putting the coefficient a_μ and x_a equal to zero if the corresponding B_μ or X_a figures in $\tilde{P}_{j,k}$ (we can set $a_\mu=0$ if $B_\mu\in\tilde{P}_{j,k}$ or $B_\mu+y_{\mu k}X_k\in\tilde{P}_{j,k}$ where $y_{\mu k}$ are real constants). Restrictions on the possible values of a_μ and x_a are obtained by requiring that $\tilde{D}\dotplus\tilde{P}_{j,k}$ forms a Lie algebra. The element $\tilde{D}$ of the algebra is then simplified using transformations belonging to the normalizer of $\tilde{P}_{j,k}$ in the similitude group, i. e., the normalizer of $\tilde{P}_{j,k}$ in the Poincaré group, listed in Table IV of I, supplemented by the discrete element D in the similitude group and transformations of the type $\exp\{D+b_\mu B_\mu+y_a X_a\}$ with b_μ and y_a so chosen as to leave $\tilde{P}_{j,k}$ invariant.

We shall consider some examples and then list all subalgebras of S obtained in this manner in Table IV above.

Consider the algebras $S_{6,k}$ of Table II. The element $\tilde{D}$ can be of the form $D+aB_2+bB_5+cB_6+x_\mu X_\mu$. Commuting with B_1+X_4, B_1 or B_1+X_1, as the case may be, we find $b=c=0$. Consider first case $S_{6,5}$, i. e.,

$$\tilde{D}=D+aB_2+xX_4,\ B_1+X_4, B_3, B_4, X_1, X_2, X_3. \tag{29}$$

We have

$$[\tilde{D}, B_1+X_4]=2(1-a)X_4$$

and hence $a=1$. Algebra (29) with $a=1$, x arbitrary real should be further simplified, i. e., we must attempt to restrict further possible values of x. The normalizer of $S_{6,5}$ contains transformations generated by $D+B_2$, B_1 and X_4 (in addition to the inner automorphisms $\exp S_{6,5}$). Using the commutation relations of Table I, it is easy to see that none of these change the value of x and hence (29) cannot be further simplified. Similar results are obtained for $S_{6,6}$ and $S_{6,7}$ (see Table IV).

It can be verified directly that none of the algebras $S_{7,k}$ or $S_{8,k}$ of Table II can be extended by dilatations. Now consider algebras $S_{10,6}$ and $S_{10,8}$ involving B_3+X_4, B_4, X_1, X_2 and in the case of $S_{10,6}$, also X_3. In the case $S_{10,6}$ we find that the most general operator $\tilde{D}$ forming a Lie algebra with $S_{10,6}$ is

$$\tilde{D}=D+\tfrac{1}{2}B_2+xX_4.$$

The normalizer of $S_{10,6}$ is generated by B_3, B_4, X_1, X_2, X_3, X_4 and $D+\frac{1}{2}B_2$. We have

$$\exp(yX_4)\tilde{D}\exp(-yX_4)=D+\tfrac{1}{2}B_2$$

if we put $y=x$. We thus obtain a single algebra generated by

$$D+\tfrac{1}{2}B_2, B_3+X_4, B_4, X_1, X_2, X_3.$$

Similarly, for $S_{10,8}$ we find that

$$\tilde{D}=D+\tfrac{1}{2}B_2+xX_3$$

provides an extension for all x. However, $\exp yX_3$ belongs to the normalizer of $S_{10,8}$ and

$$\exp(yX_3)\tilde{D}\exp(-yX_3)=D+\tfrac{1}{2}B_2$$

if we put $y=x/2$. We again obtain a single algebra

$$D+\tfrac{1}{2}B_2, B_3+X_4, B_4, X_1, X_2.$$

Continuing along the same lines we obtain the results presented in Table IV. The first column simply

enumerates the subalgebras of this type, the second tells us which subalgebra of $LSL(2, C)$ they were derived from, the third lists their intersections with the Poincaré algebra using the notations of Table II, the fourth and fifth column give all the generators and the last column gives the dimensions of the subalgebras.

This completes the list of all conjugacy classes of subalgebras of the similitude algebra.

Since the subalgebras of the homogeneous similitude algebra (the algebra of the homogeneous Lorentz group extended by dilatations) represent separate interest we provide a separate table of these (Table V). We suggest the name "scaling group" for this group. In Table V we use somewhat different conventions than in the rest of this article, in order to be able to show the mutual inclusions of the subalgebras. In this table $B_x = \cos x B_1 + \sin x B_2$ with $0 \leq x < \pi$, i. e., we *include* the points $x = 0$ and $x = \pi/2$. Subgroups of $D \otimes SL(2, C)$ that are contained in $SL(2, C)$ are separated out graphically. The lines connect each subalgebra (or continuous subgroup) with its maximal subalgebras. A full line indicates that the inclusion holds always, a dotted line indicates inclusion for specified values of the parameters only. Note that the way of writing the subalgebras in Table V corresponds more directly to Sec. 4 of article I than to the conventions of the rest of the present article.

4. CONCLUSIONS

The result of this paper is the complete classification of all subalgebras of the Lie algebra S of the similitude group SG. These subalgebras are of several types.

1. Subalgebras of S that are also subalgebras of the Poincaré algebra P and are splitting extensions of subalgebras of $LSL(2, C)$ by translations. Conjugacy classes of such algebras under the similitude group coincide with conjugacy classes under the Poincaré group. Representatives of all such algebras are listed in Table III of I and are not reproduced here. Their labels $S_{j,k}$ are obtained by setting j and k equal to the values they take in Table III of I.

2. Subalgebras of S that are also subalgebras of P and are nonsplitting extensions of $LSL(2, C)$ by translations. Many independent conjugacy classes under the Poincaré group coalesce under the similitude group. Representatives of all conjugacy classes of such algebras (under the similitude group) are given in Table II of this paper.

3. Subalgebras of S that contain D (the dilatation) as a generator. Representatives of all such algebras are obtained by taking Table III of I and adding the element D itself to the generators. We do not reproduce these subalgebras here; they are however assigned labels $S_{j,k}$ [see (24)].

4. Subalgebras of S such that (i) they contain an element $\tilde{D} = D + \Sigma a_\mu B_\mu + \Sigma x_\alpha X_\alpha$, but no SG-conjugate of D, (ii) their intersection with P splits over the translations. Representatives of all such algebras are listed in Table III above.

5. Subalgebras of S satisfying condition 4(i) above, but such that their intersection with P does not split over the translations. Representatives of all such algebras are listed in Table IV above.

The notations of this article are not entirely self-evident. It is, however, quite trivial to return to the usual physical notations. For the generators, indeed, the connection is given in formulas (13) and (14). Note that in our tables we have sometimes let the continuous parameters range through closed regions, e. g., $0 \leq c < 2\pi$ in $S_{15,25}$, sometimes through open ones like $0 < c < \pi/2$, $\pi/2 < c < \pi$ in $S_{5,9}$. In the last case the end points are separated out and listed separately. We could clearly have bunched more algebras together under one heading, but we did not find this appropriate, since the algebras, corresponding to the limiting values of the parameters often have quite specific properties.

The homogeneous similitude group $\exp D \otimes SL(2, C)$ is of separate interest and has already been treated in I. Indeed, in Table V of I we gave a complete list of subalgebras of $D \oplus LSL(2, C)$, obtained by using a version of the "Goursat twist method,"[17-19] also presented in I. The results of Table V of I are actually contained in the tables of this paper in a somewhat different, but equivalent form. Table V of the present paper is new and shows the mutual inclusions of various conjugacy classes of subgroups of the homogeneous similitude group.

Let us just mention some related work on the classification of continuous subgroups of real Lie groups. All one-dimensional subgroups of $U(p, q)$ and $SU(p, q)$ groups are known.[20] A classification of the real semisimple subgroups of real semisimple groups was performed.[21] Subgroups of the Poincaré group were also considered by other authors[22] and some work has been done on certain subgroups of the conformal group, Galilei group and others.[23]

In the following papers of this series we plan to provide similar lists of subalgebras and continuous subgroups for further groups of interest (de Sitter, conformal and others). We shall also return to the subgroups of the Poincaré and similitude groups and discuss some of their properties (mutual inclusions, isomorphisms, existence of Casimir operators, etc.).

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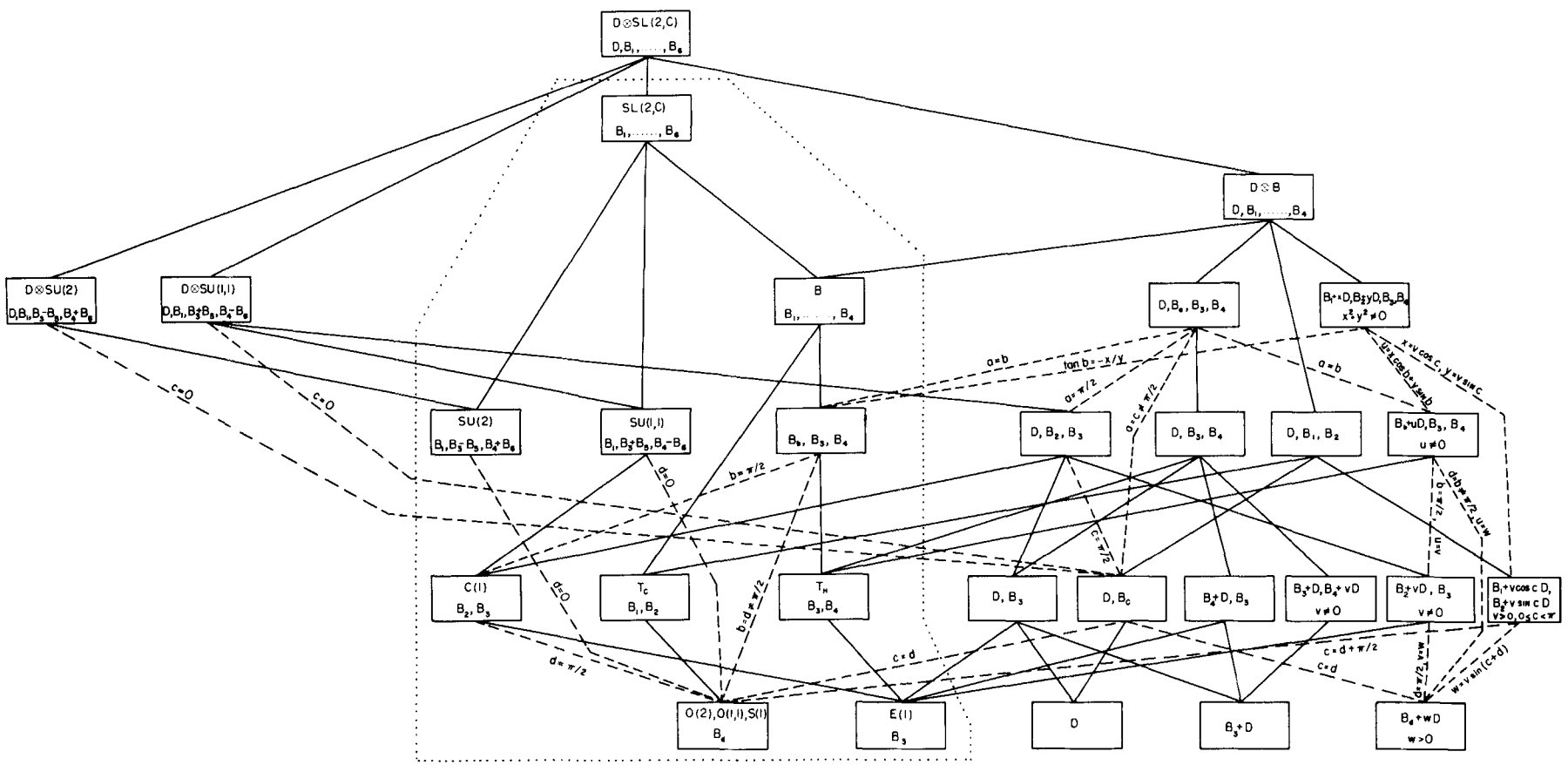

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Structural equations for Killing tensors of order two. II*

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In a preceding paper, a new form of the structural equations for any Killing tensor of order two were derived; these equations constitute a system analogous to the Killing vector equations $\nabla_\alpha K_\beta = \omega_{\alpha\beta} = -\omega_{\beta\alpha}$ and $\nabla_\gamma \omega_{\alpha\beta} = R_{\alpha\beta\gamma\delta} K^\delta$. The first integrability condition for the Killing tensor structural equations is now derived. Our structural equations and the integrability condition have forms which can readily be expressed in terms of a null tetrad to furnish a Killing tensor parallel of the Newman–Penrose equations; this is briefly described. The integrability condition implies the new result, for any given space-time, that the dimension of the set of second order Killing tensors attains its maximum possible value of 50 only if the space-time is of constant curvature. Potential applications of the structural equations are discussed.

1. INTRODUCTION

Lower case Greek letter scripts with values 1, 2, 3, 4 will be used to designate components. The signature of our metric is + 2, and we choose the sign of the Riemann tensor so that $2\nabla_{[\gamma}\nabla_{\beta]}K_\alpha = R_{\beta\gamma\alpha\mu}K^\mu$, where ∇_β is the covariant differentiation operator, and K_α is any vector field.

In the precursor I[1] of this paper, we introduced the following two tensors corresponding to any given symmetric tensor $K_{\alpha\beta}$ of order two:

$$L_{\alpha\beta\gamma} = \nabla_\alpha K_{\beta\gamma} - \nabla_\beta K_{\alpha\gamma}, \tag{1}$$

$$M_{\alpha\beta\gamma\delta} = \tfrac{1}{8}\Delta^{\phi\chi\psi\omega}_{\alpha\beta\gamma\delta}(\nabla_\omega L_{\phi\chi\psi}), \tag{2}$$

where

$$\Delta^{\phi\chi\psi\omega}_{\alpha\beta\gamma\delta} = \delta^{\phi\chi}_{\alpha\beta}\delta^{\psi\omega}_{\gamma\delta} + \delta^{\psi\omega}_{\alpha\beta}\delta^{\phi\chi}_{\gamma\delta}. \tag{3}$$

$L_{\alpha\beta\gamma}$ has the symmetries $L_{\alpha\beta\gamma} = L_{[\alpha\beta]\gamma}$ and $L_{[\alpha\beta\gamma]} = 0$, and $M_{\alpha\beta\gamma\delta}$ has the same symmetries as the Riemann tensor.[1] If $K_{\alpha\beta}$ is regarded as a small perturbation on $g_{\alpha\beta}$, then $L_{\alpha\beta\gamma}$ and $M_{\alpha\beta\gamma\delta}$ can be simply related to the corresponding first order perturbations in the affine connection and Riemann tensor, respectively. This geometric interpretation is giving in Appendix A.

When $K_{\alpha\beta}$ is a Killing tensor, the following equations were shown[1,2] to be satisfied by $K_{\alpha\beta}$, $L_{\alpha\beta\gamma}$, and $M_{\alpha\beta\gamma\delta}$ and were called the *structural equations for a Killing tensor of order two*:

$$\nabla_\gamma K_{\alpha\beta} = \tfrac{1}{3}(L_{\gamma\alpha\beta} + L_{\gamma\beta\alpha}), \tag{4}$$

$$\nabla_\delta L_{\alpha\beta\gamma} = \delta^{\phi\chi}_{\alpha\beta}\left[\tfrac{5}{8}R_{\phi\chi\delta\nu}K^\nu{}_\gamma + \tfrac{3}{8}R_{\phi\chi\gamma\nu}K^\nu{}_\delta + \tfrac{3}{4}R_{\delta\chi\gamma\nu}K^\nu{}_\phi + \tfrac{1}{4}R_{\gamma\chi\delta\nu}K^\nu{}_\phi\right] + M_{\alpha\beta\gamma\delta}, \tag{5}$$

$$\nabla_\lambda M_{\alpha\beta\gamma\delta} = \Delta^{\phi\chi\psi\omega}_{\alpha\beta\gamma\delta}\left[\tfrac{1}{8}(\nabla_\nu R_{\phi\chi\psi\omega})K^\nu{}_\lambda + \tfrac{1}{2}(\nabla_\nu R_{\phi\chi\psi\lambda})K^\nu{}_\omega - \tfrac{3}{8}(\nabla_\lambda R_{\phi\chi\psi\nu})K^\nu{}_\omega - \tfrac{1}{4}R_{\phi\chi\lambda}{}^\nu L_{\psi\omega\nu} + \tfrac{1}{3}R_{\phi\psi\lambda}{}^\nu L_{\chi\nu\omega} + \tfrac{1}{3}R_{\phi\psi\lambda}{}^\nu L_{\omega\chi\nu} + \tfrac{1}{24}R_{\phi\chi\psi}{}^\nu(5L_{\lambda\nu\omega} + 7L_{\omega\lambda\nu})\right]. \tag{6}$$

Equation (4) is equivalent to the definition of a Killing tensor, Eq. (5) is the integrability condition for Eq. (4), and Eq. (6) is the integrability condition for Eqs. (4) and (5). These equations are to be regarded[1] as a system of linear homogeneous first order equations in $K_{\alpha\beta}$, $L_{\alpha\beta\gamma}$, and $M_{\alpha\beta\gamma\delta}$, in the same way that the Killing vector equations

$$\nabla_\alpha K_\beta = \omega_{\alpha\beta}, \quad \nabla_\gamma \omega_{\alpha\beta} = R_{\alpha\beta\gamma\delta}K^\delta,$$

are often regarded as a system of first order equations in the Killing vector K_β and the corresponding bivector $\omega_{\alpha\beta} = -\omega_{\beta\alpha}$. The tensors $L_{\alpha\beta\gamma}$ and $M_{\alpha\beta\gamma\delta}$ are Killing tensor analogs of $\omega_{\alpha\beta}$.

The structural equations can be used to attack the problem of computing the second order Killing tensors of any given space—time. They also constitute a tool for the attempts to classify and discover new space-times which admit Killing tensors and which are perhaps subject to some additional constraints on the metric tensor, the Killing tensor, or both. Examples of suitable constraints are the demands that the matter tensor vanish or be that of a perfect fluid, restriction of the Weyl conform tensor to some algebraic special type, specification of the Jordan canonical form of the Killing tensor, and the existence of some symmetry group.

The objective of this paper is to augment our general formalism until it is ready for such specific applications. The new addition to our formalism is the integrability condition for Eq. (6). This is derived in Sec. 2. The result is a system of equations of the form

$$S_{[\alpha\beta][\gamma\delta][\lambda\mu]} = 0,$$

where $S_{[\alpha\beta][\gamma\delta][\lambda\mu]}$ is totally symmetric in its three bivector scripts $[\alpha\beta]$, $[\gamma\delta]$, $[\lambda\mu]$ and is a linear combination of the components $K_{\alpha\beta}$, $L_{\alpha\beta\gamma}$, and $M_{\alpha\beta\gamma\delta}$. The coefficients in this linear combination depend only on the Riemann tensor and its first and second covariant derivatives.

The basic idea of the structural equations and of their integrability condition is far from new. In 1923 Veblen and Thomas[2] considered quadratic first integrals $K_{\alpha\beta}\dot{x}^\alpha\dot{x}_\beta$ along the paths of an affinely connected space and calculated equations analogous to ours, using the first and second extensions of $K_{\alpha\beta}$ in place of our $L_{\alpha\beta\gamma}$ and $M_{\alpha\beta\gamma\delta}$, respectively. Their results can be specialized to a Riemannian geometry, and equations which are equivalent to ours but quite different in form would thereby be obtained.

In fact, in 1971, Collinson[3] did consider the problem for an n-dimensional Riemannian space and obtained an equation which is algebraically equivalent to our Eq. (6). He used the first and second covariant derivatives of $K_{\alpha\beta}$ in place of our $L_{\alpha\beta\gamma}$ and $M_{\alpha\beta\gamma\delta}$, respectively, and he derived an expression for $\nabla_\mu\nabla_\delta\nabla_\gamma K_{\alpha\beta}$ as a linear combination of the components of $\nabla_\gamma K_{\alpha\beta}$ and $\nabla_\delta\nabla_\gamma K_{\alpha\beta}$. Collinson also briefly described the process of deriving the integrability condition, but he chose to give its explicit form only for a special type of Killing tensor, viz., one which satisfies the equation $\nabla_\delta\nabla_\gamma K_{\alpha\beta}=2R^\mu{}_{\delta\gamma(\alpha}K_{\beta)\mu}$.

The difference between our forms of the structural equations and those introduced by Collinson[3] derives from our employment of the tensors $L_{\alpha\beta\gamma}$ and $M_{\alpha\beta\gamma\delta}$. These tensors were deliberately chosen to make the equations amenable to the use of a null tetrad basis and of the corresponding bivector basis whose members are eigenvectors of the duality operator. What we are proposing here is a null tetrad formalism for second order Killing tensors in space—time similar to that used by Kerr and Debney[4] in their study of the Killing vectors of algebraically special space—times. Some technical aspects of this null tetrad formalism[5] for Killing tensors are given in Appendix B.

In the discussion of Sec. 3, we point out that there is a natural isomorphism between the linear space of all second order Killing tensors $K_{\alpha\beta}$ and the linear space of all ordered triples of the tensors $K_{\alpha\beta}$, $L_{\alpha\beta\gamma}$, $M_{\alpha\beta\gamma\delta}$. With the aid of this fact and the integrability condition, we prove the new theorem that the dimension of the set of second order Killing tensors in space—time attains its maximum value of 50 only if the space—time is of constant curvature. Finally, we suggest how the structural equations and their integrability condition can be used. In particular, current efforts on axially symmetric stationary space—times (vacuum and nonvacuum) which admit Killing tensors having the same Segre characteristic as the Carter Killing tensor for the Kerr metric are described. Also, current efforts on some algebraically special vacuums are described. Results will be given in a sequel to this paper.

We now return to the structural equations and briefly outline the derivation of their integrability condition.

2. THE INTEGRABILITY CONDITION

We start by expressing $\nabla_{[\mu}\nabla_{\lambda]}M_{\alpha\beta\gamma\delta}$ as the usual linear combination of components of $M_{\alpha\beta\gamma\delta}$ with Riemann tensor coefficients; this linear combination is set equal to that expression for $\nabla_{[\mu}\nabla_{\lambda]}M_{\alpha\beta\gamma\delta}$ which is obtained by applying the operator ∇_μ to the right side of Eq. (6) and then replacing the covariant derivatives of $K_{\alpha\beta}$ and $L_{\alpha\beta\gamma}$ with the right sides of Eqs. (4) and (5). After much use of the tensor symmetries, the Bianchi identity, and simple doggedness we obtain the following final result[2]:

$$\Delta^{[\phi\chi][\psi\omega][\lambda\mu]}_{[\alpha\beta][\gamma\delta][\rho\sigma]}\Big[\tfrac{1}{4}R_{\phi\chi\lambda}{}^\tau M_{\psi\omega\mu\tau}+\tfrac{1}{6}R_{\phi\psi\lambda}{}^\tau M_{\chi\omega\mu\tau}$$
$$-\tfrac{1}{16}(\nabla_\nu R_{\phi\chi\psi\omega})L_{\lambda\mu}{}^\nu-\tfrac{1}{6}(\nabla_\mu R_{\phi\chi\psi\nu}+\nabla_\nu R_{\phi\chi\psi\mu})L^\nu{}_{\omega\lambda}$$
$$+\big(-\tfrac{1}{8}\nabla_\nu\nabla_\lambda R_{\phi\chi\psi\omega}+\tfrac{3}{16}R_{\phi\chi\lambda}{}^\tau R_{\psi\omega\nu\tau}+\tfrac{3}{8}R_{\phi\chi\psi}{}^\tau R_{\lambda\nu\omega\tau}$$
$$+\tfrac{1}{4}R_{\phi\lambda\psi}{}^\tau R_{\chi\nu\omega\tau}+\tfrac{1}{8}R_{\phi\psi\lambda}{}^\tau R_{\chi\omega\nu\tau}\big)K^\nu{}_\mu\Big]=0, \tag{7}$$

where

$$\Delta^{ABC}_{DEF}=3!\,\delta^{(A}_{D}\delta^{B}_{E}\delta^{C)}_{F} \tag{8}$$

for any bivector scripts A, B, C, D, E, F. The above result is applicable, as are Eqs. (4), (5), and (6), to an arbitrary Riemannian space.

It is easily verified and is important to note that, in Eqs. (5), (6), and (7), the Killing tensor $K_{\alpha\beta}$ *may be replaced with its traceless part*,

$$\mathring{K}_{\alpha\beta}=K_{\alpha\beta}-\tfrac{1}{4}g_{\alpha\beta}K,\quad K=K_\alpha{}^\alpha; \tag{9}$$

i.e., the isotropic part of the Killing tensor drops out of Eqs. (5), (6), (7). However, it must be retained in Eq. (4).

It is now time to assess our results. We start our discussion with an aerial view of the structural equations and with some elementary observations on the number of linearly independent solutions of these equations. Then, we will consider possible applications.

3. DISCUSSION

Consider the structural equations as an example of a system of linear homogeneous partial differential equations of the first order.[6] As such, they can be lumped into a single matrix equation

$$d\bar{K}=\Gamma\bar{K}, \tag{10}$$

where $\bar{K}$ is a column matrix with fifty elements consisting of ten independent components of $K_{\alpha\beta}$, twenty independent components of $L_{\alpha\beta\gamma}$, and twenty independent components of $M_{\alpha\beta\gamma\delta}$. As regards Γ, it is a square matrix whose elements are 1-forms depending on the metric tensor and its partial derivatives up to the fourth order. The exact dependences can be read off from Eqs. (4), (5), and (6).

The second order Killing tensors in any given space—time constitute a real linear space $V(K, 2)$. We let $V(K,$ red, $2)$ denote that linear manifold which is spanned by the set consisting of $g_{\alpha\beta}$ and of all Killing tensors of the form $A_{(\alpha}B_{\beta)}$ where A_α and B_β are any Killing vectors. The Killing tensors in $V(K,$ red, $2)$ will be called *redundant*.

The set of all ordered triples of the tensors $K_{\alpha\beta}$, $L_{\alpha\beta\gamma}$, and $M_{\alpha\beta\gamma\delta}$ is also a real linear space $V(\bar{K}, 2)$, which is represented by the column matrix solution set of Eq. (10). Any member of $V(\bar{K}, 2)$ will be called a *Killing tensor data set*.[7]

There is an obvious linear isomorphism of $V(K, 2)$ *onto* $V(\bar{K}, 2)$; *hence, the dimensions of* $V(K, 2)$ *and* $V(\bar{K}, 2)$ *are equal*. Furthermore, it is a standard theorem concerning differential equations such as Eq. (10) that, for any given point x_0, and for any given specification of the value of $\bar{K}$ at x_0, there exists not more than one solution of Eq. (10). Since the set of all column matrices $\bar{K}(x_0)$ is a 50-dimensional real linear space, it follows that the dimension of $V(K, 2)$ is ≤ 50. In other words, the general solution for $K_{\alpha\beta}$ will contain not more than 50 essential real parameters.[8] This is a special case of a theorem which was proven by Thomas[9] and which applies to arbitrary n-dimensional affine

spaces. An elegant alternative proof for n-dimensional Riemannian spaces has been given by Sommers. [10]

Flat space is an example where the dimension[8] of $V(K, 2)$ is 50. This was proven by Thomas. [9] Katzin and Levine[11] have given another proof, which is more in tune with the soul of a physicist and which uses the natural linear isomorphism between $V(K, 2)$ and the set of all quadratic constants of geodesic motion $K^{\alpha\beta}(x)p_\alpha p_\beta$. ($p_\alpha$ is particle momentum). The proof proceeds by introducing rectilinear coordinates x^α and noting that Minkowski space admits exactly 10 linearly independent first order constants of geodesic motion, viz., p_α and $L_{\alpha\beta}=x_\alpha p_\beta - x_\beta p_\alpha$. Therefore, $V(K, 2)$ is spanned by the Killing tensors corresponding to the following 56 quadratic constants of geodesic motion:

$$g^{\alpha\beta}p_\alpha p_\beta, \quad p_\alpha p_\beta, \quad L_{\alpha\beta}p_\gamma, \quad L_{\alpha\beta}L_{\gamma\delta}.$$

On account of the identities $g^{\alpha\beta}p_\alpha p_\beta = p_1p_1 + p_2p_2 + p_3p_3 - p_4p_4$, and

$$L_{[\alpha\beta}p_{\gamma]}=0, \quad L_{[\alpha\beta}L_{\gamma]\delta}=0,$$

we are left with a maximum of 50 linearly independent quadratic constants of geodesic motion. A detailed and fairly straightforward argument,[11] which we do not reproduce here, shows that the residual 50 quadratic constants of geodesic motion are linearly independent. Therefore, the dimension of $V(K, \text{red}, 2)$ is 50. Therefore, the dimension of $V(K, 2)$ is 50.

More generally, the dimension of $V(K, 2)$ is 50 for any space—time of constant curvature. This is a special case[8] of a theorem which was proven by Katzin and Levine[11] for n-dimensional Riemannian spaces. An alternative proof was given by Collinson. [3] We will now give still another proof which is in the same spirit as the proof given above for flat spaces and which uses that model of the de Sitter space in which it is represented as a hypersphere in a five-dimensional flat space with rectilinear coordinates z_i. The equation of the hypersphere is $\epsilon_{ij}z_iz_j=k=\text{const}$, where $\epsilon_{ij}=0$ if $i\neq j$, and $\epsilon_{ij}=\pm 1$ if $i=j$. There are exactly 10 linearly independent first order constants of geodesic motion, viz.,

$$L_{ij}=z_ip_j - z_jp_i, \quad p_i=\dot{z}_i.$$

Therefore, $V(K, \text{red}, 2)$ is spanned by the Killing tensors corresponding to the following 56 quadratic constants of geodesic motion[12]:

$$\epsilon_{ij}p_ip_j, \quad L_{ij}L_{kl}$$

However, if we use the constraint equations, $\epsilon_{ij}z_iz_j=k$ and $\epsilon_{ij}z_i\dot{z}_j=0$, we obtain

$$\epsilon_{ik}\epsilon_{jl}L_{ij}L_{kl}=2k\epsilon_{kl}p_kp_l.$$

Also, there is the identity, $L_{[ij}L_{kl]}=0$. Therefore, there is a maximum of 50 linearly independent quadratic constants of geodesic motion in $V(K, \text{red}, 2)$. A detailed argument, which we do not reproduce here,[13] shows that the residual 50 quadratic constants of geodesic motion are linearly independent. Therefore, the dimension of $V(K, \text{red}, 2)$ is 50, and $V(K, \text{red}, 2) = V(K, 2)$.

Conversely, if the dimension of $V(K, 2)$ *is* 50, *then the space—time is of constant curvature.* As in the case of the analogous theorem for Killing vectors, the proof[8,14] employs the integrability condition. If the dimension of $V(K, 2)$ is 50 (case of complete integrability), then the coefficient of each independent component of $\bar{K}$ in Eq. (7) must vanish identically. In particular, if this requirement is applied to the $M_{\alpha\beta\gamma\delta}$ terms of Eq. (7), an explicit calculation of these terms reveals that the Weyl conform tensor and the traceless part of the Ricci tensor vanish. So,

$$R_{\alpha\beta\gamma\delta}=\tfrac{1}{12}(g_{\alpha\gamma}g_{\beta\delta}-g_{\beta\gamma}g_{\alpha\delta})R,$$

whereupon the Bianchi identity yields $R=\text{const}$. Therefore, the space—time is of constant curvature. In summary, we have established *the new result that the dimension of* $V(K, 2)$ *is equal to* 50 *only if the space—time is of constant curvature.*

When the dimension of $V(K, 2)$ is less than 50, i.e., when the integrability condition is not satisfied identically, the classification of space—times according to the number and types of Killing tensors which they admit is an open field of investigation. We have in mind something analogous to what has been done on the classification of space—times by the groups of motions which they admit. [15] However, the hierarchy of compatibility conditions for the Killing tensor structural equations are so complex compared with their Killing vector counterparts[16] that we are uncertain about the practicality of such a program at the present time.

We are more interested in definitive programs, which can be handled in a reasonable time with tools presently at our disposal. One feasible program would be a partial return to the early treatment[17] of Killing tensors, wherein an orthonormal tetrad was chosen such that the Killing tensor assumed its Jordan canonical form relative to that tetrad. We would like to see this approach tried in terms of a null tetrad. In addition, the space—time may be required to be axially symmetric, stationary, or both axially symmetric and stationary. For example, as a first simple step, one of us is now looking at those axially symmetric stationary space—times (vacuum and nonvacuum) which admit a nonredundant Killing tensor whose Lie derivatives with respect to the given Killing vectors vanish and whose Segre characteristic is [(11) (11)]. These are the same conditions which are satisfied by the nonredundant Killing tensor associated with the Kerr metric and discovered by Carter. [18]

Another feasible program is the systematic search for algebraically special vacuums which admit nonredundant Killing tensors. Anyone who is interested in this program may find it helpful to refer to a paper of Debney, Kerr, and Schild[19] on algebraically special electrovacs and to another closely related paper of Kerr and Debney[4] on symmetry groups of algebrically special vacuums. On the basis of simplicity, it is wise to consider only one Petrov type at a time; types II_d, III, and I_d (Ref. 20) are simplest. Each calculation should start by substituting into the null tetrad form of Eq. (7) and exploring those implications which derive from the definition of the Petrov type and from the known dependences of the affine connection and the conform tensor on the complex divergence.

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APPENDIX A

We want to interpret the tensors defined by Eqs. (1) and (2) in terms which regard $K_{\alpha\beta}$ as a small perturbation on the metric. Consider the alternative metric

$$g'_{\alpha\beta} = g_{\alpha\beta} + \epsilon K_{\alpha\beta},$$

where ϵ is a real parameter. The difference of the Christoffel symbols corresponding to the two metrics is a tensor,[21]

$$\Gamma'^{\mu}_{\alpha\beta} - \Gamma^{\mu}_{\alpha\beta} = b^{\mu}_{\alpha\beta}, \tag{A1}$$

where[21]

$$g'_{\gamma\mu}\, b^{\mu}_{\alpha\beta} = \tfrac{1}{2}\epsilon(\nabla_\beta K_{\alpha\gamma} + \nabla_\alpha K_{\beta\gamma} - \nabla_\gamma K_{\alpha\beta}). \tag{A2}$$

The corresponding Riemann tensor increment is[21]

$$R'_{\alpha\beta\mu}{}^{\nu} - R_{\alpha\beta\mu}{}^{\nu} = \nabla_\alpha b^{\nu}_{\beta\mu} - \nabla_\beta b^{\nu}_{\alpha\mu} + b^{\nu}_{\alpha\lambda} b^{\lambda}_{\beta\mu} - b^{\nu}_{\beta\lambda} b^{\lambda}_{\alpha\mu}. \tag{A3}$$

Let

$$\delta f = \left(\frac{\partial f}{\partial \epsilon}\right)_{\epsilon=0}$$

for any function f of ϵ. Then, Eqs. (A1) to (A3) yield the usual first order equations

$$g_{\gamma\mu}\,\delta\Gamma^{\mu}_{\alpha\beta} = \tfrac{1}{2}(\nabla_\beta K_{\alpha\gamma} + \nabla_\alpha K_{\beta\gamma} - \nabla_\gamma K_{\alpha\beta}), \tag{A4}$$

$$\delta R_{\alpha\beta\mu}{}^{\nu} = \nabla_\alpha(\delta\Gamma^{\nu}_{\beta\mu}) - \nabla_\beta(\delta\Gamma^{\nu}_{\alpha\mu}). \tag{A5}$$

From Eqs. (1), (2), (A4), and (A5), we obtain our results,

$$L_{\alpha\beta\gamma} = -2 g_{\mu[\alpha}\,\delta\Gamma^{\mu}_{\beta]\gamma}, \tag{A6}$$

$$M_{\alpha\beta\gamma\delta} = -\tfrac{1}{8}\Delta^{\phi\chi\psi\omega}_{\alpha\beta\gamma\delta}(\delta R_{\phi\chi\psi}{}^{\nu}) g_{\nu\omega}. \tag{A7}$$

We have thus shown how $L_{\alpha\beta\gamma}$ and $M_{\alpha\beta\gamma\delta}$ can be defined in terms of the first order changes in the affine connection and the Riemann tensor, respectively. This result is worth noting, but its importance for the subject of Killing tensors is unknown and may be nonexistent.

APPENDIX B

We shall here sketch some of the relations required for expressing Eqs. (4) to (7) in a null tetrad form.[5] This appendix covers only the problem of the null tetrad components of the tensors $K_{\alpha\beta}$ and $L_{\alpha\beta\gamma}$, since these subjects cannot easily be found in the literature. Full details on the null tetrad forms of Eqs. (4) to (7) are available in the form of a seminar report[5] by the authors.

Let k, m, t, t^* denote any null tetrad which consists of 1-forms such that k and m are real, t^* is the complex conjugate of t, and $k\cdot m = t\cdot t^* = 1$. Various null tetrad components of tensors are designated by using k, m, t, and t^* as scripts. For example, $K_{kk} = k^\alpha k^\beta K_{\alpha\beta}$ and $K_{kt} = k^\alpha t^\beta K_{\alpha\beta}$. There is no loss of generality in assuming that $K_{\alpha\beta}$ is real. Thereupon, the Killing tensor has four real components K_{kk}, K_{km}, K_{mm}, and K_{tt^*} and three independent complex components K_{kt}, K_{mt}, K_{tt}, with the remaining complex components equal to $(K_{kt})^*$, $(K_{mt})^*$, $(K_{tt})^*$.

As regards $L_{\alpha\beta\gamma}$, the condition $L_{[\alpha\beta\gamma]} = 0$ can be shown to be equivalent to the set of four equations

$$L_{kmk} + L_{tt^*}{}_k = -2L_{ktt^*} + L_k,$$

$$L_{kmk} + L_{tt^*}{}_m = 2L_{mt^*}{}_t - L_m,$$

$$L_{kmt} + L_{tt^*}{}_t = 2L_{ktm} + L_t,$$

$$L_{kmt^*} + L_{tt^*}{}_{t^*} = -2L_{mt^*}{}_k - L_{t^*}$$

where L_k, L_m, L_t, L_{t^*} are the null tetrad components of $L_\alpha = L_{\alpha\beta}{}^{\beta}$. With the aid of the above identities, each component of $L_{\alpha\beta\gamma}$ can be reduced to a simple linear combination of the two real fields L_k and L_m, the nine complex fields L_t, L_{ktk}, L_{ktm}, L_{ktt}, L_{ktt^*}, $L_{mt^*}{}_k$, $L_{mt^*}{}_m$, $L_{mt^*}{}_t$, $L_{mt^*}{}_{t^*}$, and the complex conjugates of these nine fields.

As regards $M_{\alpha\beta\gamma\delta}$, it has the same symmetries as the Riemann tensor. So, we can express any null tetrad component of this tensor in terms of five complex fields which are analogous to the Newman–Penrose[22] components ψ_0, ψ_1, ψ_2, ψ_3, ψ_4 of the Weyl conform tensor, the null tetrad components of an analog of the traceless part of the Ricci tensor, and an analog of the curvature scalar. This is the same kind of decomposition which is applied to the Riemann tensor in the Newman–Penrose equations.[22]

*A preliminary report of this paper was published in Bull. Am. Phys. Soc. **19**, 108 (1974).

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[7] This term was suggested by the term "Killing vector data set" as used in a similar context (R. Geroch, seminar) for the ordered pairs consisting of any Killing vector K_α and its corresponding bivector $\omega_{\alpha\beta} = \nabla_\alpha K_\beta$.

[8] Clearly, these statements also hold for an arbitrary n-dimensional Riemannian space if we replace 50 with $n(n+1)^2(n+2)/12$. However, we do not know how to complete the proof [based on Eq. (7)] that the Riemannian space is of constant curvature if the dimension of $V(K,2)$ is $n(n+1)^2(n+2)/12$; we have proven this theorem only for

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Variational method and nonlinear oscillations and waves

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A direct variational method is developed for studying the asymptotic behavior of a wide class of nonlinear oscillation and wave problems. From some judiciously chosen trial solutions with adjustable parameters, equations governing the change of amplitudes and phases are derived and solved. The method is simple in concept and straightforward in application. Different aspects of the method are illustrated by applications to various examples: the oscillation of a pendulum with changing length; the motion of a charged particle in a strong magnetic field; the linear and nonlinear Klein-Gordon equations; and the linear and nonlinear Korteweg-de Vries equations.

1. INTRODUCTION

An approximate, direct variational method has been developed to deal with the forced oscillations of nonlinear systems.[1] The method starts with reformulating the problem by an equivalent variational problem; then some judiciously chosen asymptotic trial solutions with adjustable parameters are substituted into the functional to be varied. The examples chosen to illustrate the scheme in that previous study all had sinusoidal functions as the forcing term. Therefore, it was natural also to assume that the solutions to behave in a similar manner. In this paper, we shall extend the method to treat other class of problems whose intrinsic oscillatory behavior is not necessarily sinusoidal, and thus it is a part of problem to determine the oscillatory behavior. The examples treated in the previous study are all second order ordinary differential equations. In this paper, we shall extend our method to partial differential equations, hence the study of wave propagations.

The basic idea underlying this method is to make use of whatever prior information there is as much as possible and incorporating it into the form of the trial solution. Thus it is expected that the system of equations governing the adjustable unknown parameters would be much simpler than the original problem. In this paper as well as in the previous study, we are mainly interested in the asymptotic oscillatory solutions. Therefore, approximate solutions for the amplitude and phase can be obtained by singling out the secular terms. In this sense the spirit of this method is similar to the methods developed by others.[2,3] Our basic approach is very close to Whitham's variational method,[4] especially to his application of the variational method to the problem of water waves.[5] However, the details are different. Moreover, as demonstrated in our treatment of the Korteweg–de Vries equations, the existence of Lagrangian is not required.

In the following, we shall again employ various examples to illustrate the procedure of the scheme.

We begin with a linear ordinary differential equation for the study of adiabatic invariants to illustrate how the intrinsic oscillatory behavior can be determined. Then we apply the same method to find the adiabatic invariant for the nonlinear problem of the motion of a charged particle in a magnetic field. Next we apply the same idea to linear and nonlinear dispersive waves, using Klein–Gordon equations and Korteweg–de Vries equations as examples.

2. ADIABATIC INVARIANT

Let us first consider the simple example of the linear oscillation of a pendulum whose length is changed at a very slow rate. Thus, the differential equation is

$$\ddot{x} + \omega^2(t)x = 0, \tag{2.1}$$

where ω is a slowly varying function of t. Equation (1) is equivalent to the statement that the following functional J is stationary:

$$J = \int_0^t \tfrac{1}{2}(\dot{x}^2 - \omega^2 x^2)\,dt. \tag{2.2}$$

Let us now look for solutions such that

$$x = A(t)\phi(S(t)), \tag{2.3}$$

where A and S are both slowly varying functions of t and $\phi(S)$ is a periodic function such that

$$\phi(S + 2\pi) = \phi(S), \tag{2.4}$$

$$\langle\phi\rangle = \frac{1}{2\pi}\int_0^{2\pi} \phi(S)\,dS = 0, \tag{2.5}$$

$$\langle\phi^2\rangle = 1. \tag{2.6}$$

Since A and S are yet to be determined, conditions (2.4) and (2.6) can be imposed without loss of any generality. Condition (2.5) is, however, dictated by our anticipation of the solution.

From (3), we obtain

$$\dot{x} = \dot{A}\phi + A\dot{S}\dot{\phi}. \tag{2.7}$$

Let us substitute (2.3) and (2.7) in (2.2), making use of the slowly varying nature of A, S, and ω, then since $\langle\phi\dot{\phi}\rangle = 0$, we obtain for large t, as we have done in the previous study,[1] that

$$J \approx \tfrac{1}{2}\int_0^t [\dot{A}^2 + (\alpha\dot{S}^2 - \omega^2)A^2]\,dt, \tag{2.8}$$

where

$$\alpha = \langle\dot{\phi}^2\rangle.$$

By varying A and S in the approximate functional as given by (2.8), we obtain the Euler's equation

$$\ddot{A} - (\alpha\dot{S}^2 - \omega^2)A = 0 \tag{2.9}$$

and

$$\frac{d}{dt}(\alpha \dot{S} A^2) = 0. \tag{2.10}$$

Now the periodic function ϕ is yet not determined. As a direct variational method, any ϕ satisfying (2.4)—(2.6) will do to achieve various degrees of accuracy for our approximate solution. To obtain best results, we shall seek our guidance from the original equation (2.1) or (2.2). Thus the natural choice is

$$\phi(S) = \sqrt{2}\sin S. \tag{2.11}$$

Then

$$\alpha = \langle \dot{\phi}^2 \rangle = 1. \tag{2.12}$$

Now since A is a slowly varying function of t, we thus obtain from (2.9) the first approximation:

$$S = \int^t \omega(t)\, dt. \tag{2.13}$$

Equation (2.10) then yields

$$\omega A^2 = \text{const}. \tag{2.14}$$

The last two equations are the familiar results for adiabatic invariants. As we can see here, the procedure is very straightforward once the trial solution of the form (2.3) is chosen. Corrections to the first approximation may also be carried out based on Eqs. (2.9) and (2.10).

3. MOTION OF A CHARGED PARTICLE IN A STRONG MAGNETIC FIELD

The equation of motion of a particle of charge q and mass m acted on by an electric field $\mathbf{E}(\mathbf{r}, t)$, a magnetic field $\mathbf{B}(\mathbf{r}, t)$ and a gravitational potential $G(\mathbf{r}, t)$ is (see, for example, Bernstein[6])

$$\ddot{\mathbf{x}} = \mathbf{a} - \Omega \times \dot{\mathbf{x}}, \tag{3.1}$$

where

$$\mathbf{a} = q\mathbf{E}(\mathbf{x}, t)/m - \nabla G(\mathbf{x}, t), \tag{3.2}$$

$$\Omega = q\mathbf{B}(\mathbf{x}, t)/mc. \tag{3.3}$$

Now the magnetic field B and the electric field E can be expressed in terms of the vector potential A and the scalar potential ϕ:

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial A}{\partial t}.$$

Let us denote

$$\mathbf{V} = q\mathbf{A}/mc, \quad F = q\phi/m + G;$$

then Eq. (3.1) is equivalent to the statement that the following functional J is stationary subject to the variation of $\mathbf{x}$:

$$J = \int_0^t (\tfrac{1}{2}\dot{\mathbf{x}}^2 + \dot{\mathbf{x}} \cdot \mathbf{V} - F)\, dt. \tag{3.4}$$

The physical problem we are concerned with has a strong magnetic field in one direction, say the x_3 direction. The electric and gravitational fields as well as the magnetic field in other directions are assumed to be weak. Thus we may take

$$\mathbf{V} = (-\Omega x_2, V_2, V_3), \tag{3.5}$$

$$F = f_1 x_1 + f_2 x_2 + f_3 x_3, \tag{3.6}$$

where Ω, V_2, V_3, f_1, f_2, and f_3 are all slowly varying functions of $(\mathbf{x}, t)$, and f_1, f_2, and f_3 are not large.

Now let us look for trial solution in the form

$$x_i = R_i(t) + \rho_i(t)\sin[2\pi\theta(t) + \phi_i(t)], \quad i = 1, 2, 3, \tag{3.7}$$

where R_i, ρ_i, and ϕ_i are all slowly varying functions of t and we can take $\phi_1(t) = 0$ without loss of any generality. We have taken the sinusoidal function to represent the periodic behavior directly to simplify the computation somewhat. They are indeed suggested by a crude analysis taking external fields as constant. From (3.7) we obtain

$$\dot{x}_i = \dot{R}_i + \dot{\rho}_i \sin(2\pi\theta + \phi_i) + (2\pi\dot{\theta} + \dot{\phi}_i)\,\rho_i \cos(2\pi\theta + \phi_i), \quad i = 1, 2, 3, \tag{3.8}$$

Now we substitute (3.5)—(3.8) into (3.4) and evaluate the integral. To evaluate the integral, let us consider one term to illustrate the procedure. Take

$$\int_0^t \dot{x}_1 V_1\, dt = \int_0^t -\Omega[R_2(t) + \rho_2(t)\sin(2\pi\theta + \phi_2)] \times [\dot{R}_1 + \dot{\rho}_1 \sin 2\pi\theta + 2\pi\dot{\theta}\rho_1 \cos 2\pi\theta]\, dt.$$

Now Ω is a slowly varying function of $(\mathbf{x}, t)$; thus we can expand as follows:

$$\Omega(\mathbf{x}, t) = \Omega(\mathbf{R}(t), t) + \sum_i \rho_i \sin(2\pi\theta + \phi_i) \cdot \frac{\partial \Omega}{\partial R_i}(\mathbf{R}, t) + \cdots.$$

If we only take two terms of expansion of Ω, then for large t, since only the secular terms dominate, we obtain approximately

$$\int_0^t \dot{x}_1 V_1\, dt \approx \int_0^t \Big(-\Omega(\mathbf{R}, t)(R_2\dot{R}_1 + \tfrac{1}{2}\rho_2\dot{\rho}_1\cos\phi_2 + \pi\rho_2\rho_1\dot{\theta}\sin\phi_2) - \tfrac{1}{2}\sum_i \rho_i \frac{\partial\Omega}{\partial R_i}(\mathbf{R}, t) \times [\rho_2\dot{R}_1\cos(\phi_i - \phi_2) + \dot{\rho}_1 R_2 \cos\phi_i + 2\pi\dot{\theta}\rho_1 R_2 \sin\phi_i] \Big)\, dt.$$

To make the phrase "slowly varying function" more precise, let us take ϵ as a small parameter, and consider in general $\partial/\partial R_i = O(\epsilon)$, $d/dt = O(\epsilon)$. Furthermore, assume Ω, ρ_i, ϕ_i, R_1, and R_2 are $O(1)$; f_i, V_2, and V_3 are $O(\epsilon)$; and $\dot{\theta}$ and $\dot{R}_3$ are $O(1)$. Then after some straightforward computations, we obtain up to $O(\epsilon)$:

$$J = \int_0^t \mathcal{J}\, dt, \tag{3.9}$$

where

$$\mathcal{J} \approx \pi^2\dot{\theta}^2(\rho_1^2 + \rho_2^2 + \rho_3^2) + \pi\dot{\theta}(\rho_2^2\dot{\phi}_2 + \rho_3^2\dot{\phi}_3) + \tfrac{1}{2}\dot{R}_3^2 - \Omega(\mathbf{R}, t)(R_2\dot{R}_1 + \tfrac{1}{2}\rho_2\dot{\rho}_1\cos\phi_2 + \pi\rho_1\rho_2\dot{\theta}\sin\phi_2) - \pi\rho_1 R_2\dot{\theta}\Big(\rho_2\frac{\partial\Omega}{\partial R_2}\sin\phi_2 + \rho_3\frac{\partial\Omega}{\partial R_3}\sin\phi_3\Big) + V_3\dot{R}_3 - f_1R_1 - f_2R_2 - f_3R_3. \tag{3.10}$$

The variation of the functional J with respect to R_i, ρ_i, ϕ_i, and θ then leads to the following Euler equations:

$$\delta\rho_3: \quad 2\pi^2\dot{\theta}^2\rho_3 = -2\pi\dot{\theta}\dot{\phi}_3\rho_3 + \pi\rho_1 R_2\dot{\theta}\frac{\partial\Omega}{\partial R_3}\sin\phi_3, \tag{3.11}$$

$$\delta\phi_3: \quad -\frac{d}{dt}(\pi\dot{\theta}\rho_3^2) - \pi\rho_1\rho_3 R_2\dot{\theta}\frac{\partial\Omega}{\partial R_3}\cos\phi_3 = 0. \tag{3.12}$$

Since the right-hand side of (3.11) is $O(\epsilon)$, we obtain that, for the leading order,

$$\rho_3 = 0. \tag{3.13}$$

Thus the term associated with ρ_3 can be ignored from further consideration. The variation with respect to ϕ_2 now leads to

$$-\Omega\pi\rho_1\rho_2\dot{\theta}\cos\phi_2 = \frac{d}{dt}(\pi\dot{\theta}\rho_2^2) - \tfrac{1}{2}\Omega\rho_2\dot{\rho}_1\sin\phi_2 + \pi\rho_1 R_2\dot{\theta}\rho_2\frac{\partial\Omega}{\partial R_2}\cos\phi_2. \tag{3.14}$$

Again the right-hand side is $O(\epsilon)$, thus if we assume ρ_1, ρ_2, and $\dot{\theta}$ to be nonzero, we obtain for the leading order that

$$\phi_2 = \pi/2. \tag{3.15}$$

The variation with respect to ρ_1 and ρ_2 now gives

$$\delta\rho_1: \quad 2\pi^2\rho_1\dot{\theta}^2 - \pi\rho_2\Omega\dot{\theta}\sin\phi_2 = -\frac{1}{2}\frac{d}{dt}(\rho_2\Omega\cos\phi_2) + \pi R_2\dot{\theta}\left(\rho_2\frac{\partial\Omega}{\partial R_2}\sin\phi_2 + \rho_3\frac{\partial\Omega}{\partial R_3}\sin\phi_3\right), \tag{3.16}$$

$$\delta\rho_2: \quad 2\pi^2\rho_2\dot{\theta}^2 - \pi\rho_1\Omega\dot{\theta}\sin\phi_2 = -2\pi\rho_2\dot{\theta}\dot{\phi}_2 + \tfrac{1}{2}\dot{\rho}_1\Omega\cos\phi_2 + \pi\rho_1 R_2\dot{\theta}\frac{\partial\Omega}{\partial R_2}\sin\phi_2. \tag{3.17}$$

Again the right-hand sides are $O(\epsilon)$. Thus the leading order equations are

$$2\pi^2\rho_1\dot{\theta}^2 = \pi\rho_2\Omega\dot{\theta}$$

and

$$2\pi^2\rho_2\dot{\theta}^2 = \pi\rho_1\Omega\dot{\theta},$$

which lead to

$$\rho_1 = \rho_2 \equiv \rho \tag{3.18}$$

and

$$\dot{\theta} = \Omega/2\pi, \quad \text{or} \quad \theta = (1/2\pi)\int_0^t \Omega(\mathbf{R}(t), t)\,dt. \tag{3.19}$$

The variation with respect to θ now yields

$$\frac{d}{dt}[2\pi^2\dot{\theta}(\rho_1^2+\rho_2^2) - \pi\Omega\rho_1\rho_2\sin\phi_2] = -\frac{d}{dt}\left[\pi(\rho_2^2\dot{\phi}_2 + \rho_3^2\dot{\phi}_3) - \pi\rho_1 R_2\left(\rho_2\frac{\partial\Omega}{\partial R_2}\sin\phi_2 + \rho_3\frac{\partial\Omega}{\partial R_3}\sin\phi_3\right)\right]. \tag{3.20}$$

Setting the leading order left-hand side to zero and using (3.18) and (3.19), we obtain

$$\frac{d}{dt}(\Omega\rho^2) = 0, \quad \text{or} \quad \Omega\rho^2 = \text{const}. \tag{3.21}$$

$\Omega\rho^2$ is known as an adiabatic invariant.

The variations with respect to R_1, R_2, and R_3 now yields, to the leading order,

$$\delta R_1: \quad \frac{d}{dt}(\Omega R_2) - f_1 - \pi\rho_1\rho_2\dot{\theta}\frac{\partial\Omega}{\partial R_1}\sin\phi_2 = 0,$$

$$\delta R_2: \quad -\Omega\dot{R}_1 - f_2 - 2\pi\rho_1\rho_2\dot{\theta}\frac{\partial\Omega}{\partial R_2}\sin\phi_2 = 0,$$

$$R_3: \quad \ddot{R}_3 + f_3 + \pi\rho_1\rho_2\dot{\theta}\frac{\partial\Omega}{\partial R_3}\sin\phi_2 = 0.$$

These equations give the well-known motion of guiding center as well as the first order correction of the motion.[6] We can also find the next order correction for ρ_1, ρ_2, θ, and ϕ_2 by making use of the right-hand side of Eqs. (3.14), (3.16), (3.17), and (3.20). The details will not be presented here.

4. NONLINEAR DISPERSIVE WAVES—THE KLEIN-GORDON EQUATION

Let us now turn to partial differential equations and consider the following nonlinear wave equation:

$$u_{tt} - u_{xx} + f(u) = 0. \tag{4.1}$$

When $f(u) = u$, we have the usual Klein—Gordon equation. This equation has been investigated by Whitham[3] and Moser.[7] Here we shall employ the variational method to study the problem.

Let us define the function $F(u)$ by

$$F'(u) = f(u). \tag{4.2}$$

Then Eq. (4.1) is equivalent to the statement that the following functional J is an extremum:

$$J = \int_0^t dt\int_{-\infty}^{+\infty} dt[-\tfrac{1}{2}u_t^2 + \tfrac{1}{2}u_x^2 + F(u)]. \tag{4.3}$$

Our purpose is again to find asymptotic solution for large t, which exhibits certain oscillatory behavior. Thus let us look for trial solution of the following form:

$$u = A(x,t)\phi(S(x,t)), \tag{4.4}$$

where A and the derivatives of S are both slowly varying functions of (x,t) and ϕ is a periodic function of S which satisfies the following conditions:

$$\phi(S+2\pi) = \phi(S), \tag{4.5}$$

$$\langle\phi\rangle \equiv (1/2\pi)\int_0^{2\pi}\phi\,dS = 0, \tag{4.6}$$

$$\langle\phi^2\rangle = 1. \tag{4.7}$$

The conditions (4.5) and (4.7) are made specific without loss of generality since A and S are yet to be determined. It follows from (4.5) that

$$\langle\phi\phi'\rangle = 0, \tag{4.8}$$

and we shall denote

$$\langle\phi'^2\rangle = \alpha. \tag{4.9}$$

From (4.4) we have

$$u_t = A_t\phi + AS_t\phi', \tag{4.10}$$

$$u_x = A_x\phi + AS_x\phi'. \tag{4.11}$$

Substituting (4.4), (4.10), and (4.11) into (4.3), making use of the periodic properties of ϕ and slowly varying behavior of A and S, we obtain for large t

$$J = \int_0^t dt\int_{-\infty}^{+\infty} dx[\tfrac{1}{2}(-A_t^2 - \alpha A^2 S_t^2 + A_x^2 + \alpha A^2 S_x^2) + G(A)], \tag{4.12}$$

where

$$G(A) = \langle F(A\phi) \rangle. \tag{4.13}$$

The variation with respect to A and S then lead to

$$\delta A: \quad A_{tt} - A_{xx} - \alpha A(S_t^2 - S_x^2) + G'(A) = 0, \tag{4.14}$$

$$\delta S: \quad (\alpha A^2 S_t)_t - (\alpha A^2 S_x)_x = 0. \tag{4.15}$$

Since A is supposed to be a slowly varying function of (x, t), (4.14) can be approximated by

$$A(S_t^2 - S_x^2) - G'(A) = 0. \tag{4.16}$$

In order to determine α and $G(A)$, we need to find ϕ explicitly. In the spirit of the direct variational method, we have a great deal of freedom for the determination of ϕ. Of course, the closer ϕ approaches the real solution, the better is our approximate solution as a whole. We could artificially take $\phi(S) = (1/\sqrt{2}) \sin S$, but it may not be a very good trial solution for many cases. We shall instead use the original equation as a guide to suggest a better solution.

Let us write

$$u = \phi(s(x, t)), \tag{4.17}$$

and substitute into (4.1) or (4.3). If we use (4.1), we obtain

$$(s_t^2 - s_x^2)\phi'' + f(\phi) = (s_{xx} - s_{tt})\phi'. \tag{4.18}$$

Assume s_t and s_x to be constants and write

$$s_t^2 - s_x^2 = \omega^2;$$

we thus obtain

$$\omega^2 \phi'' + f(\phi) = 0. \tag{4.19}$$

In (4.19), ω^2 is a parameter still to be determined. However, the conditions (4.5), (4.6), and (4.7) will usually determine ϕ completely. When ϕ is found, α and $G(A)$ can be obtained. Then (4.15) and (4.16) can be used to find A and S.

Let us consider a few examples to illustrate some of the details.

(i) *The Klein–Gordon equation*: $f(u) = u$. The equation we consider is

$$u_{tt} - u_{xx} + u = 0. \tag{4.20}$$

For this case, it is evident from (4.19), (4.5), (4.6), and (4.7) that

$$\phi(S) = \sqrt{2} \sin(S + \psi), \tag{4.21}$$

where ψ is a constant. Then from (4.9) and (4.13), we obtain

$$\alpha = 1, \quad G'(A) = A.$$

Thus (4.16) becomes

$$S_t^2 - S_x^2 = 1. \tag{4.22}$$

Use the Charpit's method (see, for example, Sneddon[8]); a complete integral of the above equation is

$$S = \sqrt{1 + a^2}\, t + ax + b, \tag{4.23}$$

where a and b are two arbitrary constants. They represent the ordinary travelling wave solutions. A more interesting solution is the singular solution which is the envelope of the family of solutions represented by (4.23). This gives

$$S = (t^2 - x^2)^{1/2}, \tag{4.24}$$

which is also that given by Moser.[7]

Substituting (4.24) into (4.15), we obtain

$$t(A^2)_t + x(A^2)_x + A^2 = 0. \tag{4.25}$$

The general method for solving linear partial differential equations of the first order (see, for example, Sneddon[8]) then leads to the general solution

$$A = (1/\sqrt{t})P(x/t), \tag{4.26}$$

where P is any arbitrary function. This solution is consistent with the asymptotic expression for large t of the general solution of (4.20). In particular, if we assume A is a function of S as Moser[7] did, or equivalently take

$$P(Z) = (A_0/\sqrt{2})(1 - Z^2)^{-1/4},$$

then we obtain

$$A = (A_0/\sqrt{2})(t^2 - x^2)^{-1/4}. \tag{4.27}$$

Hence

$$u = [A_0/(t^2 - x^2)^{1/4}] \sin[(t^2 - x^2)^{1/2} + \psi]. \tag{4.28}$$

(ii) *A nonlinear Klein–Gordon equation*: $f(u) = u^3$. The equation we consider now is

$$u_{tt} - u_{xx} + u^3 = 0. \tag{4.29}$$

The function $\phi(S)$ is to be determined from

$$\omega^2 \phi'' + \phi^3 = 0. \tag{4.30}$$

Thus

$$(\omega \phi')^2 = \tfrac{1}{2}(C^4 - \phi^4),$$

where C is an integration constant, which will be taken as real for ϕ to be periodic. Thus, ϕ is an elliptic function, or

$$\frac{S}{\omega} = \int^{\phi} \frac{dy}{(\frac{1}{2}C^4 - \frac{1}{2}y^4)^{1/2}}. \tag{4.31}$$

The condition (4.5) is now

$$2\pi = 2\omega \int_{-C}^{C} \frac{dy}{(\frac{1}{2}C^4 - \frac{1}{2}y^4)^{1/2}}, \tag{4.32}$$

and the condition (4.7) now determines completely the value of ω and C. Then the value α as well as $\langle \phi^4 \rangle$ can also be explicitly determined.

From (4.13) we obtain

$$G'(A) = \langle \phi^4 \rangle A^3. \tag{4.33}$$

Equations (4.16) thus becomes

$$S_t^2 - S_x^2 = (\langle \phi^4 \rangle / \alpha) A^2. \tag{4.34}$$

To solve the coupled equations (4.34) and (4.15), let us first use the linear example as a guide and look for particular solutions such that S and A are both functions of λ, where

$$\lambda = (t^2 - x^2)^{1/2}. \tag{4.35}$$

Then Eqs. (4.34) and (4.15) become

$$\left(\frac{dS}{d\lambda}\right)^2 = \frac{\langle\phi^4\rangle}{\alpha} A^2, \tag{4.36}$$

and

$$\frac{d}{d\lambda}\left(A^2\frac{dS}{d\lambda}\right) + \frac{A^2}{\lambda}\frac{dS}{d\lambda} = 0. \tag{4.37}$$

From (4.37), we obtain

$$\lambda A^2 \frac{dS}{d\lambda} = \text{const.} \tag{4.38}$$

Substituting (4.36) into (4.38), we obtain

$$S = a\lambda^{2/3} + b \tag{4.39}$$

and

$$A = \tfrac{2}{3}a(\langle\phi^4\rangle/\alpha)^{1/2}\lambda^{-1/3}, \tag{4.40}$$

where a and b are integration constants. Thus

$$u = \tfrac{2}{3}a(\langle\phi^4\rangle/\alpha)^{1/2}(t^2 - x^2)^{-1/6}\phi[a(t^2 - x^2)^{1/3} + b]. \tag{4.41}$$

We can also try another approach. If we substitute (4.34) into (4.15), we obtain

$$[(S_t^2 - S_x^2)S_t]_t - [(S_t^2 - S_x^2)S_x]_x = 0. \tag{4.42}$$

Let us now look for solutions of the following form:

$$S = t^\mu h(w), \tag{4.43}$$

where $w = x/t$ and μ is some constant. After some straightforward calculation, we obtain

$$\begin{aligned}&[3(w^2-1)^2h'^2 - 6\mu w(w^2-1)h'h + \mu^2(3w^2-1)h^2]h'' \\ &- 6(\mu-1)w(w^2-1)h'^3 + 5\mu(\mu-1)(3w^2-1)h'^2h \\ &- 12\mu^2(\mu-1)wh'h^2 + 3\mu^3(\mu-1)h^3 = 0.\end{aligned} \tag{4.44}$$

If we take $\mu = \frac{2}{3}$, then (4.44) becomes

$$\begin{aligned}&[3(w^2-1)^2h'^2 - 4\mu w(w^2-1)h'h + \tfrac{4}{9}(3w^2-1)h^2]h'' \\ &+ 2w(w^2-1)h'^3 - \tfrac{10}{9}(3w^2-1)h'^2h + \tfrac{16}{9}wh'h^2 - \tfrac{8}{27}h^3 = 0.\end{aligned} \tag{4.45}$$

It may be verified that

$$h = a(1 - w^2)^{1/3} \tag{4.46}$$

is a solution, which agrees with (4.39).

If we take $\mu = 1$, (4.44) becomes

$$h''[3(w^2-1)^2h'^2 - 6w(w^2-1)h'h + (3w^2-1)h^2] = 0. \tag{4.47}$$

If $h'' = 0$, then we obtain

$$h = aw + b,$$

or

$$S = at + bx, \tag{4.48}$$

and

$$A^2 = (\alpha/\langle\phi^4\rangle)(a^2 - b^2). \tag{4.49}$$

If $h'' \neq 0$, then

$$(w^2-1)^2h'^2 - 2w(w^2-1)h'h + (w^2 - \tfrac{1}{3})h^2 = 0. \tag{4.50}$$

Thus

$$(w^2 - 1)h' = (w \pm 1/\sqrt{3})h,$$

which leads to

$$h = a(1 - w^2)^{1/2}\left|(1+w)/(1-w)\right|^{\mp 1/2\sqrt{3}}. \tag{4.51}$$

(iii) *The spherical Klein–Gordon equation*: Let us now consider the following equation:

$$u_{tt} - u_{rr} - (2/r)u_r + f(u) = 0. \tag{4.52}$$

Then the functional to be varied will be

$$J = \int_0^t dt \int_0^\infty dr\, r^2[\tfrac{1}{2}(-u_t^2 + u_r^2) + F(u)], \tag{4.53}$$

where again

$$F'(u) = f(u). \tag{4.54}$$

Take the trial function in the form

$$u = A(r,t)\phi(S(r,t)), \tag{4.55}$$

where ϕ again satisfies the conditions (4.5), (4.6), and (4.7). Then corresponding to Eqs. (4.15) and (4.16), we have

$$(r^2A^2S_t)_t - (r^2A^2S_r)_r = 0 \tag{4.56}$$

and

$$\alpha A(S_t^2 - S_r^2) = G'(A), \tag{4.57}$$

where α and $G(A)$ are given again by (4.9) and (4.13).

Assume $u = \phi(s(r,t))$ and substitute into (4.53); then the function ϕ again is suggested to be derived from the same equation as (4.19).

For the linear equation when $f(u) = u$, we obtain thus

$$u = (A_0/r\sqrt{t})P(r/t)\sin[(t^2 - r^2)^{1/2} + \psi]. \tag{4.58}$$

For the nonlinear case, we can also try to look for solutions of the form

$$S = t^\mu h(r/t), \tag{4.59}$$

and obtain from (4.56) and (4.57) a second order ordinary differential equation for h.

5. THE KORTEWEG-DE VRIES EQUATION

We now extend the application of the variational method to another important nonlinear dispersive wave equation, i.e., the Korteweg–de Vries equation:

$$u_t + uu_x + u_{xxx} = 0. \tag{5.1}$$

Before we deal directly with this equation, let us consider first the linear dispersive wave equation:

$$u_t + u_{xxx} = 0. \tag{5.2}$$

Contrary to the previous cases, a functional J cannot be found for the equivalent variational formulation of the problem. Therefore, we shall state the equivalent variational problem in the following form:

$$\Delta J \equiv \int_0^t dt \int_{-\infty}^{+\infty} dx(u_t + u_{xxx})\Delta u = 0. \tag{5.3}$$

The form (5.3), though unremarkable in appearance, yet surprisingly serves the purposes very well.

Let us now take the trial solution again like (4.4):

$$u = A(x,t)\phi(S(x,t)), \tag{5.4}$$

where ϕ again satisfies the conditions (4.5)–(4.9). From (5.4), we obtain

$$u_t = A_t\phi + AS_t\phi', \tag{5.5}$$

$$u_{xxx} = A_{xxx}\phi + (3A_{xx}S_x + 3A_xS_{xx} + AS_{xxx})\phi' + 3[A_x(S_x)^2 + AS_xS_{xxx}]\phi'' + A(S_x)^3\phi''', \tag{5.6}$$

and

$$\Delta u = \phi\Delta A + A\phi'\Delta S. \tag{5.7}$$

To find ϕ, let us again take

$$u = \phi(s(x,t)). \tag{5.8}$$

Substitute in (5.1), and we obtain

$$s_t\phi' + s_{xxx}\phi' + 3s_{xx}s_x\phi'' + s_x^3\phi''' = 0. \tag{5.9}$$

Assume s_t and s_x to be constants; then we see the suggested $\phi(S)$ is

$$\phi = \sqrt{2}\sin(S+\psi). \tag{5.10}$$

Then we obtain immediately that

$$\langle\phi'^2\rangle = 1, \quad \langle\phi\phi''\rangle = \langle\phi'\phi'''\rangle = -1,$$

$$\langle\phi\phi'''\rangle = \langle\phi'\phi''\rangle = 0.$$

Now substituting (5.5), (5.6), and (5.7) into (5.3) and carrying out the approximate integration scheme, we obtain

$$\Delta J \approx \int_0^t dt \int_{-\infty}^{+\infty} dx \{\Delta A[A_t + A_{xxx} - 3A_x(S_x)^2 - 3AS_xS_{xx}] + \Delta S[A^2S_t + 3AA_{xx}S_x + 3AA_xS_{xx} + A^2S_{xxx} - A^2(S_x)^3]\}. \tag{5.11}$$

Now S_t, S_x, and A are assumed to be slowly varying function of (x,t); thus, to the lowest order of approximation, the independent variation of ΔA as ΔS leads to

$$\Delta A: \quad A_t - 3A_x(S_x)^2 - 3AS_xS_{xx} = 0, \tag{5.12}$$

$$\Delta S: \quad S_t - (S_x)^3 = 0. \tag{5.13}$$

A complete integral of (5.13) is

$$S = a^3t + ax + b, \tag{5.14}$$

where a and b are arbitrary constants. They represent the travelling wave solutions or the Fourier components of the general solution. The singular solution from (5.14) is easily found to be

$$S = \tfrac{2}{3}[-x/(3t)^{1/3}]^{3/2}. \tag{5.15}$$

Substituting (5.15) into (5.12), we obtain

$$tA_t + xA_x + A/2 = 0, \tag{5.16}$$

which is the same as (4.15). Thus the general solution is again

$$A = (1/\sqrt{t})P(x/t). \tag{5.17}$$

This solution is again consistent with the asymptotic expression for large t of the general solution of (5.2). In particular, if we take $P(Z) = (A_0/\sqrt{2})Z^{1/4}$, then we obtain

$$u = \frac{A_0}{(xt)^{1/4}}\sin\left[\frac{2}{3}\left(\frac{-x}{(3t)^{1/3}}\right)^{3/2} + \psi\right], \tag{5.18}$$

which represents the asymptotic oscillatory solution from an initial δ-function disturbance.

Now we turn our attention to the nonlinear equation (5.1). From considerations of the physical circumstances in connection with the Korteweg–de Vries equation such as water waves, the trial solution we seek will be in the form:

$$u = A(x,t)\phi(S(x,t)) + B, \tag{5.19}$$

where B is a given constant and ϕ again satisfies the conditions (4.5)–(4.9). u_t, u_{xxx}, and Δu are also given by (5.5), (5.6), and (5.7), while

$$uu_x = AA_x\phi^2 + A^2S_x\phi\phi' + BA_x\phi + BAS_x\phi'. \tag{5.20}$$

Now we substitute (5.5), (5.6), (5.7), and (5.20) into

$$\Delta J \equiv \int_0^t dt \int_{-\infty}^{+\infty} dx(u_t + uu_x + u_{xxx})\Delta u = 0. \tag{5.21}$$

Thus we obtain approximately

$$\Delta J \approx \int_0^t dt \int_{-\infty}^{+\infty} dx \{\Delta A[A_t + A_{xxx} + (3A_xS_x^2 + 3AS_xS_{xx})\langle\phi\phi''\rangle + BA_x + AA_x\langle\phi^3\rangle] + \Delta SA[\alpha(AS_t + 3A_{xx}S_x + 3A_xS_{xx} + AS_{xxx} + ABS_x) + AS_x^3\langle\phi'\phi'''\rangle + AA_x\langle\phi^2\phi'\rangle]\}. \tag{5.22}$$

For most cases, due to the antisymmetry of ϕ about its nodal point, i.e.,

$$\phi(S) = -\phi(2S_0 - S), \tag{5.23}$$

where

$$\phi(S_0) = 0,$$

we have

$$\langle\phi^3\rangle = \langle\phi^2\phi'\rangle = 0. \tag{5.24}$$

Since we also have $\langle\phi\phi''\rangle = -\langle\phi'^2\rangle$, thus, to the lowest order of approximation, we obtain from (5.21)

$$A_t + BA_x - 3\alpha(A_xS_x^2 + AS_xS_{xx}) = 0 \tag{5.25}$$

and

$$\alpha(S_t + BS_x) - \beta S_x^3 = 0, \tag{5.26}$$

where

$$\beta = \langle\phi''^2\rangle = -\langle\phi'\phi'''\rangle. \tag{5.27}$$

The function $\phi(S)$ will again be suggested from the original equation. Let us take

$$u = \phi(s(x,t)) + B, \tag{5.28}$$

and assume that s_x and s_t are constants; then we obtain

$$\phi' + a\phi\phi' + b\phi''' = 0, \tag{5.29}$$

where a and b are constant parameters. Thus ϕ is an elliptic function. Even though ϕ has to satisfy the conditions (4.5)–(4.7), it still contains adjustable free parameters. However, once the parameters are chosen from whatever considerations, α and β can be readily determined, and we can proceed to solve (5.25) and (5.26).

By following the similar procedure we used for the linear case, it is found that a complete integral of (5.26) is

$$S = C_1x + [(\beta/\alpha)C_1^3 - BC_1]t + C_2, \tag{5.30}$$

where C_1 and C_2 are arbitrary constants. They again represent the travelling wave solution. The singular solution from (5.30) is readily found to be

$$S = \tfrac{2}{3}[-(x - Bt)/(3\beta t/\alpha)^{1/3}]^{3/2}. \tag{5.31}$$

Substituting the last expression into (5.25), we obtain

$$A_t + BA_x + (\alpha^2/\beta)[A_x(x - Bt) + A/2]/t = 0. \quad (5.32)$$

Let us introduce the new independent variables

$$\xi = x - Bt \quad \text{and} \quad \tau = t.$$

Then (5.32) becomes

$$\tau A_\tau + (\alpha^2/\beta)(\xi A_\xi + A/2) = 0.$$

By a similar procedure for the solution of (5.16), we obtain the general solution

$$A = (1/\sqrt{\xi})P(\xi/\tau^{\alpha^2/\beta}),$$

or

$$A = [1/(x - Bt)^{1/2}]P((x - Bt)/t^{\alpha^2/\beta}),$$

where P is some arbitrary function.

6. DISCUSSION

The method presented above is simple in concept and straightforward in application; yet it yields a great deal of information. Since it is basically a direct variational method, the more we know previously about the solution of the problem, the better would be the result and simpler the analyses involved. On the other hand, one drawback of the method is the difficulty in estimating the errors involved. So far we have only applied the method to oscillatory solutions of the nonlinear waves. Whether this approach can be adapted to find nonoscillatory solutions of the nonlinear wave problems is still a subject of continuing investigation.

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Representations of the three-dimensional rotation group by the direct method

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The irreducible representations of the three-dimensional rotation group are obtained directly from the irreducible representations of its infinitesimal generators (the spin matrices), parametrized in terms of the rotation angle and the direction of the rotation axis. Expressions are given for the rotation operator $\exp(i\psi\mathbf{n}\cdot\mathbf{S})$ in terms of two different bases of $2j+1$ elements for spin j. The results are related to the spectral decomposition of the rotation operator and expressions obtained for spin projection operators along any spatial direction for arbitrary spin.

1. INTRODUCTION

A fundamental result of the theory of Lie groups is that any continuous linear group can be generated from its infinitesimal generators by exponentiation. Likewise, every irreducible representation of the covering group is obtained in this way from the irreducible representations of the corresponding Lie algebra. This is not, however, the usual way of obtaining explicit expressions for the representation coefficients of those continuous groups of interest to physicists. In the case of $O(3)$, to which we restrict ourselves in what follows, the usual method consists of considering the transformation properties under rotations of homogeneous monomials constructed from the components of a basic spinor, the transformation properties of which are known explicitly.[1]

The direct method of calculating the exponential of the spin matrices, which are the irreducible representations of the generators of the Lie algebra of $O(3)$, is well known only for the two-dimensional (spin $\frac{1}{2}$) and the three-dimensional (spin 1) representations (c.f. Sec. 2, below). For any dimensionality, a derivation of the rotation matrix for rotations about the y axis (the middle rotation in the usual parametrization in terms of Euler angles) by the direct method has been given by Lehrer-Ilamed.[2] The derivation, however, is somewhat cumbersome, requiring the solution of a linear differential equation of order equal to the dimensionality of the representation.

In this paper the representations of $O(3)$ are obtained by the direct method, the rotations being parametrized in terms of the rotation angle and the direction of the axis of rotation. That is, explicit expressions are given for $\exp(i\psi\mathbf{n}\cdot\mathbf{S})$, where $\mathbf{n}$ is a unit vector in the direction of the rotation axis and $\mathbf{S}=(S_1,S_2,S_3)$ are the angular momentum spin matrices for spin j, for rotations about the three Cartesian axes. In Sec. 3 the results of Ref. 2 are simplified (being obtained by purely algebraic methods) and generalized to an arbitrary rotation axis. The special case of a rotation about the y axis is discussed further, and the usual symmetries of the corresponding rotation matrix are shown to follow directly from the symmetries of S_2.

In Sec. 4 a more suitable basis for expressing the dependence on $\mathbf{n}$, consisting of irreducible tensors constructed from the spin matrices, is introduced. The orthogonality properties of these operators lead in an extremely direct way to the representation matrices, the dependence on the angle of rotation being expressed in terms of Gegenbauer polynomials. The resulting expressions resemble the Rayleigh expansion of a plane wave, and are formally equivalent in the limit $j\to\infty$.

In Sec. 5 the results of the two preceeding ones are related to the spectral decomposition of the rotation operator. This leads to expressions for spin projection operators along an arbitrary spatial direction.

2. PRELIMINARIES

In this section we review the usual derivation of the two-and three-dimensional representations of $O(3)$ by the direct method, pointing out the limitation inherent in the procedure and the implications for the general case.

The $(2j+1)$-dimensional irreducible representation of $O(3)$, parametrized in terms of the angle of rotation ψ and a unit vector $\mathbf{n}$ in the direction of the axis of rotation is given by the set of rotation matrices

$$D^{(j)}(\psi,\mathbf{n})=\exp(i\psi\mathbf{n}\cdot\mathbf{S}) \tag{2.1}$$

(the index j on S_k will be understood). The matrix elements of S_k are defined by

$$(S_k)_{m',m}=\langle jm'|J_k|jm\rangle, \qquad -j\leq m\leq j,$$

where

$$[J_k,J_l]=i\epsilon_{klm}J_m$$

and

$$J_3|jm\rangle=m|jm\rangle.$$

Equation (1) remains purely formal until a way of determining explicitly its matrix elements is given. The usual definition of the exponential

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S})=\sum_{k=0}^{\infty}\frac{1}{k!}(i\psi\mathbf{n}\cdot\mathbf{S})^k \tag{2.2}$$

is useful for this purpose only if the series can be summed in some way. There are two well-known cases in which this can be readily done, namely, the two-dimensional (spin $\frac{1}{2}$) and the three-dimensional (spin 1) representations.

In the first case, $S_k = \frac{1}{2}\sigma_k$ where σ_k are the Pauli matrices, which satisfy

$$(\mathbf{n}\cdot\sigma)^2 = \mathbb{I} \tag{2.3}$$

where $\mathbb{I}$ is the 2×2 unit matrix. Powers of $\mathbf{n}\cdot\mathbf{S}$ higher than the first are thus reducible to $\mathbb{I}$ or $\mathbf{n}\cdot\mathbf{S}$ and (2) leads to the well-known result

$$\exp(i\tfrac{1}{2}\psi\mathbf{n}\cdot\sigma) = \mathbb{I}\cos\tfrac{1}{2}\psi + i(\mathbf{n}\cdot\sigma)\sin\tfrac{1}{2}\psi. \tag{2.4}$$

Similarly, the spin one matrices satisfy

$$(\mathbf{n}\cdot\mathbf{S})^3 = \mathbf{n}\cdot\mathbf{S} \tag{2.5}$$

giving, for the three-dimensional representation,

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S}) = \mathbb{I} + i(\mathbf{n}\cdot\mathbf{S})\sin\psi + (\mathbf{n}\cdot\mathbf{S})^2(\cos\psi - 1). \tag{2.6}$$

This procedure is not feasable for higher-dimensional representations. The generalization of Eqs. (3) and (5) for spin j is given by

$$\prod_{m=-j}^{j}(\mathbf{n}\cdot\mathbf{S} - m\,\mathbb{I}) = 0 \tag{2.7}$$

where the $2j+1$ numbers m, the eigenvalues of $\mathbf{n}\cdot\mathbf{S}$, vary in unit increments from $-j$ to j. It follows that $(\mathbf{n}\cdot\mathbf{S})^{2j+1}$ is expressible as a linear combination

$$(\mathbf{n}\cdot\mathbf{S})^{2j+1} = \sum_{k=0}^{2j} d_k(\mathbf{n}\cdot\mathbf{S})^k \qquad (\text{spin}\,j), \tag{2.8}$$

where the d_k are numerical coefficients. For integer j only odd values of k contribute to the sum, while for half-odd integer j even values of k contribute. Thus for $j > 1$ the sum contains two or more nonzero terms, and substitution from (8) into (2) leads to hopelessly complicated expressions.

However, Eq. (8) implies that one can write

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S}) = \sum_{k=0}^{2j} c_k(\psi)\,(\mathbf{n}\cdot\mathbf{S})^k \tag{2.9}$$

where the expansion coefficients $c_k(\psi)$ depend only on the angle of rotation.

The last equation is a better starting point than (2) for the explicit determination of the representations, since it involves a finite sum of independent terms.

3. DETERMINATION OF THE EXPANSION COEFFICIENTS

To solve for the $c_k(\psi)$ we invoke an invariance argument: As the $c_k(\psi)$ are independent of $\mathbf{n}$, we may simplify (2.9) by setting $\mathbf{n} = (0, 0, 1)$ which diagonalizes both sides, leading to

$$\exp(im\psi) = \sum_{k=0}^{2j} m^k c_k(\psi), \qquad -j \le m \le j. \tag{3.1}$$

This set of linear equations can be inverted for the $c_k(\psi)$. We first simplify further by noting that unitarity of the representation, together with the Hermitian character of $(\mathbf{n}\cdot\mathbf{S})^k$, implies that $c_k(\psi)$ is real for k even, imaginary for k odd. Thus defining real coefficients $a_k(\psi)$ by

$$c_k(\psi) = \begin{cases} a_k(\psi), & k \text{ even}, \\ ia_k(\psi), & k \text{ odd}, \end{cases} \tag{3.2}$$

one obtains, taking real and imaginary parts of (3.1), separate sets of equations for k even and k odd.

We consider the cases for j integer and j half-odd integer separately.

j integer: In this case $m = 0$ is an eigenvalue and $a_0(\psi) = 1$. Equation (3.1) gives

$$\cos m\psi - 1 = \sum_{k=1}^{j} m^{2k} a_{2k}(\psi), \tag{3.3a}$$

$$m\sin m\psi = \sum_{k=1}^{j} m^{2k} a_{2k-1}(\psi). \tag{3.3b}$$

j half-odd integer:

$$\cos m\psi = \sum_{k=0}^{j-1/2} m^{2k} a_{2k}(\psi), \tag{3.4a}$$

$$m^{-1}\sin m\psi = \sum_{k=0}^{j-1/2} m^{2k} a_{2k+1}(\psi). \tag{3.4b}$$

Thus solution requires inversion of the $j\times j$ matrix M whose elements are defined by

$$M_{m,k} = m^{2k} \tag{3.5}$$

where for j integer $m, k = 1, 2, \ldots, j$ and for j half-odd integer $m = \frac{1}{2}, \ldots, j$, and $k = 0, 1, \ldots, j - \frac{1}{2}$. The matrix M can be inverted analytically (see Appendix A). Denoting by ω_{km} the elements of the inverse of M, we have

$$\omega_{km} = \frac{(-1)^{k+m} p^{(m)}_{j-k}(1^2, \ldots, j^2)}{m^2 \Pi_{s\neq m}(s^2 - m^2)}, \qquad j \text{ integer}, \tag{3.6a}$$

$$\omega_{km} = \frac{(-1)^{k+2m} p^{(m)}_{j-k-1/2}((\tfrac{1}{2})^2, \ldots, j^2)}{\Pi_{s\neq m}(s^2 - m^2)}, \qquad j \text{ half-odd integer} \tag{3.6b}$$

where $p^{(m)}_J(a, b, \ldots z)$ is a sum over permutations of products of its arguments, J at a time, without repetition and omitting m.[3]

Inverting Eqs. (3.3) and (3.4) and returning to (2.9), we obtain for the representations:

j integer:

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S}) = \mathbb{I} + \sum_{m=1}^{j}(\cos m\psi - 1)P^+_m + i\sum_{m=1}^{j} m\sin m\psi\, P^-_m. \tag{3.7}$$

j half-odd integer:

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S}) = \sum_{m=1/2}^{j}\cos m\psi\, P^+_m + i\sum_{m=1/2}^{j} m^{-1}\sin m\psi\, P^-_m, \tag{3.8}$$

where

$$P^+_m = \sum_k \omega_{km}(\mathbf{n}\cdot\mathbf{S})^{2k} \qquad (\text{all } j), \tag{3.9a}$$

$$P^-_m = \sum_k \omega_{km}(\mathbf{n}\cdot\mathbf{S})^{2k-1} \qquad (j \text{ integer}), \tag{3.9b}$$

$$P^-_m = \sum_k \omega_{km}(\mathbf{n}\cdot\mathbf{S})^{2k-1} \qquad (j \text{ half-odd integer}). \tag{3.9c}$$

The summation is from $k=1$ to j for integer j, and from $k=0$ to $j-\frac{1}{2}$ for half-odd integer j.

These equations generalize, to arbitrary spins, Eqs. (2.4) and (2.6) above. The rotations are parametrized in terms of the angle of rotation and the direction of the axis of rotation. The dependence on the first is quite simple; the dependence on the axis as defined by n, on the other hand, is not in a very convenient form. In the next section a more suitable basis for expressing this dependence will be introduced.

A particular important case, however, in which the expressions for the matrix elements simplify is that of a rotation about the y axis, which appears as the middle rotation in the usual parametrization in terms of Euler angles. These are obtained by setting $\mathbf{n}=(0,1,0)$, that is $\mathbf{n}\cdot\mathbf{S}=S_y$. In the basis in which S_z is diagonal, the nonvanishing elements of S_y are

$$(S_y)_{m+1,m}=-\tfrac{1}{2}i[(j-m)(j+m+1)]^{1/2},$$
$$(S_y)_{m-1,m}=\tfrac{1}{2}i[(j-m)(j+m+1)]^{1/2},$$

from which it follows that

$$(S_y)_{m',m}=0 \qquad \text{unless } m'-m=1, \tag{3.10a}$$
$$(S_y)_{m',m}=-(S_y)_{m,m'}, \tag{3.10b}$$
$$(S_y)_{m',m}=(S_y)_{-m,-m'}. \tag{3.10c}$$

The last symmetry corresponds to invariance under "skew reflection," i.e., reflection on the skew diagonal.

It follows from these symmetries of S_y that S_y^{2k} is symmetric, invariant under skew reflection, and has nonvanishing matrix elements only for $m-m'$ even, while S_y^{2k+1} is antisymmetric, invariant under skew reflection, and has nonvanishing elements only for $m-m'$ odd.

Thus in Eqs. (3.7) and (3.8), in the case of rotations about the y axis, P_m^+ will contribute to matrix elements with $m'-m''$ even, P_m^- to matrix elements with $m'-m''$ odd, and the angular dependence of the corresponding elements will be linear combinations of $\cos m\psi$ in the first case, of $\sin m\psi$ in the second. The resulting expressions are quite practical for determining the representation coefficients (P_m^+ and P_m^- can be readily programmed for computer calculation). As mentioned by Wigner,[4] the dependence on the angle of rotation appearing in (3.7) and (3.8) lends itself more readily to visualizing the general behavior of the coefficients than the usual representation in terms of powers of $\cos\frac{1}{2}\psi$ and $\sin\frac{1}{2}\psi$.

The symmetry properties of $d^{(j)}(\psi)=\exp(i\psi S_2)$ follow readily from those of S_y^{2k} and S_y^{2k+1} and the discussion of the last paragraph. In particular, one has

$$d^{(j)}_{m',m}(\psi)=(-1)^{m-m'}\,d^{(j)}_{m,m'}(\psi), \tag{3.11a}$$
$$d^{(j)}_{m',m}(\psi)=d^{(j)}_{-m,-m'}(\psi). \tag{3.11b}$$

These relations are usually derived by considering succesive rotations through $\pm\pi$ and $\psi\pm\pi$ and making use of the group property.[6]

4. EXPANSION IN SPHERICAL BASIS

The basis $(\mathbf{n}\cdot\mathbf{S})^k$, $0\le k\le 2j$, in terms of which the representations have been obtained is not the most convenient for exhibiting explicitly the dependence of the matrix elements on the direction of the rotation axis, which is specified by

$$\mathbf{n}=(\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta). \tag{4.1}$$

The obvious choice of functions in which to express this dependence are the spherical harmonics $Y_{lm}(\theta,\varphi)\equiv Y_{lm}(\mathbf{n})$, with l running from 0 to $2j$ for the $(2j+1)$-dimensional representation. We complement these with operator spherical harmonics generated by "polarization" from the ordinary solid harmonics[7] $\mathcal{Y}_{lm}(\mathbf{r})$. For spin j they are defined by[8]

$$Y_{lm}(\mathbf{S})=\frac{2^l}{l!}\left(\frac{(2j-l)!}{(2j+l+1)!}\right)^{1/2}(\mathbf{S}\cdot\mathrm{grad})^l\,\mathcal{Y}_{lm}(\mathbf{r}). \tag{4.2}$$

These operators, which are irreducible tensors, appear in the formulation of interactions of spin systems, as well as in the theory of angular correlations.[9]

The matrix elements of these operators are given in terms of Wigner's 3-j symbols by[8]

$$\langle jm''|Y_{lm}(\mathbf{S})|jm'\rangle=\delta_{m,m''-m'}\left(\frac{2l+1}{4\pi}\right)^{1/2}\begin{pmatrix}j & j & l\\ m' & -m'' & m\end{pmatrix}\times(-1)^{j-m'+m}. \tag{4.3}$$

It follows from the orthogonality properties of the $3-j$ symbols that

$$\mathrm{tr}\,Y^\dagger_{l'm'}(\mathbf{S})\,Y_{lm}(\mathbf{S})=(4\pi)^{-1}\delta_{ll'}\delta_{m,m'}. \tag{4.4}$$

Forming the product, invariant under a simultaneous rotation of n and a corresponding similarity transformation of the S_k, defined by

$$Y_l(\mathbf{n})\cdot Y_l(\mathbf{S})=\sum_{m=-l}^{l}Y_{lm}(\mathbf{n})^*Y_{lm}(\mathbf{S}), \tag{4.5}$$

we write, for spin j, instead of (2.9)

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S})=\sum_{l=0}^{2j}a_l(\psi)\,Y_l(\mathbf{n})\cdot Y_l(\mathbf{S}). \tag{4.6}$$

To evaluate the expansion coefficients we first simplify by setting $\mathbf{n}=(0,0,1)$. The product (4.5) then reduces to the single term

$$[(2l+1)/4\pi]^{1/2}\,Y_{l0}(S_3)$$

and Eq. (4.6) to

$$\exp(i\psi S_3)=\sum_{l=0}^{2j}a_l(\psi)\left(\frac{2l+1}{4\pi}\right)^{1/2}Y_{l0}(S_3). \tag{4.7}$$

The orthogonality relations then give at once

$$a_l(\psi)=4\pi\left(\frac{4\pi}{2l+1}\right)^{1/2}\mathrm{tr}\,(Y_{l0}(S_3)\exp(i\psi S_3)). \tag{4.8}$$

Since both $Y_{l0}(S_3)$ and $\exp(i\psi S_3)$ are diagonal in the basis $|jm\rangle$, we have

$$\begin{aligned}\mathrm{tr}(Y_{l0}(S_3)\exp(i\psi S_3))&=\sum_m\langle jm|Y_{l0}(S_3)|jm\rangle\exp(im\psi)\\&=\left(\frac{2l+1}{4\pi}\right)^{1/2}\sum_m\begin{pmatrix}j & j & l\\ m & -m & 0\end{pmatrix}(-1)^{j-m}\exp(im\psi),\end{aligned} \tag{4.9}$$

giving

$$a_l(\psi) = 4\pi H_{jl}(\psi/2), \tag{4.10}$$

where

$$H_{jl}\left(\frac{\psi}{2}\right) = \sum_m \begin{pmatrix} j & j & l \\ m & -m & 0 \end{pmatrix} (-1)^{j-m} \exp(im\psi). \tag{4.11}$$

The functions $H_{jl}(\psi/2)$ have been studied by Bander and Ytzykson[10] and by Talman[11] in connection with the representations of $O(4)$. They are related to the Gegenbauer polynomials C^{l+1}_{2j-l} by[11]

$$H_{jl}(\varphi) = l!\left(\frac{(2j-l)!}{(2j+l+1)!}\right)^{1/2} (2i\sin\varphi)^l C^{l+1}_{2j-l}(\cos\varphi), \tag{4.12}$$

and are given explicitly by

$$H_{jl}(\varphi) = i\left(\frac{(2j-l)!}{(2j+l+1)!}\right)^{1/2} (\sin\varphi)^l \frac{d^l}{d(\cos\varphi)^l} \frac{\sin(2j+1)\varphi}{\sin\varphi}. \tag{4.13}$$

The matrix elements of the representation are obtained using

$$\begin{aligned}\langle jm''|Y_l(\mathbf{n})\cdot Y_l(\mathbf{S})|jm'\rangle &= \sum_m Y_{lm}(\mathbf{n})^* \langle jm''|Y_{lm}(\mathbf{S})|jm'\rangle \\ &= \left(\frac{2l+1}{4\pi}\right)^{1/2} \begin{pmatrix} j & j & l \\ m' & -m'' & m''-m' \end{pmatrix} (-1)^{j-m'} Y_{l,m'-m''}(\mathbf{n}),\end{aligned} \tag{4.14}$$

giving

$$\langle jm''|\exp(i\psi\mathbf{n}\cdot\mathbf{S})|jm'\rangle = \sum_{l=0}^{2j} \sqrt{4\pi(2l+1)} \times \begin{pmatrix} j & j & l \\ m' & -m'' & m''-m' \end{pmatrix} (-1)^{j-m'} \times H_{jl}\left(\frac{\psi}{2}\right) Y_{l,m'-m''}(\mathbf{n}). \tag{4.15}$$

This expression for the representation matrix elements has been given by Talman[11] by considering the representations of $O(3)$ subduced by representations of $O(4)$, the latter being obtained as the direct product of two representations of $SU(2)$. This (perhaps) circuitous procedure yields, as above, the representations of $O(3)$ parametrized in terms of the rotation angle ψ and the rotation axis n. We remark that if the rotation matrix $d^{(j)}(\theta)$ for rotations about the y axis, and its properties, are considered known (as in Talman's approach), then Eq. (4.15) follows rather more simply by factoring the rotation operator $\exp(i\psi\mathbf{n}\cdot\mathbf{S})$ into a product of several rotations about the y and z axes. The details are given in Appendix B.

The present derivation, of course, requires no previous knowledge of the rotation matrices $d^{(j)}$, being based directly on the representations of the angular momentum operators and the properties of the 3-j symbols.

A different expression for the representations of $O(3)$, parametrized in terms of ψ and n has been given by Harry E. Moses[12] in terms of Jacobi polynomials (see also Ref. 13).

Equation (4.6) resembles the Rayleigh expansion for a plane wave in the direction of a vector k

$$\exp(i\mathbf{k}\cdot\mathbf{r}) = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr)\, Y_l(\hat{k})\cdot Y_l(\hat{r}) \tag{4.16}$$

where $\hat{k}$ and $\hat{r}$ are unit vectors in the directions of k and r, respectively. In fact, as $j\to\infty$ we have[14]

$$\begin{pmatrix} j & l & j \\ -m & 0 & m \end{pmatrix} \approx \frac{(-1)^{j-m}}{2j} P_l\left(\frac{m}{j}\right), \tag{4.17}$$

and in this limit

$$\begin{aligned} H_{jl}\left(\frac{\psi}{2}\right) &\approx \frac{1}{2}\int_{-1}^{1} P_l(x)\exp(ij\psi x)\,dx \\ &= i^l j_l(j\psi). \end{aligned} \tag{4.18}$$

Hence in the limit $j\to\infty$ we have, in complete analogy with the Rayleigh expansion,

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S}) \approx 4\pi\sum_l i^l j_l(j\psi)\, Y_l(\mathbf{n})\cdot Y_l(\mathbf{S}). \tag{4.19}$$

In particular, we have using (4.14)

$$\langle jj|\exp(i\psi n\cdot S)|jj\rangle \approx \exp(i\psi\mathbf{n}\cdot\mathbf{j})$$

where $\mathbf{j} = j\mathbf{e}_z$, a relation with a clear interpretation.

The limit $j\to\infty$ of the representations of $O(3)$ parametrized in terms of ψ and n is useful in the study of the spherical Bessel functions.[15] This asymptotic relationship can be given an intuitive geometrical grounding (c.f. remarks by Biedenharn and van Dam, Ref. 5, pp. 3–5).

5. SPECTRAL DECOMPOSITION OF THE ROTATION OPERATOR

Expansions (2.9) and (4.6) are closely related to the spectral decomposition of the rotation operator $\exp(i\psi\mathbf{n}\cdot\mathbf{S})$ in the $2j+1$ space spanned by the vectors $|jm\rangle$. Since the eigenvalues of $\mathbf{n}\cdot\mathbf{S}$ are the same as those of S_3, that is, the numbers m, $-j\le m\le j$, the spectral decomposition of the rotation operator is

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S}) = \sum_{m=-j}^{j} \exp(im\psi)\, P_m(\mathbf{n}) \tag{5.1}$$

where $P_m(\mathbf{n})$ is the projection operator on the eigenvector of $\mathbf{n}\cdot\mathbf{S}$ with eigenvalue m. Defining $|jm\,\mathbf{n}\rangle$ by

$$\mathbf{n}\cdot\mathbf{S}|jm\,\mathbf{n}\rangle = m|jm\,\mathbf{n}\rangle, \tag{5.2}$$

then, in Dirac notation,

$$P_m(\mathbf{n}) = |jm\,\mathbf{n}\rangle\langle\mathbf{n}\,jm|. \tag{5.3}$$

The spectral decomposition of $(\mathbf{n}\cdot\mathbf{S})^k$ for $k = 0, 1, \ldots, 2j$

$$(\mathbf{n}\cdot\mathbf{S})^k = \sum_{m=-j}^{j} m^k P_m(\mathbf{n}) \tag{5.4}$$

yields, upon inversion, formulas for the $P_m(\mathbf{n})$ in terms of the basis $(\mathbf{n}\cdot\mathbf{S})^k$. The results of section 3 give, for integer j

$$P_m(\mathbf{n}) = \frac{1}{2}\sum_{k=1}^{j} \omega_{km}[(\mathbf{n}\cdot\mathbf{S}) + m\,\mathrm{II}]\,(\mathbf{n}\cdot\mathbf{S})^{2k-1}, \tag{5.5a}$$

and for half-odd integer j

$$P_m(\mathbf{n}) = \frac{1}{2}\sum_{k=0}^{j-1/2} \omega_{km}[\mathrm{II} + m^{-1}(\mathbf{n}\cdot\mathbf{S})]\,(\mathbf{n}\cdot\mathbf{S})^{2k}. \tag{5.5b}$$

In terms of the spherical basis, comparison of (5.1) with Eqs. (4.6), (4.16), and (4.11) gives

$$P_m(\mathbf{n}) = 4\pi\sum_{l=0}^{2j} \begin{pmatrix} j & j & l \\ m & -m & 0 \end{pmatrix} (-1)^{j-m} Y_l(\mathbf{n})\cdot Y_l(\mathbf{S}). \tag{5.6}$$

These projections operators can be of use in a variety of problems involving interacting spin systems.

6. CONCLUDING REMARKS

The expressions obtained for the representations of the rotation operator $\exp(i\psi\mathbf{n}\cdot\mathbf{J})$ have, perhaps, a certain intuitive appeal. They may be seen as the generalization to the multidimensional representations of $O(3)$ of Euler's formula

$$\exp(im\varphi) = \cos m\varphi + i\sin m\varphi,$$

which gives the irreducible representations, for integer m, of the group of rotations in the plane; $\exp(i\varphi)$ is, of course, the rotation operator in the complex plane.

The ease with which the representations can be obtained from the spin matrices leads one to expect that a similar procedure will work for $O(4)$ and, in general, for $O(n)$. The spectral decomposition of the rotation operators would seem to provide an appropriate starting point.

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APPENDIX A

Inversion of the matrices M with elements $M_{mk} = m^{2k}$. We refer to Muir (Ref. 3, Chap. XI).

j integer: The values taken by m and k are $m, k = 1, 2, \ldots, j$. The matrix M can be factored as

$$M = AB, \tag{A1}$$

where

$$B = \begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{j-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{j-1} \\ & \cdot & \cdot & \cdot & \\ 1 & x_j & x_j^2 & & x_j^{j-1} \end{pmatrix} \tag{A2}$$

and A is diagonal with elements

$$A_{lm} = x_m\delta_{lm}. \tag{A3}$$

x_m is defined by

$$x_m = m^2. \tag{A4}$$

The determinant of B is a Vandermonde determinant and is given by the difference product of the x_m.

$$\det B = \prod_{k,l}{}' (x_k - x_l) \tag{A5}$$

where the prime denotes $k > l$ only in the product.

The unsigned minor of the element B_{mk} is the determinant of a matrix similar to B except that x_m and the $(k-l)$th power is missing. It is given by (Muir, p. 333)

$$\mathcal{M}_{mk} = \prod_{s\neq m} (x_s - x_m)\,p_{j-k}^{(m)}(x_1, \ldots, x_j), \tag{A6}$$

where $p_{j-k}^{(m)}(x_1, \ldots, x_j)$ is a sum of products of the x_m, $j-k$ at a time, without repetition and omitting x_m.

Hence

$$(B^{-1})_{km} = (A^{-1})_{mm}(B^{-1})_{km} = \frac{(-1)^{k+m} p_{j-k}^{m}(x_1 \ldots x_j)}{x_m \prod_{s\neq m}(x_s - x_m)} \tag{A7}$$

which is the expression given in the text.

j half-odd ineger: In this case, since $k = 0, 1, \ldots, j - \frac{1}{2}$, M is already in Vandermonde form, i.e., in the form of (A2), the only difference being in the indexing of the elements, k running as above and $m = \frac{1}{2}, \ldots j$. The same procedure (except $A = \mathrm{II}$) gives

$$(M^{-1})_{km} = \frac{(-1)^{k+2m} p_{j-1/2-k}^{(m)}(x_{1/2}, \ldots, x_j)}{\prod_{s\neq m}(x_s - x_m)}. \tag{A8}$$

APPENDIX B

To obtain Eq. (4.15) from the matrices $d^j(\theta)$ for rotations about the y axis, we write

$$\exp(i\psi\mathbf{n}\cdot\mathbf{S}) = \exp(i\varphi S_z)\exp(i\theta S_y)\exp(i\psi S_z)\exp(-i\theta S_y) \times \exp(-i\varphi S_z). \tag{B1}$$

In the basis $|jm\rangle$

$$(\exp(i\varphi S_z))_{m',m} = \exp(im\varphi)\,\delta_{m',m}.$$

and

$$(\exp(i\theta S_y))_{m',m} = d^j(\theta)_{m',m}$$

Using

$$d^j(-\theta)_{m,m''} = d^j(\theta)_{m'',m}, \tag{B2}$$

Eq. (B1) gives

$$\langle jm' \,|\, \exp(i\psi\mathbf{n}\cdot\mathbf{S}) \,|\, jm''\rangle = \exp[i(m'-m'')\varphi]\sum_{m=-j}^{j} \exp(im\psi)\,d^j(\theta)_{\widehat{m'm}}\,d^j(\theta)_{m'',m}. \tag{B3}$$

Further,

$$d^j(\theta)_{m',m}\,d^j(\theta)_{m'',m}$$

$$= (-1)^{m''-m} d^j(\theta)_{-m'',-m} d^j(\theta)_{m',m}$$

$$= (-1)^{m''-m} \sum_l (2l+1) \times \begin{pmatrix} j & j & l \\ m' & -m'' & m''-m' \end{pmatrix}$$

$$\times \begin{pmatrix} j & j & l \\ m & -m & 0 \end{pmatrix} \times d^l(\theta)_{m''-m',0}. \tag{B4}$$

Substitution in (B2) together with use of

$$d^l(\theta)_{M,0} \exp(iM\varphi) = (-1)^M \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{lM}(\theta, \varphi)$$

gives Eq. (4.15).

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The symmetrical energy–momentum tensor derived by parametrization

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With reference to a paper by Goedecke in this journal attention is drawn to the fact that already in his original paper on the subject Rosenfeld proved the equality of the results of the two general procedures of symmetrizing energy–momentum tensors, i.e., the procedure of Belinfante (1939), utilizing the angular momentum tensor, and the procedure of Rosenfeld (1940), taking the Lorentz metric limit of the manifestly symmetrical energy–momentum tensor of Riemannian space. Since Rosenfeld's presentation of his procedure may give the misleading impression that it has something to do with curved spaces, general relativity, or gravitational theory, we show in the present paper how his scheme can be recast in a form, where one merely takes resort to an infinitesimal transformation of the ordinary Lorentz coordinates to arbitrary curvilinear coordinates, describing the same original Lorentz space of zero curvature. This transformation, of course, means a parametrization of the variational principle, and the analysis can thus be performed by means of a generalization of the theory of parameter-invariant variational principles. An expression for the symmetrized energy–momentum tensor is given, which is equivalent to that given by Rosenfeld, and in which the transformation functions are seen to vanish identically. The procedure is thus seen to be not so much a limiting process as a transformation to curvilinear coordinates, construction of a symmetrical energy–momentum tensor, and a transformation back again.

In a recent paper on stress-energy tensors Goedecke[1] has mentioned that, apart from educated guesswork for special cases, there are the following two systematic schemes for symmetrizing the tensors in question: First, we have the formal procedure given by Belinfante[2] in 1939, utilizing the law of conservation of angular momentum. Second, we can calculate the Lorentz metric limit of the symmetric, canonical stress-energy tensor, derived from the actual Lagrangian, generalized to Riemannian metric.

Before applying these two schemes to various physical fields, showing in each case that the results are indeed equal, Goedecke remarks that to his knowledge the presumed equality of the results of the two procedures has never been proven in general. This remark makes it appropriate to recall the fact that such a proof was given at an early stage, namely by Rosenfeld[3] in the paper of 1940, where the method of utilizing Riemannian metric for symmetrizing the energy—momentum tensor was presented for the first time.

Now, from Rosenfeld's presentation the reader may very easily get the impression that the symmetrization of the stress-energy tensor by means of Riemannian metric has something to do with curved spaces, general relativity or gravitational theory. Since, however, this is not in the least the case, it may be of some interest to demonstrate that Rosenfeld's procedure can be readily cast in a form, where one merely takes resort to an infinitesimal transformation of the ordinary Lorentz coordinates to arbitrary curvilinear coordinates, describing the same Lorentz space of zero curvature. For such a recast, of which a brief account is given in the following, use is only made of the theory of parameter-invariant variational principles, presented, e.g., by Rund,[4] and generalized by Linder[5] as to include also a simultaneous transformation of the field components.

We start out with ordinary Lorentz coordinates $x^k = (x, y, z, t)$ with the pseudo-Cartesian metric $\eta_{kl} = \eta^{kl} = \delta_{kl} - 2\delta_{k4}\delta_{l4}$. Consider a field theory, where the Lagrangian $L(Q_A, Q_{A,k})$ is a function of certain field components Q_A and their first order derivatives $Q_{A,k} = \partial Q_A / \partial x^k$. The variational principle for the field thus reads

$$\delta_A \int L(Q_A, Q_{A,k})\, d^4x = 0 \quad (d^4x = dx^1\, dx^2\, dx^3\, dx^4), \tag{1}$$

where δ_A denotes variation with respect to the field components Q_A. We obtain

$$\delta_A L \equiv \left[\frac{\partial L}{\partial Q_A} - \left(\frac{\partial L}{\partial Q_{A,k}}\right)_{,k}\right] \delta Q_A = 0, \tag{2}$$

giving the extremal equations

$$L_A \equiv \frac{\partial L}{\partial Q_A} - \left(\frac{\partial L}{\partial Q_{A,k}}\right)_{,k} = 0. \tag{3}$$

We now make the following infinitesimal transformation of the integration parameters x^k in the variational principle:

$$x^k = x^k(u^\alpha), \quad u^\alpha = u^\alpha(x^k), \tag{4}$$

and a simultaneous transformation of the field components, being a special case of a generalization of the theory of Rund,[4] studied by Linder[5]:

$$Q_A = Q_A(Q_\Gamma, x^k_{,\alpha}), \quad Q_\Gamma = Q_\Gamma(Q_A, u^\alpha_{,k}). \tag{5}$$

With $J = |x^k_{,\alpha}|$ and $d^4u = du^1\, du^2\, du^3\, du^4$ we obtain

$$\delta \int \Lambda\, d^4u = 0, \quad \Lambda = LJ, \tag{6}$$

where the field components now are $Q_\Gamma(u^\alpha)$ and $x^k(u^\alpha)$. Thus, by means of (4) and (5), the new Lagrangian Λ is considered as a function of Q_Γ, $Q_{\Gamma,\alpha}$, $x^k_{,\alpha}$ and also, necessarily, of $x^k_{,\alpha\beta}$.

The variation δ_Γ with respect to Q_Γ is seen to be

$$\delta_\Gamma \Lambda \equiv \left[J\frac{\partial L}{\partial Q_A} - \left(J\frac{\partial L}{\partial Q_{A,k}} u^\alpha_{,k}\right)_{,\alpha}\right] \delta Q_A = 0 \tag{7}$$

with

$$\delta Q_A = \frac{\partial Q_A}{\partial Q_\Gamma}\, \delta Q_\Gamma\,. \tag{8}$$

As is seen from (5) any assigned variation of Q_A can be obtained from a suitable variation of Q_Γ. The parametrized variational principle gives thus

$$J\frac{\partial L}{\partial Q_A} - \left(J\frac{\partial L}{\partial Q_{A,k}}u^\alpha_{,k}\right)_{,\alpha} = 0. \tag{9}$$

writing $()_{,k}$ for $()_{,\alpha}u^\alpha_{,k}$ after using the first of the Piola identities

$$(Ju^\alpha_{,k})_{,\alpha} \equiv 0, \quad (J^{-1}x^k_{,\alpha})_{,k} \equiv 0, \tag{10}$$

the Eqs. (9) are seen to reduce to (3), showing that the Q_Γ-extremals of (6) are identical with the Q_A-extremals of (1), only, of course, expressed in the new independent coordinates and new field components.

Since the Lagrangian Λ is independent of x^k, the x^k-extremals of (6) are "cyclic," having the form of conservation theorems, viz.

$$\frac{\delta_x\Lambda}{\delta x^k} \equiv \left[-\frac{\partial\Lambda}{\partial x^k_{,\alpha}} + \left(\frac{\partial\Lambda}{\partial x^k_{,\alpha\beta}}\right)_{,\beta}\right]_{,\alpha} = 0, \tag{11}$$

where $\delta_x\Lambda$ is the variation with respect to x^k. Since the variational principle (6) is parameter-invariant, the x^k-extremals (11) are not independent of the Q_Γ-extremals (9), but are satisfied in virtue of the latter and can thus be deduced from them.

By choosing different forms of the transformation (4), (5) the extremals (11) can take different forms, e.g., different with respect to additive divergence-free quantities within the bracket [ ]. If, e.g., we choose $Q_\Gamma = Q_A$ and observe that

$$Q_{A,l} = Q_{A,\beta}u^\beta_{,l}, \tag{12}$$

$$\frac{\partial J}{\partial x^k_{,\alpha}} = Ju^\alpha_{,k}, \tag{13}$$

$$\frac{\partial u^\beta_{,l}}{\partial x^k_{,\alpha}} = -u^\beta_{,k}u^\alpha_{,l}, \tag{14}$$

we obtain by virtue of (10)

$$\frac{\partial_x\Lambda}{\delta x^k}J^{-1} \equiv -\left(L\frac{\partial J}{\partial x^k_{,\alpha}} + J\frac{\partial L}{\partial Q_{A,l}}Q_{A,\beta}\frac{\partial u^\beta_{,l}}{\partial x^k_{,\alpha}}\right)_{,\alpha}J^{-1}$$

$$= -\left(L\delta_{kl} - \frac{\partial L}{\partial Q_{A,l}}Q_{A,k}\right)_{,l} = 0, \tag{15}$$

i.e., the energy–momentum conservation law, expressed by means of the canonical, nonsymmetrized tensor.

Another choice of the transformation, which leads to an equivalent of Rosenfeld's procedure, is to let the transformation (5) be the transformation of the field components under a general coordinate transformation (4), according to their transformation properties as tensors or spinors. If the original theory is Lorentz-invariant, we know that under such a transformation the Lagrangian Λ takes the form of a scalar density under Riemannian transformations, the $x^k_{,\alpha}$ and $x^k_{,\alpha\beta}$, introduced by the transformation (4), (5), occurring only in the combinations given by

$$g_{\alpha\beta} = x^k_{,\alpha}x^l_{,\beta}\eta_{kl}, \quad \eta_{kl} = u^\alpha_{,k}u^\beta_{,l}g_{\alpha\beta} \tag{16}$$

and by $g_{\alpha\beta,\gamma}$, entering in the Christoffel symbols of the covariant derivatives. This is an evident fact in the case of the Q_A : s being tensor components, and by the way, in this case also valid for finite transformations. It is also seen to be true for the spinors, in any case for infinitesimal transformations, the only ones necessary for our purpose. In fact, it follows immediately, e.g., from the representations of the matrices of the Dirac equation in Riemannian metric, utilized by Goedecke.

This structure of the transformed equations being guaranteed, the variation $\delta_x\Lambda$ can be written

$$\delta_x\Lambda \equiv \frac{\delta\Lambda}{\delta g_{\alpha\beta}}\delta_x g_{\alpha\beta}, \tag{17}$$

where

$$\frac{\delta\Lambda}{\delta g_{\alpha\beta}} \equiv \frac{\partial\Lambda}{\partial g_{\alpha\beta}} - \left(\frac{\partial\Lambda}{\partial g_{\alpha\beta,\gamma}}\right)_{,\gamma}, \tag{18}$$

and where, from (16), we have

$$\delta_x g_{\alpha\beta} = \eta_{kl}x^l_{,\beta}\delta x^k_{,\alpha} + \eta_{kl}x^k_{,\alpha}\delta x^l_{,\beta}. \tag{19}$$

We thus obtain

$$\delta_x\Lambda \equiv \left(\frac{\delta\Lambda}{\delta g_{\alpha\beta}} + \frac{\delta\Lambda}{\delta g_{\beta\alpha}}\right)x^k_{,\alpha}\eta_{kl}\delta x^l_{,\beta} \equiv -\eta_{ml}\left[\left(\frac{\delta\Lambda}{\delta g_{\alpha\beta}} + \frac{\delta\Lambda}{\delta g_{\beta\alpha}}\right)x^m_{,\alpha}\right]_{,\beta}\delta x^l. \tag{20}$$

The x-extremals are thus, after multiplication with η^{kl},

$$\left[\left(\frac{\delta\Lambda}{\delta g_{\alpha\beta}} + \frac{\delta\Lambda}{\delta g_{\beta\alpha}}\right)x^k_{,\alpha}\right]_{,\beta} = 0. \tag{21}$$

Since $[\,]_{,\beta} = [\,]_{,l}x^l_{,\beta}$, we obtain by means of the second Piola identity (10)

$$T^{kl}{}_{,l} = 0 \tag{22}$$

with the manifestly symmetrical energy–momentum tensor

$$T^{kl} = T^{lk} = x^k_{,\alpha}x^l_{,\beta}\left(\frac{\delta\Lambda}{\delta g_{\alpha\beta}} + \frac{\delta\Lambda}{\delta g_{\beta\alpha}}\right)J^{-1}, \tag{23}$$

which contains Rosenfeld's result.

Evidently the T^{kl} of (23) is the same, independently of the choice of the coordinate system u^α. In fact, T^{kl} can according to (23) be interpreted as the tensor

$$T^{\alpha\beta} = \left(\frac{\delta(JL)}{\delta g_{\alpha\beta}} + \frac{\delta(JL)}{\delta g_{\beta\alpha}}\right)J^{-1}, \tag{24}$$

transformed to the original, pseudo-Cartesian Lorentz coordinate system, the result of such a transformation being the same irrespective of the coordinate system u^k, from which the transformation is made. The independence of the expression (23) of u^k can also be proven by a direct, although rather lengthy calculation, as has been made in the tensor case for a finite transformation by Sandin.[6]

The equivalence of the result (24) with that of Belinfante[2] is now proved in much the same way as made by Rosenfeld,[3] and the reader will find it easy to translate Rosenfeld's proof to the present scheme.

The actual calculation of T_{kl} according to (23) in special cases is of course conveniently performed by the

scheme, presented by Goedecke.[1] It may be pointed out, however, that it is not necessary to go to the limit of unity transformation, when the result is written in the form (23), since the transformation functions then vanish indentically in the result. The procedure is thus not so much a limiting process as a transformation to curvilinear coordinates, construction of a symmetrical energy–momentum tensor, and a transformation back again to the original coordinates.

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Heisenberg subgroups of semisimple Lie groups

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The restriction of a unitary representation of a semisimple Lie group to a Heisenberg subgroup H_n is shown to be quasiequivalent to the regular representation of H_n. Spectral properties of elements of the Heisenberg subgroup are described. Conditions under which an element of a semisimple Lie algebra may be embedded in a Heisenberg algebra are found.

INTRODUCTION

Suppose an element x in the Lie algebra $\mathcal{G}$ of a Lie group G can be embedded in a three-dimensional Heisenberg subalgebra $\{x, y, z\}$ of $\mathcal{G}$ with $[x, y] = z$, $[x, z] = [y, z] = 0$. Thus x will, together with y, satisfy the CCR. It is known that such an embedding controls to a large extent the spectrum of x in the differential of any unitary representation of G. In this paper we examine the above situation when G is a simple Lie group. More generally, we first examine the restriction of a unitary irreducible representation π of G to an arbitrary Heisenberg subgroup of G with Lie algebra $\{x_i, y_j, z\}$, $[x_i, y_j] = \delta_{ij} z$. In particular, upon restricting $d\pi$, the differential of π, to the generators x_i, y_j, we obtain a complete analysis of their spectral properties. Their spectral invariants are independent of the representation π and the semisimple group G. For a class of simple Lie groups we obtain sufficient algebraic conditions that an element of the Lie algebra be embedded in a Heisenberg algebra. We finally apply these results to Poincaré subgroups of G.

Let G be a Lie group with Lie algebra $\mathcal{G}$. Let π be a continuous irreducible unitary representation of G. If $x \in \mathcal{G}$, $\pi(\exp(tx))$ is a continuous one parameter group of unitary operators, and by Stone's theorem has a skew-adjoint infinitesimal generator $d\pi(x)$ such that $\pi(\exp(tx)) = \exp(td\pi(x))$, $\forall\ t \in R$. The $d\pi(x)$, $x \in \mathcal{G}$, have a common dense domain and $x \to d\pi(x)$ defines a representation of $\mathcal{G}$ by essentially skew-adjoint operators.

Now let G be a simple Lie group. Suppose $H_n \subset G$ is a $2n+1$ parameter Heisenberg subgroup, that is H_n is a nilpotent Lie group whose Lie algebra $\mathcal{H}$ has generators $\{x_1, \ldots, x_n, y_1, \ldots, y_n, z\}$ with commutation relations $[x_i, y_j] = \delta_{ij} z$, $[x_i, z] = [y_j, z] = 0$. We shall examine the restriction of π to H_n and $d\pi$ to the generators x_i, y_j. First, recall the dual object of H_n. The irreducible unitary representations U of H_n fall into two distinct classes, according to the scalar value of dU on the center (z). Those for which $d\pi(z) = 0$ are one-dimensional, being just lifts to H_n of characters of the vector group E^{2n} of $2n$-dimensional Euclidean space. On the other hand, for each $\lambda \neq 0$ there exists an infinite-dimensional irreducible unitary representation π_λ for which $d\pi_\lambda(z) = i\lambda$. The classification of these representations is given by the celebrated Stone–von Neuman theorem.[1]

The Hilbert space of these representations may be taken to be $L_2(E^{2n})$ and $(-i\, d\pi_\lambda(x_i),\ -i\, d\pi_\lambda(y_i))$ are realized as the usual operators of differentiation and multiplication in coordinate directions. Thus

$$d\pi_\lambda(x_i) = \frac{\partial}{\partial x_i},$$

$$d\pi_\lambda(y_i) = i\lambda y_i,$$

$$d\pi_\lambda(z) = i\lambda.$$

The representations $\{\pi_\lambda \mid \lambda \in R - \{0\}\}$ are mutually inequivalent. Thus $R - \{0\}$ parameterizes the infinite-dimensional representations and the Plancherel formula for H_n, which gives the decomposition of the regular representation of H_n, is obtained as described below.

Fix an infinite-dimensional representation π_λ. If f is a C^∞ function on H_n with compact support, define the operator

$$\pi_\lambda(f) = \int_{H_n} f(g)\, \pi_\lambda(g)\, dg, \quad dg \text{ Haar measure.}$$

Then $\pi_\lambda(f)$ is of trace class and $X_{\pi_\lambda}(f) = \mathrm{Tr}(\pi_\lambda(f))$ is a distribution on H_n called the global character of π_λ. We then have

$$f(e) = c \int_{-\infty}^{\infty} X_{\pi_\lambda}(f)\ |\lambda|^n d\lambda, \quad f \in C_c^\infty(R),$$

where e is the identity of H_n and $d\lambda$ the Lebesque measure, which is the Plancherel formula for H_n.[2] The Plancherel measure $c|\lambda|^n d\lambda$, where c is a normalization constant, is thus concentrated on the infinite-dimensional representations of H_n.

We return now to the situation outlined above. Thus $H_n \subseteq G$, G a simple Lie group, and π is a continuous irreducible unitary representation of G. Denoting the direct sum of countably infinitely many copies of a representation π by $\infty \cdot \pi$, we have:

Theorem 1: $\pi|_{H_n}$ is contained in $\infty \cdot R_n$, where R_n is the regular representation of H. If G is not a group of automorphisms of a bounded symmetric domain, $\pi|_{H_n}$ is unitarly equivalent to $\infty \cdot R_n$.

Proof: The decomposition of $\pi|_{H_n}$ is determined by the spectrum of $-id_\pi(z)$. The relations $[x_i, y_j] = \delta_{ij} z$ imply that $\mathrm{ad}z$ is nilpotent.[3] Thus z generates a noncompact one-parameter subgroup $[\exp(tz)]$, $\forall\ t \in R$. Since π is irreducible, there is no nonzero vector ψ in the Hilbert space of π such that $\pi(g)\psi = \psi$, $\forall\ g \in G$. The results of Moore[4] now imply that there is no nonzero vector $\psi \in H$ such that $\pi(\exp(tz))\psi = \psi$, $\forall\ t \in R$. In particular, $\{0\}$ is not an isolated eigenvalue of $-id\pi(z)$. Moreover,

it is shown in Ref. 4 that the self-adjoint operator $-id\pi(z)$ is unitarily equivalent to the multiplication operator acting on the space of square integrable functions from an interval I to an infinite-dimensional Hilbert space, where I is either $(0,\infty)$, $(-\infty,0)$, or $(-\infty,\infty)$. Thus $-id\pi(z)=\infty\cdot\int_I \lambda dP_\lambda$, where dP has spectral multiplicity one and is absolutely continuous with respect to Lebesgue measure.

Moreover, if G is not a group of automorphisms of a bounded symmetric domain, then $I=(-\infty,\infty)$.[5] We thus have the direct integral decomposition

$$\pi\big|_{H_\eta}=\infty\cdot\int_I \pi_\lambda\, dP_\lambda$$

and the theorem follows from the absolute continuity of dP with respect to the Plancherel measure $|\lambda|^n d\lambda$.

QED

Upon further restricting $d\pi$ to one of the generators x_i of the Lie algebra of H_n, we obtain:

Corollary 1:

$$-id\pi(x_i)\sim\infty\cdot\int_{-\infty}^{\infty}\lambda dE_\lambda$$

where $\int_{-\infty}^{\infty}\lambda\, dE_\lambda$ is the spectral resolution of the operator $-i\,d/dx$ on $L^2(R)$. Thus, in particular, $-i\,d\pi(x)$ has spectral measure absolutely continuous with respect to Lebesgue measure, and infinite multiplicity.

We next discuss when an element $x\in\mathcal{G}$ can be embedded in a Heisenberg algebra $\{x,y,z\}\subset\mathcal{G}[x,y]=z$, $[x,z]=[y,z]=0$. We shall assume $\mathcal{G}$ is either complex, of type A_l, $l>1$, D_l, $l>2$, E_6, E_7, E_8, or a split real form of one of these algebras. Listed below are the classical linear groups whose Lie algebras have the indicated type:

Type	Complex group	Real group	Dynkin diagram
A_l, $l>1$	$SL(l+1,C)$	$SL(l+1,R)$	0-0-0- ⋯ -0
D_l, $l>2$	$SO(2l,C)$	$SO(l,l)$	0-0- ⋯ -0-0-0 (with 0 above the second 0)

We can show the following theorem.

Theorem 2: Let $\mathcal{G}$ be as above. Then if $x\in\mathcal{G}$ with ad$x$ nilpotent, x can be embedded in a three-dimensional Heisenberg algebra $\{x,y,z\}\subset\mathcal{G}$ where $[x,y]=z$, $[x,z]=[y,z]=0$.

This theorem has appeared elsewhere,[6] but for completeness we sketch a proof. Let us review the root theory of $\mathcal{G}$.

Let $\mathcal{H}$ be a Cartan subalgebra of $\mathcal{G}$. Then $\mathcal{H}$ is a maximal Abelian subalgebra of $\mathcal{G}$ and by assumption the characteristic roots of ad$_{\mathcal{G}}h$ are in the base field of $\mathcal{G}$ for all $h\in\mathcal{H}$. We have

$$\mathcal{G}=\mathcal{H}+\sum_\alpha g_\alpha$$

where α runs over the nonzero linear functionals (roots) on $\mathcal{H}$ such that there exists an $e_\alpha\neq 0$ (root vector) in g_α with $\mathrm{ad}\,h(e_\alpha)=\alpha(h)e_\alpha\ \forall\ h\in\mathcal{H}$. The spaces g_α are one-dimensional. A total order can be put on the set of roots, and we denote the positive roots with respect to this order by Φ^+.

A positive root is called *simple* with respect to this order if it is not the sum of two other positive roots. Any root is of the form $\sum k_i\alpha_i$ where α_i are simple roots and k_i are integers. If $\alpha=\sum k_i$, $\sum|k_i|$ is called the *level* of α, set

$$\mathcal{N}=\sum_{\alpha\in\Phi^+} g_\alpha:$$

then $\mathcal{N}$ is a maximal nilpotent subalgebra of $\mathcal{G}$. Any ad-nilpotent element of $\mathcal{G}$ can be mapped into $\mathcal{N}$ by an automorphism of $\mathcal{G}$. If e_α, e_β are root vectors in $\mathcal{N}$, we have

$$[e_\alpha,e_\beta]=\begin{cases}N_{\alpha,\beta}\,e_{\alpha+\beta}, & \text{if } \alpha+\beta \text{ is a root,}\\ 0, & \text{otherwise.}\end{cases}$$

Moreover, since the Dynkin diagram of $\mathcal{G}$ has no double bonds, for any roots α, $\beta\in\Phi^+$, $2\alpha+\beta$ is never a root, so $[e_\alpha,\ e_{\alpha+\beta}]=0$.

Proof of Theorem 2: Suppose $x\in\mathcal{G}$, ad$x$ nilpotent. By the above remarks we may assume without loss of generality that $x\in\mathcal{N}$. Thus

$$x=\sum_{\alpha\in\Phi^+} c_\alpha e_\alpha.$$

Suppose first there exists a $c_\alpha\neq 0$, where α is not the highest root of Φ^+. Then there exists a positive root β such that $\alpha+\beta$ is a root, and for this β we have $[x,e_\beta]\neq 0$. Now let β be the positive root of highest level such that $[x,e_\beta]\neq 0$. Then $[x,e_\delta]=0$ if level$(\delta)>$level(β). We assert that $\{x,e_\beta,[x,e_\beta]\}$ is a three-dimensional Heisenberg algebra.

For the remainder of the proof, all sums run over all positive roots α such that $\alpha+\beta$ is a root. Now $[x,e_\beta]=\sum d_{\alpha+\beta}e_{\alpha+\beta}$, so $[[x,e_\beta],e_\beta]=\sum d_{\alpha+\beta}[e_{\alpha+\beta},e_\beta]=0$, since $[e_{\alpha+\beta},e_\beta]=0$ for all α. Also

$$[[x,e_\beta],x]=[\sum d_{\alpha+\beta}\,e_{\alpha+\beta},x]$$
$$=\sum d_{\alpha+\beta}[e_{\alpha+\beta},x]=0,$$

since level $(\alpha+\beta)>$ level β. Finally, if $x=c_\alpha e_\alpha$, α can be mapped onto a simple root by an element of the Weyl group, which induces an automorphism of x onto the root vector corresponding to a simple root. The above argument can now be applied. QED

We conclude with a brief discussion of simple Lie groups containing the Poincaré group P. First, suppose G is one of the simple Lie groups whose Lie algebra was discussed above. Let p_0 denote the energy operator in P. O'Raifeartaigh[7] has shown that adp_0 is nilpotent. Hence we conclude from Theorem 2 and the Corollary to Theorem 1 that the spectrum of $-i\,d\pi(p_0)$ is $(-\infty,\infty)$ and the spectral measure is absolutely continuous with respect to the Lebesque measure. In fact,[8] shows that this can happen in any simple Lie group which is not the group of automorphisms of a bounded symmetric domain. On the other hand, for certain diserete series representations of a group of bounded symmetric domain, ad-

nilpotent elements may have one-sided spectrum $(0, \infty)$ or $(-\infty, 0)$, and in these representations we may have only representations with strictly positive or strictly negative energy states occuring in $\pi|_P$. In this connection, see Ref. 9.

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Boundedness below for fermion model theories. I

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The spatially cut-off Hamiltonians for the models $(\bar{\psi}\bar{\psi}\phi)_2$ and $(\bar{\psi}\bar{\psi}\phi^N + \phi^{2M})_2$ with $M > N$ are bounded below uniformly in a momentum cutoff, by using the semi-Euclidean formulation.

1. INTRODUCTION

Two interactions are considered: the generalized Yukawa (GY_2) and the Yukawa (Y_2). These are $(\lambda\bar{\psi}\psi\phi^N + \phi^{2M})_{1+1}$ and $(\lambda\bar{\psi}\psi\phi)_{1+1}$ respectively. The corresponding spatially cut-off Hamiltonians are shown to be bounded below provided $M > N$. For Y_2, this problem was first solved by Glimm in Ref. 1. GY_2 was bounded below by Federbush in Ref. 2. The methods used in this paper constitute a considerable improvement over those in Ref. 2. In particular they can be extended to prove that the lower bound is linear in the volume. This will be given in another paper. Also Y_2 and GY_2 can be treated in a uniform manner. This being so, the proof is given for Y_2, and details for GY_2 are given only in the one place where the proofs diverge appreciably.

The lower bound is obtained by estimating, uniformly in a momentum cutoff and the expectation state,

$$E_0 = -\lim_{T\to\infty} \frac{1}{T} \ln\langle e^{-TH}\rangle, \tag{1.1}$$

where H is given by (1.3). For simplicity, E_0 is first estimated for the Fock vacuum. The details for establishing a bound uniform in the expectation state are provided in an appendix. E_0 is bounded below, uniformly in the expectation and momentum cutoff, provided

$$\langle e^{-TH}\rangle \leq C_1 C_2^T, \tag{1.2}$$

where C_2 is independent of the state and the cutoff.

In Sec. 2 $\langle e^{-TH}\rangle$ is expanded by a partly renormalized type of perturbation expansion similar to those used by Glimm and Jaffe in Refs. 3, 4. The expansion is generated by applying two identities referred to as P (perturbation) and C (contraction). As in Ref. 4, the P identity is applied in unit intervals in the time axis so that the eventual bound for $\langle e^{-TH}\rangle$ will have the form of a product of bounds over unit intervals making up $[0, T]$ as required by (1.2). The expansion achieves two objectives: First the divergent quantities are exhibited and cancelled, and secondly the kernels of the remaining nondivergent quantities are rather well behaved. To increase this good behavior, one further operation is performed after the expansion is complete: The uncontracted fermion legs are given an effective momentum cutoff by moving them a short distance across neighboring exponents. This is so arranged that no further contractions occur.

In Sec. 3, by methods outlined in Ref. 5, all fermion operators are removed by an estimate that has been called "defermiation." The total Fock space is regarded as being fibered over Nelson space, and operators are estimated by taking the norm over fermion Fock space at each point in Q space [Nelson space is $L^2(Q)$]. The result is an expression which involves only commuting boson operators, and this can be estimated in a conventional manner. The antisymmetry of fermion wavefunctions enters into this "defermiation" in an essential way. Some of the operators are bounded pointwise in Q space because of the one particle per mode property. The boundedness of the exponential operators depends on the anticommutation relations. This estimate is postponed to Sec. 7.

In Sec. 4, the convergence of the expansion and thence (1.2) is proved with the help of an estimate on boson expectations, whose proof is postponed until Secs. 5 and 6. The proof of convergence involves estimating sums over fermion graphs. These estimates closely follow procedures used by Dimock and Glimm in Ref. 6.

Section 5 contains an estimate on boson expectations. The methods are very similar to those in Ref. 6. The only modifications made are necessary to handle the more singular kernels resulting from the expansion, as compared with the kernels assumed in Ref. 4. Section 6 is devoted to the proof of some estimates on kernels which are used in Secs. 4 and 5. Finally, in Sec. 7, the estimate on exponential operators, referred to in Sec. 3, is proved. This estimate substitutes for the Wick ordering bound used in $P(\phi)_2$. A simple form of Glimm's dressing transformation, in which only the fermions are dressed, is used to bound from below the pair creation and annihilation part of the interaction (cf. Ref. 2). In a similar way, a corresponding bound for GY_2 can be proved, with the aid of the ϕ^{2M} term in the GY_2 interaction. Dressing only the fermions has the merit of giving a pointwise bound on Q space. To complete the proof, a bound on the scattering part of the interaction is required. At this point Y_2 and GY_2 seem to be different. In particular it is here that $M > N$ is needed, whereas Y_2 can be considered as a special case of $M = N$. This is in fact the only significant difference between the proofs for Y_2 and GY_2. Details have been given for both. The Hamiltonian H is given by

$$H = H_{0B} + H_{0F} + \lambda \int :\bar{\psi}_K(x)\psi_K(x): \phi(x)g(x)\,dx - \tfrac{1}{2}\delta m_K^2 \int g^2(x) :\phi^2(x): dx - E_K, \tag{1.3}$$

where H_{0B} and H_{0F} are the free boson and fermion Hamiltonians:

$$H_{0B} = \int \mu(k) a^*(k) a(k)\,dk,$$

$$H_{0F} = \int \omega(p)[b^*(p)b(p) + b'^*(p)b'(p)]\,dp.$$

The subscript K represents a sharp momentum cutoff. $g(x)$ is a nonnegative spatial cutoff satisfying

$$g \in L^p \quad \forall p : 1 \le p \le \infty,$$
$$\exists \epsilon > 0 : \int |\hat{g}(k)|^2 (1 + |k|^\epsilon)\, dk < \infty, \qquad (1.4)$$
$$\int |\hat{g}(k)|^{4/3} (1 + |k|^\epsilon)\, dk < \infty.$$

These assumptions are quite mild: g can be a characteristic function, for example. The counterterms are given by perturbation theory:

$$\delta m_K^2 = -\left(\frac{\lambda^2}{\pi}\right) \int_{|p| \le K} \frac{\omega^2 + p^2 - M^2}{\omega^2} \frac{1}{2\omega}\, dp, \qquad (1.5a)$$

$$E_K = -\left(\frac{\lambda}{4\pi}\right)^2 \int_{\substack{|p_1| \le K \\ |p_2| \le K}} \frac{\omega_1\omega_2 - p_1p_2 - M^2}{\omega_1\omega_2} \frac{1}{\omega_1 + \omega_2 + \mu(k)} \frac{1}{\mu(k)}$$
$$\times |\hat{g}(p_1 + p_2 + k)|^2\, dp_1\, dp_2\, dk. \qquad (1.5b)$$

Let

$$V = \lambda \int :\bar{\psi}_K(x)\psi_K(x): \phi(x) g(x)\, dx - \tfrac{1}{2}\delta m_K^2$$
$$\times \int g^2(x) :\phi^2(x): dx - E_K. \qquad (1.6)$$

The interaction is broken up in the following way:

$$\lambda \int :\bar{\psi}_K(x)\psi_K(x): \phi(x) g(x)\, dx$$
$$= \int_{\substack{|p_1| \le K \\ |p_2| \le K}} [b^*(p_1) b'^*(p_2) + b(-p_1) b'(-p_2)]\, W_p(p_1, p_2, k)$$
$$\times \phi(k)\, dp_1\, dp_2\, dk + \int_{\substack{|p_1| \le K \\ |p_2| \le K}} [b^*(p_1) b(-p_2) + b'^*(p_1) b'(-p_2)$$
$$\times W_s(p_1, p_2, k) \phi(k)\, dp_1\, dp_2\, dk, \qquad (1.7)$$

where

$$\phi(k) = \frac{1}{\mu^{\frac{1}{2}}(k)} [a^*(k) + a(-k)],$$

$$W_p(p_1, p_2, k) = -\frac{\lambda}{(4\pi)^{1/2}} \hat{g}(p_1 + p_2 + k) \left(\frac{\omega_1\omega_2 - p_1p_2 - M^2}{\omega_1\omega_2}\right)^{1/2}$$
$$\times \operatorname{sgn}(p_1 - p_2), \qquad (1.8)$$

$$W_s(p_1, p_2, k) = -\frac{\lambda}{(4\pi)^{1/2}} \hat{g}(p_1 + p_2 + k) \left(\frac{\omega_1\omega_2 + p_1p_2 + M^2}{\omega_1\omega_2}\right)^{1/2}.$$

The cutoffs in momentum that are used in the proof will all be selected from a sequence (K_n) where n is a positive integer. Cutoffs apply only to fermion momenta until Sec. 7, in which bosons are cut off:

$$K_n = n^\alpha. \qquad (1.9)$$

α will be chosen large. The term "lower momentum cutoff" is used to indicate a momentum cutoff of the form

$$J(p_1, p_2) = \text{characteristic function of the set } \{\text{either}$$
$$|p_1| \ge L \text{ or } |p_2| \ge L\} \text{ for some } L. \qquad (1.10)$$

2. THE EXPANSION

Firstly, $\langle e^{-TH} \rangle$ is rewritten in Nelson space N. In Sec. 7 it is shown that a quadratic boson monomial, $c(\phi)$, depending on K and an $\epsilon > 0$, can be chosen so that

$$H_{0F} + V + c(\phi) \ge -O(K^\epsilon), \quad H_{0B} - c(\phi) \ge -O(1). \qquad (2.1)$$

By the Trotter product formula,

$$\langle e^{-TH} \rangle = \lim_{N \to \infty} \langle (\exp\{-T/N[H_{0B} - c(\phi)]\}$$
$$\times \exp\{-T/N[H_{0F} + V + c(\phi)]\})^N \rangle. \qquad (2.2)$$

Define $H_{0F}(s)$, $V(s)$, and $c(\phi, s)$ by substituting in H_{0F}, V, and $c(\phi)$

$$\phi(k) \to \phi(k, s), \quad b^\#(p) \to b^\#(p, s), \qquad (2.3)$$

where $\phi(k, s)$ is the partial Fourier transform of a sharp time Euclidean boson field on Nelson space. $b^\#$ denotes b^*, b, b'^*, or b' and the time dependence in $b^\#(p, s)$ is dummy, i.e., $b^\#(p, s) = b^\#(p)$. It will be used to define a time ordering.

By the Feynman–Kac–Nelson formula, as given in Ref. 7,

$$\exp\{-t[H_{0B} - c(\phi)]\} = E_0 U(t) \exp[+\int_0^t c(\phi, \tau)\, d\tau] E_0 \qquad (2.4)$$

[where E_0 projects onto the time zero slice of Nelson space, and $U(t)$ is the unitary operator induced by translation in time by t], and the Markov property:

$$\langle e^{-TH} \rangle = \lim_{N \to \infty} T\left\langle\!\!\left\langle \prod_{j=1}^{N} \exp\{-T/N[H_{0F}(jT/N) + V(jT/N) + c(\phi, jT/N)]\right.\right.$$
$$\left.\left. \exp[+\int_0^T c(\phi, \tau)\, d\tau] \right\rangle\!\!\right\rangle_N. \qquad (2.5)$$

T is a time ordering operator applying to the noncommuting fermion operators. The subscript N means that the expectation for the boson fields is taken in Nelson space with respect to the Nelson space vacuum. (2.5) is rewritten in the following symbolic manner:

$$\langle e^{-TH} \rangle = T\langle \exp\{-\int_0^T [H_{0F}(T) + V(\tau)]\, d\tau\} \rangle_N. \qquad (2.6)$$

In order to obtain an estimate with the correct dependence on T, (2.6) is rewritten as

$$\langle e^{-TH} \rangle = T\langle \prod_I \exp\{-\int_I [H_{0F}(\tau) + V(\tau)]\, d\tau\} \rangle_N, \qquad (2.7)$$

where $\int_I$ denotes integration over the time interval $[I, I+1]$ and the product runs over integers I such that $[0, T] = \cup_I [I, I+1]$.

Define

$$A(\tau) = H_{0F}(\tau) + V(\tau), \quad A_n(\tau) = H_{0F}(\tau) + V_n(\tau), \qquad (2.8)$$

where $V_n(\tau)$ is given by replacing K by K_n in (1.6). The two identities (P) and (C) which generate the expansion are now given. The Duhamel formula

$$\exp(-A) = \exp(-A_n) - \int_0^1 ds \exp(-sA)(A - A_n)$$
$$\times \exp[-(1 - s)A_n] \qquad (2.9)$$

can be applied to factors in finite time-ordered Trotter approximants and a strong limit taken to show that

$$TE_{\sigma_2} \exp[-\int_{\sigma_1}^{\sigma_2} A(\tau)\, d\tau] E_{\sigma_1}$$
$$= TE_{\sigma_2} \exp[-\int_{\sigma_1}^{\sigma_2} A_n(\tau)\, d\tau] E_{\sigma_1}$$
$$- TE_{\sigma_2} \int_{\sigma_1}^{\sigma_2} ds [A(s) - A_n(s)]$$
$$\times \exp[-\int_{\sigma_1}^{s} A_n(\tau)\, d\tau - \int_s^{\sigma_2} A(\tau)\, d\tau] E_{\sigma_1} \qquad (P)$$

(it is hoped that T, the time-ordering operator will not be confused with the time T), where $E_{\sigma_2}, E_{\sigma_1}$ project onto time slices at σ_1 and σ_2 in Nelson space and $\sigma_1 \le \sigma_2$. This formula remains valid if there are other operators present at times in the interval $[\sigma_1, \sigma_2]$.

By integrating the derivative of $\exp\{-(1 - s)[A + \omega(p)]\}$

$\times b(p)\exp(-sA)$, where $b(p)$ is to be smeared by an L^2 function, it can be shown that

$$b(p)\exp(-A) = \exp\{-[A+\omega(p)]\}b(p) + \int_0^1 ds \exp\{-(1-s)[A+\omega(p)]\} \times [V, b(p)]\exp(-sA). \quad (2.10)$$

Since iterated applications of (P) will result in stepwise time dependent momentum cutoffs, (2.10) is extended by allowing such cutoffs. Let

$$A_K(s) = H_{0F}(s) + V_K(s), \quad (2.11a)$$

where $K = K(s)$ is a stepwise time dependent momentum cutoff and $V_K(s)$ is defined by replacing K by $K(s)$ in the definition of $V(s)$. Then it follows that for $\sigma_2 \geq \sigma \geq \sigma_1$

$$TE_{\sigma_2} b(p,\sigma)\exp[-\int_{\sigma_1}^{\sigma_2} A_K(\tau)\,d\tau]E_{\sigma_1}$$

$$= TE_{\sigma_2}\exp[-\omega(p)(\sigma-\sigma_1)]b(p,\sigma_1)\exp[-\int_{\sigma_1}^{\sigma_2} A_K(\tau)\,d\tau]E_{\sigma_1}$$

$$+ TE_{\sigma_2}\int_{\sigma_1}^{\sigma} ds \exp[-\omega(p)(\sigma-s)][V_K(s), b(p,s)]$$

$$\times\exp[-\int_{\sigma_1}^{\sigma_2} A_K(\tau)\,d\tau]E_{\sigma_1}. \quad (2.11b)$$

A monomial $R = R(b^{\#}(s_1), b^{\#}(s_2), \ldots, b^{\#}(s_n))$ can be included so that

$$TE_{\sigma_2} b(p,\sigma)R\exp[-\int_{\sigma_1}^{\sigma_2} A_K(\tau)\,d\tau]E_{\sigma_1}$$

$$= TE_{\sigma_2}\exp[-\omega(p)(\sigma-\sigma_1)]b(p,\sigma_1)R$$

$$\times\exp[-\int_{\sigma_1}^{\sigma_2} A_K(\tau)\,d\tau]E_{\sigma_1}$$

$$+ TE_{\sigma_2}R\int_{\sigma_1}^{\sigma} ds\exp[-\omega(p)\sigma - s)][V_K(s), b(p,s)]$$

$$\times\exp[-\int_{\sigma_1}^{\sigma_2} A_K(\tau)\,d\tau]E_{\sigma_1} + T\sum_{s_i\leq\sigma} E_{\sigma_2}$$

$$\times R(\ldots, \exp[-\omega(p)(\sigma-s_i)][b(p), b^{\#}(s_i)], \ldots)$$

$$\times\exp[-\int_{\sigma_1}^{\sigma_2} A_K(\tau)\,d\tau]E_{\sigma_1}. \quad (C)$$

There is a similar formula for b', and the adjoints are used to move b^*, b'^* to the left.

The expansion for $\langle e^{-TH}\rangle$ is obtained as follows: An interval I is selected and (P) is applied to the corresponding factor $\exp(-\int_I A\,d\tau)$ so as to interpolate between A and A_0, i. e., choose $n=0$ in (P). The interpolating term has a new "P" vertex. (C) is now used to move the corresponding $b^{\#}$'s over to the vacuum where they annihilate. In the course of this, new "C" vertices are formed; these are not further contracted. After renormalization, the description of which is postponed for the moment, (P) is applied again in the same interval to interpolate between A and A_1. (C) is then applied as before, followed by renormalization, and so on. If (P) has been applied in a given interval n times, then the $(n+1)$th application in I is used to interpolate between A and A_n. Eventually, the expansion will terminate for I, because, if n is large enough, $K_n \geq K$. Then a new interval is selected.

It is possible for a P vertex to contract twice to a C vertex. The corresponding factor is represented by a subgraph. See Fig. 1. The lines represent fermion contractions. $s_{\nu+1}$ and s_ν are the times of the vertices which are to be integrated over. $s_{\nu+1}$ is to be integrated over $[0, T]$. This will give a result that diverges as $K\to\infty$. Split the range of integration by

$$\int_0^T ds_{\nu+1} = \int_I ds_{\nu+1} + \int_{I^c} ds_{\nu+1}$$

The complement is with respect to $[0, T]$. I is the interval containing the P vertex. The integration over I^c is not divergent. Observe from (C) that the exponent does not depend on $s_{\nu+1}$. Furthermore, the counterterms associated with ν occur in a term with the same exponent as that in the term containing the factor R_ν, represented by Fig. 1. Hence both terms may be combined to give a new one with a factor (2.12), given below, assigned to ν. For later use note that, when ν is renormalized, the cutoff in the exponent is constant in the interval $(s_\nu, I+1)$; also R_ν vanishes unless $s_{\nu+1} \in (s_\nu, I+1)$, because otherwise the momentum cutoffs on ν and $\nu+1$ are disjoint:

$$\{\int_I R_\nu\, ds_{\nu+1} + \tfrac{1}{2}\delta m_\nu^2 \int g^2(x) : \phi^2(x, s_\nu) : dx + E_\nu\}. \quad (2.12)$$

If the P vertex was introduced during the nth application of (P) in I, then

$$\delta m_\nu^2 = \delta m_K^2 - \delta m_{K_{n-1}}^2, \quad E_\nu = E_K - E_{K_{n-1}}. \quad (2.13)$$

The expression in the curly brackets will be referred to as a "cancelled renormalization subgraph." The C vertex will be referred to as having been "integrated out." Introduce the Euclidean momentum $\bar{k} = (k^0, k^1)$ and write (2.12) as

$$\int R_\nu(\bar{k}_1, \bar{k}_2) : \phi(\bar{k}_1)\phi(-\bar{k}_2) : d\bar{k}_1\, d\bar{k}_2 + \delta E_\nu, \quad (2.14)$$

where

$$R_\nu(\bar{k}_1, \bar{k}_2) = \int_{s_\nu}^{I+1} ds_{\nu+1} \int_{\substack{|p_1|\leq K \\ |p_2|\leq K}} W_p(p_1, p_2, k_1^1)\overline{W}_p(p_1, p_2, k_2^1)\rho_n(p_1, p_2)$$

$$\times\exp[-(\omega_1+\omega_2-ik_1^0)(s_{\nu+1}-s_\nu)]\exp[i(k_1^0-k_2^0)s_\nu]\,dp_1\,dp_2$$

$$+ (\tfrac{1}{2}\delta m_\nu^2/4\pi)\hat{g}^*\hat{g}(k_1^1-k_2^1)\exp[i(k_1^0-k_2^0)s_\nu], \quad (2.15)$$

$$\delta E_\nu = \int_{s_\nu}^{I+1} ds_{\nu+1}\int |W_p(p_1, p_2, k)|^2 \times\exp\{-[\omega_1+\omega_2+\mu(k)](s_{\nu+1}-s_\nu)\} \times\rho_n(p_1, p_2)\mu^{-1}(k)\,dp_1\,dp_2 + E_\nu, \quad (2.16)$$

where $\rho(p_1, p_2)$ = characteristic function of the set: either $|p_1| \geq K_n$ or $|p_2| \geq K_n$. For a given term in the expansion, let

$$\rho(I) = \text{largest fermion cutoff in the exponent in } I. \quad (2.17a)$$

Suppose, for this term, there are $n_P(I)$ P vertices in I; then by the way in which the expansion is defined and (1.9) it follows that

$$\rho(I) = n_P(I)^\alpha. \quad (2.17b)$$

When the expansion is complete, one last operation, referred to as "smoothing the uncontracted legs," is performed. Each uncontracted fermion annihilation operator in I with momentum above $\rho(I)$ is moved to the

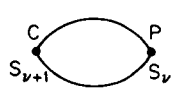


FIG. 1. A divergent subgraph.

right, or backwards in time, halfway toward the next vertex, excluding those C vertices which have been integrated out because they are part of a cancelled renormalization subgraph [see (2.12)]. Similarly, uncontracted creation operators with momentum above $\rho(I)$ move to the left. Suppose such an operator associated with vertex ν is moved halfway toward vertex ν'; then the corresponding momentum acquires an effective momentum cut-off given by

$$\exp[-\bar{\omega}(p)|s_\nu - s_{\nu'}|/2], \tag{2.18}$$

where

$$\begin{aligned}\bar{\omega}(p) &= 0 \quad \text{if } |p| \le \rho(I)\\ &= \omega(p) \quad \text{if } |p| > \rho(I)\end{aligned} \tag{2.19}$$

and $s_\nu, s_{\nu'}$, are the times of the vertices ν and ν'. No contractions can occur in the course of smoothing the uncontracted legs, because the momenta of the operators that are moved are too high to contract with the exponent, and they are not moved far enough to contract with any vertex. The expansion is written in the form

$$\langle e^{-TH}\rangle = \sum_g \int ds_g\, T\langle K_g \prod_I \exp(-\textstyle\int_I B(\tau, s_g)\, d\tau)\rangle_N, \tag{2.20}$$

where g is a label that uniquely specifies the possible vertices and their contractions. g comprises:

(1) a function $I \to n(I)$ specifying the number of vertices in I.

(2) for each I, a function from $\{1, 2, 3, \ldots, n(I)\}$ into $\{\mathrm{P}, \mathrm{C}\}$. This labels the vertices and specifies whether they are P or C vertices.

(3) a graph F on $\sum_I n(I)$ labelled vertices with two lines leaving each vertex. Each C vertex may have at most one open line, that is, a line which does not connect to another vertex. P vertices have no open lines. Open lines are labelled "low momentum" or "high momentum" to specify whether they have been moved in smoothing the uncontracted legs. (2.21a)

An open line pointing right represents an annihilation operator; an open line pointing left represents a creation operator. Lines which are not open represent contractions resulting from using (C).

To describe K_g, introduce the following notation:

$V_\nu(p_1, p_2, k)$ represents either W_p or W_s (2.21b)

[see (1.8)]; $J_\nu(p_1, p_2)$ is a cutoff on the fermion momenta associated with the vertex ν. In general J_ν will depend on g and the times of the vertices. For P vertices J_ν contains a low momentum cutoff depending on g and ν [see (P)]. Let

$$s_g = (s_\nu)_{\nu \in \{\text{vertices}\}},$$

where ν runs over the vertices that have not been integrated out [see (2.12)]. Let l denote a line in F and let t_l be the time difference associated with this line. For l connecting vertices ν and ν'

$$t_l = |s_{\nu'} - s_\nu|. \tag{2.22}$$

If l is an open line, then t_l is the quantity $|s_\nu - s_{\nu'}|$ given in (2.18).

With each vertex ν which is not part of a cancelled renormalization subgraph (note that ν can be a vertex in a renormalization subgraph with P and C vertices in different intervals) associate the kernel

$$\int Q_\nu(p_{\nu 1}, p_{\nu 2}, k)\, \phi(k, s_\nu)\, dk, \tag{2.23a}$$

where, if both lines l_1 and l_2 leaving ν are not open,

$$\begin{aligned}Q_\nu(p_{\nu 1}, p_{\nu 2}, k) &= V_\nu(p_{\nu 1}, p_{\nu 2}, k)\, J_\nu(p_{\nu 1}, p_{\nu 2})\\ &\quad \times \exp[-\omega(p_{\nu 1})\, t_{l_1}/2] \exp[-\omega(p_{\nu 2})\, t_{l_2}/2].\end{aligned} \tag{2.23b}$$

If one line, say l_1, is open, then

$$\begin{aligned}Q_\nu(p_{\nu 1}, p_{\nu 2}, k) &= V_\nu(p_{\nu 1}, p_{\nu 2}, k)\, J_\nu(p_{\nu 1}, p_{\nu 2})\\ &\quad \times \exp[-\bar{\omega}(p_{\nu 1})\, t_{l_1}/2] \exp[-\omega(p_{\nu 2})\, t_{l_2}/2].\end{aligned} \tag{2.23c}$$

If ν and ν' belong to a cancelled renormalization subgraph, and ν is the P vertex, then associate with (ν, ν') the kernel

$$\int R_\nu(\bar{k}_1, \bar{k}_2) : \phi(\bar{k}_1)\, \phi(-\bar{k}_2) : d\bar{k}_1, d\bar{k}_2 + \delta E_\nu, \tag{2.23d}$$

which is given by (2.15) and (2.26). $\tilde{K}_g$, the boson valued kernel of K_g, is formed by contracting the kernels (2.23a) according to the lines in the fermion graph F which g specifies. To contract two legs with momenta $p_{\nu 1}$, and $p_{\nu' 1}$, say, a factor $\delta(p_{\nu 1} + p_{\nu' 1})$ is inserted, and the arguments are integrated over.

The quantity $B(\tau, s_g)$ in (2.20) is defined as follows. For a given interval I, suppose that the P vertices are times $s_1 \cdots s_n$ with $I = s_0 \le s_1 \le s_2 \le \cdots \le s_n \le s_{n+1} = I + 1$; then for $\tau \in I$ let

$$B(\tau, s_g) = A_i(\tau) \text{ for } s_i \le \tau < s_{i+1}, \quad \text{where } i = 1, 2, \ldots, n. \tag{2.24}$$

The range of integration in (2.20) is such that each C vertex in the interval I is to be integrated over I. With the same definitions as in the paragraph above, the P vertices in I are to be integrated over the time ordered region

$$I = s_0 \le s_1 \le \cdots \le s_n \le s_{n+1} = I + 1. \tag{2.25}$$

3. DEFERMIATION

In (2.20), the operator K_g has the form of a kernel $\tilde{K}_g$, which is a function on the uncontracted fermion momenta and Q space, smeared against a product of $b^\#$'s at different times. Consider the special case wherein $\tilde{K}_g$ is smeared by only two $b^\#$'s and only depends on fermion modes in a finite-dimensional subspace, S, of the one particle fermion space. Furthermore, suppose that the operator $B(\tau, s_g)$ in (2.20) likewise depends only on modes in S. Then the fermion Fock space factors, and one need only consider the Fock space on S, which is a finite-dimensional Fock space. In this case, operators can be regarded as finite matrix-valued functions on Q space:

$$T\langle K_g \prod_I \exp(-\textstyle\int_I B(\tau, s_g)\, d\tau)\rangle_N$$

$$= T\langle K_g \exp(-\int_0^T B(\tau, s_g)\, d\tau)\rangle_N$$

$$\leq \langle \| T(K_g \exp(-\int_0^T B(\tau, s_g)\, d\tau) \|_F \rangle_N, \tag{3.1}$$

where $\| \ \|_F$ denotes the norm over fermion Fock space at a single point in Q space. It follows from the definition of the time ordered exponential that as an inequality almost everywhere on Q space

$$\left\| T\left[K_g \exp\left(-\int_0^T B(\tau, s_g)\, d\tau\right)\right]\right\|_F$$

$$\leq \lim_{N\to\infty} \left\| T\left(K_g \prod_{i=1}^{N} \exp\left[-\frac{T}{N} B\left(\frac{iT}{N}, s_g\right)\right]\right)\right\|_F. \tag{3.2}$$

To estimate the right-hand side, write

$$K_g = \sum_{\#} \sum_{ij} (\tilde{K}_g)_{ij} b_i^{\#} b_j^{\#} \quad \text{and} \quad \|b_i^{\#}\| = 1.$$

The sum over # is over possible ways of assigning the $b^{\#}$'s to the open lines specified by g. i and j refer to two orthonormal bases for S, and $(\tilde{K}_g)_{ij}$ is the matrix of $\tilde{K}_g$ with respect to these bases. Then (3.2) implies

$$\left\| T\left[K_g \exp\left(-\int_0^T B(\tau, s_g)\, d\tau\right)\right]\right\|_F$$

$$\leq \lim_{N\to\infty} \sum_{i,j,\#} \left|(\tilde{K}_g)_{ij}\right| \prod_{i=1}^{N} \left\| \exp\left[-\frac{T}{N} B\left(\frac{iT}{N}, s_g\right)\right]\right\|_F. \tag{3.3}$$

Suppose that as an operator estimate

$$B(\tau, s_g) \geq -d(\phi, \tau, s_g), \tag{3.4}$$

where $d(\phi, \tau, s_g)$ is a real-valued measurable function on Q space. Then from (3.3):

$$\| T(K_g \exp[-\int_0^T B(\tau, s_g) d\tau]) \|_F$$

$$\leq \sum_{i,j,\#} |(\tilde{K}_g)_{ij}| \exp[\int_0^T d(\phi, \tau, s_g) d\tau]. \tag{3.5}$$

This holds for any choice of bases in S. Taking the infimum over bases implies

$$\| T(K_g \exp[-\int_0^T B(\tau, s_g) d\tau]) \|_F$$

$$\leq \sum_{\#} \mathrm{Tr}\, |\tilde{K}_g| \exp[+\int_0^T d(\phi, \tau, s_g) d\tau], \tag{3.6}$$

where $|\tilde{K}_g| = (\tilde{K}_g^* \tilde{K}_g)^{1/2}$, identifying the kernel $\tilde{K}_g$ with the corresponding operator on $L^2(R)$. (3.1) and (3.6) imply

$$T\langle K_g \prod_I \exp[-\int_I B(\tau, s_g) d\tau]\rangle_N$$

$$\leq \sum_{\#} \langle \mathrm{Tr}\, |\tilde{K}_g| \prod_I \exp[+\int_I d(\phi, \tau, s_g) d\tau]\rangle_N. \tag{3.7}$$

When $\tilde{K}_g$ is smeared by more than two $b^{\#}$'s, it is a tensor product of two-fermion kernels as in (3.7). This is because any fermion graph is a collection of subgraphs which are either lines with two open ends or closed loops. The open lines correspond to two-fermion kernels, and the loops are functions on Q space, which only contribute numerical factors at a given point in Q space. Define the trace of a tensor product to be the product of the individual traces. The restriction to a finite number of modes is removed by a limiting argument. Therefore, the following lemma holds:

Lemma: Suppose $d(\phi, \tau, s_g)$ is a real-valued measurable function on Q space and that, as operators,

$$B(\tau, s_g) \geq -d(\phi, \tau, s_g).$$

Then

$$T\langle K_g \prod_I \exp[-\int_I B(\tau, s_g) d\tau]\rangle_N$$

$$\leq \langle \mathrm{Tr}\, |\tilde{K}_g| \prod_I \exp[\int_I d(\phi, \tau, s_g) d\tau]\rangle_N (\prod_I 2^{n(I)}). \tag{3.8}$$

Recall from (2.21a) that $n(I)$ is the number of vertices in interval I. The factor $2^{n(I)}$ overcounts sums over #.

4. CONVERGENCE OF THE EXPANSION

In Sec. 7, it is shown that, given $\epsilon > 0$, $\exists d(\phi, \tau, s_g)$ as in Lemma (3.8)

$$B(\tau, s_g) \geq -d(\phi, \tau, s_g), \tag{4.1a}$$

$$\langle \prod_I \exp[+2\int_I d(\phi, \tau, s_g) d\tau]\rangle_N \leq \prod_I [O(1)]^{\rho(I)\epsilon} \tag{4.1b}$$

[$\rho(I)$ is defined by (2.17a)]. (2.20), (4.1), Lemma (3.8), and the Cauchy–Schwartz inequality imply

$$\langle e^{-TH}\rangle \leq \sum_g \int ds_g \langle (\mathrm{Tr}\, |\tilde{K}_g|)^2\rangle_N^{1/2} (\prod_I [O(1)]^{[n(I)+\rho(I)\epsilon]} \tag{4.2}$$

Let l be a line in a graph. Define

$$d_l = \max\{1, \text{number of complete unit intervals that } l \text{ crosses}\}. \tag{4.3}$$

Let $\{g: n(I)\}$ denote the set of all g with a given $n(I)$ specified for each I. The following estimate is used to count fermion graphs:

$$\sum_{\{g:n(I)\}} (\prod_l d_l^{-5}) \leq \prod_I [O(1)]^{n(I)} [2n(I)]! \tag{4.4}$$

The product is over all lines in the fermion graph, F, specified by g [see (2.21a)]. A factor, $2^{n(I)}$, for each interval, I, overcounts the number of possible functions in (2.21a), part (2). A factor $O(1)^{n(I)}$ for each I overcounts the number of ways in which C vertices can have open lines. Therefore, the proof of (4.4) is reduced to showing that

$$\sum_G \prod_{l\in G} d_l^{-5} \leq \prod_I ([O(1)]^{n(I)} [2n(I)!), \tag{4.5}$$

where the sum runs over all graphs with no open lines, which can be drawn on $\sum_I n(I)$ vertices, where the vertices are fixed in advance to have either one leg or two legs. This is proved by Dimock and Glimm, Lemma (2.6) in Ref. 6. (4.2), (4.4), and (2.17b) imply, for $\epsilon > 0$,

$$\langle e^{-TH}\rangle \leq \sum_{\{n(I)\}} (\prod_I [O(1)]^{[n(I)+n(I)^{\epsilon\alpha}]} [2n(I)]!)$$

$$\times \sup_{\{g:n(I)\}} \{(\prod_l d_l^5) \int ds_g \langle (\mathrm{Tr}\, |\tilde{K}_g|)^2\rangle_N^{1/2}\}. \tag{4.6}$$

Define d_ν to be the sum of the contraction distances d_l over lines l that leave vertex ν. Let L_ν be the lower momentum cutoff in $J_\nu(p_1, p_2)$ [see (2.21b)]. In Secs. 5 and 6 the following lemma is proved.

Lemma: $\exists \eta > 0$: $\forall m \geq 0$,

$$\int ds_g \langle (\mathrm{Tr}\, |\tilde{K}_g|)^2\rangle_N^{1/2}$$

$$\leq \prod_I \left([O(1) \log^2 n(I)]^{n(I)} [n(I)!]^2 \prod_{\nu\in I} [1 + L_\nu]^{-\eta} d_\nu^{-m} \right). \tag{4.7}$$

The product over $\nu \in I$ means the product over all vertices in the interval I. (4.6) and (4.7) imply, for $\epsilon > 0$ and for all $m \geq 0$,

$$\langle e^{-TH} \rangle \leq \sum_{\{n(I)\}} \Big(\prod_I [O(1) \log^2 n(I)]^{[n(I)+n(I)^{\epsilon\alpha}]} [n(I)!]^4 \Big) \times \sup_{\{g : n(I)\}} \Big(\prod_I \prod_{\nu \in I} (1 + L_\nu)^{-\eta} d_\nu^{-m} \Big). \tag{4.8}$$

The m has been relabelled to include the d_i^5 in (4.6). Recall from the description of the expansion in Sec. 2 that if ν is a P vertex formed during the $(n+1)$th application of (P) in a given interval I, then $L_\nu = K_n$. If ν is a C vertex, $L_\nu = 0$. By replacing η by $\eta/3$, if necessary, the factor $(1 + L_\nu)$ in (4.8) can be replaced by $(1 + L'_\nu)$, where $L'_\nu = L_\nu$ if ν is a P vertex, but if ν is a C vertex, L'_ν is the lower momentum cutoff of a P vertex contracted to ν. If there are two such P vertices, then the largest lower momentum cutoff is chosen. The expansion is such that every C vertex is contracted to a P vertex, and, of course, no P vertex can contract to more than 2 C vertices.

For a fixed I and $n(I)$, define $\mathcal{G}(n(I))$ to be the set of all g which have $n(I)$ vertices in I. (4.8) implies, for $\epsilon > 0$ and all $m > 0$,

$$\langle e^{-TH} \rangle \leq \prod_I \Big[\sum_{n(I)} [O(1) \log^2 n(I)]^{[n(I)+n(I)^{\epsilon\alpha}]} (n(I)!)^4 \times \sup_{g \in \mathcal{G}(n(I))} \Big(\prod_{\nu \in I} [1 + L'_\nu]^{-\eta} d_\nu^{-m} \Big) \Big]. \tag{4.9}$$

In order to prove (1.2) and thereby bound (1.1) for the Fock vacuum, it suffices to show that, for sufficiently large m and α,

$$\sup_{g \in \mathcal{G}(n(I))} \Big(\prod_{\nu \in I} (1 + L'_\nu)^{-\eta} d_\nu^{-m} \Big) \leq O(1)[n(I)!]^{-5}. \tag{4.10}$$

For, given m and α such that (4.10) holds, choose ϵ small so that $\epsilon\alpha \leq 1$. Then (4.9) and (4.10) imply (1.2) for the Fock vacuum.

For the proof of (4.10) the following notation is introduced. For a fixed interval I, $n(I)$, and $g \in \mathcal{G}(n(I))$, define, for $i = 2, 3, 4, \cdots$, C_i to be the set of all C vertices in I which contract to a P vertex via a line l with $d_l = i$. [d_l is defined by (4.3).] Define C_1 to be the union of the set of P vertices in I with the set of all C vertices in I which contract to a P vertex via a line l with $d_l = 1$. The fact that a C vertex can contract to at most 2 P vertices implies that

$$\sup_{g \in \mathcal{G}(n(I))} \prod_{\nu \in I} (1 + L'_\nu)^{-\eta} d_\nu^{-m} \leq \sup_{g \in \mathcal{G}(n(I))} \Big(\prod_{i=1}^{\infty} \prod_{\nu \in C_i} (1 + L'_\nu)^{-\eta} d_\nu^{-m} \Big)^{1/2} \leq \sup_{g \in \mathcal{G}(n(I))} \Big(\prod_{i=1}^{\infty} i^{-m|C_i|} \prod_{\nu \in C_i} (1 + L'_\nu)^{-\eta} \Big)^{1/2}, \tag{4.11}$$

where $|C_i|$ = number of elements in C_i. Define $\tilde{C}_i$ to be the set of all P vertices that are either in C_i or contract to C vertices in C_i. The definition of L'_ν and the fact that at most two P vertices can contract to a given C vertex imply that

$$\prod_{\nu \in C_i} (1 + L'_\nu)^{-\eta} \leq \Big(\prod_{\nu \in \tilde{C}_i} (1 + L_\nu)^{-\eta} \Big)^{1/2}. \tag{4.12}$$

The definition of $\tilde{C}_i$ implies that there exists an interval, I', that contains at least $|C_i|/12$ of the P vertices in $\tilde{C}_i$. Since these P vertices are in the same interval, as a consequence of the way in which the expansion is generated, they must all have different cutoffs, L_ν, selected from the set $\{K_1, K_2, K_3, \cdots\}$. Recall from (1.9) that $K_j = j^\alpha$; therefore,

$$\prod_{\nu \in \tilde{C}_i} (1 + L_\nu)^{-\eta} \leq (|C_i|/12!)^{-\eta\alpha}. \tag{4.13}$$

(4.11), (4.12), and (4.13) imply that

$$\sup_{g \in \mathcal{G}(n(I))} \prod_{\nu \in I} (1 + L'_\nu)^{-\eta} d_\nu^{-m} \leq \sup_{g \in \mathcal{G}(n(I))} \prod_{i=1}^{\infty} [i^{-m|C_i|/4} (|C_i|/12!)^{-\eta\alpha/4}], \tag{4.14}$$

where $g \in \mathcal{G}(n(I))$ implies that $\sum_i |C_i| \geq n(I)$; therefore, the right-hand side of (4.14) can be majorized by taking the supremum over $|C_i|$ such that

$$\sum_i |C_i| = n(I). \tag{4.15}$$

This is done by first taking the log and using Lagrange multipliers, i.e., maximize

$$J = -\sum_{i=1}^{\infty} \Big[m \frac{|C_i|}{4} \log i + \frac{\eta\alpha}{4} \Big(\frac{|C_i|}{12} \Big) \Big(\log \frac{|C_i|}{12} - 1 \Big) \Big] + \lambda \Big(n(I) - \sum |C_i| \Big) \tag{4.16}$$

By Sterling's formula, the right-hand side of (4.15) is majorized by the supremum of e^J. On differentiating,

$$(m/4) \log i + (\eta\alpha/48) \log(|C_i|/12) + \lambda = 0 \quad \text{for } i = 1, 2, 3, \cdots,$$

$$\sum_{i=1}^{\infty} |C_i| = n(I). \tag{4.17}$$

When (4.17) hold,

$$J = \sum_{i=1}^{\infty} |C_i| (\lambda + \eta\alpha/48) = n(I)(\lambda + \eta\alpha/48). \tag{4.18}$$

If $m/\alpha \geq 2\eta/12$, λ can be eliminated from (4.18), by using (4.17), to show that

$$J \leq -n(I)[(\eta\alpha/48) \log n(I) - O(\eta\alpha)]. \tag{4.19}$$

(4.19) and (4.14) imply (4.10).

This completes the proof of boundedness below for the Hamiltonian except for the estimates (4.1), which are proved in Sec. 7, and Lemma (4.7), which is proved in Secs. 5 and 6.

5. ESTIMATE ON BOSON EXPECTATIONS

In this section the left-hand side of (4.7) is estimated in terms of norms on kernels. The estimates on these norms, needed to complete the proof of Lemma (4.7), are given in Sec. 6. The method is based on techniques from Ref. 6. A more elegant, but less elementary, method relying on L_p estimates and hypercontractivity is also outlined. This is taken from Ref. 7. The author is grateful to Ira Herbst for drawing his attention to the L_p method.

Let λ denote a vertex at time s_λ. Let $\bar{k}_i = (k_i^0, k_i^1)$ be Euclidean momenta. Define

$$H_\lambda(\bar{k}_1, \bar{k}_2) = \int Q_\lambda(p_1, p_2, k_1^1) \bar{Q}_\lambda(p_1, p_2, k_2^1)\, dp_1\, dp_2 \times \exp(i k_1^0 s_\lambda) \exp(-i k_2^0 s_\lambda), \tag{5.1}$$

where Q_λ was defined by (2.33). Consider the special case in which $\tilde{K}_g$ is the kernel of a two-particle fermion operator, as in (3.7); then the fact that the trace norm of a product of operators is majorized by the product of the Hilbert–Schmidt norms of the individual operators implies that

$$(\mathrm{Tr}\,|\tilde{K}_g|)^2 \le \prod_\lambda \int H_\lambda(\bar{k}_1,\bar{k}_2)\phi(\bar{k}_1)\phi(-\bar{k}_2)\,d\bar{k}_1\,d\bar{k}_2. \tag{5.2}$$

λ runs over the vertices specified by g. (5.2) continues to hold when $\tilde{K}_g$ is a tensor product of two-particle fermion operator kernels. Equivalently, one can say that (5.2) holds for any g with a fermion graph F [see (2.21a)] consisting of lines with open ends. In fact F may also include nondivergent closed fermion loops, because these are traces of products of operators of the form implied by the right-hand side of (5.2). Therefore, a general $\tilde{K}_g$ can be estimated by

$$(\mathrm{Tr}\,|\tilde{K}_g|)^2 \le \prod_\lambda \int H_\lambda(\bar{k}_1,\bar{k}_2)\phi(\bar{k}_1)\phi(-\bar{k}_2)\,d\bar{k}_1\,d\bar{k}_2 \times \prod_\mu \Big(\int R_\mu(\bar{k}_1,\bar{k}_2):\phi(\bar{k}_1)\phi(-\bar{k}_2):d\bar{k}_1,d\bar{k}_2+\delta E_\mu\Big)^2, \tag{5.3}$$

where λ runs over all vertices which are not part of cancelled renormalization subgraphs and μ runs over P vertices which are part of cancelled renormalization subgraphs. R_μ and δE_μ are given by (2.15) and (2.16). (5.3) can be rewritten as

$$(\mathrm{Tr}\,|\tilde{K}_g|)^2 \le \sum_S \prod_{\substack{\lambda \\ \mu_1\in S,\ \mu_2\in S^c}} \Big[\int H_\lambda(\bar{k}_1,\bar{k}_2)\phi(\bar{k}_1)\phi(-\bar{k}_2)\,d\bar{k}_1\,d\bar{k}_2\Big] \times\Big[\int R_{\mu_1}(\bar{k}_1,\bar{k}_2):\phi(\bar{k}_1)\phi(-\bar{k}_2):d\bar{k}_1\,d\bar{k}_2\Big][\delta E_{\mu_2}], \tag{5.4}$$

where S runs over subsets of the set, containing twice, P vertices which are part of cancelled renormalization subgraphs. The complement of S is with respect to this set.

Define

$$C(\bar{k}) = 1/(m^2+|\bar{k}|^2). \tag{5.5}$$

This is the Fourier transform of the covariance operator of the free boson measure. The vacuum expectation, or alternatively the integral with respect to the free measure of the right-hand side of (5.4), can be performed exactly so that

$$\langle(\mathrm{Tr}\,|\tilde{K}_g|)^2\rangle_N \le \sum_S \sum_G \int \prod_{\substack{\lambda \\ \mu_1\in S \\ \mu_2\in S^c}} H_\lambda R_{\mu_1}\delta E_{\mu_2} \prod_{l\in G} C(\bar{k}_l)\,d\bar{k}_l, \tag{5.6}$$

where G is a graph on the vertices labelled by μ_1, μ_2, and λ. Vertices labelled by λ have two legs which are allowed to contract to each other. Vertices labelled by μ_1 have two legs which are restricted to contract to legs on other vertices. Vertices labelled by μ_2 have no legs. l runs over the lines in G and $\bar{k}_l$ denotes the corresponding momenta. (More details are given in Ref. 6.) Let $\chi(t)$ be function in $C^\infty(R)$ such that $\chi(t)\equiv 1$, if $|t|\ge\frac{1}{2}$; $\equiv 0$, if $|t|\le\frac{1}{4}$. d_l is defined as in (4.3). Define, for each l,

$$\chi_l(t)\equiv 1, \quad \text{if } d_l = 1$$
$$\equiv \chi(t/d_l) \quad \text{if } d_l > 1. \tag{5.7}$$

Regard χ_l as being a function of two variables, with t being dual to k_0. Then, in the right-hand side of (5.6), $C(\bar{k}_l)$ can be replaced by $(\hat{\chi}_l * C)(\bar{k}_l)$ without changing its value, because vertices connected by lines with $d_l > 1$ are localized in separated intervals in time. (There is no momentum cutoff on k^0 components.) With this replacement made, regard the right-hand side of (5.6) as a product of operators. For example, for a given vertex λ, the corresponding operator would have the kernel

$$(\hat{\chi}_{l_1} * C)^{1/2}(\bar{k}_1) H_\lambda(\bar{k}_1,\bar{k}_2)(\hat{\chi}_{l_2} * C)^{1/2}(\bar{k}_2). \tag{5.8}$$

(It does not matter which square root is chosen.) Depending on how the lines l_1 and l_2 leave λ, this kernel is to be thought of as an operator either from $L^2(R^2)$ to $L^2(R^2)$ or from $L^2(R^4)$ to $\mathbb{C}$. [If l_1 and l_2 are the same line because λ is contracted to itself, then it is not treated this way. In this case λ gives rise to a constant.] The right-hand side of (5.6) is now majorized by taking Hilbert–Schmidt norms of operators and absolute values of constants. (This is a simple version of techniques used by Glimm and Jaffe in Ref. 4.) The Hilbert–Schmidt norms are simplified by the estimate, for $n \ge 0$,

$$|(\hat{\chi}_l * C)(\bar{k})| \le O(1) d_l^{-n} C(\bar{k}). \tag{5.9}$$

The proof of (5.9) is postponed. The Hilbert–Schmidt norm corresponding to a vertex λ, is thereby less than $O(1)d_{l_1}^{-n}d_{l_2}^{-n}\|C^{1/2}H_\lambda C^{1/2}\|_2$, which is majorized by $O(1)d_{l_1}^{-n}d_{l_2}^{-n}\times\mathrm{tr}(C^{1/2}H_\lambda C^{1/2})$ because $C^{1/2}H_\lambda C^{1/2}$ is a positive operator on $L^2(R^2)$. These remarks prove that, for $n \ge 0$,

$$\langle(\mathrm{Tr}\,|\tilde{K}_g|)^2\rangle_N \le \sum_S \prod_{\mu_1,\mu_2,\lambda} \|Q_\lambda\|_{C,2}^2 \|R_{\mu_1}\|_{C,2}|\delta E_{\mu_2}| \times \sum_G \prod_{l\in G} O(1) d_l^{-n}, \tag{5.10}$$

where μ_1 runs over S and μ_2 over S^c and, by definition,

$$\|Q_\lambda\|_{C,2}^2 = \int |Q_\lambda(p_1,p_2,\bar{k})|^2 C(\bar{k})\,d\bar{k}\,dp_1\,dp_2,$$
$$\|R_{\mu_1}\|_{C,2}^2 = \int |R_{\mu_1}(\bar{k}_1,\bar{k}_2)|^2 C(\bar{k}_1)C(\bar{k}_2)\,d\bar{k}_1\,d\bar{k}_2. \tag{5.11}$$

Note that $\|Q_\lambda\|_{C,2} = \mathrm{tr}(C^{1/2}H_\lambda C^{1/2})$ by (5.1). From Ref. 6, Lemma (2.6),

$$\sum_G \prod_{l\in G} O(1) d_l^{-5} \le \prod_I O(1)^{n(I)}[2n(I)]!; \tag{5.12}$$

therefore, (5.10) implies

$$\langle(\mathrm{Tr}\,|\tilde{K}_g|)^2\rangle_N \le \sum_S \prod_{\mu_1,\mu_2,\lambda} \|Q_\lambda\|_{C,2}^2 \|R_{\mu_1}\|_{C,2}|\delta E_{\mu_2}| \times \prod_I O(1)^{n(I)}[2n(I)]!. \tag{5.13}$$

The proof of Lemma (4.7) will now follow from estimates on the norms in (5.13). These are given in the next section.

(5.9) is proved by

$$\|C^{-1}(\hat{\chi}_l * C)\|_\infty \le \|(m^2-\Delta)\chi_l \hat{C}\|_1 \le O(1) d_l^{-n},$$

where the last inequality follows from the exponential decay of $\hat{C}$ away from the origin.

The L_p method is now given. Suppose f_i are two particle polynomials on Nelson space, whose time supports are localized in unit intervals denoted by I in the usual way. Suppose $n(I)f_i$'s are localized in I in this manner:

$$\langle \prod_i f_i \rangle_N = \langle \prod_I \prod_{i\in I} f_i \rangle_N$$
$$= \left\langle \prod_I \left[E_{I+1} \left(\prod_{i\in I} f_i \right) E_I \right] \right\rangle_N, \tag{5.14}$$

where E_I denotes the projection onto the time slice $t = I$ in Nelson space. This is not to be confused with the projection onto the interval I. This notation is described in Ref. 7:

$$\leq \prod_I \left\| E_{I+1} \left(\prod_{i\in I} f_i \right) E_I \right\|. \tag{5.15}$$

The bars denote the operator norm on $L^2(Q)$, i. e., Nelson space. By hypercontractivity (see Chap. III, Ref. 7), (5. 15) is overestimated by

$$\prod_i \left\| \prod_{i\in I} f_i \right\|_p \tag{5.16}$$

provided p sufficiently large. Applying the Hölder inequality to (5. 16) implies

$$\langle \prod_i f_i \rangle \leq \prod_I \prod_{i\in I} \|f_i\|_{pn(I)}. \tag{5.17}$$

Since f_i is a two-particle operator for each i, Nelson's best estimate applied to the operator $\exp(-tN)$ for sufficiently large t shows that

$$\|f_i\|_{pn_I} \leq (pn(I) - 1)\|f_i\|_2. \tag{5.18}$$

Nelson's best estimate is also described in Ref. 7, Chap. III. (5. 17) and (5. 18) imply that

$$\langle \prod_i f_i \rangle \leq \prod_I \left(O(1)^{n(I)} n(I)! \prod_{i\in I} \|f_i\|_2 \right); \tag{5.19}$$

(5. 19) applied to (5. 4) implies (5. 13).

6. ESTIMATES ON KERNELS

In this section the five estimates (6. 1)—(6. 5) given below, are proved. For (6. 1), suppose λ is a completely contracted vertex, i. e., in the fermion graph F, neither of the lines l_1 and l_2 which leave λ are open. Then, for $n \geq 0$ and some $\eta > 0$ independent of n,

$$\|Q_\lambda\|_{C,2} \leq O(1)(1 + L_\lambda)^{-\eta} d_{l_1}^{-n} d_{l_2}^{-n} t_{l_1}^{-5/16} t_{l_2}^{-5/16}, \tag{6.1}$$

where L_λ is the low momentum cutoff associated with λ ($L_\nu \neq 0$ only for P vertices). t_l is defined by (2. 22). For (6. 2), suppose λ is not completely contracted so that l_1 is an open line in F. Then, for $n \geq 0$,

$$\|Q_\lambda\|_{C,2} \leq O(1)(1 + L_\lambda)^{-\eta} \log^2 n(I)^\alpha d_{l_2}^{-n} t_{l_1}^{-1/16} t_{l_2}^{-1/2}. \tag{6.2}$$

The factor $(1 + L_\lambda)^{-\eta}$ is put in merely to make the notation uniform. In fact, since λ has an open line, λ is a C vertex and therefore $L_\lambda = 0$. For (6. 3) and (6. 4) suppose μ_1 and μ_2 are P vertices in cancelled renormalization subgraphs; then

$$\|R_{\mu_1}\|_{C,2} \leq O(1)(1 + L_{\mu_1})^{-\eta} (I + 1 - s_{\mu_1})^{-1/32}, \tag{6.3}$$
$$|\delta E_{\mu_2}| \leq O(1)(1 + L_{\mu_2})^{-\eta} (I + 1 - s_{\mu_2})^{-1/32}, \tag{6.4}$$

where s_{μ_1} and s_{μ_2} are the times of the P vertices and I, as usual, is the integer that labels the unit interval containing μ_1 (μ_2). For (6. 5) the notation $I(\mu)$ is used to indicate the interval containing a vertex μ and μ runs over all P vertices which are part of cancelled renormalization subgraphs:

$$\int ds_g \prod_{l\in F} t_l^{-\sigma_l} \prod_\mu (I(\mu) + 1 - s_\mu)^{-1/32} \leq \prod_I O(1)^{n(I)} n(I)!, \tag{6.5}$$

where if l is open, $\sigma_l = \frac{1}{16}$; if l connects two completely contracted vertices, $\sigma_l = \frac{10}{16}$; if l connects to a vertex which is not completely contracted, $\sigma_l = \frac{13}{16}$. The case in which l connects two vertices which are both not completely contracted cannot occur by the way the expansion is defined.

Lemma (4. 7) is proved by combining (6. 1)—(6. 5) with (5. 13) and noting that the number of subsets S summed over in (5. 13) is less than $\prod_I 2^{n(I)}$.

Proof of (6. 1): from (2. 23b), (1. 8), and (5. 11), for $n \geq 0$,

$$\|Q_\lambda\|_{C,2}^2 \leq O(1) \int |\hat{g}(p_1 + p_2 + k^1)|^2 J_\lambda(p_1, p_2) \exp(-\omega_1 t_{l_1})$$
$$\times \exp(-\omega_2 t_{l_2}) C(\bar{k})\, dp_1\, dp_2\, d\bar{k} \tag{6.6}$$
$$\leq O(1) \int |\hat{g}(p_1 + p_2 + k^1)|^2 J_\lambda(p_1, p_2) \omega_1^{-10/16} \omega_2^{-10/16}$$
$$\times \mu^{-1}(k^1)\, dp_1\, dp_2\, dk^1\, d_{l_1}^{-2n} d_{l_2}^{-2n} t_{l_1}^{-10/16} t_{l_2}^{-10/16}. \tag{6.7}$$

J_λ contains a lower cutoff at L_λ; therefore,

$$\|Q_\lambda\|_{C,2}^2 \leq O(1) \int_{\substack{|p_1| \geq L_\lambda \\ \text{or} \\ |p_2| \geq L_\lambda}} |\hat{g}(p_1 + p_2 + k^1)|^2 \omega_1^{-10/16} \omega_2^{-10/16}$$
$$\times \mu^{-1}(k^1)\, dp_1\, dp_2\, dk^1\, d_{l_1}^{-2n} d_{l_2}^{-2n} t_{l_1}^{-10/16} t_{l_2}^{-10/16} \tag{6.8}$$
$$\leq O(1)(1 + L_\lambda)^{-2\eta} d_{l_1}^{-2n} d_{l_2}^{-2n} t_{l_1}^{-10/16} t_{l_2}^{-10/16}. \tag{6.9}$$

(1. 4) is used to obtain the last inequality. η is some small number > 0.

Proof of (6. 2): from (2. 23c), (1. 8), (5. 11), and the fact that $\rho(I) \leq n(I)^\alpha$ [see (2. 17) for the definition of $\rho(I)$]

$$\|Q_\lambda\|_C^2 \leq O(1) \int_{|p_1| \leq n(I)^\alpha} |\hat{g}(p_1 + p_2 + k^1)|^2 J_\lambda(p_1, p_2)$$
$$\times \exp(-\omega_2 t_{l_2}) C(\bar{k})\, dp_1\, dp_2\, d\bar{k}$$
$$+ O(1) \int_{|p_1| \geq n(I)^\alpha} |\hat{g}(p_1 + p_2 + k^1)|^2 J_\lambda(p_1, p_2)$$
$$\times \exp(-\omega_1 t_{l_1}) \exp(-\omega_2 t_{l_2}) C(\bar{k})\, dp_1\, dp_2\, d\bar{k} \tag{6.10}$$
$$\leq O(1) \int_{|p_1| \leq n(I)^\alpha} |\hat{g}(p_1 + p_2 + k^1)|^2 \omega_2^{-1} \mu(k^1)^{-1}\, dp_1\, dp_2\, dk^1$$
$$\times d_{l_2}^{-2n} t_{l_2}^{-1} + O(1) \int_{|p_1| \geq n(I)^\alpha} |\hat{g}(p_1 + p_2 + k^1)|^2 \omega_2^{-1} \omega_1^{-1/8}$$
$$\times \mu(k^1)^{-1}\, dp_1\, dp_2\, dk^1\, d_{l_2}^{-2n} t_{l_2}^{-1} t_{l_1}^{-1/8}. \tag{6.11}$$

The proof of (6. 2) is completed by the elementary estimates:

$$\int_{|p_1| \leq n(I)^\alpha} |\hat{g}(p_1 + p_2 + k^1)|^2 \omega_2^{-1} \mu(k^1)^{-1}\, dp_1\, dp_2\, dk^1$$
$$\leq O(1) \log^2 n(I)^\alpha,$$
$$\int_{|p_1| \geq n(I)^\alpha} |\hat{g}(p_1 + p_2 + k^1)|^2 \omega_2^{-1} \omega_1^{-1/8} \mu(k^1)^{-1}\, dp_1\, dp_2\, dk^1$$
$$\leq O(1).$$

Proof of (6. 3): By (2. 15) and the triangle inequality it is sufficient to prove (6. 3) with R_{μ_1} replaced in turn by the following three kernels:

$$\int_{\substack{|p_1| \leq K \\ |p_2| \leq K}} dp_1\, dp_2 W_p(p_1, p_2, k_1^1) \overline{W}_p(p_1, p_2, k_2^1) \rho(p_1, p_2)$$
$$\times \frac{\exp[-(\omega_1 + \omega_2 - ik_1^0)(I + 1 - s_{\mu_1})]}{\omega_1 + \omega_2 - ik_1^0} \exp[i(k_1^0 - k_2^0) s_{\mu_1}] \tag{6.12}$$

$$\int_{\substack{|p_1|\le K\\ |p_2|\le K}} dp_1\,dp_2 W_\rho(p_1,p_2,k_1^1)\overline{W}_\rho(p_1,p_2,k_2^1)\rho(p_1,p_2)$$
$$\times\left(\frac{1}{\omega_1+\omega_2-ik_1^0}-\frac{1}{\omega_1+\omega_2}\right)\exp[i(k_1^0-k_2^0)s_{\mu_1}] \tag{6.13}$$

$$\int_{\substack{|p_1|\le K\\ |p_2|\le K}} dp_1\,dp_2\left(W_\rho(p_1,p_2,k_1^1)\overline{W}_\rho(p_1,p_2,k_2^1)\rho(p_1,p_2)\right.$$
$$\left.\times\frac{1}{\omega_1+\omega_2}\exp[i(k_1^0-k_2^0)s_{\mu_1})]\right)+\frac{\frac{1}{2}\delta m_{\mu_1}^2}{4\pi}\hat{g}*\hat{g}(k_1'-k_2')$$
$$\times\exp[i(k_1^0-k_2^0)s_{\mu_1}], \tag{6.14}$$

where $\rho(p_1,p_2)$ is a lower cutoff at L_{μ_1} [see (1.10)]. These corresponding inequalities are respectively implied by (6.15)–(6.17) below. For $\epsilon>0$, $\exists\,\eta>0$ such that for all K

$$\left|\int_{\substack{p_1+p_2=\xi\\ |p_1|,\,|p_2|\le K}}\rho(p_1,p_2)\frac{\exp[-(\omega_1+\omega_2-ik_1^0)(I+1-s_{\mu_1})]}{\omega_1+\omega_2-ik_1^0}\right|$$
$$\le O(1)(1+L_{\mu_1})^{-\eta}(I+1-s_{\mu_1})^{-1/32}, \tag{6.15}$$

$$\int_{\substack{p_1+p_2=\xi\\ |p_1|,\,|p_2|\le K}}\rho(p_1,p_2)\left|\frac{1}{\omega_1+\omega_2-ik_1^0}-\frac{1}{\omega_1+\omega_2}\right|$$
$$\le O(1)(1+L_{\mu_1})^{-\eta}|k_1^0|^{\epsilon}, \tag{6.16}$$

$$\left|\int_{\substack{p_1+p_2=\xi\\ |p_1|,\,|p_2|\le K}}\frac{\omega_1\omega_2-p_1p_2-M^2}{\omega_1\omega_2}\rho(p_1,p_2)\frac{1}{\omega_1+\omega_2}\right.$$
$$\left.-\int_{\substack{p_1+p_2=0\\ |p_1|,\,|p_2|\le K}}\frac{\omega_1\omega_2-p_1p_2-M^2}{\omega_1\omega_2}\rho(p_1p_2)\frac{1}{\omega_1+\omega_2}\right|$$
$$\le O(1)(1+L_{\mu_1})^{-\eta}|\xi|^{\epsilon}. \tag{6.17}$$

For example, by (6.17) the absolute value of (6.14) is majorized by

$$O(1)(1+L_{\mu_1})^{-\eta}\int d\xi\,|\hat{g}(k_1^1-\xi)|\,|\xi|^{\epsilon}|\hat{g}(\xi-k_2^1)|$$
$$\le O(1)(1+L_{\mu_1})^{-\eta}\mu^{\epsilon/2}(k_1^1)\mu^{\epsilon/2}(k_2^1)\int d\xi \tag{6.18}$$
$$\times|\mu^{\epsilon/2}(k_1^1-\xi)\hat{g}(k_1^1-\xi)|\,|\mu^{\epsilon/2}(\xi-k_2^1)\hat{g}(\xi-k_2^1)|. \tag{6.19}$$

Therefore, the $(C,2)$ norm of (6.14) is majorized by

$$O(1)(1+L_{\mu_1})^{-\eta}\{\int d\bar{k}_1\,d\bar{k}_2[\mu^{\epsilon/2}|\hat{g}|*\mu^{\epsilon/2}|\hat{g}|(k_1^1-k_2^1)]^2$$
$$\times\mu^{\epsilon/2}(k_1^1)C(\bar{k}_1)\mu^{\epsilon/2}(k_2^1)C(\bar{k}_2)\}^{1/2}. \tag{6.20}$$

By doing the integrals over k_1^0 and k_2^0 and changing the integration variables (6.20) is less than

$$O(1)(1+L_{\mu_1})^{-\eta}\{\int d\eta[\mu^{\epsilon/2}|\hat{g}|*\mu^{\epsilon/2}|\hat{g}|(\eta)]^2$$
$$\times\int_{k_1'-k_2'=\eta}\mu^{-1+\epsilon/2}(k_1')\mu^{-1+\epsilon/2}(k_2')\}^{1/2} \tag{6.21}$$
$$\le O(1)(1+L_{\mu_1})^{-\eta}\|\mu^{\epsilon/2}|\hat{g}|*\mu^{\epsilon/2}|\hat{g}|\,\|_2 \tag{6.22}$$
$$=O(1)(1+L_{\mu_1})^{-\eta}\|[(\mu^{\epsilon/2}|\hat{g}|)^{\vee}]^2\|_2. \tag{6.23}$$

In the last equality "$\vee$" denotes the inverse Fourier transform. By the Tichmarsh theorem (6.23) is majorized by

$$O(1)(1+L_{\mu_1})^{-\eta}\|\mu^{\epsilon/2}|\hat{g}|\,\|_{4/3}^2\le O(1)(1+L_{\mu_1})^{-\eta}$$

by (1.4). This completes the proof that, given (6.17), (6.3) holds with R_{μ_1} replaced by (6.14). In a similar way (6.15) and (6.16) imply that (6.3) holds with R_{μ_1} replaced by (6.12) and (6.13) respectively. Therefore, the proof of (6.3) reduces to proving (6.15)–(6.17). (6.15) and (6.16) are elementary. (6.17) is implied by the following three elementary inequalities. For $\epsilon>0$, $\exists\eta>0$ such that

$$\int dp\left|\frac{\omega(p)\omega(\xi-p)-p(\xi-p)-M^2}{\omega(p)\omega(\xi-p)}-\frac{\omega^2(p)+p^2-M^2}{\omega^2(p)}\right|$$
$$\times\rho(p,\xi-p)\frac{1}{\omega(p)+\omega(\xi-p)}\le O(1)(1+L_{\mu_1})^{-\eta}|\xi|^{\epsilon}, \tag{6.24}$$

$$\int dp\left|\frac{1}{\omega(p)+\omega(\xi-p)}-\frac{1}{2\omega(p)}\right|\rho(p_1,\xi-p)$$
$$\le O(1)(1+L_{\mu_1})^{-\eta}|\xi|^{\epsilon}, \tag{6.25}$$

$$\int dp\frac{1}{\omega(p)}\,|\chi_\xi(p)-\chi_0(p)|\le O(1)(1+L_{\mu_1})^{-\eta}|\xi|^{\epsilon}, \tag{6.26}$$

where $\chi_\xi(p)$ is the characteristic function of the set $\{|p|\le K,\,|\xi-p|\le K\}\cap\{\text{either }|p|\ge L_{\mu_1}\text{ or }|\xi-p|\ge L_{\mu_1}\}$ and χ_0 is given by putting $\xi=0$. This completes the proof of (6.3).

Proof of (6.4): From (2.16), (2.13), and (1.8)

$$\delta E_{\mu_2}=\left(\frac{\lambda}{4\pi}\right)^2\int_{\substack{|p_1|\le K\\ |p_2|\le K}}|\hat{g}(p_1+p_2+k)|^2\frac{\omega_1\omega_2-p_1p_2-M^2}{\omega_1\omega_2}$$
$$\times\rho(p_1,p_2)\mu^{-1}(k)\frac{\exp\{-[\omega_1+\omega_2+\mu(k)](I+1-s_{\mu_2})\}}{\omega_1+\omega_2+\mu(k)}$$
$$\times dp_1\,dp_2\,dk \tag{6.27}$$
$$\le O(1)\int d\xi|\hat{g}(\xi)|^2\int_{p_1+p_2+k=\xi}$$
$$\times\frac{\exp\{-[\omega_1+\omega_2+\mu(k)](I+1-s_{\mu_2})\}}{\omega_1+\omega_2+\mu(k)}\frac{1}{\mu(k)}\rho. \tag{6.28}$$

(6.4) now follows from (1.4) and

$$\int_{p_1+p_2+k=\xi}\frac{\exp\{-[\omega_1+\omega_2+\mu(k)](I+1-s_{\mu_2})\}}{\omega_1+\omega_2+\mu(k)}\frac{\rho}{\mu(k)}$$
$$\le O(1)(1+L_{\mu_2})^{-\eta}(I+1-s_{\mu_2})^{-1/32}. \tag{6.29}$$

Proof of (6.5): From (2.25) P vertices are time ordered, but C vertices are not. First assume that all vertices are time ordered and labelled in that order by $\nu=1,2,3,\cdots$. By (2.25) each vertex is also restricted to lie in a certain interval. Suppose, for example, that a vertex ν in $[I-1,I]$ is contracted by a line l to ν'' in $[I,I+1]$. Let $s_\nu\le s_{\nu+1}\le\cdots s_{\nu'}\le I\le s_{\nu'+1}\le\cdots\le s_{\nu''}$ be the times of the intervening vertices. Then, for $\sigma_\nu,\sigma_{\nu+1}\cdots\sigma_{\nu''-1}$ positive numbers with $\sigma_\nu+\sigma_{\nu+1}+\cdots+\sigma_{\nu''-1}=\sigma_l$,

$$t^{-\sigma_l}=(s_{\nu''}-s_\nu)^{-\sigma_l}\le(s_{\nu+1}-s_\nu)^{-\sigma_\nu}(s_{\nu+2}-s_{\nu+1})^{-\sigma_{\nu+1}}$$
$$\times\cdots(I-s_{\nu'})^{-\sigma_{\nu'}}(s_{\nu'+1}-I)^{-\sigma_I}\cdots(s_{\nu''}-s_{\nu''-1})^{-\sigma_{\nu''-1}}. \tag{6.30}$$

By use of estimates similar to (6.30) it follows that

$$\int_{\text{time ordered}}ds_g\prod_{l\in F}t_l^{-\sigma_l}\prod_\mu(I(\mu)+1-s_\mu)^{-1/32}$$
$$\le\prod_I\left[\int\prod_{i=1}^{i=n(I)+1}\frac{dt_i}{t_i^{31/32}}\,\delta\left(\sum_{i=1}^{n(I)+1}t_i-1\right)\right] \tag{6.31}$$

$$= \prod_I \frac{\Gamma(1/32)^{n(I)}}{\Gamma(\sum_I n(I)/32)} \leq \prod_I O(1)^{n(I)}, \tag{6.32}$$

where the σ_I are chosen as in (6.5). There are less than $\prod_I n(I)!$ ways of time ordering the region of integration on the right-hand side of (6.5); therefore, (6.5) follows from (6.32).

7. ESTIMATES ON THE EXPONENT

In this section it is proved that, given K and $\epsilon > 0$ there exists a function $c(\phi)$ such that

$$H_{0F} + V + c(\phi) \geq -O(K^{\epsilon}), \tag{7.1a}$$

$$H_{0B} - 2c(\phi) \geq -O(1). \tag{7.1b}$$

A corresponding estimate is also proved for GY_2. This proves the claim made in (2.1). By replacing K with K_i and referring to (2.24), (2.8), and (2.17a), the proof of (4.1) also follows.

Define the quantities

$$N_{\tau F} = \int \omega^{\tau}(p)[b^*(p)b(p) + b'^*(p)b'(p)]\,dp \quad \text{on } \Omega^{\perp}$$
$$= 1 \quad \text{on } \Omega, \tag{7.2a}$$

$$N_{\tau B} = \int \mu^{\tau}(k)a^*(k)a(k)\,dk \quad \text{on } \Omega^{\perp}$$
$$= 1 \quad \text{on } \Omega. \tag{7.2b}$$

Ω is the Fock vacuum.

$r(p_1, p_2)$ = characteristic function of the set

$$\{|p_1| \geq L \text{ or } |p_2| \geq L\}. \tag{7.3}$$

L will be chosen later.

$$V_{pr} = \int_{|p_1|,\,|p_2| \leq K} [b^*(p_1)b'^*(p_2) + b(-p_1)b'(-p_2)]r(p_1, p_2)$$
$$\times W_p(p_1, p_2, k)\phi(k)\,dp_1\,dp_2\,dk - \tfrac{1}{2}(\delta m_K^2 - \delta m_L^2)$$
$$\times \int g^2(x) : \phi^2(x) : dx - (E_K - E_L), \tag{7.4}$$

$$V_{sr} = \int_{|p_1|,\,|p_2| \leq K} [b^*(p_1)b(-p_2) + b'^*(p_1)b'(-p_2)]r(p_1, p_2)$$
$$\times W_s(p_1, p_2, k)\phi(k)\,dp_1\,dp_2\,dk, \tag{7.5}$$

$$\Gamma V_{pr} = \int_{|p_1|,\,|p_2| \leq K} [b^*(p_1)b'^*(p_2) - b(-p_1)b'(-p_2)]\frac{1}{\tilde{\omega}_1 + \tilde{\omega}_2}$$
$$\times r(p_1, p_2)W_p(p_1, p_2, k)\phi(k)\,dp_1\,dp_2\,dk, \tag{7.6}$$

where $\tilde{\omega}(p) = \omega(p) - \omega^{\tau}(p)$, $\tau < 1$. In order that $\tilde{\omega} > 0$, assume the fermion mass is larger than unity. This is not an essential restriction. Note that ΓV_{pr} is an antisymmetric operator designed so that

$$[\Gamma V_{pr}, H_{0F} - N_{\tau F}] + V_{pr} + \tfrac{1}{2}(\delta m_K^2 - Sm_L^2)$$
$$\times \int g^2(x) : \phi^2(x) : dx + (E_K - E_L) = 0. \tag{7.7}$$

(7.1a, b) are obtained by adding the inequalities (7.8) given below.

Given $\tau \in (0, 1)$, for sufficiently large L, there exists $c_1(\phi)$ such that

$$H_{0F} - N_{\tau F} + V_{pr} + c_1(\phi) \geq -O(\log K), \tag{7.8a}$$

$$\tfrac{1}{3}H_{0B} - 2c_1(\phi) \geq 0. \tag{7.8b}$$

Given $\epsilon > 0$, for L sufficiently large and τ close enough to 1 ($\tau < 1$), there exists $c_2(\phi)$ such that

$$\tfrac{1}{2}N_{\tau F} + V_{sr} + c_2(\phi) \geq -O(K^{\epsilon}), \tag{7.8c}$$

$$\tfrac{1}{3}H_{0B} - 2c_2(\phi) \geq 0. \tag{7.8d}$$

Given L there exists $c_3(\phi)$ such that

$$\tfrac{1}{2}N_{\tau F} + V_L + c_3(\phi) \geq -O(1), \tag{7.8e}$$

$$\tfrac{1}{3}H_{0B} - 2c_3(\phi) \geq -O(1), \tag{7.8f}$$

where V_L is defined by replacing K by L in the definition of V in (1.6).

A proof for (7.8e, f) may easily be constructed using the following remarks. (1) The mass counterterm in V_L is formally positive. (2) Each kernel of V_L can be written as the sum of products of Hermite functions plus remainder in such a way that the term corresponding to the remainder can be estimated by an $N_{\tau F}$ estimate as will be demonstrated for (7.8c, d). The other term can be majorized by a suitable boson function by

$$\left|\sum W_{ijk}b^{\#}(h_i)b^{\#}(h_j)\phi(h_k)\right| \leq \sum |W_{ijk}|\,|\phi(h_k)|,$$

where h_i are Hermite functions with unit L_2 norm.

(7.8a, b) will now be proved by Glimm's dressing transformation (Ref. 1).

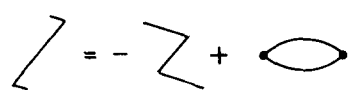
Define

$$\tilde{b}(p) = b(p) - [\Gamma V_{pr}, b(p)], \quad \tilde{b}'(p) = b'(p) - [\Gamma V_{pr}, b'(p)] \tag{7.9}$$

and calculate, using (7.7), the operator $\int \tilde{\omega}(p)[\tilde{b}^*(p)\tilde{b}(p) + \tilde{b}'^*(p)\tilde{b}'(p)]dp$. Then, since this operator is positive,

$$0 \leq H_{0F} - N_{\tau F} + V_{pr} + \tfrac{1}{2}(\delta m_K^2 - \delta m_L^2)\int g^2(x) : \phi^2(x) : dx$$
$$+ (E_K - E_L) + \int \tilde{\omega}(p)\{[\Gamma V_{pr}, b^*(p)][\Gamma V_{pr}, b(p)]$$
$$+ [\Gamma V_{pr}, b'^*(p)][\Gamma V_{pr}, b'(p)]\}dp. \tag{7.10}$$

The result of normal ordering the fermion operators in the second order term in (7.10) can be represented graphically as



(7.11)

The first term on the right-hand side of (7.11) is the negative of a positive operator; therefore, (7.10) implies

$$H_{0F} - N_{\tau F} + V_{pr} + \tfrac{1}{2}(\delta m_K^2 - \delta m_L^2)\int g^2(x) : \phi^2(x) : dx$$
$$+ \int dk_1\,dk_2 : \phi(k_1)q(k_1, k_2)\phi(-k_2) : \tag{7.12}$$
$$\geq -(E_K - E_L) - \int dk\,q(k, k)\mu^{-1}(k),$$

where q denotes the kernel of the last term on the right-hand side of (7.11). The boson fields in this term have also been normal ordered in obtaining (7.12). The right-hand side of (7.12) is equal to [see (1.5b)]

$$\left(\frac{\lambda}{4\pi}\right)^2 \int_{|p_1|,\,|p_2| \leq K} \frac{\omega_1\omega_2 - p_1p_2 - M^2}{\omega_1\omega_2} r(p_1, p_2)$$
$$\times \left(\frac{1}{\omega_1 + \omega_2 + \mu(k)} - \frac{1}{\tilde{\omega}_1 + \tilde{\omega}_2}\right)\mu^{-1}(k)\left|\hat{g}(p_1 + p_2 + k)\right|^2 \tag{7.13}$$
$$\times dp_1\,dp_2\,dk.$$

It can readily be checked that this behaves as $-O(\log K)$. For large L, $c_1(\phi)$ can be chosen to be the last two terms on the left-hand side of (7.12), i.e.,

$$\left(\frac{\lambda}{4\pi}\right)^2 \int d\xi : \phi(k_1)\hat{g}(k_1-\xi)\Bigg(\int_{\substack{p_1+p_2=\xi \\ |p_1|,\,|p_2|\le K}} \frac{\omega_1\omega_2 - p_1p_2 - M^2}{\omega_1\omega_2}$$

$$\times r(p_1,p_2)\frac{1}{\tilde{\omega}_1+\tilde{\omega}_2} - \int_{\substack{p_1+p_2=0 \\ |p_1|,\,|p_2|\le K}} \frac{\omega_1\omega_2 - p_1p_2 - M^2}{\omega_1\omega_2} r(p_1,p_2) \tag{7.14}$$

$$\times \frac{1}{\omega_1+\omega_2}\Bigg)\hat{g}(\xi-k_2)\phi(-k_2) : dk_1\,dk_2.$$

(7.8b) is a consequence of an $N_{\tau B}$ estimate (Ref. 8). Let $q'(k_1,k_2)$ denote the kernel of (7.14) so that (7.14) equals

$$\int dk_1\,dk_2 : \phi(k_1)q'(k_1,k_2)\phi(-k_2):. \tag{7.15}$$

Then (7.8b) holds if the L^2 norm of $\mu^{-1}(k_1)q'(k_1,k_2)\mu^{-1}(k_2)$ can be made arbitrarily small, uniformly in K, by choosing L large. The estimates for this are omitted. See (6.17).

Next it is shown that, in (7.8c, d), $c_2(\phi)$ can be chosen to be

$$c_2(\phi) = \tfrac{1}{2}\int_{|p_1|,\,|p_2|\le K} r(p_1,p_2)W_s(p_1,p_2,k_1)\frac{1}{\omega_2^\tau}\overline{W}_s(p_1,p_2,k_2) \tag{7.16}$$

$$\times : \phi(k_1)\phi(-k_2) : dp_1\,dp_2\,dk.$$

For, by an $N_{\tau F}$ estimate to V_{sr}, regarding the ϕ's as numerical quantities,

$$\| V_{sr}N_{\tau F}^{-1/2}\|_F \le \{2[c_2(\phi)+O(K^\epsilon)]\}^{1/2}. \tag{7.17}$$

The $O(K^\epsilon)$ arises when the bosons are normal ordered to comply with (7.16). (7.17) implies

$$V_{sr}^2 \le 2[c_2(\phi)+O(K^\epsilon)]N_{\tau F},$$

and since operator inequalities are preserved in the taking of square roots,

$$\pm V_{sr} \le \sqrt{2}\,[c_2(\phi)+O(K^\epsilon)]^{1/2}N_{\tau F}^{1/2} \le c_2(\phi)+O(K^\epsilon)+\tfrac{1}{2}N_{\tau F}. \tag{7.18}$$

The expression under the square root is equal to (7.16) with the ϕ's not normal ordered. This is a positive operator so the square root is well-defined. (7.18) is equivalent to (7.8c).

(7.8d) is proved by an $N_{\tau B}$ estimate. From (7.16), it suffices to show that the L^2 norm of (7.19) can be made arbitrarily small, uniformly in K, by choosing L large:

$$\mu(k_1)^{-1}\int_{|p_1|,\,|p_2|\le K} W_s(p_1,p_2,k_1)\omega^{-\tau}(p_2)\overline{W}_s(p_1,p_2,k_2)r(p_1,p_2)$$

$$\times dp_1\,dp_2\,\mu(k_2)^{-1}. \tag{7.19}$$

Since this is the kernel of a positive operator on $L^2(R)$, the L^2 norm is less than its trace which is less than

$$O(1)\int d\xi\,|\hat{g}(\xi)|^2\int_{p_1+p_2+k=\xi}\frac{\omega_1\omega_2+p_1p_2+M^2}{\omega_1\omega_2} \tag{7.20}$$

$$\times r(p_1,p_2)\omega^{-\tau}(p_2)\mu^{-2}(k).$$

The following estimate applied to (7.20) completes the proof of (7.8d). For $0<\epsilon\le 1$

$$(\omega_1\omega_2+p_1p_2+M^2)/\omega_1\omega_2 \le O(1)\omega(p_1+p_2)^{2\epsilon}\omega(p_1-p_2)^{-\epsilon}. \tag{7.21}$$

Generalized Yukawa

The estimates that substitute for (7.1a, b) are: Given K and $\epsilon>0$ there exists $c(\phi)$ such that

$$H_{0F}+V+c(\phi) \ge \int g(x) : \phi^{2M}(x) : dx - O(K^\epsilon), \tag{7.22a}$$

$$H_{0B}+\int g(x) : \phi^{2M}(x): dx - 2c(\phi) \ge -O(K^\epsilon), \tag{7.22b}$$

where $M>N$ and

$$V = \lambda\int : \bar{\psi}_K(x)\psi_K(x): : \phi^N(x) : g(x)\,dx$$

$$-\tfrac{1}{2}\delta m^2_{K,0}\int g^2(x) : \phi^{2N}(x) : dx$$

$$-\tfrac{1}{2}\delta m^2_{K,1}\int g^2(x): \phi^{2N-2}(x): dx$$

$$-\cdots-\tfrac{1}{2}\delta m^2_{K,N-1}\int g^2(x): \phi^2(x): dx$$

$$-E_K+\int g(x) : \phi^{2M}(x) : dx. \tag{7.23}$$

E_K is not the same as that in (1.5b). The extra counterterms are added to cancel diagrams like

(7.24)

Glimm's dressing transformation is used to bound the pair creation and annihilation part of V by a function $c_1(\phi)$ without using a lower momentum cutoff $r(p_1,p_2)$. To bound the scattering part, a function $c_2(\phi)$ is found so that for τ close enough to 1

$$\tfrac{1}{2}N_{\tau F}+V_s+c_2(\phi) \ge 0, \tag{7.25}$$

where

$$V_s = \int_{|p_1|,\,|p_2|\le K}[b^*(p_1)b(-p_2)+b'^*(p_1)b'(-p_2)]W_s(p_1,p_2,k) \tag{7.26}$$

$$: \phi^N(k) : dp_1\,dp_2\,dk.$$

$: \phi^N(k):$ denotes the kth Fourier component of $: \phi^N(x):$. To obtain $c_2(\phi)$, begin by estimating, for $\alpha>1/2$,

$$\|N_{\tau F}^{-\alpha/2}V_sN_{\tau F}^{-\alpha/2}\|_F. \tag{7.27}$$

Let

$$y(p_1,p_2) = \int W_s(p_1,p_2,k): \phi^N(k) : dk. \tag{7.28}$$

Then

$$N_{\tau F}^{-\alpha/2}\int_{\substack{p_1\ge p_2 \\ |p_1|,\,|p_2|\le K}} y(p_1,p_2)b^*(p_1)b(-p_2)\,dp_1\,dp_2N_{\tau F}^{-\alpha/2} \tag{7.29}$$

$$= O(1)\int_0^\infty dt\,t^{-1+\alpha/2}\exp(-tN_{\tau F})\int_{\substack{p_1\ge p_2 \\ |p_1|,\,|p_2|\le K}} \tag{7.30}$$

$$\times y(p_1,p_2)b^*(p_1)b(-p_2)\,dp_1\,dp_2\,N_{\tau F}^{-\alpha/2}$$

$$= O(1)\int_0^\infty dt\,t^{-1+\alpha/2}\int_{\substack{p_1\ge p_2 \\ |p_1|,\,|p_2|\le K}} y(p_1,p_2)$$

$$\times\exp[-(2\omega_1^\tau-\omega_2^\tau)t/2]b^*(p_1) \tag{7.31}$$

$$\times\exp[-t/2)N_{\tau F}]\,b(-p_2)\exp[(-t/2)N_{\tau F}]\,dp_1\,dp_2N_{\tau F}^{-\alpha/2}.$$

Therefore, the $\|\ \|_F$ norm of (7.29) is bounded by

$$O(1)\int_0^\infty dt\, t^{-1+\alpha/2}\| \sum_{\substack{p_1\geq p_2\\ |p_1|,\,|p_2|\leq K}} y(p_1,p_2)$$

$$\times\exp[-(2\omega_1^\tau-\omega_2^\tau)t/2]\,b^*(p_1) \tag{7.32}$$

$$\times\exp[(-t/2)]N_{\tau F}]b(-p_2)N_{\tau F}^{-1/2}\|_F\|N_{\tau F}^{1/2-\alpha/2}$$

$$\times\exp[(-t/2)N_{\tau F}]\|$$

Despite the fact that $\exp[(-t/2)N_{\tau F}]$ is sandwiched between the $b^{\#}$'s in (7.32), a glance at the proof given in Ref. 8 shows that an N_τ estimate can still be applied so that (7.32) is bounded by

$$O(1)\int_0^\infty dt\, t^{-1+\alpha/2}\exp[-O(1)t]\,t^{-1/2+\alpha/2}$$

$$\times\left(\sum_{\substack{p_1\geq p_2\\ |p_1|,\,|p_2|\leq K}}|y(p_1,p_2)|^2\exp[-(2\omega_1^\tau-\omega_2^\tau)t]\omega_2^{-\tau}\,dp_1\,dp_2\right)^{1/2} \tag{7.33}$$

$$\leq O(1)\Big[\int|y(p_1,p_2)|^2\,\omega_1^{-\epsilon\tau}\omega_2^{-\tau}\,dp_1\,dp_2\Big]^{1/2} \tag{7.34}$$

provided $\alpha-\frac{3}{2}-\epsilon<1$. It is also necessary that $\epsilon\tau+\tau>1$ so that the boson fields in (7.34) can be normal ordered. Clearly the same estimate can be derived for a term with $p_1\leq p_2$; also antifermions can be included so that

$$\|N_{\tau F}^{-\alpha/2}V_s N_{\tau F}^{-\alpha/2}\|_F\leq O(1)\Big[\int|y(p_1,p_2)|^2$$

$$\times(\omega_1^{-\epsilon\tau}\omega_2^{-\tau}+\omega_1^{-\tau}\omega_2^{-\epsilon\tau})\,dp_1\,dp_2\Big]^{1/2}. \tag{7.35}$$

(7.35) implies

$$\pm V_s\leq O(1)\Big[\int|y(p_1,p_2)|^2(\omega_1^{-\epsilon\tau}\omega_2^{-\tau}+\omega_1^{-\tau}\omega_2^{-\epsilon\tau})\,dp_1\,dp_2\Big]^{1/2}N_{\tau F}^{\alpha} \tag{7.36}$$

and therefore

$$-V_s\leq\tfrac{1}{2}N_{\tau F}+O(1)\Big[\int|y(p_1,p_2)|^2$$

$$\times\ (\omega_1^{-\epsilon\tau}\omega_2^{-\tau}+\omega_1^{-\tau}\omega_2^{-\epsilon\tau})\,dp_1\,dp_2\Big]^{1/2(1-\alpha)}, \tag{7.37a}$$

where

$$\alpha-\tfrac{3}{2}-\epsilon<1,\quad \epsilon\tau+\tau>1. \tag{7.37b}$$

Consequently, (7.25) holds with $c_2(\phi)$ chosen to be the last term on the right-hand side of (7.37). Since the dressing transformation only works for $\tau<1$, (7.37b) requires $\alpha>\frac{1}{2}$.

To prove (7.22b), one needs, for suitable α,

$$H_{0B}+\int g(x)\colon\phi^{2M}(x)\colon dx-2c_1(\phi)-2c_2(\phi)\geq-O(K^\epsilon), \tag{7.38}$$

where $c_1(\phi)$ is the term arising from the dressing transformation. Instead, it is now proved that α can be chosen so that

$$\tfrac{1}{2}H_{0B}+\tfrac{1}{2}\int g(x)\colon\phi^{2M}(x)\colon dx-2c_2(\phi)\geq-O(K^\epsilon) \tag{7.39}$$

because the estimate with c_2 replaced by c_1 in (7.39) can be proved in a similar way to (7.39). $c_2(\phi)$ has the form

$$\Big[\int Y(k_1,k_2)\colon\phi^N(k_1)\colon\colon\phi^N(-k_2)\colon dk_1\,dk_2\Big]^{1/2(1-\alpha)},$$

where

$$Y(k_1,k_2)=O(1)\int d\xi\,\hat g(k_1-\xi)\sum_{p_1+p_2=\xi}\frac{1}{\omega_1^{\epsilon\tau}}\frac{1}{\omega_2^{\tau}}+\frac{1}{\omega_2^{\tau}}\frac{1}{\omega_1^{\epsilon\tau}}$$

$$\times\frac{\omega_1\omega_2+p_1p_2+M^2}{\omega_1\omega_2}\,\hat g(\xi-k_2). \tag{7.40}$$

By using the hypothesis $M>N$, α is picked so that

$$\alpha>\tfrac{1}{2},\quad 1/2(1-\alpha)<M/N. \tag{7.41}$$

Let $\gamma=1/2(1-\alpha)$. Note that $1<\gamma<M/N$.

By hypercontractivity and the F. K. N. formula (Ref. 7), it is sufficient to prove

$$\exp(-\int_0^1[U(t)-O(1)T^\gamma(t)]dt)\in L^p \tag{7.42}$$

for $1\leq p<\infty$, where

$$U(t)=\int g(x)\colon\phi^{2M}(x,t)\colon dx, \tag{7.43}$$

$$T(t)=\int Y(k_1,k_2)\colon\phi^N(k_1,t)\colon\phi^N(-k_2,t)\colon dk_1\,dk_2. \tag{7.44}$$

[$\phi(x,t)$, $\phi(k,t)$ refer to Euclidean fields.] Define $U_L(t)$ and $T_L(t)$ by introducing a sharp momentum cutoff at L into each field in the spatial momentum. Let

$$\delta U_L(t)=U(t)-U_L(t),\quad \delta T_L(t)=T(t)-T_L(t). \tag{7.45}$$

The following estimate is easy to show, for each L:

$$\int_0^1 dt[U(t)-O(1)T^\gamma(t)]\geq\int_0^1 dt[U_L(t)-O(1)T_L^\gamma(t)] \tag{7.46}$$

$$+\int_0^1 dt[\delta U_L(t)-O(1)\,|\delta T_L(t)|^\gamma].$$

Suppose the estimates

$$\int_0^1 dt[U_L(t)-O(1)T_L^\gamma(t)]$$

$$\geq O(1)\log^M L\|\int_0^1 dt[\delta U_L(t)-O(1)\,|\delta T_L(t)|^\gamma]\|_q \tag{7.47a}$$

$$\leq O(1)(q\gamma)^M L^{-\eta} \tag{7.47b}$$

hold for some $\eta>0$ and all L; then Nelson's method (Ref. 9) can be applied to prove (7.42). Therefore, it suffices to prove (7.47a,b).

Proof of (7.47a): In (7.40), $\epsilon\tau+\tau>1$; therefore,

$$\int_{p_1+p_2=\xi}\frac{1}{\omega_1^{\epsilon\tau}}\frac{1}{\omega_2^{\tau}}+\frac{1}{\omega_2^{\tau}}\frac{1}{\omega_1^{\epsilon\tau}}\leq O(1). \tag{7.48}$$

This implies that, considered as operators on $L^2(R)$,

$$Y\leq O(1)\hat g*\hat g; \tag{7.49}$$

therefore,

$$T_L(t)\leq O(1)\int g^2(x)(:\phi_L^N(x,t):)^2\,dx. \tag{7.50}$$

(7.50) implies

$$[U_L(t)-O(1)T_L^\gamma(t)]\geq U_L(t)-O(1)\Big[\int g^2(x)(:\phi_L^N(x,t):)^2\,dx\Big]^\gamma. \tag{7.51}$$

Since $\gamma>1$ and by hypothesis (1.4) $g\in L^p$ for all p ($1\leq p\leq\infty$), the "Hölder" inequality can be applied to (7.51) so that

$$U_L(t)-O(1)T_L^\gamma(t)\geq U_L(t)-O(1)\int g(x)\,|:\phi_L^N(x,t):|^{2\gamma}\,dx \tag{7.52}$$

$$=\int g(x)[:\phi_L^{2M}(x,t):-O(1)\,|:\phi_L^N(x,t):|^{2\gamma}]\,dx. \tag{7.53}$$

Therefore, (7.47a) is proved if it is shown that

$$:\phi_L^{2M}(x,t):-O(1)[:\phi_L^N(x,t):\colon:\phi_L^N(x,t):]^\gamma\geq O(1)\log^M L. \tag{7.54}$$

This follows from Wick's theorem since $\gamma<M/N$.

Proof of (7.47b): This is a consequence of hypercontractivity, e.g.,

$$\| \int_0^1 dt(\delta U_L(t) - O(1)|\delta T_L(t)|^\gamma)\|_q \leq \int_0^1 dt\|\delta U_L(t)\|_q + O(1)\int_0^1 dt\|\delta T_L(t)\|_{q\gamma}^\gamma. \quad (7.55)$$

Now apply Nelson's best estimate to each term separately on the right-hand side. (For Nelson's best estimate, see Ref. 10).

APPENDIX: UNIFORMITY IN THE EXPECTATION STATE

It is sufficient to find a uniform lower bound for

$$-\lim_{T\to\infty}(1/T)\ln\langle s'e^{-TH}s\rangle, \quad (A1)$$

where s and s' have the form of a product of a Wick monomial in Fermi fields with an L^∞ function on Q space depending on time zero fields. Finite sums of quantities of this type are dense, and, by virtue of the T limit, (1.1) evaluated for such a sum is bounded below by the infimum over cross product contributions. The L^∞ functions can be majorized by their sup norms during "defermiation." The resulting constant gives no contribution in the T limit. The fermion parts of s and s' can be introduced in the calculation by allowing the "P" vertices to contract with the "external" fields in s and s'. Suppose the latter have been labelled $1,2,\ldots,p$, then the inclusion of a factor $(\Pi_I A^{n(I)})(p!)$ in (4.4) is sufficient to count the extra fermion graphs. A "P" vertex has two legs, each of which can be external or internal, hence the $\Pi_I A^{n(I)}$. In the set of external legs, the first has p choices of external fields with which to contract, the second has $p-1$, etc.; hence the $p!$. The $\Pi_I 4^{n(I)}$ can be absorbed into the $O(1)^{n(I)}$ in (4.4). The T limit annihilates the $p!$; hence a uniform bound holds for (1.1), and the Hamiltonian is bounded below.

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Decay of correlations for infinite-range interactions

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Strong cluster properties are proved at low activity and in various other situations for classical systems with infinite-range interactions. The decay of the correlations is exponential, resp. like an inverse power of the distance, if the potential decreases itself exponentially, resp. like an inverse power of the distance. The results allow us to extend to the case of exponentially decreasing potentials the equivalence theorem between strong cluster properties and analyticity with respect to the activity, previously proved for finite-range interactions.

I. INTRODUCTION

There has been a recent interest in the rigorous study of the decay properties of correlations in classical statistical mechanics.

The main results have been obtained, up to now, for finite-range interactions. An exponential decay has then been proved in various situations, either in the framework of the transfer-matrix method,[1] or by making use of series expansions of the connected correlations ρ_Λ^T with respect to the activity z.[2–4] In this latter case, the results have been obtained at low activity and in a number of other situations where analyticity is known (or assumed).

In Ref. 4 "strong cluster properties" have been proved in the form

$$|\rho_\Lambda^T(x_1, \ldots, x_N)| \leq C^N N_1! \cdots N_p! \exp[-\mu L(X)], \qquad (1)$$

where $L(X)$ is the minimal length of all connected trees T joining $x_1, \ldots, x_N$ and possibly arbitrary other vertices, and where C and μ are independent of N, of $X=(x_1, \ldots, x_N)$ and of the box Λ. (They depend on the activity z, the reciprocal temperature β and the potential Φ). The factor $N_1! \cdots N_p!$ arises if the points $x_1, \ldots, x_N$ occupy only p different positions $y_1, \ldots, y_p$ occurring respectively $N_1, \ldots, N_p$ times.

For infinite-range potentials, the connected correlations are known to tend to zero when some points are separated from each other[2] and to satisfy various integrability properties[6,7]. The decay has been proved in [8] to be exponential for one-dimensional systems with exponentially decreasing potentials, through the use of a generalization of the transfer-matrix method. On the other hand, a decay of the same type as that of the potential (exponential, resp. like an inverse power of the the distance, according to the potential) has been proved at low activity for the 2-point function $\rho^T(x_1, x_2)$ in[9,10] through the use of a series expansion method. Finally, it has been proved in Ref. 11 that the decay cannot in general be exponential if the potential does not decrease exponentially.

In the present paper, strong cluster properties of the N-point functions are again proved in the form (1) for exponentially decreasing potentials. When the potential decreases like r^{-s} $(s > \nu)$, analogous results are obtained:

$$|\rho_\Lambda^T(x_1, \ldots, x_N)| < C^N N_1! \cdots N_p! \exp[-s' L_\alpha(X)] \qquad (2)$$

where $L_\alpha(X)$ is now the minimal length of all connected trees joining $x_1, \ldots, x_N$ and possibly other arbitrary vertices, with respect to the new "distance" $\log(1 + \alpha|l|)$; $\alpha > 0$ and $s' > 0$ are again independent of X, N, Λ (and may depend on z, β, Φ).

The bound (2) also yields

$$|\rho_\Lambda^T(x_1, \ldots, x_N)| < C^N \sum_{T\,(x_1, \ldots, x_N)} \prod_{l \in T} u_{\alpha, s'}(|l|) \qquad (3)$$

where the sum $\sum$ runs over all connected trees joining $x_1, \ldots, x_N$ (without supplementary vertices), and where $u_{\alpha,s'}(|l|) = (1 + \alpha|l|)^{-s'/2}$; (3) is a strong cluster property in the sense of Ref. 5 if $\sum_{x \in z^\nu} u_{\alpha,s'}(|x|) < \infty$ (i.e. if $s'/2 > \nu$). (This last condition ensures the integrability of $|\rho_\Lambda^T|$.)

In Sec. II, the results are first proved at low activity. They are derived in Sec. III by an extension of the conformal mapping method of Refs. 2–4 when the correlations remain analytic in a connected domain D of the complex z-space containing $z=0$, and satisfy in D the additional boundedness condition

$$|z^{-N} \rho_\Lambda^T(x_1, \ldots, x_N)| < C^N N_1! \cdots N_p! \qquad (4)$$

where C is independent of X, N, Λ and of z in D.

The analyticity of ρ_Λ^T and the bound (4) hold in particular in the following situations, as already proved in Ref. 4 by using, in cases (ii) and (iii), results on the zeroes of $Z_\Lambda(z_1, \ldots, z_N, z)$ (more generally, they seem to be linked with the analyticity with respect to $z_1, \ldots, z_N$):

(i) for positive potentials, in the region of convergence of the Mayer z-expansion;

(ii) for lattice systems at arbitrary activity and high temperature;

(iii) for lattice ferromagnets when $\mathrm{Re}\, H \neq 0$, β arbitrary, or at $H=0$, as soon as the partition function $Z_\Lambda(\beta, H) \neq 0$ in some complex neighborhood of $H=0$.

The results allow the extension to exponentially de-

caying interactions of the equivalence theorem of Ref. 4 between (i) strong cluster properties (at real values of z) and (ii) analyticity with respect to z and the bounds (4).

For simplicity, only lattice gases are considered in Secs. II and III. However, the results can be adapted without difficulty to continuous systems, with slight modifications. This adaptation is briefly outlined in Sec. IV.

II. STRONG CLUSTER PROPERTIES AT LOW ACTIVITY

Let $K(x-y)=\exp[-\beta\Phi(x-y)]-1$. The Ursell function $\varphi(x_1,\ldots,x_N)$, which is the connected part of the Boltzmann factor $\exp[-\beta U(X)]$ (and is the value of $z^{-N}\rho_\Lambda^T$ at $z=0$), has the well-known explicit form

$$\varphi(x_1,\ldots,x_N)=\sum_{\Gamma^c}\prod_{l\in\Gamma^c}K(l), \tag{5}$$

where the sum $\sum$ runs over all connected graphs Γ^c joining the vertices $x_1,\ldots,x_N$.

The following result which holds for continuous systems is proved in Refs. 9 and 10 for positive and hard-core potentials, and in Appendix B for general stable potentials [the stability constant B which appears in (6) is replaced in Ref. 10 by $A/2$, where A is defined below Eq. (7)]:

Theorem 1:

$$|\varphi(x_1,\ldots,x_N)|\leq(\exp(2\beta B))^{N-2}\sum_{\mathcal{T}}\prod_{l\in\mathcal{T}}|K(l)| \tag{6}$$

where B is the stability constant and where the sum $\sum_{\mathcal{T}}$ runs over all (connected) trees joining $x_1,\ldots,x_N$.

Remark: A somewhat different bound which is slightly better in some situations can also be derived for hard-core potentials (see Appendix B):

$$|\varphi(x_1,\ldots,x_N)|<(\exp(\beta B))^{N-2}\sum_{\mathcal{T}}\prod_{l\in\mathcal{T}}\hat{K}(l) \tag{7}$$

where

$$\hat{K}(x-y)=\sup\{1-\exp[-\beta\Phi(x-y)],$$
$$\exp[\beta A](1-\exp(\beta\Phi(x-y))\},$$
$$A=\sum_{y\in Z^\nu}\Phi_-(x-y),\quad \Phi_-=\sup(0,-\Phi).$$

The following series expansion of the connected correlations is known[12]:

$$z^{-N}\rho_\Lambda^T(X;\beta,z)=\sum_{n\geq 0}z^n C_{\Lambda,n}(X;\beta), \tag{8}$$

where

$$C_{\Lambda,n}(X,\beta)=\frac{1}{n!}\sum_{Y\in\Lambda^n}\varphi(X,Y;\beta),$$

$$X=(x_1,\ldots,x_N),\quad Y=(y_1,\ldots,y_n).$$

A direct derivation of this formula is given in Appendix A.

When the potential Φ decreases like $\exp(-\chi r)$, resp. like r^{-s} $(s>\nu)$, it is useful to introduce the class of functions $u_\alpha(r)=\exp(-\alpha\chi r)$, resp. $u_\alpha(r)=(1+\alpha r)^{-s+\nu+\epsilon}$, where $0<\alpha<1$ and $\epsilon>0$ is a given arbitrarily small number. We note that $-\log u_\alpha(r)$ is always a distance, i.e.,

(i) $-\log u_\alpha(r)\geq 0$, $-\log u_\alpha(r)=0\Rightarrow r=0$,

(ii) $-\log u_\alpha(|x-y|)-\log u_\alpha(|y-z|)\geq-\log u_\alpha(|x-z|)$.

Below we shall generally denote by $\mathcal{L}_\alpha(X)$ the minimal length of all (connected) trees joining $x_1,\ldots,x_N$ and possibly other arbitrary vertices, with respect to the distance $-\log u_\alpha(r)$. [$\mathcal{L}_\alpha(X)=\alpha\chi L(X)$, resp. $\mathcal{L}_\alpha(X)=s'L_\alpha(X)$, $s'=s-\nu-\epsilon$, where $L(X)$, resp. $L_\alpha(X)$ is the minimal length given in the Introduction with respect to the usual distance r, resp. with respect to the distance $\log(1+\alpha r)$].

The following bound is then derived from (6):

Lemma 1:

$$|C_{\Lambda,n}(X;\beta)|\leq(\exp(2\beta B))^{N+n-2}\frac{(N+n)^{N+n-2}}{(N-1)!n!}N_1!\cdots N_p!$$
$$\times[C_\alpha(\beta)]^{N+n-1}\exp[-\mathcal{L}_\alpha(X)]. \tag{9}$$

where $C_\alpha(\beta)=\sum_{x\in Z^\nu}|K_\alpha(x)|$, and $K_\alpha(x)=K(x)\cdot u_\alpha(|x|)^{-1}$.

Proof:

$$|C_{\Lambda,n}(X;\beta)|\leq\frac{1}{n!}\sum_{Y^n}|\varphi(x_1,\ldots,x_N,y_1,\ldots,y_n)|$$
$$\leq\frac{1}{n!}(\exp(2\beta B))^{N+n-2}\max_{Y,\mathcal{T}}\prod_{l\in\mathcal{T}}u_\alpha(|l|)$$
$$\times\sum_{Y^n}\sum_{\mathcal{T}(x_1,\ldots,x_N,y_1,\ldots,y_n)}\prod_{l\in\mathcal{T}}K_\alpha(l).$$

The term $\max_{Y,\mathcal{T}}\prod_{l\in\mathcal{T}}u_\alpha(|l|)$ is clearly bounded by $\exp[-\mathcal{L}_\alpha(X)]$. On the other hand,

$$\sum_{Y^n}\left(\sum_{\mathcal{T}}\prod_{l\in\mathcal{T}}K_\alpha(l)\right)\leq\frac{N_1!\cdots N_p!}{(N-1)!}\sum_{\substack{x_2,\ldots,x_N\\ y_1,\ldots,y_n}}\left(\sum_{\mathcal{T}}\prod_{l\in\mathcal{T}}K_\alpha(l)\right).$$

The bound (9) then follows from the fact that the number of trees joining $N+n$ points is $(N+n)^{N+n-2}$.[13] QED

Theorem 2: Let $R_\alpha(\beta)=\exp(-2\beta B-1)(C_\alpha(\beta))^{-1}$. For $|z|<R_\alpha(\beta)$, the following strong cluster property holds for Λ finite or infinite:

$$|z^{-N}\rho_\Lambda^T(x_1,\ldots,x_N)|\leq\frac{e^2C_\alpha(\beta)}{N-1}\frac{1}{1-\eta|z|/R_\alpha(\beta)}$$
$$\times\left(\frac{\eta}{\eta-1}\times\frac{1}{R_\alpha(\beta)}\right)^{N-2}$$
$$\times N_1!\cdots N_p!\exp[-\mathcal{L}_\alpha(X)] \tag{10}$$

where η is an arbitrary real number such that $1<\eta<R_\alpha(\beta)/|z|$.

Proof: The bound (10) is readily derived from Lemma 1 together with the inequalities

$$(N+n)^{N+n-2}\leq(N+n-2)!\exp(N+n), \tag{11}$$

$$\sum_{n\geq 0}|t|^n\frac{(k+n)!}{n!}\leq k!\frac{1}{1-\eta|t|}\left(\frac{\eta}{\eta-1}\right)^k. \tag{12}$$

Remarks: $R_\alpha(\beta)$ tends to the usual Kirkwood–Salzburg radius of convergence $R(\beta)=\exp(-2\beta B-1)\left(\sum_{y\in Z^\nu}|K(x-y)|\right)^{-1}$, when $\alpha\to 0$.

Therefore, Theorem 2 exhibits a strong cluster property for each point z in the region $|z|<R(\beta)$.

A similar result with slightly different coefficients in front of $\exp[-\mathcal{L}_\alpha(X)]$ is derived in the same way from (7).

III. STRONG CLUSTER PROPERTIES IN MORE GENERAL SITUATIONS

In a number of situations, it can be proved that the connected correlations $\rho_\Lambda^T(X;\beta,z)$ remain analytic with respect to z not only at low activity but in larger domains in complex z-space where, moreover, they satisfy the bounds (4). Results of this type have been proved in Ref. 4 and recalled in the Introduction. The following theorem, which is an extension to infinite range potentials of Theorem 3 of Ref. 4, is then of interest.

Theorem 3: Suppose that the connected correlations $\rho_\Lambda^T(X;\beta,z)$ are analytic in a connected domain D in complex z-space, containing $z=0$, and satisfy there the bound (4)

$$|z^{-N}\rho_\Lambda^T(X;\beta,z)| \leq C^N N_1! \cdots N_p!$$

where C is independent of X, N, Λ, and of z in D.

Then the following decay properties hold for $|t(z)| > (t_\alpha)^\delta$:

$$|\rho_\Lambda^T(X;z,\beta)| < E_\delta^N N_1! \cdots N_p! \exp\left(-\mathcal{L}_\alpha(X)\frac{\log|t(z)|}{\delta \log t_\alpha}\right) \quad (13)$$

where $z \to t(z)$ is a conformal mapping of D onto the interior of the unit circle $|t(z)| < 1$, such that $t(0)=0$, t_α is the largest value for which $|t(z)| < t_\alpha$ implies $|z| < R_\alpha(\beta)$, $\mathcal{L}_\alpha(X)$ and $R_\alpha(\beta)$ are those of formula (10) in Sec. II ($0 < \alpha < 1$), δ is an arbitrary real number such that $\delta > 1$, and E_δ is independent of X, N, and Λ.

Remarks: The bounds (13) are strong cluster properties in the sense of Refs. 4, 5 whenever they ensure the integrability of $|\rho_\Lambda^T(X;z,\beta)|$. (This is, in particular, always true for exponentially decreasing potentials.)

The proof below makes use of the conformal mapping method of Refs. 2–4. Alternatively, a method using results on subharmonic functions, which is introduced in Ref. 9, would also allow one to extend the strong cluster properties from the low activity region to the domain D. However, this last method does not seem, so far, to provide any information on the rates of fall-off.

Proof: The following series expansion holds and is convergent for $|t| < 1$, in view of the analyticity of $\rho_\Lambda^T(X;\beta,z)$ in D:

$$(z^{-N}\rho_\Lambda^T)(X;\beta,t) = \sum_{n\geq 0} t^n \gamma_n(X;\beta). \quad (14)$$

By using a Cauchy formula and the bound (4), resp. the bound (10), one gets

$$|\gamma_n(X;\beta)| < C^N N_1! \cdots N_p!, \quad (15)$$

resp.

$$|\gamma_n(X;\beta)| < E'_N N_1! \cdots N_p! \exp[-\mathcal{L}_\alpha(X)] \frac{1}{(t_\alpha)^{\delta n}} \quad (16)$$

where

$$E'_N = \frac{e}{N}\left(\frac{\eta}{\eta-1}\right)^{N-1}\left(\frac{1}{R_\alpha(\beta)}\right)^N \frac{1}{1-\eta[R'_{\alpha,\delta}/R_\alpha(\beta)]}, \quad 1 < \eta < R_\alpha(\beta)/R'_{\alpha,\delta} \quad (17)$$

and $R'_{\alpha,\delta}$ is the largest value of $|z|$ such that $|t(z)| < (t_\alpha)^\delta$.

Let $n_0(X) = \mathcal{L}_\alpha(X) \times |\log(t_\alpha)^\delta|^{-1}$. In view of (15), resp. of (16), the following bounds are obtained

$$\left|\sum_{n\geq n_0(X)} t^n \gamma_n(X;\beta)\right| \leq C^N N_1! \cdots N_p! \frac{1}{1-|t(z)|}|t(z)|^{n_0(X)}, \quad (18)$$

resp.

$$\sum_{n<n_0(X)} t^n \gamma_n(X;\beta) \leq E'_N N_1! \cdots N_p! \left(1-\frac{(t_\alpha)^\delta}{|t(z)|}\right)^{-1} |t(z)|^{n_0(X)} \quad (19)$$

from which (13) is readily derived with a suitable choice of E_δ.

The same methods also provide the following theorem:

Theorem 3′: Let $t \to (\beta(t), z(t))$ be an analytic mapping of the unit circle $|t| < 1$ with values in $\mathbb{C}^2$, such that the correlations (i) are analytic w.r.t t and satisfy the bounds (4) for $|t| < 1$, (ii) satisfy strong cluster properties in a neighborhood of $t=0$.

Then strong decay properties, which are always strong cluster properties for exponentially decreasing potentials, hold in the whole region $|t| < 1$.

When $z(0)=0$, (ii) can be *proved*; when $\beta(t) \equiv \beta_0$, (ii) is ensured by the strong cluster property *at* $(\beta_0, z(0))$ (see the proof of Theorem 6 in Ref. 4).

Equivalence theorem: Theorems 2, 3 allow the extension to exponentially decreasing potentials of the equivalence Theorem 6 of Ref. 4 between

(i) analyticity with respect to z of the correlations and the bounds (4) in a complex neighborhood of the real segment $[0, z_0]$, and

(ii) the strong cluster properties at *real* points z of $[0, z_0]$.

For potentials which decrease like r^{-s}, the analogous result is not completely proved so far in view of the fact that the bounds (13) do not always ensure the integrability of $|\rho_\Lambda^T|$.

IV. STRONG CLUSTER PROPERTIES FOR CONTINUOUS SYSTEMS

In this section, we briefly mention the extensions of the previous results to the case of continuous gases.

A. Ursell functions

Theorem 1 applies directly to continuous systems with stable potentials such that $C(\beta) = \int_{\mathbb{R}^\nu} |\exp[-\beta\Phi(x)]|\, dx < \infty$; it has been proved in Ref. 10 for hard-core potentials and is proved in Appendix B for general stable potentials.

The bound (7) is proved in Appendix II for hard-core or positive potentials such that

$$\hat{C}(\beta) = \int_{\mathbb{R}^\nu} |\hat{K}(x)|\, dx < \infty$$

where

$$\hat{K}(x) = \sup\{|1-\exp[-\beta\Phi(x)]|, \exp[\beta A](1+\exp(\beta\Phi(x))\}$$

and

$$A = \begin{cases} \sup_{\{x_i\}_{i\in\mathbb{N}}} \sum_{i\in\mathbb{N}} \Phi_-(x_i), & \text{for hard-core potentials with diameter } \delta \text{ and} \\ |x_i - x_j| \geq \delta & \Phi_- = \sup(0, -\Phi) \\ 0, & \text{for positive potentials.} \end{cases}$$

B. Strong cluster properties at $z \neq 0$

The results of Secs. II and III apply to smeared out connected correlations of the form

$$\bar{\rho}^T_\Lambda(x_1, \ldots, x_N) = \frac{1}{a^{\nu(N+1)}} \int dx'_1 \cdots dx'_N \chi_{x_1}(x'_1) \cdots \chi_{x_N}(x'_N) \rho^T_\Lambda(x'_1 \cdots x'_N)$$

where $x_1, \ldots, x_N \in Z^\nu$ and where χ_x is the characteristic function of the cubic cell of side a, centered at ax (a is an arbitrary positive number); in the same way we define

$$\bar{C}_{\Lambda,n}(X;\beta) = \frac{1}{n!} \frac{1}{a^{\nu(N+1)}} \times \int dx'_1 \cdots dx'_N \, dy_1 \cdots dy_n \chi_{x_1}(x'_1) \cdots \chi_{x_N}(x'_N) \times \varphi(X', Y),$$

so that the method of Lemma 1 applies with

$$\bar{L}_\alpha(X) = \inf_{X' : |x_i - x'_i| \leq a/2} L_\alpha(X').$$

The results are then obtained without further restrictions.

We finally note that more general smearing functions χ can also be used.

V. DISCUSSION

As a conclusion, we would like to mention the following remarks:

(1) For reasons which are discussed in Ref. 5, it is also useful to consider strong cluster properties for partially connected correlations, i.e., correlations which are connected only with respect to clusters of points. (These functions and their cluster properties are involved in the problems of analyticity with respect to β or other parameters of the interaction.) The results of the present paper are correspondingly extended in a coming work.[14]

(2) The results obtained for potentials which decrease like r^{-s} are not completely satisfactory: They indicate a decrease like $r^{-s'}$ of the correlations, where $s' = s - \nu - \epsilon$ at low activity and $s' \to 0$ near the boundary of the analyticity domain, outside the Kirkwood–Salzburg region. This type of decay does not always ensure the integrability of the connected correlations $|\rho^T_\Lambda|$, which has been proved directly in Refs. 6 and 7 at least at low activity.

For the 2-point function, a decrease like r^{-s} has indeed been proved at low activity in Refs. 9 and 10. Work is in progress to obtain corresponding results for the N-point functions, at low activity and more generally in the analyticity domain.

(3) In $P(\Phi)_2$ field theories, strong decay properties of the connected Schwinger functions can also be obtained for small $|\lambda|$ and Re $\lambda > 0$,[16] (with $C^N N_1! \cdots N_p!$ being replaced by a different constant A_N).

Theorem 3′ of Sec. III allows extension of these strong decay properties in the connected domain in complex λ-space, containing the above region, where the Schwinger functions remain analytic and satisfy bounds of the form $|S^T_N| < A'_N$.

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APPENDIX A

The Mayer expansion of the connected correlations are proved in Ref. 6 by an algebraic method. In this appendix, we give an alternative method which is based on graph expansions and takes explicitly into account the connected character of $\rho^T_\Lambda(X)$. This method is an adaptation of analogous method of Ref. 15.

The nonconnected correlations are given by

$$\rho_\Lambda(X;z,\beta) = Z^{-1}_\Lambda(z;\beta) z^N \sum_{n \geq 0} \frac{z^n}{n!} \int_{\Lambda^n} dY \exp[\beta U(X, Y)]$$

where the Boltzmann factor has the graph expansion

$$\exp[-\beta U(X,Y)] = \sum_\Gamma (x,y) f(\Gamma).$$

Here the sum $\sum_\Gamma$ runs over all graphs constructed on (X, Y) and

$$f(\Gamma) = \prod_{l \in \Gamma} (\exp[-\beta \Phi(|l|)] - 1).$$

The consideration of the connected parts of the graphs leads to

$$\exp[-\beta U(X,Y)] = \sum_{Y' \subset Y} \exp[-\beta U(Y \setminus Y')] \times \sum_{(X)}{}_{\{X_1 \cdots X_k\}} \sum_{(Y')}{}_{\{Y_1 \cdots Y_k\}} \prod_{i=1}^k \varphi(X_i, Y_i)$$

where the sum $\sum_{(X)}{}_{\{X_1 \cdots X_k\}}$ runs over all partitions of X into nonempty subsets and $\sum_{(Y')}{}_{\{Y_1 \cdots Y_k\}}$ runs over all partitions of Y' into k subsets (with possibly empty ones).

Then using the symmetry of $\exp[-\beta U(X, Y)]$ with respect to Y, we get the following equality between formal expressions:

$$\sum_{n \geq 0} \frac{z^n}{n!} \int_{\Lambda^n} dY \exp[-\beta U(X,Y)] = \left(\sum_{n \geq 0} \frac{z^n}{n!} \int_{\Lambda^n} dY \exp[-\beta U(Y)] \right) \sum_{(X)}{}_{\{X_1 \cdots X_k\}} \prod_{i=1}^k \times \left(\sum_{n \geq 0} \frac{z^n}{n!} \int_\Lambda dY \varphi(X_i, Y) \right);$$

and, consequently, we obtain

$$\rho_\Lambda(X) = \sum_{(X)}{}_{\{X_1 \cdots X_k\}} \prod_{i=1}^k z^{N_i} \left(\sum_{n \geq 0} \frac{z^n}{n!} \int_{\Lambda^n} dY \varphi(X_i, Y) \right).$$

Since

$$\rho_\Lambda(X) = \sum_{(X)}{}_{\{X_1 \cdots X_k\}} \prod_{j=1}^k \rho^T_\Lambda(X_j),$$

we have the formal equation

$$\rho^T_\Lambda(X) = z^N \sum_{n \geq 0} \frac{z^n}{n!} \int_{\Lambda^n} dY \varphi(X, Y).$$

The proof is achieved if this last formal expansion has a nonvanishing radius of convergence; this follows for

instance from bounds on the integrals of the Ursell functions.

APPENDIX B

The methods presented below are adaptations of methods previously used to prove bounds (without decay properties) on the Ursell functions or their integrals: See Chap. IV. in Ref. 6 and also Ref. 11.

They are extended to Ursell functions $\varphi(X_0;X_1, \ldots, X_p)$ which are connected only with respect to clusters $X_0, \ldots, X_p$ in Ref. 14.

Proof of Theorem 1 in Sec. II

It is useful to introduce the Ursell functions $\varphi(X_0;x_1, \ldots, x_N)$ which is connected with respect to a set X_0 of N_0 points $x_{01}, \ldots, x_{0N_0}$ and to the points $x_1, \ldots, x_N$ (but not with respect to the points of X_0) and has the following explicit form:

$$\varphi(X_0;x_1, \ldots, x_N)=\sum_{\Gamma} {}_c(X_0;x_1, \ldots, x_N) \sum_{l\in\Gamma} K(l), \quad \text{(B1)}$$

where the sum $\sum$ runs over all graphs Γ on the points $x_1, \ldots, x_N, x_{01}, \ldots, x_{0N_0}$, which are such that the points $x_1 \cdots x_N$ and the *cluster* X_0 are linked in a connected way.

The following recurrence relations of the Kirkwood–Salzburg type (see for instance Ref. 6) are easily checked from the above definition:

$$\varphi(X_0;x_1, \ldots, x_N)=\exp[-\beta W(x_0,\tilde{X}_0)] \times \sum_{I\subset\{1,\ldots,N\}} \prod_{i\in I} K(x_0-x_i)\varphi(\{\tilde{X}_0,x_I\};x_{CI}), \quad \text{(B2)}$$

where $x_0\in X_0$, $\tilde{X}_0=X_0\backslash x_0$, $W(x_0,\tilde{X}_0)=\sum_{y\in\tilde{X}_0}\Phi(x_0-y)$, $x_I=\{x_i, i\in I\}$, and CI is the complement of I in $\{1\cdots N\}$.

It is always possible[6] to choose a point $x_0\in X_0$ such that

$$\exp[-\beta W(x_0,\tilde{X}_0)]\leq \exp(2\beta B). \quad \text{(B3)}$$

Then, the following inequality is easily derived from (B2) by induction on the total number $N+N_0$ of points:

$$|\varphi(X_0;x_1, \ldots, x_N)| \leq (\exp(2\beta B))^{N+N_0-1} \sum_{\Gamma(x_0;x_1,\ldots,x_N)} \prod_{l\in\Gamma} |K(l)|, \quad \text{(B4)}$$

where the sum $\sum$ runs over all graphs on the points $x_1, \ldots, x_N, x_{01}, \ldots, x_{0N_0}$ such that

(i) there are no internal lines inside X_0,

(ii) the graph Γ^v induced by contraction of X_0 (i.e., by identifying all its vertices) is a connected tree.

The bound (6) of Theorem 1 is the particular case of (B4) obtained when $N_0=1$. [The bound derived from (B4) includes a further factor $\exp(2\beta B)$. This factor is however easy to remove.]

Proof of the bound (7) in Sec. II

The bound (7) is proved similarly by using the following recurrence relations of the Mayer–Montroll type, which are also easily checked from the definition (B1):

$$\varphi(X_0;x_1, \ldots, x_N)= =\exp[-\beta U(X_0)] \sum_{I\subset\{1\cdots N\}} \prod_{i\in I} K(X_0,x_i)\varphi(\{x_I\};x_{CI}) \quad \text{(B5)}$$

where $K(X_0,x)=\exp[-\beta W(x,X_0)-1]$, with $I\neq\phi$.

The following inequality, proved in Ref. 11, is to be used:

$$|K(X_0,y)| \leq \sum_{i=1}^{N_0} \hat{K}(x_0-y) \quad \text{(B6)}$$

(when all points of X_0 are different from each other). (Note that $\varphi=0$ otherwise.)

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The conditional entropy in the microcanonical ensemble

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The existence of the configurational microcanonical conditional entropy in classical statistical mechanics is proved in the thermodynamic limit for a class of long-range multiparticle observables. This result generalizes a theorem of Lanford for finite range observables.

Although a considerable amount of research has been directed in recent years toward proving the existence of the thermodynamic limit for the classical ensembles, the microcanonical ensemble for long-range interactions has presented certain difficulties. In this article we provide a proof of the existence of the configurational conditional entropy for a class of systems including long-range interactions falling off in ν dimensions faster than $1/r^{\nu}$.

Griffiths, using arguments of Fisher,[1,2] has outlined proofs of the existence of the microcanonical entropy for variously tempered two-body interactions. There the microcanonical energy is studied as a function of the entropy, and the entropy is recovered implicitly after the infinite volume limit has been taken. Similar results for two-body interactions were obtained by Minlos and Povzner.[3]

Lanford[4] has pointed out that methods of Ruelle[5] can be employed to obtain the entropy directly, and has used this approach to prove the existence of the configurational conditional entropy for strictly finite-range observables.

We use the Lanford approach to extend the existence theorem to observables with long-range behavior.

1. LIMIT ALONG A SPECIAL SEQUENCE OF CUBES

Let T^{ν} designate either the ν-dimensional lattice Z^{ν} or ν-dimensional real Euclidean space $\mathbb{R}^{\nu}$ with counting or Lebesgue measure μ, and denote the corresponding phase space by $\mathcal{G}$, $\mathcal{G}=\cup_{n=1}^{\infty}(T^{\nu})^n$. The extension of μ to $(T^{\nu})^n$ and $\mathcal{G}$ will also be written μ. If $Q_i\in\mathcal{G}\cap(T^{\nu})^{n_i}$, $Q_i=(q_{i1},\ldots,q_{in_i})$, $i=1,2$, write $N(Q_i)=n_j$, $q_{ij}\in Q_i$, and $d(Q_1,Q_2)=\inf\{\tilde{d}(q_1,q_2)\mid q_i\in Q_i\}$, where $\tilde{d}:T^{\nu}\times T^{\nu}\to\mathbb{R}$ is the Euclidean metric. Let $\mathcal{S}$ be the set of bounded, measurable subsets of T^{ν}, and $\mathcal{C}_t$, the set of bounded open convex subsets of $\mathbb{R}^t$, $t\in Z_+$. If $J\in\mathcal{C}_t$ and $\epsilon>0$, then $J^{\epsilon}=\{x\in J\mid\|x-y\|>\epsilon,\ \forall\, y\in\mathbb{R}^t/J\}$ is the ϵ-contraction of J, and $J^{-\epsilon}=\{x\in\mathbb{R}^t\mid\|x-y\|<\epsilon \text{ for some } y\in J\}$.

Definition 1.1: The real linear space $\mathcal{A}_t^{\lambda}$ of t-valued observables, $t\in Z_+$ and $\lambda\in\mathbb{R}$, is the set of μ-measurable functions $f:\mathcal{G}\to\mathbb{R}^t$ satisfying the following:

(i) $f(Q+q)=f(Q)$, $Q\in\mathcal{G}$, $q\in T^{\nu}$, and $Q+q=\{p\in T^{\nu}\mid p-q\in Q\}$;

(ii) $f(Q)=f(Q')$ if Q' is a permutation of Q;

(iii) there exist $A>0$ and $R_0>0$ such that, for all $m\in Z_+$ and $Q_1,\ldots,Q_m\in\mathcal{G}$, $d(Q_i,Q_j)\geq r\geq R_0$ for all $i\neq j$ implies

$$\left\| f(Q_1,\ldots,Q_m)-\sum_{i=1}^{m} f(Q_i)\right\| \leq \frac{A}{r^{\lambda}}\left(\sum_{i=1}^{m} N(Q_i)\right)^2.$$

For $\Lambda\in\mathcal{S}$, $J\in\mathcal{C}_t$, $n\in Z_+$, and $f\in\mathcal{A}_t^{\lambda}$, the conditional phase space volume $\mathcal{V}_f$ is

$$\mathcal{V}_f(\Lambda,n,J)=(1/n!)\,\mu\{Q\in\Lambda^n\mid(1/n)f(Q)\in J\}.$$

The vector-valued observable f is to be viewed as a set of t translation-invariant symmetric scalar-valued observables, with a decrease condition (tempering) for each at large distances. For example, tempering would require a pair potential interaction generating a Hamiltonian to fall off at least as fast as $r^{-\lambda}$. Since the observable f will be fixed, the subscript on $\mathcal{V}$ will be dropped. Also, throughout it will be necessary to assume that $\lambda>\nu$.

Proposition 1.2: (a) If $J\in\mathcal{C}_t$ and $\Lambda\subset\Lambda'$, Λ, $\Lambda'\in\mathcal{S}$, then $\mathcal{V}(\Lambda',n,J)\geq\mathcal{V}(\Lambda,n,J)$.

(b) If $\{\Lambda_i\}_{i=1}^m\subset\mathcal{S}$, $d(\Lambda_i,\Lambda_j)\geq r\geq R_0$ for $i\neq j$, $n=\sum_{i=1}^m n_i$, $n_i\in Z_+$, and $\{J_i\}_{i=1}^m\subset\mathcal{C}_t$, then

$$\mathcal{V}\left(\bigcup_{i=1}^{m}\Lambda_i,\ \sum_{i=1}^{m} n_i,\ \sum_{i=1}^{m}\left(\frac{n_i}{n}\right)J_i\right)\geq\prod_{i=1}^{m}\mathcal{V}(\Lambda_i,n_i,J_i^{An^{-\lambda}}).$$

Proof: The first part is obvious. If $Q_i\in\Lambda_i^{n_i}$, then for $J=\sum_{i=1}^m(n_i/n)J_i$, $(1/n_i)f(Q_i)\in J_i^{An^{-\lambda}}$ implies $(1/n)f(Q_1,\ldots,Q_m)\in J$ by 1.1 (iii), since

$$\frac{1}{n}\sum_{i=1}^{m} f(Q_i)\in\sum_{i=1}^{m}\left(\frac{n_i}{n}\right)J_i^{An^{-\lambda}}=J^{An^{-\lambda}}.$$

Hence

$$\left\{(Q_1,\ldots,Q_m)\,\middle|\, Q_i\in\Lambda_i^{n_i}\text{ and }\frac{1}{n_i}f(Q_i)\in J_i^{An^{-\lambda}}\right\}$$

$$\subset\left\{Q\in\left(\bigcup_{i=1}^{m}\Lambda_i\right)^n\,\middle|\,\frac{1}{n}f(Q)\in\sum_{i=1}^{m}\left(\frac{n_i}{n}\right)J_i\right\}.$$

Define the density $\rho=n/\mu(\Lambda)$, the specific volume $v=1/\rho$, and $l_v=v^{1/\nu}$. For $\epsilon=\lambda-\nu>0$ as in 1.1 (ii), $\kappa\in(0,1)$, and $m\in Z_+$, let $\theta_{\kappa}=2^{(\nu+\kappa\epsilon)/\lambda}$, $\varphi_{\kappa}=[1-(2^{\nu}/\theta_{\kappa}^{\lambda})]^{-1}$, $R_{\kappa}=R_0(2-\theta_{\kappa})^{-1}$, $R_{\kappa,m}=\theta_{\kappa}^m R_0$, and $\Delta_{\kappa,m}=A\varphi_{\kappa}2^{(m+1)\nu}/R_{\kappa,m}^{\lambda}$. Denote the cube $\Lambda_{\kappa,m}(v)=\{q=(q_1,\ldots,q_{\nu})\in T^{\nu}\mid 0<q_k<2^m l_v-\theta_{\kappa}^m R_{\kappa},\ k=1,\ldots,\nu\}$.

The reasons for choosing $\Lambda_{\kappa,m}(v)$ and $R_{\kappa,m}$ in this manner will be apparent from Proposition 1.3. In particular, φ_κ is chosen to make valid the last equality in the proof of that proposition. Note that as $m \to \infty$ $\Delta_{\kappa,m}$ goes to zero as $2^{-\kappa\epsilon m}$, and $J^{\Delta_{\kappa,m}} \to J$. The parameter κ is specified, since later some control will be needed over the rate of convergence of $\Delta_{\kappa,m}$ to zero.

Proposition 1.3: If $J \in \mathcal{C}_t$, then

$$\not\parallel(\Lambda_{\kappa,m+1}(v),\ 2^{(m+1)\nu}, J^{\Delta\kappa,m+1}) \geq \{\not\parallel(\Lambda_{\kappa,m}(v), 2^{m\nu}, J^{\Delta\kappa,m})\}^{2^\nu}.$$

Proof: Since $R_{\kappa,m} = (2^{m+1}l_v - \theta_\kappa^{m+1}R_\kappa) - 2(2^m l_v - \theta_\kappa^m R_\kappa)$, 2^ν disjoint translates of $\Lambda_{\kappa,m}(v)$ with mutual separation equal to or greater than $R_{\kappa,m}$ can be placed inside $\Lambda_{\kappa,m+1}(v)$. Further,

$$(J^{\Delta\kappa,m+1})^{A2^{(m+1)\nu}/R^\lambda_{\kappa,m}} = J^{\Delta_{\kappa,m}}.$$

The proof is completed using 1.2.

Corollary 1.4:

$$\frac{1}{2^{(m+1)\nu}} \log \not\parallel(\Lambda_{\kappa,m+1}(v),\ 2^{(m+1)\nu},\ J^{\Delta\kappa,m+1})$$

$$\geq \frac{1}{2^{m\nu}} \log \not\parallel(\Lambda_{\kappa,m}(v), 2^{m\nu}, J^{\Delta\kappa,m})$$

and the limit as $m \to \infty$ is equal to the supremum over $m \in Z_+$.

Definition 1.5: For $J \in \mathcal{C}_t$ and $x \in \mathbb{R}^t$, let

$$S_\kappa(v,J) = \lim_{m\to\infty} \frac{1}{2^{m\nu}} \log \not\parallel(\Lambda_{\kappa,m}(v), 2^{m\nu}, J^{\Delta\kappa,m})$$

and

$$s_\kappa(v,x) = \inf_{x\in J\in\mathcal{C}_t} \{S_\kappa(v,J)\}.$$

Proposition 1.6: (i) If $J \subset J'$, $J, J' \in \mathcal{C}_t$, then $S_\kappa(v,J) \leq S_\kappa(v,J') \leq 1 + \log v$.

(ii) If $\{J_i\}_{i=1}^k \subset \mathcal{C}_t$, $J_0 = \cup_{i=1}^k J_i \in \mathcal{C}_t$, and for $\Delta > 0$ sufficiently small, $\cup_{i=1}^k J_i^\Delta = J_0^\Delta$, then $S_\kappa(v, \cup_{i=1}^k J_i) = \sup_{1\leq i\leq k} S_\kappa(v, J_i)$.

(iii) If $J \in \mathcal{C}_t$, then $S_\kappa(v,J) = \sup\{S_\kappa(v,\hat{J}) \mid \hat{J} \in \mathcal{C}_t, \hat{J}^- \subset J\}$.

(iv) $S_\kappa(v,J) = \sup_{x\in J} S_\kappa(v,x)$.

Proof: Routine, using 1.2 and properties of μ.

Corollary 1.7: (i) $x \to s_\kappa(v,x)$ is upper semicontinuous and concave on $\mathbb{R}^t$.

(ii) $v \to s_\kappa(v,x)$ is nondecreasing and concave on $\mathbb{R}_+$, and continuous on (v_x, ∞), where $v_x = \inf\{v \mid s_\kappa(v,x) > -\infty\}$.

When the tempering condition in the definition of $\mathcal{A}_t^\lambda$ is replaced by a finite range condition (additivity: $A = 0$), then the interior of Γ_κ is nonempty if the components of f are linearly independent. More generally, a sort of asymptotic openness is required.

Proposition 1.8: Let $\Omega_\kappa(v)$ be the convex set

$$\Omega_\kappa(v) = \{x \in \mathbb{R}^t \mid s_\kappa(v,x) > -\infty\},$$

and, for $m \in Z_+$, let $E_m(v) = \text{ess range}\ ((1/2^{m\nu}) f_{\kappa,m})$, where $f_{\kappa,m}$ is the restriction of f to $[\Lambda_{\kappa,m}(v)]^{2^{m\nu}}$. Write

$$\lim_{n\to\infty} \text{s. } E_m(v)$$
$$= \{x \in \mathbb{R}^t \mid 0 \cap E_m(v) \neq \phi \text{ for infinitely many } m, \text{ for each open } 0 \subset \mathbb{R}^t,\ x \in 0\}.$$

Then

$$\Omega_\kappa(v)^- = \lim_{m\to\infty} \text{s. } E_m(v).$$

Proof: If $x_0 \notin \Omega_\kappa(v)^-$, then there exists $J \in \mathcal{C}_t$ such that $x_0 \in J$ and $S_\kappa(v,J) = -\infty$, hence $J^{\Delta\kappa,m} \cap E_m(v) = \phi$ and $x_0 \in J^{\Delta\kappa,m}$ for m sufficiently large. Therefore, $x_0 \notin \lim\text{ s.}_{m\to\infty} E_m(v)$.

On the other hand, $x_0 \notin \lim\text{ s.}_{m\to\infty} E_m(v)$ implies $J \cap E_m(v) = \phi$ for some $J \in \mathcal{C}_t$, $x_0 \in J$, and all sufficiently large m. Passing to the contraction $J^{\Delta\kappa,m}$ gives the desired result.

Definition 1.9: We say that f is asymptotically open if there exists $v > 0$ and $\kappa = K$ such that $(\lim\text{ s.}_{m\to\infty} E_m(v))^0 \neq \phi$. We denote by $v_0(\kappa)$ the infimum over all such v for any $\kappa \leq K$. In the remainder we will always assume that $\kappa \leq K$.

If f is asymptotically open and $v > v_0(\kappa)$, then $\Omega_\kappa(v)^0 \neq \phi$. Let $\Gamma_\kappa = \Gamma_\kappa(f)$ be the set $\{(v,x) \in \mathbb{R}_+ \times \mathbb{R}^t \mid s_\kappa(v,x) > -\infty\}$.

Corollary 1.10: (i) Γ_κ^0 is convex.

(ii) If f is asymptotically open, then Γ_κ^0 is nonempty and dense in Γ_κ.

(iii) $(v,x) \to s_\kappa(v,x)$ is continuous and concave on Γ_κ^0.

Corollary 1.11: If f is asymptotically open and $0 < v < v_0(\kappa)$, then $\Omega_\kappa(v) = \phi$. Hence $v_0(\kappa) = \inf_x v_x$.

2. INDEPENDENCE OF THE PARAMETER

We shall show in this section that the contraction parameter κ can be removed, and that the result coincides with the conditional entropy defined without contractions, at least for the limit taken along a special sequence of cubes.

Lemma 2.1: Let $f: \mathbb{R}^t \to \mathbb{R} \cup \{-\infty, \infty\}$ be upper semicontinuous and concave, $J_1, J_2 \in \mathcal{C}_t$ with $J_1 \cap J_2 \neq \phi$, $f(J_1 \cap J_2) \cap \mathbb{R} \neq \phi$, and $\{d_i\}_{i=1}^\infty$ a sequence of positive real numbers with $d_i \to 0$. Then

$$\inf_i \sup_{x\in J_1^{-d_i} \cap J_2} f(x) = \sup_{x\in J_1\cap J_2} f(x).$$

Proof: Since $J^{-d_i} \supset J$,

$$\inf_i \sup_{x\in J_1^{-d_i}\cap J_2} f(x) \geq \sup_{x\in J_1\cap J_2} f(x).$$

So assume $(J_1^{-d_i}/J_1) \cap J_2 \neq \phi$ for all i, $\sup_{x\in J_1\cap J_2} f(x) < \infty$, and suppose

$$\inf_i \sup_{x\in J_1^{-d_i}\cap J_2} f(x) > \sup_{x\in J_1\cap J_2} f(x) + \tfrac{3}{2}\epsilon, \quad \epsilon > 0.$$

Then, for each i,

$$\sup_{x\in (J_1^{-d_i}/J_1)\cap J_2} f(x) > \sup_{x\in J_1\cap J_2} f(x) + \tfrac{3}{2}\epsilon.$$

Let $y_i' \in (J_1^{-d_i}/J_1) \cap J_2$ be such that

$$f(y_i') > \sup_{x \in (J_1^{-d_i}/J_1) \cap J_2} f(x) - \epsilon/2$$

and $\{y_i\}_{i=1}^{\infty}$ a subsequence convergent to $y \in \partial(J_1 \cap J_2)$. If $z_i \to y$, by upper semicontinuity,

$$f(y) \geq \lim_{i \to \infty} \sup f(z_i) \geq \lim_{i \to \infty} \sup f(y_i) \geq \sup_{x \in J_1 \cap J_2} f(x) + \epsilon$$

and by concavity

$$\sup_{x \in (J_1 \cap J_2)^-} f(x) = \sup_{x \in J_1 \cap J_2} f(x),$$

which yields a contradiction.

Definition 2.2: For $v > 0$ and $\kappa \in (0, K)$, let $\tilde{C}_t(v, \kappa) = \{J \in C_t \mid (\{v\} \times J) \cap \Gamma_\kappa \neq \emptyset$ or $d(\{v\} \times J, \Gamma_\kappa) > 0\}$. For $J \in \tilde{C}_t(v, \kappa)$ and $x \in \mathbb{R}^t$, define

$$S_{\kappa,0}(v, J) = \lim_{m \to \infty} \frac{1}{2^{m\nu}} \log \mathcal{V}(\Lambda_{\kappa,m}(v), 2^{m\nu}, J),$$

$$s_{\kappa,0}(v, x) = \inf_{x \in J \in \tilde{C}_i} S_{\kappa,0}(v, J),$$

and for $\kappa_1, \kappa_2 \in (0, K)$, $\alpha > 0$,

$$S_{\kappa_1,\kappa_2,\alpha}(v, J) = \lim_{m \to \infty} \frac{1}{2^{m\nu}} \log \mathcal{V}(\Lambda_{\kappa_1,m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_2,m}}$$

Theorem 2.3: If $0 < v \neq v_0(\kappa_i)$, $\alpha > 0$, $\kappa_1, \kappa_2 \in (0, K)$, and $J \in \tilde{C}_t(v, \kappa_1) \cap \tilde{C}_t(v, \kappa_2)$, then

(i) $S_{\kappa_1,0}(v, J) = S_{\kappa_1}(v, J)$,

(ii) $S_{\kappa_1}(v, J) = S_{\kappa_2}(v, J)$,

(iii) $S_{\kappa_1,\kappa_2,\alpha}(v, J) = S_{\kappa_1}(v, J)$.

Proof: For each $d > 0$ there exists a positive integer $m(d)$ satisfying

$$(1/2^{m\nu}) \log \mathcal{V}(\Lambda_{\kappa,m}(v), 2^{m\nu}, J) \leq (1/2^{m\nu}) \log \mathcal{V}(\Lambda_{\kappa,m}(v), \times 2^{m\nu}, J^{-d+\Delta_{\kappa,m}})$$

for $m > m(d)$. Hence, if $\{d_i\}_{i=1}^{\infty}$ is a sequence of positive numbers with $d_i \to 0$,

$$\lim_{m \to \infty} \sup (1/2^{m\nu}) \log \mathcal{V}(\Lambda_{\kappa,m}(v), 2^{m\nu}, J) \leq \inf_i S_\kappa(v, J^{-d_i}).$$

Now, by Proposition 1.6(iv) and the concavity of $x \to s_\kappa(v, x)$,

$$S_\kappa(v, J^{-d_i}) = \sup\{s_\kappa(v, x) \mid x \in J^{-d_i} \cap \Omega_\kappa(v)^0\}.$$

Therefore, for $(\{v\} \times J) \cap \Gamma_\kappa^0 \neq \emptyset$, by 1.7 and 2.1, $\inf_i S_\kappa(v, J^{-d_i}) = S_\kappa(v, J)$, and so

$$\lim_{m \to \infty} \sup (1/2^{m\nu}) \log \mathcal{V}(\Lambda_{\kappa,m}(v), 2^{m\nu}, J) \leq S_\kappa(v, J).$$

In the case $d(\{v\} \times J, \Gamma_\kappa) > 0$, if δ satisfies $(\{v\} \times J^{-\delta}) \cap \Gamma_\kappa = \emptyset$, then $S_\kappa(v, J^{-\delta}) = -\infty$, so that $S_\kappa(v, J) = -\infty$.

Assuming $\kappa_2 > \kappa_1$ and noting $\Lambda_{\kappa_2,m}(v) \subset \Lambda_{\kappa_1,m}(v)$, obtain $S_{\kappa_2,0}(v, J) \leq S_{\kappa_1,0}(v, J)$. On the other hand, letting $0 < v' < v$ if $v < v_0(\kappa_1)$, or $v_0(\kappa_1) < v' < v$ otherwise, compute

$$\lim_{m \to \infty} \frac{2^{m+1} l_v - \theta_{\kappa_2}^{m+1} R_{\kappa_2}}{2(2^m l_{v'})} = \frac{l_v}{l_{v'}} > 1,$$

so that 2^ν disjoint translates of the cube with sides $(0, 2^m l_{v'})$ can be placed inside $\Delta_{\kappa_2,m+1}(v)$ for all sufficiently large m, and hence 2^ν disjoint translates of $\Lambda_{\kappa,m}(v')$ with mutual separations equal to or greater than $R_{\kappa_1,m}$. Since

$$J^{\Delta_{\kappa_1,m+1}} \subset J^{\Delta_{\kappa_2,m+1}}$$

for sufficiently large m, therefore

$$\mathcal{V}(\Lambda_{\kappa_2,m+1}(v), 2^{(m+1)\nu}, J^{\Delta_{\kappa_2,m+1}}) \geq [\mathcal{V}(\Lambda_{\kappa_1,m}(v'), 2^{m\nu}, J^{\Delta_{\kappa_1,m}})]^{2^\nu}$$

and so

$$S_{\kappa_2}(v, J) \geq \sup_{v' < v} S_{\kappa_1}(v', J) = S_{\kappa_1}(v, J).$$

Thus (ii) follows from (i).

Finally, for $\kappa_2 > \kappa_1$, $d > 0$, and m sufficiently large,

$$\mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\Delta_{\kappa_2,m}}) \geq \mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1,m}})$$

and

$$\mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1,m}}) \geq \mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{d+\Delta_{\kappa_2,m}})$$

so that

$$S_{\kappa_2}(v, J) \geq \lim_{m \to \infty} \sup (1/2^{m\nu}) \log \mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1,m}})$$

and

$$\lim_{m \to \infty} \inf (1/2^{m\nu}) \log \mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1,m}}) \geq \sup_{d > 0} S_{\kappa_2}(v, J^d)$$

$$\geq \sup\{S_{\kappa_2}(v, \hat{J}) \mid \hat{J} \in C_t \text{ and } \hat{J}^- \subset J\} = S_{\kappa_2}(v, J).$$

If $\kappa_2 < \kappa_1$, then, for m large,

$$\mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1,m}}) \geq \mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\Delta_{\kappa_2,m}})$$

so that

$$\lim_{m \to \infty} \inf (1/2^{m\nu}) \log \mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1,m}}) \geq S_{\kappa_2}(v, J).$$

On the other hand,

$$S_{\kappa_2}(v, J) = S_{\kappa_2,0}(v, J) \geq \lim_{m \to \infty} \sup (1/2^{m\nu}) \log \mathcal{V}(\Lambda_{\kappa_2,m}(v), 2^{m\nu}, J^{\alpha \Delta_{\kappa_1,m}}).$$

Corollary 2.4: For all $v > 0$, $v \neq v_0(\kappa_1)$, $\kappa_1, \kappa_2, \kappa_3 \in (0, K)$, and $x \in \mathbb{R}^t$,

$$S_{\kappa_1}(v, x) = S_{\kappa_2}(v, x) = S_{\kappa_3,0}(v, x).$$

Corollary 2.5: $\Gamma(f) = \Gamma_\kappa(f)$, $\tilde{C}_t(v) = \tilde{C}_t(v, \kappa)$, and $v_0 = v_0(\kappa)$ are independent of κ.

3. LIMIT ALONG GENERAL SEQUENCES

We wish to extend the results of the previous sections, derived for limits taken along the *standard* sequences of cubes $\{\Lambda_{\kappa,m}\}_{m=1}^{\infty}$, to limits along a more general sequence of domains.

For $\Lambda \in \mathcal{S}$ with boundary $\partial\Lambda$, let $V_\partial(r; \Lambda)$

$= \mu\{x \in T^\nu \mid d(x, \partial\Lambda) \leq r\}$. A sequence $\{\Lambda_i\}_{i=1}^\infty \subset \mathcal{S}$ is said to tend to infinity in the sense of Fisher, $\Lambda_i \to \infty$ (Fisher) if[6] $V(\Lambda_i) \to \infty$ and there exists an $i_0 \in Z_+$ such that

$$\lim_{\alpha \to 0} \sup_{i \geq i_0} V_\partial(\alpha V(\Lambda_i)^{1/\nu}; \Lambda_i)/V(\Lambda_i) = 0.$$

Lemma 3.1[1]: If $\Lambda \in \mathcal{S}$ is filled with cubes of edge-length d lying entirely within Λ, the volume remaining after maximal filling is less than $V_\partial(\nu^{1/\nu} d; \Lambda)$.

Suppose $\{\Lambda_i\}_{i=1}^\infty \subset \mathcal{S}$, $\Lambda_i \to \infty$ (Fisher), and $\{n_i\}_{i=1}^\infty \subset Z_+$ satisfy $\lim_{i\to\infty} V(\Lambda_i)/n_i = v \in (0, \infty)$. Then we will say that $\{(\Lambda_i, n_i)\}_{i=1}^\infty$ is a Fisher system tending to density $1/v$. In this case, let $\kappa, \kappa', \kappa'' \in (0, K)$ be such that $\kappa'' > \kappa' > \kappa$ and $\kappa'' - \kappa' > \kappa$, for $n \in Z_+$; let $m(n) = \mathcal{N}((\log_2 n)[\nu + \kappa'(\lambda - \nu)]^{-1})$, where $\mathcal{N}(x)$ is the greatest integer in x, and define $n_i = m_i 2^{m(n_i)\nu} + r_i$ with $0 \leq r_i < 2^{m(n_i)\nu}$ and

$$r_i = \sum_{j=0}^{m(n_i)-1} C_{ij} 2^{j\nu}$$

For $0 < v' < v$, let $\zeta > 1$ satisfy $v' < \zeta^\nu v' < v$, and write $\Lambda_m(\zeta^\nu v')$, $m \in Z_+$, for the cube in T^ν with edges $(0, 2^m \zeta l_{v'})$. Finally, let $\mathcal{J}_i$ be the number of cubes in a maximal filling of Λ_i with translates of cubes $\Lambda_{m(n_i)}(\zeta^\nu v')$.

Lemma 3.2: For i sufficiently large, $m_i + \sum_{j=0}^{m(n_i)-1} C_{ij}$ disjoint translates of $\Lambda_{m(n_i)}(\zeta^\nu v')$ may be placed inside Λ_i.

Proof: Observe

$$\lim_{i\to\infty} \frac{\mathcal{J}_i 2^{m(n_i)\nu}}{n_i} = \frac{v}{\zeta^\nu v'} \lim_{i\to\infty} \frac{\mathcal{J}_i V(\Lambda_{m(n_i)}(\zeta^\nu v'))}{V(\Lambda_i)}.$$

Therefore, if $\lim_{i\to\infty} \mathcal{J}_i V(\Lambda_{m(n_i)}(\zeta^\nu v'))/V(\Lambda_i) = 1$, then $\lim_{i\to\infty} \mathcal{J}_i/m_i \geq v/\zeta^\nu v'$, and so there exists $\xi \in \mathbb{R}$, $\zeta^\nu v'/v < \xi < 1$ such that $\mathcal{J}_i > m_i + (\xi v/\zeta^\nu v' - 1)m_i$ for all large enough i. Hence $m_i + \mathcal{N}(m_i \xi v/\zeta^\nu v' - m_i)$ disjoint translates of $\Lambda_{m(n_i)}(\zeta^\nu v')$ may be placed inside Λ_i, and the lemma follows from obvious estimates.

Using 3.1 for $i \geq i_0$ and

$$H(\alpha) = \sup_{i \geq i_0} V_\partial(\alpha V(\Lambda_i)^{1/\nu}, \Lambda_i)/V(\Lambda_i),$$

$$1 - \frac{\mathcal{J}_i V(\Lambda_{m(n_i)}(\zeta^\nu v'))}{V(\Lambda_i)} \leq \frac{V_\partial(\nu^{1/\nu} 2^{m(n_i)} \zeta l_{v'}; \Lambda_i)}{V(\Lambda_i)}$$

$$\leq H\left(\frac{\nu^{1/\nu} 2^{m(n_i)} \zeta l_{v'}}{V(\Lambda_i)^{1/\nu}}\right).$$

Choose $w \in \mathbb{R}$, $\zeta l_{v'}/l_v < w < 1$, so that, for i large, $V(\Lambda_i)^{1/\nu} > w l_v n_i^{1/\nu}$. Then $\zeta l_{v'}/V(\Lambda_i)^{1/\nu} < n_i^{-1/\nu}$, and

$$H(\nu^{1/\nu} 2^{m(n_i)} \zeta l_{v'}/V(\Lambda_i)^{1/\nu}) \leq H(\nu^{1/\nu} n_i^{1/[\nu+\kappa'(\lambda-\nu)]-1/\nu}).$$

But

$$\lim_{i\to\infty} n_i^{1/[\nu+\kappa'(\lambda-\nu)]-1/\nu} = 0.$$

Theorem 3.3: Suppose $\{(\Lambda_i, n_i)\}_{i=1}^\infty$ is a Fisher system tending to density $1/v$, $v \neq v_0$. Let $\{d_i\}_{i=1}^\infty$ be a sequence of nonnegative real numbers, $d_i \to 0$, $\kappa \in (0, K)$, and $J \in \tilde{C}_t(v)$. Then

$$\liminf_{i\to\infty} \frac{1}{n_i} \log \mathcal{V}(\Lambda_i, n_i, J^{d_i}) \geq S_{\kappa,0}(v, J).$$

Proof: From 1.6 and 2.3, it is sufficient to show that there exists $\kappa'' \in (0, K)$ such that for all $v_0 < v' < v$ and $\hat{J} \in C_t$ with $\hat{J}^- \subset J$,

$$\liminf_{i\to\infty} (1/n_i) \log \mathcal{V}(\Lambda_i, n_i, J^{d_i}) \geq S_{\kappa''}(v', \hat{J}).$$

Suppose $\kappa, \kappa', \kappa'' \in (0, K)$ as before, Lemma 3.2. By that lemma, for sufficiently large i, $m_i + \sum_{j=0}^{m(n_i)-1} C_{ij}$ disjoint translates of $\Lambda_{\kappa'', m(n_i)}(\zeta^\nu v')$ with mutual separation at least $\theta_{\kappa''}^{m(n_i)} R_0$ may be placed inside Λ_i. Therefore, for any $\tilde{J} \in C_t$ and i sufficiently large,

$$\mathcal{V}_i \equiv \mathcal{V}\left(\Lambda_i, n_i, \frac{m_i 2^{m(n_i)\nu}}{n_i} \hat{J} + \sum_{j=0}^{m(n_i)-1} \left(\frac{C_{ij} 2^{j\nu}}{n_i}\right) \tilde{J}\right)$$

$$\geq [\mathcal{V}(\Lambda_{\kappa'', m(n_i)}(\zeta^\nu v'), 2^{m(n_i)\nu}, \hat{J}^{\Delta_i})]^{m_i}$$

$$\times \prod_{j=0}^{m(n_i)-1} [\mathcal{V}(\Lambda_{\kappa'', m(n_i)}(\zeta^\nu v'), 2^{j\nu}, \tilde{J}^{\Delta_i})]^{C_{ij}},$$

where $\Delta_i = A n_i/\theta_{\kappa''}^{\lambda m(n_i)} R_0^\lambda$.

A short computation gives $\Delta_i < C\Delta_{\kappa''-\kappa', m(n_i)}$ for $C = 2^{\kappa'(\lambda-\nu)} \varphi_{\kappa''-\kappa'}^{-1}$, and $\Delta_{\kappa,j} \geq A\varphi_\kappa 2^{\nu+\kappa(\lambda-\nu)}/R_0^\lambda 2^{\kappa(\lambda-\nu)m(n_i)}$ for $0 \leq j < m(n_i)$. Hence, for large enough i, $\Delta_i < \Delta_{\kappa,j}$, so that $\tilde{J}^{\Delta_{\kappa,j}} \subset \tilde{J}^{\Delta_i}$. Similarly, it is seen that $\Lambda_{\kappa,j}(v') \subset \Lambda_{\kappa'', m(n_i)}(\zeta^\nu v')$ and $\Lambda_{\kappa'', m(n_i)}(v') \subset \Lambda_{\kappa'', m(n_i)}(\zeta^\nu v')$. Writing $N_1 = \inf\{m \in Z_+ \mid \Lambda_{\kappa,m}(v') \neq \emptyset\} \in \{0, 1, \ldots, m(n_i) - 1\}$, we obtain

$$\mathcal{V}_i \geq [\mathcal{V}(\Lambda_{\kappa'', m(n_i)}(v'), 2^{m(n_i)\nu}, \hat{J}^{C\Delta_{\kappa''-\kappa', m(n_i)}})]^{m_i}$$

$$\times \prod_{j=0}^{N_1-1} [\mathcal{V}(\Lambda_{\kappa, N_1}(v'), 2^{j\nu}, J^{\Delta_{\kappa,j}})]^{C_{ij}}$$

$$\times \prod_{j=N_1}^{m(n_i)-1} [\mathcal{V}(\Lambda_{\kappa,j}(v'), 2^{j\nu}, \tilde{J}^{\Delta_{\kappa,j}})]^{C_{ij}}.$$

Next $\tilde{J} \in C_t$ will be fixed to guarantee that each of the factors above will be nonzero. Choose $x_0 \in \mathbb{R}^t$ such that $s_\kappa(v', x_0) > -\infty$ and let $J_{-1} \in C_t$ be a rectangular solid with edges $\{(a_{-1k}, b_{-1k})\}_{k=1}^t$ containing x_0. Then, for all $j \geq N_2$, $\mathcal{V}(\Lambda_{\kappa,j}(v'), 2^{j\nu}, J_{-1}^{\Delta_{\kappa,j}}) > 0$, where $N_2 = \inf\{j \in Z_+ \mid \mathcal{V}(\Lambda_{\kappa,j}(v'), 2^{j\nu}, J_{-1}^{\Delta_{\kappa,j}}) > 0\}$, and, for i large, $0 \leq N_2 < m(n_i)$. Let $J_j \in C_t$ be a rectangular solid with edges $\{(a_{jk}, b_{jk})\}_{k=1}^t$ such that $\mathcal{V}(\Lambda_{\kappa,N_1}(v'), 2^{j\nu}, J_j^{\Delta_{\kappa,j}}) > 0$ for $0 \leq j < N_1$, and $\mathcal{V}(\Lambda_{\kappa,j}(v'), 2^{j\nu}, J_j^{\Delta_{\kappa,j}}) > 0$ for $N_1 \leq j < N_2$. Then define J to be a rectangle with sides $\{(a_k, b_k)\}_{k=1}^t$, where

$$a_k = (\inf_{-1 \leq j < N_3} a_{jk}) - \Delta_{\kappa,0}, \quad b_k = (\inf_{-1 \leq j < N_3} b_{jk}) + \Delta_{\kappa,0},$$

$$N_3 = \sup\{N_1, N_2\}.$$

Since

$$\lim_{i\to\infty} \sum_{j=0}^{m(n_i)-1} \frac{C_{ij} 2^{j\nu}}{n_i} = 0 \quad \text{and} \quad \lim_{i\to\infty} \frac{m_i 2^{m(n_i)\nu}}{n_i} = 1,$$

for i large enough,

$$\frac{m_i 2^{m(n_i)\nu}}{n_i}\hat{J}+\sum_{j=0}^{m(n_i)-1}\left(\frac{C_{ij}2^{j\nu}}{n_i}\right)\tilde{J}\subset J^{d_i}.$$

Using this and 2.3(iii),

$$\liminf_{i\to\infty}\frac{1}{n_i}\log\not|(\Lambda_i,n_i,J^{d_i})\geq s_{\kappa,\rho}(v',\hat{J})+\liminf_{i\to\infty}\sigma_i$$

for

$$|\sigma_i|=\frac{1}{n_i}\left|\sum_{j=0}^{N_1-1}C_{ij}2^{j\nu}\frac{1}{2^{j\nu}}\log\not|(\Lambda_{\kappa,N_1}(v'),2^{j\nu},\tilde{J}^{\Delta_{\kappa,j}})+\sum_{j=N_1}^{m(n_i)-1}C_{ij}2^{j\nu}\frac{1}{2^{j\nu}}\log\not|(\Lambda_{\kappa,j}(v'),2^{j\nu},\tilde{J}^{\Delta_{\kappa,j}})\right|$$

$$\leq\frac{m(n_i)2^{m(n_i)\nu}}{n_i}\sup\left\{\sup_{0\leq j<N_1}\left|\frac{1}{2^{j\nu}}\log\not|(\Lambda_{\kappa,N_1}(v'),2^{j\nu},\tilde{J}^{\Delta_{\kappa,j}})\right|,\sup_{N_1\leq j<m(n_i)}\left|\frac{1}{2^{j\nu}}\log\not|(\Lambda_{\kappa,j}(v'),2^{j\nu},\tilde{J}^{\Delta_{\kappa,j}})\right|\right\}.$$

But the first term in the supremum is finite by construction of $\tilde{J}$ and nondependence of N_1 on i, and the second term is equal to

$$\sup\left\{\frac{1}{2^{N_1\nu}}\left|\log\not|(\Lambda_{\kappa,N_1}(v'),2^{N_1\nu},\tilde{J}^{\Delta_{\kappa,N_1}})\right|,\frac{1}{2^{(m(n_i)-1)\nu}}\left|\log\not|(\Lambda_{\kappa,m(n_i)-1}(v'),2^{[m(n_i)-1]\nu},\tilde{J}^{\Delta_{\kappa,m(n_i)-1}})\right|\right\}.$$

Here again the first term is finite by choice of $\tilde{J}$, and the second term is bounded by $2+\log v'$, hence $\lim_{i\to\infty}|\sigma_i|=0$.

Lemma 3.4[1]: If $\{\Lambda_i\}_{i=1}^{\infty}\subset\mathcal{S}$, each Λ_i is connected, and $\Lambda_i\to\infty$ (Fisher), then $\inf_i V(\Lambda_i)/V(\tilde{\Lambda}_i)>0$, where $\tilde{\Lambda}_i$ is any minimal cube containing Λ_i.

Theorem 3.5: Suppose $\{(\Lambda_i,n_i)\}_{i=1}^{\infty}$ is a Fisher system tending to density $1/v$, each Λ_i is connected, $\kappa\in(0,K)$, $J\in\tilde{\mathcal{C}}_t(v)$, and $s_\kappa(v,J)>-\infty$. Then there exists a decreasing sequence $\{d_i\}_{i=1}^{\infty}$ of strictly positive real numbers converging to zero, such that

$$s_{\kappa,0}(v,J)\geq\limsup_{i\to\infty}\frac{1}{n_i}\log\not|(\Lambda_i,n_i,J^{d_i}).$$

Proof: For $i\in Z_+$, let $p(i)=1+\inf\{m\in Z_+\mid\Lambda_{\kappa,m}(v)$ contains a translate Λ_i' of $\Lambda_i\}$, so that $\Lambda_{\kappa,p(i)-1}(v)$ is the minimal *standard* cube containing Λ_i. Writing $d_i=A\varphi_\kappa 2^{p(i)\nu}/\theta_\kappa^{\lambda p(i)}R_\kappa$, if $\tilde{\Lambda}_i$ is any minimal cube containing Λ_i, then

$$2^\nu\leq V(\Lambda_{\kappa,p(i)}(v))/V(\tilde{\Lambda}_i)\leq(2^\nu+1)^2$$

for i sufficiently large, so

$$\frac{1}{2^\nu}\geq\frac{V(\Lambda_i)}{V(\Lambda_{\kappa,p(i)}(v))}>\frac{1}{(2^\nu+1)^2}\inf_i\frac{V(\Lambda_i)}{V(\tilde{\Lambda}_i)}>0.$$

Now pass to a subsequence $\{\Lambda_{i_j}\}_{j=1}^{\infty}$ such that

$$\lim_{j\to\infty}\frac{V(\Lambda_{i_j})}{V(\Lambda_{\kappa,p(i_j)}(v))}=\beta$$

and

$$\lim_{j\to\infty}\frac{1}{n_{i_j}}\log\not|(\Lambda_{i_j},n_{i_j},J^{d_{i_j}})=\lim_{i\to\infty}\sup\frac{1}{n_i}\log\not|(\Lambda_i,n_i,J^{d_i}).$$

Let $\Lambda_i''=\{q\in\Lambda_{\kappa,p(i)}(v)/\Lambda_i'\mid d(q,\Lambda_i')>\theta_\kappa^{p(i)}R_\kappa\}$ and $n_{i_j}''=2^{p(i_j)\nu}-n_{i_j}$. It can be shown, as in Ref. 1, that $\Lambda_i''\to\infty$ (Fisher) and it is easy to see that $\lim_{j\to\infty}V(\Lambda_{i_j}'')/V(\Lambda_{\kappa,p(i_j)}(v))=1-\beta$. By computing $\lim_{j\to\infty}n_{i_j}''/2^{p(i_j)\nu}=1-\beta$, therefore $\lim_{j\to\infty}V(\Lambda_{i_j}'')/n_{i_j}''=v$. Since Λ_{i_j}' and Λ_{i_j}'' may be translated inside $\Lambda_{\kappa,p(i_j)}(v)$ with mutual separation $\theta_\kappa^{p(i_j)}R_\kappa\geq R_0$, for large enough j,

$$\frac{1}{2^{p(i_j)\nu}}\log\not|(\Lambda_{\kappa,p(i_j)}(v),2^{p(i_j)\nu},J)\geq\frac{n_{i_j}}{2^{p(i_j)\nu}}\frac{1}{n_{i_j}}\log\not|(\Lambda_{i_j},n_{i_j},J^{d_{i_j}})+\frac{n_{i_j}''}{2^{p(i_j)\nu}}\frac{1}{n_{i_j}''}\log\not|(\Lambda_{i_j}'',n_{i_j}'',J^{d_{i_j}}).$$

The theorem follows from 3.3.

Corollary 3.6: Suppose $\{(\Lambda_i,n_i)\}_{i=1}^{\infty}$ is a Fisher system tending to density $1/v$, $v\neq v_0$, with each Λ_i connected, and f is an asymptotically open t-valued observable with $\lambda>\nu$. Then, if $J\in\tilde{\mathcal{C}}_t(v)$,

$$\lim_{i\to\infty}\frac{1}{n_i}\log\not|(\Lambda_i,n_i,J)=s(v,J)$$

exists, and

$$s(v,x)=\inf_{x\in J\in\tilde{\mathcal{C}}_t}s(v,J)$$

is given by

$$s(v,x)=s_{\kappa,0}(v,x),\quad\kappa\in(0,K).$$

Therefore, s has the continuity and concavity properties of Corollaries 1.7 and 1.10.

The existence of the limit follows from 3.3 and 3.5 by removal of the contractions from J^{d_i} as in 2.3, and from an argument similar to 3.5.

We note that when $t=1$ and f is the potential energy U of a tempered interaction, $s(v,\epsilon)$ is the usual microcanonical configurational entropy per particle for a system at density $1/v$ and interaction energy per particle ϵ.

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Foundations of a quantum probability theory*

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Statistical physical theories are frequently formulated in terms of probabilistic structures founded on a "logic of experimentally verifiable propositions." It is argued that to each experimentally verifiable proposition there corresponds an experimental procedure which, in general, alters the state of the system, and is completely characterized by a "measurement transformation" or "operation." An analysis of the relations among these experimental procedures leads us to a "logic of operations" which is quite different from the "lattice theoretic logics" that are often considered (albeit inadequate empirical justification), as models for the calculus of experimentally verifiable propositions of quantum theory. It is seen that the quantum probability theory based on the logic of operations provides the proper mathematical framework for discussing the statistics of successive observations in quantum theory. We also indicate how a theory of quantum stochastic processes can be formulated in a way similar to the Kolmogorov formulation of the classical theory.

1. INTRODUCTION

It has been widely recognized[1] that the theory of probability as has been systematized by Kolmogorov[2] is not suitable for a discussion of situations that arise in quantum mechanics. It is also a common belief that probabilistic concepts appear in quantum mechanics in an entirely different way, as compared to classical statistical mechanics. In fact, there are many striking illustrations of the nonconformity of quantum theory with traditional probability theory. We may cite, for example, Feynman's discussion of the double slit experiment,[1] recent investigations of the nonexistence of joint distributions for noncommuting observables,[3-9] de Broglie's discussion of the "quantum interference of probabilities,"[10] etc.

The attempts to construct a generalized probability theory that would be appropriate for quantum mechanics, originated with the work of Birkhoff and von Neumann[11] on the logic of quantum mechanics. Their basic idea was that the formalism of a statistical physical theory is that of a probability theory founded on a calculus of events or what are called the experimentally verifiable propositions of the theory. The structure of this calculus is to be deduced from empirical considerations. Birkhoff and von Neumann argued that the experimentally verifiable propositions of quantum theory form a nondistributive lattice in contrast to the Boolean algebraic structure of the classical (experimentally verifiable) propositions. This has inspired several investigations on generalized probability theories founded on lattice structures.[4,12-16]

In recent years, an alternative approach to quantum theoretic probability, called the "operational approach," has been investigated (mainly) by Davies, Davies and Lewis, and Edwards.[17-19] This is based on the observation that von Neumann's theory of successive measurements[20] can be used to introduce statistical concepts into quantum theory. By suitably generalizing von Neumann's theory of measurement transformations (also called the "collapse expression"), Davies and Lewis were able to develop certain basic notions of a generalized probability theory.

In this paper we attempt to formulate the operational approach to statistical physical theories as a probabilistic theory based on a "logic of operations." Our contention is that the empirical basis that has been provided for adopting the lattice structure for the experimentally verifiable propositions in quantum theory is totally inadequate. Also, it gives rise to a representation of each experimentally verifiable proposition in terms of the set of all states that assign unit probability to the proposition—a representation which fails to characterize the corresponding experimental procedure completely. We propose a representation of the experimentally verifiable propositions in terms of the "measurement transformations" or "operations" that completely characterize the corresponding experimental procedures. The propositional connectives can now be more directly correlated with empirical procedures, and the ensuing "logic of operations" is seen to have a structure quite different from various lattice structures considered hitherto. We also find that the resulting probability theory has a very rich structure and goes well beyond the ordinary statistical interpretation in discussing statistical correlations among several random variables.

2. STATISTICS OF SUCCESSIVE MEASUREMENTS IN QUANTUM THEORY

One of the basic features of quantum theory is that the measurement of an observable causes a transformation of the state. A theory of such transformations due to measurement was initiated by von Neumann via his "projection postulate." We will briefly describe von Neumann's theory, for the case where it is ideally applicable—measurement of an observable with discrete spectrum.

Let A be the self-adjoint operator representing an observable, with the spectral resolution

$$A=\sum_i \lambda_i P_i, \tag{2.1}$$

where P_i are projection operators onto the eigensubspaces of A. The basic postulate of von Neumann can be stated as follows.

If, after the measurement of the observable A, all the information that is extracted is that the result lies

in a Borel subset E of the real line, then the act of measurement transforms the state ρ, of the system before measurement, into the state ρ' (unnormalized) given by

$$\rho' = \sum_{\lambda_i \in E} P_i \rho P_i. \tag{2.2}$$

In particular, if we ascertain that the eigenvalue λ_i is obtained then $\rho' = P_i \rho P_i$. Also if we make a "complete measurement" or what has been called a "measurement without sorting" where no information is extracted, then

$$\rho' = \sum_i P_i \rho P_i, \tag{2.3}$$

which corresponds to a mixed state in general.

If the spectrum of the observable is nondegenerate, the projection postulate can be obtained from the hypothesis of repeatability—"If, on a measurement of the observable A in a state ρ, the result is found to lie in the Borel set E, then an immediate repetition of the measurement will lead to the same result." If the spectrum of the observable is degenerate, then, in order to obtain the unique measurement transformation (2.2) (usually called the collapse expression), an additional assumption of "least interference" or "minimum distrubance" is also necessary.[20, 21]

The projection postulate of von Neumann is sufficient to give all the statistical correlations between successive measurements, as long as we restrict ourselves to observables with discrete spectrum only. For example, the joint probability $P_2(\lambda_1 t_1, \lambda_2 t_2)$ that a measurement of A at time t_1, gives the value λ_1, and a measurement at a later time t_2 gives the value λ_2, can be given by

$$P_2(\lambda_1 t_1, \lambda_2 t_2) = P(\lambda_1 t_1) W(\lambda_2 t_2 | \lambda_1 t_1), \tag{2.4}$$

where $P(\lambda_1 t_1)$ is the probability for obtaining λ_1 at t_1 and $W(\lambda_2 t_2 | \lambda_1 t_1)$ is the conditional probability for obtaining λ_2 at t_2, given that λ_1 has been obtained at t_1. $W(\lambda_2 t_2 | \lambda_1 t_1)$ is calculated by performing the appropriate measurement transformation (2.2) on the initial state at t_1 and calculating the probability of obtaining λ_2 when this state has evolved to the time t_2. If we consider Hamiltonian time evolutions given by the unitary operator $U(t_2, t_1)$, we have

$$P_2(\lambda_1 t_1, \lambda_2 t_2) = \mathrm{Tr}[P_2 V(t_2, t_1) P_1 \rho(t_1) P_1 V^\dagger(t_2, t_1) P_2]. \tag{2.5}$$

Equation (2.5) can be generalized to the rth order joint probability distribution

$$P_r(\lambda_1 t_1, \ldots, \lambda_r t_r) = \mathrm{Tr}[P_r V(t_r, t_{r-1}) \cdots P_2 V(t_2, t_1) P_1 \rho(t_1) \times P_1 V^\dagger(t_2, t_1) P_2 \cdots V^\dagger(t_r, t_{r-1}) P_r]. \tag{2.6}$$

If we had considered the evolution in the Heisenberg picture, we would have

$$P_r(\lambda_1 t_1, \ldots, \lambda_r t_r) = \mathrm{Tr}[P_r(t_r) \cdots P_1(t_1) \rho \times P_1(t_1) \cdots P_r(t_r)]. \tag{2.7}$$

Equations (2.6), (2.7) contain all the relevant statistical information for studying the correlations of successive measurements. In this context we can recall the dictum of Wigner[22] that one obtains a consistent formulation of quantum mechanics (free from the well-known duality in the change of the state vector), if one adopts the viewpoint that "quantum mechanics gives only probability connection between successive observations on a system." Wigner also emphasizes that: "This formulation frankly gives primacy to the act of observation; it considers it as the basic quantity between the values of which physics establishes regularities, though, according to quantum mechanics only of a statistical, that is probabilistic nature." An analysis of the nature of these probabilistic connections is thus very basic to the understanding of quantum theory.

de Broglie[10] studied particular cases of the joint probabilities (2.6), (2.7) and pointed out that they do not satisfy all the properties of joint distributions in the classical theory of stochastic processes (see also Ref. 6, 23, 24). In fact as the projection operators $P_i(t_i)$ do not, in general, commute among themselves, we have

(i) $P_r(\lambda_1 t_1, \ldots, \lambda_r t_r)$ are not symmetric in general.

(ii) They satisfy marginal probability conditions only when summed over the variable corresponding to the final time t_r, i.e., though we have

$$\sum_{\lambda_r} P_r(\lambda_1 t_1, \ldots, \lambda_{r-1} t_{r-1}, \lambda_r t_r) = P_{r-1}(\lambda_1 t_1, \ldots, \lambda_{r-1} t_{r-1}), \tag{2.8}$$

we also have, for example,

$$\sum_{\lambda_1} P_2(\lambda_1 t_1, \lambda_2 t_2) \neq P(\lambda_2 t_2). \tag{2.9}$$

de Broglie pointed out that these nonclassical features reflected a certain "interference of probabilities" in quantum theory, which is due to the fact that the measurement of one quantity can influence the values of the other. This led him to the conclusion that the "usual mathematical statistics is based on postulates which cease to be exact in wave mechanics in such a way that, to make the formalism of wave mechanics enter into the general picture of the calculus of probabilities, it is necessary to construct a mathematical statistical theory more comprehensive than that of which use is generally made—by abandoning certain too restricted postulates."[10] For a realization of this program it is very necessary to overcome first the limitations on the theory imposed by von Neumann's projection postulate.

We can list some of the arguments that show that the projection postulate of von Neumann, or equivalently the collapse expression (2.2), is at best, only of limited applicability.[17,18,23] Firstly the collapse expression (2.2) cannot be used for observables with a continuous spectrum, as there are no projectors P_i available for this case. von Neumann proposed (what he himself acknowledged to be) a "temporary" way to circumvent this difficulty by partitioning the spectrum of the observable into nonoverlapping intervals. This procedure is quite unsatisfactory as the partitioning is arbitrary and usually destroys the invariance properties of the original observable. Secondly, von Neumann's projection postulate is based on the repeatability hypothesis; existence of measurements which are not repeatable has been widely accepted, and these have been termed the "measurements of the second kind."[25] (For example, the system changes, due to the first measurement, in

such a way that it is not available for a repetition of the measurement.)

A suitable generalization of von Neumann's projection postulate, which is also free from the above limitations, was proposed by Davies and Lewis.[18] They generalized the notion of "operation" as formulated by Schwinger[26] and Haag and Kastler,[27] to obtain a general class of collapse expressions which he called "Instruments." Each instrument completely characterizes the measurement transformations associated with a unique observable which is in general a positive operator valued measure. This constitutes also a generalization of the standard formulation of quantum mechanics which admits only projection valued measures for observables.

An instrument is defined as a mapping

$$I: B(R)\times V \to V,$$

where $B(R)$ is the set of all Borel sets of a value space R (usually the real line), and V is the set $\mathcal{T}_s(H)$ of the self-adjoint trace class operators on a Hilbert space H. The requirements on the mapping I for it to define an instrument are

(i) $I(E, v) \geq 0$

whenever $v \in V^+$ for all $E \in B(R)$ and

$$\text{(ii)}\quad I(\bigcup_i E_i, v) = \sum_i I(E_i, v), \tag{2.10}$$

for each countable family $\{E_i\}$ of pairwise disjoint sets $E_i \in B(R)$.

$$\text{(iii)}\quad I(E, \alpha_1 v_1 + \alpha_2 v_2) = \alpha_1 I(E, v_1) + \alpha_2 I(E, v_2), \tag{2.11}$$

for each $E \in B(R)$ and $v_1,\ v_2 \in v$.

$$\text{(iv)}\quad \mathrm{Tr} I(R, v) = \mathrm{Tr} v, \tag{2.12}$$

for each $v \in V$.

Davies and Lewis[18] proved that given two instruments I_1 and I_2 on value spaces R_1 and R_2 (which satisfy certain requirements like, for example, that of a complete metric space), we can consider their composition as a unique instrument I defined on $R_1 \times R_2$. Also, given an instrument I on a value space R, there corresponds a unique positive operator valued measure

$$\omega: B(R) \to B_s^+(H) \tag{2.13}$$

where $B_s^+(H)$, is the set of all bounded positive operators on H, such that

$$\mathrm{Tr}[I(E, v)] = \mathrm{Tr}[v\omega(E)], \tag{2.14}$$

for all $v \in V$. Conversely, given any positive operator valued measure ω, there exists *at least one* instrument I such that (2.14) is satisfied.

This shows that if, by the representation of an observable, we also intend to characterize the corresponding measurement transformation or the collapse expression uniquely, then a proper (and necessary) generalization of the standard formalism of quantum theory would be to identify the set of all observables with the set of all instruments. The notions of generalized measurement transformations and the associated instruments will be fundamental to a discussion of the foundations of the probability theory appropriate to the analysis of statistical connection between successive measurements in quantum theory. Davies and Lewis have called this the "operational approach to quantum probability."

3. LATTICE THEORETIC APPROACH TO QUANTUM PROBABILITY

The general framework that has been used to analyze the logical structure of physical theories, ever since the pioneering work of Birkhoff and von Neumann, is one where the basic notions are those of "states," "observables," and the "experimentally verifiable propositions" of physical systems. The experimentally verifiable propositions are of the form: "A measurement of a given observable, on the system, yields a result in a given Borel subset of the value space of the observable." Thus the general features of a system which are independent of the particular state of the system are to be found among the relations between the different propositions—the so-called "propositional calculus."

The propositional calculus or the structure of the "experimentally verifiable propositions" (or what are also called the "events") of the system is a basic constituent, which might vary from one theory to another, depending on basic phenomenological considerations. The states of a system are usually defined as some kind of probability measures on the set of propositions. The observables are defined as some kind of measurable functions—random variables—from the Borel subsets of the value space (usually the real line) of the observable, into the set of propositions. It is thus clear that the basic notions of Kolmogorov's theory of probability, are also basic to the logical structure of any physical theory, and as Kolmogorov's axioms are rooted in empirical experience, any change in our basic conceptions of the universe will be reflected by a corresponding modification of the basic probabilistic structure.

A. The "logic" of propositions in classical theory

It was Birkhoff and von Neumann who precisely stated that the experimental propositions concerning any system in classical theory correspond to a Boolean algebra of subsets of its phase space. Consequently, the logical structure of classical statistical mechanics coincides with that of Kolmogorov's probability theory, and we will describe it briefly.[14-16]

The set B of all propositions form a Boolean algebra, which can be characterized by the following properties.

(P1) B is partially ordered by a reflexive, asymmetric, transitive relation $\leq$, i.e., we have

(a) $A \leq A$ for all $A \in B$,

(b) $A_1 \leq A_2$ and $A_2 \leq A_1$ implies $A_1 = A_2$ for all $A_1,\ A_2 \in B$,

(c) $A_1 \leq A_2$ and $A_2 \leq A_3$ implies $A_1 \leq A_3$ for all $A_1, A_2, A_3 \in B$.

The relation $\leq$ corresponds to the notion of implication of experimental propositions.

(P2) B contains a "null" element $\emptyset$ and a "unit"

element Ω, such that

(a) $\phi \leq A$ for all $A \in B$,

(b) $A \leq \Omega$ for all $A \in B$. The null element ϕ corresponds to the absurd proposition which is always false, and the unit element Ω corresponds to the trivial proposition which is always true.

(P3) B is a complemented distributive lattice, i.e.,

(a) Given a finite set $\mathcal{J}$ of elements $A_i \in B$, B contains a unique infimal element $C = \bigwedge_{A_i \in \mathcal{J}} A_i$ and also a unique supremal element $D = \bigvee_{A_i \in \mathcal{J}} A_i$; i.e., $C \leq A_i$ for all $A_i \in \mathcal{J}$ and $P \leq A_i$ for all $A_i \in \mathcal{J}$ implies $P \leq C$; and $A_i \leq D$ for all $A_i \in \mathcal{J}$ and $A_i \leq Q$ for all $A_i \in \mathcal{J}$ implies $D \leq Q$.

We denote $\bigwedge_{i=1,2} A_i$ by $A_1 \wedge A_2$ and $\bigvee_{i=1,2} A_i$ by $A_1 \vee A_2$. We may note that $\wedge$ corresponds to conjunction and $\vee$ corresponds to disjunction of propositions. (b) For any A_1, A_2, $A_3 \in B$, we have the distributive laws

$$A_1 \vee (A_2 \wedge A_3) = (A_1 \vee A_2) \wedge (A_1 \vee A_3), \tag{3.1}$$

$$A_1 \wedge (A_2 \vee A_3) = (A_1 \vee A_2) \wedge (A_1 \vee A_3). \tag{3.2}$$

(c) For any element $A \in B$, there exists an $A' \in B$ such that

$$A \wedge A' = \phi, \tag{3.3}$$

and

$$A \vee A' = \Omega. \tag{3.4}$$

A' represents negation of the proposition A. B will be called a Boolean σ algebra, if in addition to (P1), (P2) and (P3), we also have (it should be noted that we have not given an axiomatic characterization of Boolean algebra.)

$\bigwedge_{A_i \in \mathcal{J}} A_i$ and $\bigvee_{A_i \in \mathcal{J}} A_i$ exist and belong to B, for every countable subset $\mathcal{J}$ of B.

We can deduce from (P1)–(P3) that the negation of each proposition is unique and satisfies the following properties:

$$(A')' = A, \tag{3.5}$$

$$A_1 \leq A_2 \quad \text{implies} \quad A_2' \leq A_1', \tag{3.6}$$

and

$$\left(\bigwedge_{A_i \in \mathcal{J}} A_i\right)' = \bigvee_{A_i \in \mathcal{J}} A_i'. \tag{3.7}$$

Two elements A_1, $A_2 \in B$ are said to be disjoint, a relation that is usually denoted as $A_1 \perp A_2$ iff $A_1 \leq A_2'$. $\perp$ is a symmetric irreflexive transitive relation for a complemented distributive lattice.

There are general results on the representations of abstract Boolean algebras[14–16] as a Boolean algebra of subsets of some phase space. [For Boolean σ algebras, such a representation is not possible in general. The implications of this on the foundations of (traditional) probability theory may be found in Refs. 28, 29.] In classical mechanics this will be the phase space of all pure states of the system, and each proposition will now be represented by the subset composed of all the states that assign unit probability to the proposition. The connectives $\leq$, $\vee$, and $\wedge$ now correspond respectively to set theoretic inclusion, union, and intersection.

For the sake of the abstract theory, it is sufficient to assume that the set of all experimental propositions of a classical system is given by a Boolean σ algebra B. The states of the system are probability measures on B, i.e., a state μ is a real valued function

$$\mu : B \to [0, 1]$$

such that

$$(S1)\ \mu(\phi) = 0; \tag{3.8}$$

$$(S2)\ \mu(\Omega) = 1; \tag{3.9}$$

(S3) If $\mathcal{J}$ is a countable set of mutually disjoint elements $A_i \in B$, then

$$\mu\left(\bigvee_{A_i \in \mathcal{J}} A_i\right) = \sum_{A_i \in \mathcal{J}} \mu(A_i). \tag{3.10}$$

The "observables" of the system are the "random variables"

$$X : B(R) \to B,$$

where $B(R)$ are Borel subsets of the value space R, such that

$$(O1)\ X(\phi) = \phi; \tag{3.11}$$

$$(O2)\ X(R) = \Omega; \tag{3.12}$$

(O3) If E_i are mutually disjoint Borel subsets of R, then the $X(E_i)$ are mutually disjoint elements of B such that

$$X\left(\bigcup_i E_i\right) = \bigwedge_i X(E_i). \tag{3.13}$$

We just note that in the standard Kolmogorov model, the random variables are defined as measurable functions from the phase space into the value space.

It is well known that the rich structure of traditional probability theory is based on the above formalism.[2] Birkhoff and von Neumann's analysis thus relates the discussion of logical notions presupposed in classical statistical theory with the empirical foundations of classical probability theory.

B. The "logic" of quantum propositions—the lattice approach

In generalizing the structure of classical propositional calculus, to obtain a "logic" of quantum experimental propositions, Birkhoff and von Neumann's main objective was to provide a phenomenological basis at a very fundamental level for the well-known Hilbert space formalism of quantum theory. The two main observations on which they based their analysis were the Heisenberg uncertainty principle and von Neumann's conclusion that two noncommuting observables cannot be measured simultaneously.[11] It should, of course, be noted that the latter result is widely contested by many authors,[30,31] and it has also been argued that the projection postulate and the nonclassical nature of the joint probabilities are among the main arguments in favor of such results on incompatibility.

von Neumann's main conclusion was that the set of experimental propositions in quantum theory do not form a Boolean σ algebra, but an "abstract projective geometry." Without going into the technicalities of lattice theory, we just note that the properties (P1),

(P2), (P3a), and (P3c) are assumed to hold in quantum propositional calculus also, where as the property (P3b) of distributivity is given up. Instead of (P4) one now assumes,

(P4′) If $\{A_i\}$ is a sequence of mutually disjoint propositions, then $\bigvee_i A_i$ exists.

[Recall that propositions A_1 and A_2 were defined to be mutually disjoint ($A_1 \perp A_2$) whenever $A_1 \leq A_2'$. For the quantum case $A_1 \wedge A_2 = \phi$ is only a necessary condition for A_1 and A_2 to be disjoint, whereas in the classical case it is also a sufficient condition.]

There has been an extensive study[32] on the additional axioms one has to impose in order to finally realize specifically the (so-called) standard representation of quantum propositional calculus—the orthocomplemented nondistributive lattice $\mathcal{L}$ of all the closed subspaces of a Hilbert space H over the field of complex numbers. For our purposes, it suffices to consider $\mathcal{L}$ as representing the logic of quantum propositions.

In $\mathcal{L}$, the relation $\leq$ is again realized by one of inclusion. The orthocomplement A' of a given closed subspace $A \in \mathcal{L}$ is given by

$$A' = \{\psi \in H \mid (\psi, \varphi) = 0 \text{ for all } \varphi \in A\},$$

where (,) denotes the inner product in H. The improper subspace H and the null subspace ϕ function as the unit and null elements, respectively. From the lattice structure of $\mathcal{L}$, we can immediately conclude that $A_1 \wedge A_2$ is represented by the subspace obtained by the set theoretic intersection of the subspaces A_1 and A_2; $A_1 \vee A_2$ is represented by the smallest subspace containing both A_1 and A_2. Two subspaces A_1, A_2 are 'disjoint' ($A_1 \perp A_2$) whenever they are orthogonal.

Two subspaces A_1 and A_2 are said to be compatible (denoted by $A_1 \leftrightarrow A_2$), if there exist mutually disjoint subspaces D_1, D_2, and D_3 such that

$$A_1 = D_1 \vee D_2 \quad \text{and} \quad A_2 = D_1 \vee D_3$$

If A_1, A_2, and A_3 are mutually compatible subspaces, then the distributive laws (3.1) and (3.2) are valid. Since there is a one-to-one correspondence between the set of all closed subspaces of a Hilbert space and the set of all projection operators, we might as well consider the projection operator P_A onto the subspace A as representing the corresponding proposition. A_1 and A_2 are compatible iff P_{A_1} and P_{A_2} commute.

The states of a quantum system can now be represented by probability measures on $\mathcal{L}$ that satisfy (S1)—(S3). It is a celebrated result of Gleason[33] that to each such measure μ on $\mathcal{L}$ (the lattice of closed subspaces of a Hilbert space H), there corresponds a unique density operator ρ_μ on H (i.e., a self-adjoint positive trace class operator with trace unity), such that

$$\mu(A) = \mathrm{Tr}(\rho_\mu P_A), \tag{3.14}$$

for all $A \in \mathcal{L}$.

The random variables or observables are mappings from Borel sets on the value space into $\mathcal{L}$, which satisfy (O1)—(O3). Thus an observable X can be identified with the projection valued measure

$$P_X : E \to P_{X(E)}$$

and therefore corresponds to a unique self-adjoint operator. Also, each observable X generates a probability measure on the value space, for each state μ, given by

$$p_X^\mu(E) = \mu(X(E)) = \mathrm{Tr}(\rho_\mu P_{X(E)}). \tag{3.15}$$

Thus, an identification of the propositional calculus of quantum theory with the orthocomplemented nondistributive lattice $\mathcal{L}$ generates the complete orthodox formalism of quantum theory including its statistical interpretation as given by (3.15). The objective of obtaining a generalized probability theory is also fulfilled. However, it is well known that this probability theory lacks the rich structure of Kolmogorov's theory in that notions like joint distributions, conditional expectations, stochastic processes, etc., can be defined only under highly restricted circumstances.

In fact, if x_1 and x_2 are two observables, one can, of course, form

$$p^\mu_{x_1,x_2}(E_1, E_2) = \mu(x_1(E_1) \wedge x_2(E_2)), \tag{3.16}$$

for each state. But $p^\mu_{x_1,x_2}$ does not define an additive measure on R^2 in general. This phenomenon can be directly traced to the nonvalidity of the distributive law in $\mathcal{L}$. For example, if $E_1 \cap E_3 = E_2 \cap E_4 = \phi$, $p^\mu_{x_1,x_2}$ will be a probability measure on R^2 only if

$$p^\mu_{x_1,x_2}(E_1 \cup E_3, E_2 \cup E_4) = p^\mu_{x_1,x_2}(E_1, E_2) + p^\mu_{x_1,x_2}(E_1, E_4) + p^\mu_{x_1,x_2}(E_3, E_2) + p^\mu_{x_1,x_2}(E_3, E_4). \tag{3.17}$$

From (3.16) it is clear that the validity of (3.17) depends on the validity of the distributive law among the subspaces $x_1(E_i)$ and $x_2(E_i)$; the distributive law is a consequence of commutability of the corresponding projection operators. There are general results due to Varadarajan,[4,14] Gudder,[34] *et al.*, which enumerate the conditions under which joint distributions exist.

Also, the time evolution of an observable can be considered as a stochastic process only when x_{t_1}, x_{t_2}, etc., have joint distributions. For Hamiltonian evolution this would be the case if the operators corresponding to x_t and dx_t/dt commute.[35]

C. Critique of the lattice theoretic approach

We will now analyze some of the arguments given by von Neumann and others in favor of the nondistributive lattice structure for the quantum propositional calculus. First of all, we should point out that there are many divergent views on the interpretation of the calculus of the experimentally verifiable propositions and its relation to the similar calculi of mathematical logic. One school of thought is best summarized by the following excerpt from Jauch's book[15]: The calculus of experimentally verifiable propositions is "the formalization of a set of empirical relations, which are obtained by making measurements on a physical system. It expresses an objectively given property of the physical world. —The calculus of formal logic, on the other hand, is obtained by making an analysis of the meaning

of propositions. It is true under all circumstances and even tautologically so. Thus ordinary logic is used even in quantum mechanics of systems with a propositional calculus mostly different from that of formal logic. The two need have nothing in common." Thus the nondistributive lattice of experimentally verifiable propositions is viewed purely as an algebraic structure, which bears certain formal resemblance to logical structure, but does not function as a vehicle for logical reasoning. Another viewpoint,[36,37] which can be traced back to the paper of Birkhoff and von Neumann, is that the canons of classical logic are violated by quantum theory, and hence, there are empirical grounds for adopting a "deviant logic" as embodied in the nondistributive lattice structure of the quantum propositional calculus. Recently, there have been many discussions[38-41] on the syntactical and semantical notions associated with the above viewpoints, apart from the basic philosophical question as to whether logic is an empirical science.[42]

As our intentions are to examine the probabilistic structure associated with quantum mechanics, we only need to start from the guiding principle that the formal structure of statistical physical theories is that of a probability theory founded on the calculus of experimentally verifiable propositions of the theory. The experimentally verifiable propositions have to be related to the experimental procedures that can be carried out on physical systems. The propositional calculus is a structure that reflects the relations among these experimental procedures. Thus the justification for choosing a particular set of axioms for the propositional calculus has to come from a heuristic discussion of the relations between experimental procedures—relations which are independent of the state of the system. Our main contention is that the axioms proposed by Birkhoff and von Neumann fail to satisfy this criterion. We should also note that there are several other critiques of the Birkhoff—von Neumann proposal, from various standpoints.[38-41,43]

Among the postulates, the postulate (P1), that the relation of implication in a propositional calculus defines a partial ordering, is generally uncontestable. One has just to point out the experimental procedures of measuring the position of a particle to be in Borel sets E_1 and E_2; whenever $E_1 \subseteq E_2$, the first proposition implies the second, and this does generate a partial ordering.

In this context, it should be emphasized that the partial ordering $\leq$, should not be identified with implication ($\rightarrow$) in formal logic, which is a propositional connective; i.e., if A_1 and A_2 are propositions, so is the implication $A_1 \rightarrow A_2$. In order to understand this difference clearly, we have only to note that the algebraic structure that is usually called the calculus of experimentally verifiable propositions is actually what is called the Lindenbaum—Tarski algebra[44] of a corresponding propositional logic (the algebraic structure that is obtained from the propositional calculus after identifying equivalent propositions). Also, it is well known[45] that probability measures on a sentential calculus are equivalent to probability measures on the Lindenbaum—Tarski algebra of that calculus. We may also note that mathematicians have also considered logical systems, whose Lindenbaum—Tarski algebras are not Boolean[46]—for example, the intuitionistic logics which correspond to pseudo-Boolean algebras and some systems of modal logic which correspond to more general lattice structures.

We now come to the definition of the connectives $\wedge$ and $\vee$. In the lattice theoretic approach, it is not only assumed that these are defined for any two propositions, but are also related to the partial ordering $\leq$, as lattice operations; thus they also are associative and commutative operations. The main problem lies in relating these connective to specific combinations of experimental procedures. Birkhoff and von Neumann[11] left this as a suggested question at the end of their paper: "What experimental meaning can one attach to the meet and join of two given experimental propositions?" Let us first discuss the connective $\wedge$—the conjunction. Birkhoff and von Neumann recognized the basic difference between conjunction in a classical propositional system, "which just involves independent observers read off the measurements which either proposition involves and combining these results logically," and conjunction in quantum theory; the latter can be treated in the same way as conjunction in formal logic only under exceptional circumstances—"only when all the measurements involved commute (are compatible)." In spite of this, the only justification provided for continuing with a commutative and associative conjunction is that these are the well-known formal properties of conjunction in classical logic or lattice theory. The reasons for doing away with the distributive law were: (i) A distributive complemented lattice would become a Boolean algebra, so that one returns to the formalism of classical theory, and (ii) distributivity is a property that relates different experimental propositions which may not obey classical relations whenever the corresponding measurements are not compatible. We should emphasize that the same arguments can be repeated in favor of giving up any property that involves different experimental propositions.

The preceding analysis clearly shows that there is no justification for assuming lattice theoretic properties for the connectives $\wedge, \vee$, of quantum propositional calculus, unless combinations of experimental procedures are constructed, and they are verified to satisfy these properties. In fact, it can be argued that the postulates of Birkhoff and von Neumann arise either from an analogy with formal logic or an analogy with the structure of the set of all closed subspaces of a Hilbert space, rather than as a result of a specific consideration of the nature of quantum mechanical measurement—the study of which owes a lot to the contributions of von Neumann.

The problem of devising an experimental procedure for the proposition $A \wedge B$ (when the procedures for A and B are given) has also been discussed by various other authors. Jauch[15] has suggested the following schematic procedure, and postulates that "the proposition $A \wedge B$ is true if the system passes the ... filter" in Fig. 1. If we assume the projection postulate, it can be shown that the experimental procedures for proposi-

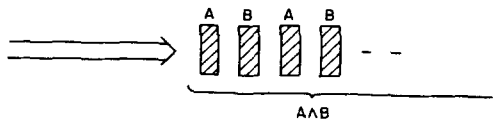

FIG. 1. Jauch's scheme for testing the proposition $A \wedge B$.

tions $A \wedge B$ and $B \wedge A$ are the same, i.e., transform all the systems in the same way. This is based on the well-known formula for the projection operator $P_{A \wedge B}$,

$$P_{A \wedge B} = \lim_{n \to \infty} (P_A P_B)^n. \tag{3.18}$$

However, if we restrict to any finite chain in the filter proposed for $A \wedge B$, the commutativity of the conjunction is no longer valid. Apart from the fact that it is dependent on the projection postulate, our main objection to Jauch's proposal is that it is an idealization which is not what is usually achieved in correlation measurements; the correlations among observables are directly related to the properties of the conjunction of corresponding experimental propositions.

Birkhoff[47] has suggested that the experimental procedure for the proposition $A \wedge B$ may be taken to be the sequence of experimental procedure for A and B taken in that order. This is a perfectly legitimate empirical definition (and in fact the one that we will adopt in the next section), and makes the conjunction noncommutative. However, for the propositional calculus Birkhoff advocates the lattice theoretic commutative conjunction arguing that the set of all states that have unit probability for satisfying the experimental procedure $\{A, B\}$ also have unit probability for satisfying the sequence $\{B, A\}$. Firstly, in general this is true only when we restrict to measurements that satisfy the projection postulate. It is more important to emphasize that the set of all states that assign unit probability to a proposition do not completely characterize the corresponding experimental procedure. The experimental procedure can be completely characterized only by designating how it transforms different states of the system. Two experimental propositions can have the same set of (all) the states that assign unit probability to a proposition do not different experimental procedures if the associated measurement transformations are different.

[We should mention that if one restricts the set of allowed measurements only to those that are described by the projection postulate, Jauch's scheme gives a valid definition of conjunction. However, apart from the limitations of the projection postulate itself, we cannot even include a simple succession of two experimental procedures, to be represented in the theory. This is directly related to the well-known fact that a composition of measurement transformations of the form (2.2) cannot, in general, be recast as a measurement transformation of the form (2.2).]

Instead of continuing with a repetition of our arguments on specific proposals, we can summarize our viewpoint as follows. To each experimental proposition, there corresponds an experimental procedure which is designed to test the proposition. The experimental procedures (in quantum theory) in general alter the state of the system, and are completely characterized by the corresponding "measurement transformation" or "operation." In fact, this is the basic reason why the experimentally verifiable propositions of classical theory are related as in formal logic, while those of quantum theory are not.

In a statistical theory each state of the system provides an assignment of probabilities to the propositions. We can model this situation by saying that if we subject an ensemble of systems to a given experimental procedure, only a part of the ensemble (depending on the probability) satisfies the test (triggers the apparatus). However, the ensemble that emerges after the test need not be a subensemble of the original ensemble, but a new "distorted" or "collapsed" ensemble, with the total number of copies diminished by a factor equal to the probability. In the classical theory, this distortion due to measurement is absent, and hence after carrying out an experimental procedure, a genuine subensemble of the original ensemble emerges. This allows us to identify the experimental procedures, and hence the corresponding propositions of classical statistical theory, with the set of all states that satisfy the proposition. This allows us to reformulate classical propositional calculus as a calculus of subsets of a phase space. The quantum propositions, as we have explained, do not admit such a representation; they are to be directly correlated with a complete description of the experimental procedures, as is accomplished by the "measurement transformations" or "operations."

4. "LOGIC" OF QUANTUM MECHANICAL OPERATIONS

We have argued that the experimentally verifiable propositions of a physical theory, correspond to the (measurement) operations on physical systems. The structure of the corresponding propositional calculus will now be analyzed on the basis of a heuristic discussion of the relations between the experimental procedures that these operations characterize. Our discussion of the propositional calculus of quantum theory is based on the generally accepted notion of "operations" in the Hilbert space formalism of quantum theory, and will be mainly confined to the definition of propositional connectives and the corresponding experimental procedures. The procedure is similar to what Finkelstein[37] characterizes as "taking a well-known theory and distilling its logic." Discussions of general axiomatic approaches to statistical physical theories, based on similar notions, can be found in the works of Davies, Edwards,[19,48,49] Hellwig and Krauss,[50,51] Lewis, Ludwig[52–54] Pool,[55] *et al.*[56]

In the standard formulation of quantum theory, the states are represented by the density operators, which are positive trace class operators on a Hilberg space H, normalized to unit trace. The set of self-adjoint trace class operators on H, which we denote by V (also denoted by $\mathcal{T}_s(H)$ in the literature), is a Banach space under the trace norm. The set of positive (self-adjoint) trace class operators $V^+ = \mathcal{T}_s^+(H)$ forms a closed cone in V. This generates a partial ordering

$$v_1 \leq v_2 \quad \text{for} \quad v_1, v_2 \in V \quad \text{iff} \quad v_1 - v_2 \in V^+.$$

From our discussion of the measurement transformations in Sec. 1, it is clear that an operation is to be defined as a positive norm-nonincreasing linear operator on V, i.e., if $\mathcal{O}$ is the set of all operations on V, then $\mathcal{E}\in\mathcal{O}$ is a mapping

$$\mathcal{E}: V \to V,$$

such that

$$\begin{aligned} &(C1)\ \mathcal{E} \text{ is linear,} \\ &(O2)\ \text{If } v\in V^+, \text{ then } \mathcal{E}(v)\in V^+ \text{ also,} \\ &(O3)\ \mathrm{Tr}\mathcal{E}(v) \leq \mathrm{Tr}v \quad \text{for all } v\in V^+. \end{aligned} \tag{4.1}$$

Also, it is well known[18,19] that the set V^* of continuous linear functionals on V can be identified with the set $B_S(H)$ of all bounded self-adjoint operators on H. Thus to each operation, we can associate an adjoint $\mathcal{E}^*$ which is a positive norm-nonincreasing linear mapping

$$\mathcal{E}^*: B_S(H) \to B_S(H).$$

The set of all operations $\mathcal{O}$ will now correspond to the set of experimental propositions of a physical system. We will now discuss the ensuing structure of the propositional calculus.

A. Implication

The relation of implication is again a partial ordering on $\mathcal{O}$, which can be interpreted as follows. "An experimental proposition $\mathcal{E}_1$ is said to imply another experimental proposition $\mathcal{E}_2$, whenever the experimental procedure for $\mathcal{E}_1$ is a subprocedure of the experimental procedure for $\mathcal{E}_2$." This may be formalized via the following definition:

$$\mathcal{E}_1 \leq \mathcal{E}_2 \quad \text{iff} \quad \mathcal{E}_1 v \leq \mathcal{E}_2 v, \tag{4.2}$$

for all $v\in V^+$. $\leq$ can immediately be verified to be a reflexive, asymmetric, transitive relation, defining a partial order.

B. Absurd and trivial propositions

As in classical logic, $\mathcal{O}$ also contains a unique absurd proposition θ. θ is the operation such that

$$\theta(v) = 0 \quad \text{for all} \quad v\in V. \tag{4.3}$$

We also have

$$\theta \leq \mathcal{E}, \quad \text{for all} \quad \mathcal{E}\in\mathcal{O}. \tag{4.4}$$

The quantum logic $\mathcal{O}$, however, does not admit a unique "trivial proposition" that is implied by all propositions. Actually, $\mathcal{O}$ has a subset Σ of maximal propositions with the property

$$\mathrm{Tr}[\xi(v)] = \mathrm{Tr}v, \tag{4.5}$$

for all $\xi\in\Sigma$. Of course, the set Σ contains the identity operation I, which leaves all the elements of V unchanged. Also, given an operation $\mathcal{E}\in\mathcal{O}$, there always exists a $\xi\in\Sigma$ such that $\theta \leq \mathcal{E} \leq \xi$ (see the discussion in the Appendix). Such a ξ is not unique in general. We should also note that a general operation $\mathcal{E}$ does not satisfy the relation $\mathcal{E} \leq I$. In fact, the operations that satisfy the relation $\mathcal{E} \leq I$ correspond to experimental procedures which pass a subset of the set of all states unchanged, and do not pass the rest of the states; in this respect, they are analogous to classical experimental procedures.

C. Disjoint propositions

Since $\mathcal{O}$ is a set of mappings on a linear space, there is a natural operation of addition defined on it. But as $\mathcal{O}$ only contains the set of all positive norm-nonincreasing maps, it is only a convex set under addition. A countable set of propositions $\{\mathcal{E}_i\}$ is said to be a disjoint set of propositions iff $\Sigma_i \mathcal{E}_i \in \mathcal{O}$.

If the set $\{\mathcal{E}_1, \mathcal{E}_2\}$ is a disjoint set of propositions, we also write $\mathcal{E}_1 \perp \mathcal{E}_2$. We may note that $\perp$ is a symmetric relation, which is not transitive or irreflexive in general. In the classical logic, as well as in lattice structures, the notion of disjoint propositions was defined using the notion of "negation" or "orthocomplement" as in Sec. 3. Since we do not have a unique unit element in our logic of propositions, we have to define a complement or negation of the proposition $\mathcal{E}$, to be a proposition $\mathcal{E}'$ such that

$$\mathcal{E} + \mathcal{E}' \in \Sigma.$$

This criterion, of course, does not lead to a unique negation for each proposition. For instance, all the elements of Σ act as negations of θ, which in turn serves as the negation for all of them. The notion of negation is not a very useful concept unless one restricts oneself to the range of a single random variable (instrument).

D. Conjunction

We have extensively argued in Sec. 3 that the propositional connnectives have to be defined by a specific reference to the corresponding experimental procedures. This actually constituted our main objection to the lattice theoretic definition of propositional connectives. We define the proposition $\mathcal{E}_1 \wedge \mathcal{E}_2$ as follows.

"The experimental procedure corresponding to the proposition $\mathcal{E}_1 \wedge \mathcal{E}_2$ is the procedure in which the system is subjected to the sequence of procedures $\mathcal{E}_1, \mathcal{E}_2$ in that order." Schematically this can be depicted as shown in Fig. 2.

The operation $\mathcal{E}_1 \quad \mathcal{E}_2$ is hence given by the composition of $\mathcal{E}_2$ and $\mathcal{E}_1$; i.e.,

$$(\mathcal{E}_1 \wedge \mathcal{E}_2)(v) = (\mathcal{E}_2 \circ \mathcal{E}_1)(v) = \mathcal{E}_2(\mathcal{E}_1(v)), \tag{4.6}$$

for all $v\in V$ where $\circ$ denotes composition of operations. It is immediate that $\mathcal{E}_1 \wedge \mathcal{E}_2$ is a well-defined operation for any two given operations $\mathcal{E}_1, \mathcal{E}_2$.

From the definition it is obvious that $\wedge$ is an associative operation, which is not commutative in general.

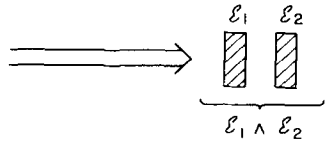

FIG. 2. Experimental procedure for the proposition $\mathcal{E} \wedge \mathcal{E}_2$.

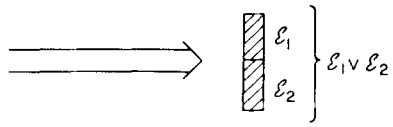

FIG. 3. Experimental procedure for the proposition $\mathcal{E}_1 \vee \mathcal{E}_2$, when $\mathcal{E}_1 \perp \mathcal{E}_2$.

This noncommutativity of conjunction constitutes a fundamental departure from the structure of classical propositional calculus. (We should note that a noncommutative conjunction has been advocated by P. Jordan[57] also. Based on this, he has formulated a theory of noncommutative or skew lattices as a structure appropriate to quantal propositional calculus. As our propositional calculus is not based on a lattice theoretic framework, we will not discuss Jordan's approach in this paper.) We can define two propositions to be compatible (denoted by $\longleftrightarrow$), whenever $\mathcal{E}_1 \wedge \mathcal{E}_2 = \mathcal{E}_2 \wedge \mathcal{E}_1$.

The conjunction satisfies the properties

$$\mathcal{E} \wedge I = I \wedge \mathcal{E} = \mathcal{E} \quad \text{and} \quad \mathcal{E} \wedge \theta = \theta \wedge \mathcal{E} = \theta \tag{4.7}$$

for all $\mathcal{E} \in \mathcal{O}$. However, we do not have $\mathcal{E} \wedge \mathcal{E} = \mathcal{E}$ in general. We can define a proposition to be repeatable (for lack of better terminology), if $\mathcal{E} \wedge \mathcal{E} = \mathcal{E}$ is satisfied.

E. Disjunction

In classical logic or in Birkhoff and von Neumann lattice theoretic approach to propositions, disjunction is defined using the negation and conjunction, via De-Morgan's laws (3.7), and turns out to be well defined for any pair of propositions; this, of course, is based on the belief that one can provide experimental procedures that justify a lattice theoretic conjunction.

Since we have no apriori justification for employing lattice theoretic constructs, we have to define disjunction separately and provide an empirical counterpart. We may note that the connective disjunction is mainly encountered in joining two propositions which refer to obtaining values in disjoint subsets of the value space of an observable (as in the case of two geiger counters which are active for disjoint volumes). Therefore, we define disjunction as a connective which is defined only for disjoint propositions and refers in some sense to the "fusing" or physical adjoining of the corresponding experimental procedures (the terminology should be changed when we talk of position measurements). Schematically we can represent this as in Fig. 3. Mathematically, the disjunction $\mathcal{E}_1 \vee \mathcal{E}_2$ of two operations is defined only when they are mutually disjoint ($\mathcal{E}_1 \perp \mathcal{E}_2$), and is given by

$$\mathcal{E}_1 \vee \mathcal{E}_2 = \mathcal{E}_1 + \mathcal{E}_2, \tag{4.8}$$

whenever $\mathcal{E}_1 \perp \mathcal{E}_2$. $\vee$ is a well defined operation in $\mathcal{O}$ and can be extended to any countable disjoint set of propositions. In an abstract characterization of the logic $\mathcal{O}$, the extension to countable sets will have to be accomplished via regularity assumptions.

We see that the disjunction is commutative and associative whenever defined. Also

$$\mathcal{E} \vee \theta = \mathcal{E}. \tag{4.9}$$

However, note that $\mathcal{E} \perp \mathcal{E}$ implies that

$$\mathcal{E} \vee \mathcal{E} = 2\mathcal{E}.$$

A very important feature of these definitions is that $\wedge$ is distributive with respect to $\vee$ whenever the latter is defined. In fact, if $\mathcal{E}_2 \perp \mathcal{E}_3$, then $(\mathcal{E}_1 \wedge \mathcal{E}_2) \perp (\mathcal{E}_1 \wedge \mathcal{E}_3)$ and $(\mathcal{E}_2 \wedge \mathcal{E}_1) \perp (\mathcal{E}_3 \wedge \mathcal{E}_1)$ for all $\mathcal{E}_1 \in \mathcal{O}$, and we have

$$\begin{aligned} &\mathcal{E}_1 \wedge (\mathcal{E}_2 \vee \mathcal{E}_3) = (\mathcal{E}_1 \wedge \mathcal{E}_2) \vee (\mathcal{E}_1 \wedge \mathcal{E}_3), \\ &(\mathcal{E}_2 \vee \mathcal{E}_3) \wedge \mathcal{E}_1 = (\mathcal{E}_2 \wedge \mathcal{E}_1) \vee (\mathcal{E}_3 \wedge \mathcal{E}_1). \end{aligned} \tag{4.10}$$

However, is not, in general, distributive with respect to $\wedge$. Finally, if $\mathcal{E}'$ is a negation of $\mathcal{E}$, then

$$\mathcal{E} \vee \mathcal{E}' \in \Sigma. \tag{4.11}$$

But $\mathcal{E} \vee \mathcal{E}'$ is not the identity operation in general. Thus two complementary propositions will only give us a maximal proposition, but not the identity proposition in general, unless the propositions are classical.

F. States

Having given a brief sketch of the "logic" of the set $\mathcal{O}$ of experimental propositions of a quantum system, we can now define the states on the logic $\mathcal{O}$. These are functions $\mu : \mathcal{O} \to [0,1]$, with

$$\text{(QS1)} \quad \mu(\theta) = 0, \tag{4.12}$$

$$\text{(QS2)} \quad \mu(\xi) = 1 \quad \text{for all } \xi \in \Sigma, \tag{4.13}$$

(QS3) $\{\mathcal{E}_i\}$ is a countable disjoint set of propositions, then

$$\mu(\bigvee_i \mathcal{E}_i) = \sum_i \mu(\mathcal{E}_i). \tag{4.14}$$

Note that the properties (QS1) and (QS3) are the same as the assumptions (S1) and (S3) for the states in a classical theory except that the notion of disjointness is specific to the propositional calculus. However, (QS2) differs from (S2) in that we assign unit probability to all the maximal propositions $\xi \in \Sigma$ in quantum theory.

Since the disjunction in (4.14) is the same as addition of operations, every state will define a linear continuous functional on $\mathcal{O}$. Since our characterization of $\mathcal{O}$ has not been axiomatic, we do not consider the precise determination of the set of all states on an abstract logic of operations. Instead, we only note that for the particular realization of the logic under consideration, all the quantum mechanical density operator states satisfy (QS1)–(QS3). These are states of the form

$$\mu(\mathcal{E}) = \mathrm{Tr}\mathcal{E}(\rho), \tag{4.15}$$

where $\rho \in V^+$ and $\mathrm{Tr}\rho = 1$.

In this context, we may also note that we have

$$\begin{aligned} \mu(\mathcal{E} \wedge \xi) &= \mathrm{Tr}[\xi(\mathcal{E}(\rho))] \\ &= \mathrm{Tr}\mathcal{E}(\rho) \\ &= \mu(\mathcal{E}), \end{aligned} \tag{4.16}$$

for all $\mathcal{E} \in \mathcal{O}$, and $\xi \in \Sigma$. This property will prove to be of importance in the discussion of joint distributions of random variables.

We can follow the traditional terminology and call the ordered pair $(\mathcal{O}, \mu)$, where $\mathcal{O}$ is the quantum logic of

operations, and μ a state on $\mathcal{O}$, a "quantum probability space." The random variables in the present theory will coincide with the "instruments" defined by Davies and Lewis.

G. Random variables—Instruments

By following the general program outlined in Sec. 3, a random variable or an instrument can be defined as a map from the set of all Borel subsets $B(R)$ of a value space R (usually the real line, or a general completely separable metric space), into the "logic" $\mathcal{O}$, such that

$$(QO1)\ X(\phi)=\theta, \tag{4.17}$$

$$(QO2)\ X(R)\in\sum, \tag{4.18}$$

(QO3) if $\{E_i\}$ is a sequence of mutually disjoint Borel sets in $B(R)$, then $\{X(E_i)\}$ is a disjoint sequence of propositions and

$$X(\cup_i E_i)=\bigvee_i X(E_i). \tag{4.19}$$

Let us first note that (QO_1) and (QO3) imply that

$$X(E_1)\leq X(E_2), \tag{4.20}$$

whenever $E_1\subseteq E_2$. This shows that if we had assumed $X(R)=I$, as in classical probability theory, instead of (QO2), then all the operations associated with the instrument X would have been constrained to satisfy the classical relation $X(E)\leq I$. Our requirement (QO2) on the instruments clearly reflects the basic feature of quantum instruments that even when the measurement is such that minimum information is extracted (that the result is somewhere in the value space of the instrument), more than often the state of the system undergoes an alteration.

H. Quantum probability theory

The quantum probability spaces $(\mathcal{O},\mu)$ and instruments defined on them, constitute the basis for a generalized probability theory appropriate to quantum systems. The basic features of such a theory has been set forth by Davies and Lewis in their pioneering work[18] on the subject.

First of all, each state of the system μ associates, with every instrument X, a probability measure on the value space of the instrument, given by

$$p_x^\mu(E)=\mu(X(E)), \tag{4.21}$$

for each Borel subset E of the value space. (It is immediate to check that p_x^μ is a probability measure on R, the value space.) As we have already noted, this coincides with the statistical interpretation of quantum mechanics.

If X_1 and X_2 are any two instruments, the natural definition of the joint distribution of the ordered pair (X_1,X_2) in the state μ, would be

$$p^\mu_{x_1,x_2}(E_1,E_2)=\mu(X_1(E_1)\wedge X_2(E_2)). \tag{4.22}$$

That $p^\mu_{x_1,x_2}$ as defined above can be extended to a unique probability measure on the Cartesian product $R_1\times R_2$ of the value spaces, is a direct consequence of Davies and Lewis' result on the composition of instruments noted in Sec. 2. In fact, any ordered n-tuple of instruments gives rise to a unique joint probability measure on the Cartesian product of the value spaces. One of the properties crucial for the existence of these joint probability measures is, of course, the distributive law (4.10).

These joint probability measures exhibit all the typical features of the "quantum interference of probabilities," i.e., we have

$$p^\mu_{x_1,x_2}(E_1,E_2)\neq p^\mu_{x_2,x_1}(E_1,E_2)$$

$$p^\mu_{x_1,x_2}(R_1,E_2)\neq p^\mu_{x_2}(E_2)$$

$$p^\mu_{x,x}(E_1,E_2)\neq p^\mu_x(E_1\cap E_2),$$

in general, unless the instruments satisfy special conditions. However, we still have the marginal probability condition

$$p^\mu_{x_1,x_2}(E_1,R_2)=p^\mu_{x_1}(E_1), \tag{4.23}$$

as can be directly verified using (4.16).

Thus all the nonclassical features of quantum probability theory (as summarized in Sec. 2), arise as a natural consequence of the quantum logic of experimental propositions.

5. QUANTUM STOCHASTIC PROCESSES

In classical probability theory, a stochastic process[58] is a family of classical random variables $\{C_t\}_{t\in T}$ indexed by a set T. In a physical theory T could be taken to be the interval $(0,\infty)$ or a subset thereof. Thus it is natural to define a quantum stochastic process as a family of instruments $\{Q_t\}_{t\in T}$ on a quantum probability space $(\mathcal{O},\mu)$, as defined in Sec. 4. We will only consider the case when all the instruments Q_t have the real line R for their value space.

In classical probability theory, there is a basic construction (due to Kolmogorov) which reduces the study of the stochastic processes to a study of probability measures on the space of paths—i.e., on the space of suitable class of functions

$$f: T\to R.$$

This is achieved by considering the so-called "measures on finite dimensional cylinder sets," which can be derived from the joint distributions of the form

$$\mu_{t_1,t_2,\ldots,t_r}(E_1,E_2,\ldots,E_r)$$
$$=\mu(C_{t_1}(E_1)\cap C_{t_2}(E_2)\cap\ldots\cap C_{t_r}(E_r)) \tag{5.1}$$

These "finite-dimensional distributions" satisfy the well-known consistency conditions

(C1) $\mu_{t_1,t_2,\ldots,t_r}(E_1,E_2,\ldots,E_r)$ are invariant if $\{E_i\}$ and $\{t_i\}$ are permuted together in the same way.

$$(C2)\ \mu_{t_1,\ldots,t_{r-1},t_r}(E_1,\ldots,E_{r-1},R)=\mu_{t_1,\ldots,t_{r-1}}(E_1,\ldots,E_{r-1}). \tag{5.2}$$

$$(C3)\ \mu_{t_1,\ldots,t_{r-1},t_r}(E_1,\ldots,E_{r-1},E_r)$$
$$=\mu_{t_1,\ldots,t_{r-1}}(E_1,\ldots,E_{r-1}\cap E_r), \tag{5.3}$$

whenever $t_{r-1}=t_r$. From (C1) and (C2) we can conclude

that the marginal distribution condition (5.2) is valid for the other time variables t_i $(i<r)$ also.

The basic result of Kolmogorov is that,[58] given a family of finite-dimensional distributions $\mu_{t_1,\ldots,t_r}$ which satisfy the consistency conditions (C1)–(C3), there exists a classical probability space (B,μ) and a stochastic process $\{C_t\}_{t\in T}$ such that $\mu_{t_1,\ldots,t_r}$ will be its finite-dimensional distributions.

We will now consider how a similar formulation can be attempted for quantum stochastic processes. Let $\{Q_t\}_{t\in T}$ be a family of instruments on a quantum probability space $(\mathcal{O},\mu)$. The finite-dimensional distributions of this quantum stochastic process will be given by

$$\mu_{t_1,\ldots,t_r}(E_1,\ldots,E_r)=\mu(Q_{t_1}(E_1)\wedge\cdots\wedge Q_{t_r}(E_r)). \tag{5.4}$$

If the state μ is characterized by the density operator ρ, then

$$\mu_{t_1,\ldots,t_{r-1},t_r}(E_1,\ldots,E_{r-1},E_r)=\mathrm{Tr}[\{Q_{t_r}(E_r)\circ Q_{t_{r-1}}(E_{r-1})\circ\cdots\circ Q_{t_1}(E_1)\}\rho]. \tag{5.5}$$

We can rewrite (5.5) also in terms of the so-called "expectations" Q_t^*, which are nothing but adjoints of instruments, being mappings from $B(R)$ into the corresponding adjoint operations. We get the well-known result

$$\mu_{t_1,\ldots,t_r}(E_1,\ldots,E_r)=\mathrm{Tr}[\{(Q_{t_1}^*(E_1)\circ\cdots\circ Q_{t_r}^*(E_r))1\}\rho]. \tag{5.6}$$

It was stated in Sec. 4, that (5.5) or (5.6) define a joint probability measure on R^r. The equation (5.6) may be used to analyze these joint distributions in terms of the positive operator valued measures,[59] which associate each Borel subset $E_1\times\cdots\times E_r$, or R^r, with the bounded positive operator $\{Q_{t_1}^*(E_1)\circ\cdots\circ Q_{t_r}^*(E_r)\}1$.

Before analyzing the properties of these distributions, we should note that if "t" is interpreted as a physical time, then the finite-dimensional distributions (5.4) can be given an operational meaning iff $t_1\leq t_2\leq\cdots\leq t_r$. One could argue that the same will be true of the finite-dimensional distributions (5.1) of a classical stochastic process in a physical context. However, the basic difference is that the finite-dimensional distributions (5.1), considered as functions parametrized by t_i, have the property of symmetry as given by (C1) whereas the quantum finite-dimensional distributions (5.4) are not symmetric in general, because the conjunction $\wedge$ is not commutative. Similarly, we can see that (C3) is not a general property of the finite-dimensional distributions (5.4). In fact, the validity of (C3) depends on whether the instruments Q_t satisfy a "repeatability property" of the form

$$Q_t(E_{r-1})\wedge Q_t(E_r)=Q_t(E_{r-1}\cap E_r). \tag{5.7}$$

Still we can show that (C2) is valid for finite distributions (5.4) also. We have only to note that $Q_{t_r}(R)\in\Sigma$ and use (4.16) to obtain

$$(Q)\quad \mu_{t_1,\ldots,t_{r-1},t_r}(E_1,\ldots,E_{r-1},R)=\mu_{t_1,\ldots,t_{r-1}}(E_1,\ldots,E_{r-1}). \tag{5.8}$$

Since (1) is no longer valid, we cannot deduce from (5.8) the marginal probability condition for other time variables t_i, $i<r$. Thus we conclude that the only consistency condition on the finite-dimensional distributions of a quantum stochastic process is given by (Q).

We can pose the Kolmogorov problem for the quantum stochastic process as follows: "Given a set of finite-dimensional distributions $\mu_{t_1,\ldots,t_r}$ which satisfy the consistancy condition (Q), does there exist a quantum probability space $(\mathcal{O},\mu)$ and a stochastic process such that $\mu_{t_1,\ldots,t_r}$ will be its finite-dimensional distributions?"

One result that may be considred as being related to this problem is the result of Benioff[59] that "operator valued measures on finite Cartesian product spaces R^r, which obey a consistency condition similar to (Q), can be extended uniquely to the space of all infinite real sequences." We may also note that in the theory of classical stochastic processes, if we just restrict to the consistancy condition (C2) [or (Q)] alone, as is sometimes done in the study of functions of Markov chains using "stochastic modules," then we obtain a representation of the process in terms of probability spaces similar to quantum probability spaces. This remarkable feature, which has been pointed out by Kingman,[60] may be of considerable significance in the study of quantum stochastic processes.

A rigorous analysis of a closely related class of quantum stochastic processes has been carried out by Davies[61–63] in a series of papers, which also initiated the general operational approach. He has obtained several analytical results, including a characterization of these processes in terms of infinitesimal generators. However, as his analysis is not based on a quantum probability space, the characterization of quantum stochastic processes from their finite-dimensional distributions and the corresponding consistency conditions is not immediate. We should also emphasize that a formulation in terms of quantum probability spaces facilitates further considerations of conditional expectations, Markovicity, etc., which are basic to a probability theory.

Quantum Markov processes

A rigorous formulation of the condition of Markovicity would involve a discussion of conditional expectations on quantum probability spaces. We will restrict ourselves here only to a few remarks on some differences between quantum and classical Markov processes. For this, we will only consider finite-dimensional measures on R^r, of a quantum stochastic process, which are obtainable via finite-dimensional distribution functions of the form $P_r(\lambda_1 t_1,\ldots,\lambda_r t_r)$. The consistency condition (Q) will be

$$\sum_{\lambda_r}P_r(\lambda_1 t_1,\ldots,\lambda_{r-1}t_{r-1},\lambda_r t_r)=P_{r-1}(\lambda_1 t_1,\ldots,\lambda_{r-1}t_{r-1}), \tag{5.9}$$

where the sum will be replaced by an integral for the continuous case. We can define the conditional proba-

bilities in the usual way, by

$$W_r(\lambda_r t_r \mid \lambda_{r-1} t_{r-1} \cdots \lambda_1 t_1) = \frac{P_r(\lambda_1 t_1, \ldots, \lambda_r t_r)}{P_{r-1}(\lambda_1 t_1, \ldots, \lambda_{r-1} t_{r-1}}, \quad (5.10)$$

As in the classical theory, we can say that a process is Markovian if

$$W_r(\lambda_r t_r \mid \lambda_{r-1} t_{r-1}, \ldots, \lambda_1 t_1) = W(\lambda_r t_r \mid \lambda_{r-1} t_{r-1}), \quad (5.11)$$

for all $\{\lambda_i t_i\}$ with $t_i < t_{i+1}$ for all r.

This is, of course, equivalent to

$$P_r(\lambda_1 t_1, \ldots \lambda_r t_r) = P(\lambda_1 t_1) W(\lambda_2 t_2 \mid \lambda_1 t_1) \cdots \times W(\lambda_r t_r \mid \lambda_{r-1} t_{r-1}). \quad (5.12)$$

To obtain an example of a quantum Markov process, let us consider an instrument which obeys the collapse expreesion (2.2) of von Neumann and corresponds to a self-adjoint operator A, with a discrete spectrum as given by (2.1). If we assume that the system undergoes Hamiltonian evolution, then we can obtain a quantum stochastic process given by the family of instruments $\{Q_t\}_{t \in T}$ defined by

$$Q_t(E)\rho = \sum_{\lambda_i \in E} P_i(t) \rho P_i(t), \quad (5.13)$$

with

$$P_i(t) = V^{-1}(t) P_i(0) V(t). \quad (5.14)$$

We can immediately see that the finite-dimensional measures (5.5) of this process correspond to the joint distribution function (2.7); i.e.,

$$P_r(\lambda_1 t_1, \ldots, \lambda_r t_r) = \mathrm{Tr}[P_r(t_r) \cdots P_1(t_1) \rho \times P_1(t_1) \cdots P_r(t_r)]. \quad (5.15)$$

If, in addition, the spectrum of A is nondegenerate, then $\{P_i\}$ will be a orthonormal set of projection operators onto one-dimensional subspace; now using (5.14), we can rewrite (5.15) as

$$P_r(\lambda_1 t_1, \ldots, \lambda_r t_r) = P(\lambda_1 t_1) W(\lambda_2 t_2 \mid \lambda_1 t_1) \cdots \times W(\lambda_r t_r \mid \lambda_{r-1} t_{r-1}), \quad (5.16)$$

where

$$W(\lambda_r t_r \mid \lambda_{r-1} t_{r-1}) = \mathrm{Tr}[P_r(t_r) P_{r-1}(t_{r-1})]. \quad (5.17)$$

Equations (5.16) and (5.17) show that we have a quantum Markov process. However, we also have

$$\sum_{\lambda_2} W(\lambda_3 t_3 \mid \lambda_2 t_2) W(\lambda_2 t_2 \mid \lambda_1 t_1) \neq W(\lambda_3 t_3 \mid \lambda_1 t_1), \quad (5.18)$$

in general. In fact it is a general characteristic of quantum Markov processes that the Smoluchowski, Chapman, Kolmogorov (SCK) equation is not valid in general. In the study of classical Markov processes, the SCK equation is usually derived using the consistancy conditions (1), (2), together with the condition for Markovicity (5.11) or (5.12). The failure of SCK equation for quantum Markov processes is again a direct consequence of the "quantum interference of probabilities" and can be illustrated by several such examples.

We may also note that if the instrument Q_t corresponds to a self-adjoint operator A as in (2.1) but with a degenerate spectrum, then we can no longer derive (5.16) from (5.15), and actually we obtain a quantum stochastic process which is non-Markovian in general. In this context we can recall an observation of Goldberger and Watson[21] that in the measurement of observables with a spectral degeneracy, the previous information (memory) persists even after a new measurement is made. The preceding discussion also makes it clear that Markovicity is a special property of certain instruments and the dynamics of the system, and is not a general feature of all quantum stochastic processes.

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APPENDIX: "OPERATIONS" AND "EFFECTS" OR "SIMPLE OBSERVABLES"

Apart from the lattice theoretic approach, there are other axiomatic studies in which each experimental procedure is associated with a positive operator $F \in B_s^+(H)$ such that $0 < F < 1$. Such operators have been called "effects" or "simple observables." The set of all effects may be denoted by Q. It can be shown[19] that, to each operation $\mathcal{E} \in O$, there corresponds a unique effect $F_{\mathcal{E}} \in Q$ such that

$$\mathrm{Tr}[\mathcal{E}(v)] = \mathrm{Tr}(F_{\mathcal{E}} v), \quad (A1)$$

for all $v \in V^+$. However, given any effect $F \in Q$, there exists several operations in O, which are all related to F in the manner of Eq. (A1). For example, we may define operations $\mathcal{E}_1$ and $\mathcal{E}_2$, by

$$\mathcal{E}_1(v) = \mathrm{Tr}(Fv)\rho, \quad (A2)$$

where ρ is an arbitrary density operator, and

$$\mathcal{E}_2(v) = F^{1/2} v F^{1/2}, \quad (A3)$$

so that we have

$$\mathrm{Tr}[\mathcal{E}_1(v)] = \mathrm{Tr}[\mathcal{E}_2(v)] = \mathrm{Tr}(Fv), \quad (A4)$$

for all $v \in V^+$. Therefore, a representation of the experimentally verifiable propositions by elements of Q will not provide a complete characterization of the corresponding experimental procedures. This can be demonstrated more clearly, by showing that the logical relations among the experimental procedures cannot all be inferred just by a study of the set Q of all effects alone.

Two operations $\mathcal{E}_1, \mathcal{E}_2 \in O$ are said to be isotonic[19] if

$$\mathrm{Tr}[\mathcal{E}_1(v)] = \mathrm{Tr}[\mathcal{E}_2(v)], \quad (A5)$$

for all $v \in V^+$. The set of all operations isotonic to a given operation $\mathcal{E}$ is an equivalence class (termed "isotony class"), which may be denoted by $[\mathcal{E}]$. From (A1) and (A5), it is clear that to each element of Q there corresponds a unique isotony class and conversely. In this context we should also note the following property of the logic O of quantum mechanical operations. The condi-

tion

$$\mu(\mathcal{E}_1)=\mu(\mathcal{E}_2), \tag{A6}$$

for all the density operator states μ, will only allow us to conclude that $\mathcal{E}_1$ and $\mathcal{E}_2$ belong to the same isotony class. This is significantly different from the lattice theoretic logics (and some of the algebraic approaches to axiomatic quantum theory), where probabilistically indiscernable propositions are assumed to be identical.

In fact, it has been emphasized by Edwards[48] that the properties of operations (and hence of the corresponding experimental procedures) can be classified into two categories, namely those which are shared by all the members of an isotony class (isotonic properties) and those which are not. The transmission probability or the factor by which the size of an ensemble is diminished when it is subjected to the experimental procedure is a property of the first category, whereas the purely quantum mechanical "distortion" or the "collapse" of the ensemble is a property which varies with the different members of an isotony class. We can show that, in each isotony class $[\mathcal{E}]$, there exists a unique operation $\mathcal{E}_0$ given by

$$\mathcal{E}_0(v)=\{\mathrm{Tr}[\mathcal{E}(v)]/\mathrm{Tr}(v)\}v, \tag{A7}$$

for all $v\in V^*$, which satisfies the condition of distortion-free measurement,

$$\mathcal{E}_0\leq I. \tag{A8}$$

Such operations have been called "reflections" by Edwards,[48,49] who has also given a detailed analysis of different classes of operations.

We now examine the structure of the logic $\mathcal{O}$ of quantum mechanical operations in relation to the structure of the set Q of all effects—or equivalently the set of all isotony classes of operations. The relation of implication is not an isotonic relation. If $\mathcal{E}_1\leq\mathcal{E}_2$, we evidently have $F_{\mathcal{E}_1}\leq F_{\mathcal{E}_2}$, where $F_{\mathcal{E}_i}$ is defined in (A1). However, the converse

The absurd proposition forms an isotony class by itself. The set of all maximal operations form an isotony class containing the identity operation, i.e.,

$$[\theta]=\{\theta\}, \tag{A9}$$

$$[I]=\Sigma. \tag{A10}$$

The set of all negations of an operation $\mathcal{E}$ is the isotony class $[I-\mathcal{E}_0]$ where $\mathcal{E}_0$ is given by (A7). For each $\mathcal{E}'\in[I-\mathcal{E}_0]$, we have

$$\mathcal{E}+\mathcal{E}'\in\Sigma. \tag{A11}$$

Also every element of the isotony class $[\mathcal{E}]$ is a negation of every element of the isotony class $[I-\mathcal{E}_0]$ and vice versa.

The relation of disjointness is isotonic, as

$$\mathcal{E}_1\perp\mathcal{E}_2 \quad \text{iff} \quad F_{\mathcal{E}_1}+F_{\mathcal{E}_2}\leq 1. \tag{A12}$$

Also, if $\mathcal{E}_1\perp\mathcal{E}_2$ and $\mathcal{E}_3\in[\mathcal{E}_1]$ and $\mathcal{E}_4\in[\mathcal{E}_2]$ then $\mathcal{E}_3\perp\mathcal{E}_4$ and

$$\mathcal{E}_3\vee\mathcal{E}_4\in[\mathcal{E}_1\vee\mathcal{E}_2]. \tag{A13}$$

However, the conjunction $\mathcal{E}_1\wedge\mathcal{E}_2$ of two operations is a connective that is crucially dependent on the "distortion" produced by the experimental procedure $\mathcal{E}_1$, and hence cannot be characterized in terms of isotonic properties alone.

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Elementary systems in general relativity

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The problem of definition of elementary systems in general relativity is analyzed and some current theories are compared. A definition of dynamically free local elementary systems in general relativity is proposed, taking into account the influence of the gravitational field arising from the intrinsic dependence of the symmetry groups on the field.

1. INTRODUCTION

By an elementary system we shall understand the collection of structureless objects which are obtained from the classification of the unitary irreducible representations of some symmetry group in a physical theory.[1] In the case of the special theory of relativity the elementary systems defined by the group of isometries of Minkowski space–time (the Poincaré group) gives a very close approximation to what is presently known as elementary particles. When we deal with general relativity we have a collection of space–times instead of the single Minkowski space–time of special relativity. This change in the geometrical structure compels us to ask if the structure of elementary systems in general relativity should be different from that in special relativity, what are the changes in structure, and finally what are the physical implications of the new structure.

The definition of elementary systems in general relativity depends on a characterization of a certain symmetry group to be defined in the general theory of relativity.

Unlike the case of special relativity, in general relativity we do not have a previously given space–time. However, given a certain space–time of general relativity we should also be able to define elementary systems in this space–time. Therefore we have two problems. On the one hand, the definition of elementary systems in general relativity without the previous choice of a certain space–time and, on the other hand, the definition of elementary systems in a given space–time of general relativity. These two problems must be compatible. One way to ensure this compatibility is to choose a group of symmetries such that it holds true in both problems. This solution imposes strong restrictions on the choice of the group of symmetries. A more general solution is to consider a group of symmetries defined in general relativity and project it on each space–time. In this case the compatibility condition is that the projected group should coincide with the appropriate group of symmetries defined in the space–time.

2. KINEMATICAL COUPLING

We proceed to review briefly and comment on some currently proposed theories of elementary systems in general relativity, labeled according to the adopted groups of symmetry.

A. The Poincaré theory

This theory is based on the assumption that the gravitational force is too weak to produce any significant change in the structure of the elementary systems as defined in special relativity. Therefore the elementary systems are defined by the representations of the Poincaré group. This group can be defined in general relativity in different ways. It can be considered as the fiber group of the tangent bundle plus translations. It may also be considered as the holonomy group of orthogonal tetrads plus translations.

The fact that translations have to be added separately on the Poincaré group in general relativity seems to be pathological.[2] While there may be some mathematical means of introducing the Poincaré group in general relativity, this should not be done too artificially. The Poincaré group in special relativity has a clear meaning as the group of isometries of the space–time.

On the physical side it can be said that the weakness of the gravitational force should not be taken too seriously when we are considering a group theoretic definition where no dynamical considerations take place. One example of a theory of this type is the one proposed by Ne'eman and Rosen[3] which assumes a Poincaré type definition for the elementary systems and uses a local embedding technique to define internal symmetries. Another example is the recently proposed f–g theory of Salam which assumes a Poincaré type definition of spin two mesons but curiously enough assumes dynamical interaction when a strong gravitational field is present.[4]

B. The BMS theory

The second proposed structure of elementary systems is based on a group which is closely associated with the group of isometries of the space–times of general relativity[2]; since the Poincaré group is the group of isometries of Minkowski space–time it is natural to search for a group structure with similar properties in general relativity. Unfortunately, exact isometries are not always present in the space–times of general relativity. However, in the cases of asymptotically flat space–times an approximate isometry group can be defined. This group is the BMS group of asymptotic isometries and it differs from the Poincaré group by the fact that translations are replaced by supertranslations in the semidirect product with the Lorentz group.[5,6]

Since the elementary systems associated with the BMS group are asymptotically defined they can be assumed to be dynamically free from gravitation. How-

ever, the fact that the BMS group differs from the Poincaré group is one indication that the elementary systems defined by this group are not entirely free from the gravitational field. This can be seen from the following thought experiment. Supposing that the gravitational field could be switched off (i.e., not simply "made zero" by taking its sources to a far away distance), then the group of isometries in this new situation would be the Poincaré group which would lead to the gravitational free elementary systems of special relativity. In actual fact the switching off cannot be done and the elementary systems feel the effects of the gravitational field even if they are very far away from the sources of this field. Therefore the elementary systems defined by the BMS group are indirectly coupled to the gravitational field. This is not a dynamical coupling. It is due only to the dependence of the considered group of symmetries (BMS) on the gravitational field and is independent of the strength of that field.

The above conclusion lead us to the concept of kinematical coupling. *Any physical structure defined by a group of symmetries is said to be kinematically coupled to the field upon which the group depends.* Thus both the BMS and the Poincaré structures of elementary systems in general relativity are dynamically free from the gravitational field. However, in the BMS case they are kinematically coupled to that field.

One difficulty of the BMS theory lies on the asymptotic character of the elementary systems, leaving unsolved the problem of definition of elementary systems near a gravitational source. Further difficulties are the limitation to asymptotically flat space–times and the infinite number of Casimir operators of the BMS group.[6]

C. The de Sitter theory

The most extensively studied model of elementary systems in general relativity is based on the de Sitter group. The cosmological implications of the de Sitter space–time, the easy comparison with the flat space–time case and the ten parameters of the de Sitter group are the main attributes of this model. Some representations of the de Sitter group were calculated using the local isometric embedding of de Sitter space–time.[7,8] The resulting elementary systems are obviously kinematically coupled to the gravitational field which characterizes the geometry of the de Sitter space–time. Further properties of these elementary systems were studied in analogy with the elementary systems of the Minkowski space–time.[9]

A negative aspect of this theory, when it is viewed from the standpoint of the theory of general relativity, is its restriction to a single and specifically chosen space–time. Thus it would be desirable to have an extension of this model of elementary systems to the whole of general relativity.

3. ISOMETRIC LOCAL ELEMENTARY SYSTEMS

The extension of the de Sitter model of elementary systems to all space–times of general relativity can be made provided the following observations are made.

Since the de Sitter model of elementary systems is defined on a previously chosen space–time, its extension to general relativity requires in the first place that Einstein's equations hold throughout the process of definition as defining the set of space–times to be used.

Secondly, we notice that the de Sitter model is based on an exact isometry. This seems to be too restrictive since not all space–times of general relativity admit a Killing vector field. Nevertheless there are some good physical justifications for the use of isometries. In a physical theory based on a metric geometry, the physical measurements are performed during intervals of time when the measuring rods are expected to remain invariant, an indication that a timelike Killing vector field should exist. Physical theories without isometries or even without a metric can be defined but the notions of observable and the measurment conditions should be revised (Newtonian theory is based on an affine geometry but with a metric on the space sections).

The elementary systems so far known to agree with physics are defined by a group of isometries. Thus, at least in a first attempt on a theory of elementary systems in general relativity it seems reasonable that they should be defined by some group structure associated to isometries as in the last two theories analysed in the previous section. Observe that we are not restricting the definition of elementary systems to space–times with isometries but only stating that they are more likely to agree with present day physics when restricted to space–times with isometries.

The third remark to be made is that the elementary systems of the de Sitter model are locally defined, in the sense that they hold for a neighborhood of an arbitrary point of the space–time.

With these observations we conclude that to obtain an extension of the de Sitter model to general relativity we need a group structure with the following properties:

(a) It is a subgroup of the manifold mapping group of general relativity, defined independently of the previous choice of a specific space–time.

(b) The restriction of this group to a certain space–time of general relativity is local and must result in the full group of isometries of the space–time if the space–time admit isometries and is completely innocuous otherwise (that is, if the space–time does not admit isometries the restriction of the group to this space–time results only on the identity transformation).

(c) In the flat limit the group should reduce to the Poincaré group.

4. THE GROUPS $L(p, r, s)$

We shall show that for each of the minimal isometric embedding classes of the space–times of general relativity the homogeneous fiber group of the embedding bundle satisfies the required conditions for the extension of the de Sitter theory of elementary systems.

If $R4$ denotes any space–time of general relativity, the minimal isometric embedding bundle $E(R4)$ is the Whitney sum of the tangent bundle and a minimal normal bundle whose dimension is given by the Gauss–

Codazzi equations of $R4$. The typical fiber $M(p, r, s)$ is a pseudo-Euclidean space with dimension $p \geq 4$ and metric signature $r+s$. $R4$ is the base space and each fiber is locally defined on $R4$. The minimal condition not only specifies the smallest embedding space but also gives the uniqueness of the embedding, provided the space–time metric is not changed.

The use of embedding formalism is regarded here as in the de Sitter case, not a result of physical imposition, but as a convenient mathematical tool, useful to deal with group representations.

It is important to notice that an embedding bundle is not a property of a single space–time but a property of a class of space–times, so that $M(p, r, s)$ is the same for all space–time of that class. In general relativity there are 22 distinct minimal isometric embedding bundles.

On each fiber $M(p, r, s)$ we may use Cartesian coordinates denoted by X^μ (all Greek indices run from 1 to p) and Gaussian coordinates based on the space–time hypersurface, denoted by x^α. The Gaussian coordinates may be separated into coordinates on the space–time, denoted by x^1 (lower case, boldface Latin indices run from 1 to 4) and coordinates orthogonal to the space–time, denoted by $x^\mathbf{A}$ (capital boldface Latin indices run from 5 to p). In the Gaussian system the space–time hypersurface embedded in $M(p, r, s)$ is defined by the equations $x^\mathbf{A}=0$. The Cartesian components of the metric tensor of $M(p, r, s)$ are denoted by $\eta_{\mu\nu}$ and its Gaussian components are $g_{\alpha\beta}$.

If $f(x^\alpha)$ is a function defined on $M(p, r, s)$, its space–time projection is

$$f(x^\alpha)\big|_{R4} = \lim_{x^\mathbf{A}\to 0} f(x^\alpha).$$

The embedding is obtained when the functions $X^\mu = X^\mu(x^\alpha)$ and its Jacobian matrix with elements $X^\mu{}_\alpha$ are given. Let

$$X'^\mu = X^\mu + U^\mu, \quad U^\mu = \epsilon^\mu{}_\nu X^\nu, \quad U^{(\mu,\nu)} = 0 \tag{4.1}$$

be an infinitesimal transformation of the homogeneous fiber group $L(p, r, s)$ of $M(p, r, s)$. In Gaussian coordinates we have

$$x'^\alpha = x^\alpha + \xi^\alpha, \tag{4.2}$$

where $\xi^\alpha = x^\alpha{}_\mu U^\mu$, $x^\alpha{}_\mu$ being the components of the inverse of the Jacobian matrix $x^\alpha{}_\mu X^\mu{}_\beta = \delta^\alpha{}_\beta$. The last of Eq. (4.1) corresponds to

$$\xi^{(\alpha;\beta)} = 0. \tag{4.3}$$

Semicolon denotes covariant derivative and round brackets on indices denote complete symmetrization. In order to obtain Killing's equations in $R4$ by projection of (4.3) on the space–time we require the additional conditions[10]

$$\xi^\mathbf{A}\big|_{R4} = 0. \tag{4.4}$$

We may write

$$\xi^\mathbf{A} = x^\mathbf{A}{}_\mu U^\mu = x^\mathbf{A}{}_\mu \epsilon^{\mu\nu} X_\nu = X^\nu{}_\beta \epsilon^{\mathbf{A}\beta} X_\nu,$$

where we used the fact that $x^\mathbf{A}{}_\mu X^\mu{}_\alpha = \delta^\mathbf{A}{}_\alpha$ and

$$\epsilon^{\alpha\beta} = x^\alpha{}_\mu x^\beta{}_\nu \epsilon^{\mu\nu}.$$

Since $X^\nu{}_\beta X_\nu = \frac{1}{2}(\eta_{\mu\nu} X^\mu X^\nu)_{,\beta}$, we have

$$\xi^\mathbf{A} = \tfrac{1}{2}(X^\nu X_\nu)_{,\beta} \epsilon^{\mathbf{A}\beta}.$$

Thus (4.4) is equivalent to

$$\tfrac{1}{2}(X^\nu X_\nu)_{,\beta} \epsilon^{\mathbf{A}\beta}\big|_{R4} = 0. \tag{4.4'}$$

With these conditions we get vector fields in $M(p, r, s)$, projected on $R4$, which are defined by the set of equations

$$\xi^{(\mathbf{i};\mathbf{j})}\big|_{R4} = 0, \quad \xi^{(\mathbf{i};\mathbf{A})}\big|_{R4} = 0, \quad \xi^{(\mathbf{A};\mathbf{B})}\big|_{R4} = 0. \tag{4.5}$$

The first equations give the descriptors of the homogeneous part of the group of isometries of the space–time. To understand the meaning of the second set of equations we may consider the Lie algebra of $L(p, r, s)$. The operators of this algebra $L_{\mu\nu}$, in the Cartesian frame, satisfy the commutation relations

$$[L_{\mu\nu} L_{\rho\sigma}] = (\eta_{\mu\rho} L_{\nu\sigma} + \eta_{\nu\sigma} L_{\mu\rho} - \eta_{\mu\sigma} L_{\nu\rho} - \eta_{\nu\rho} L_{\mu\sigma}). \tag{4.6}$$

The Gaussian components of these operators are

$$L_{\alpha\beta} = X^\mu{}_\alpha X^\nu{}_\beta L_{\mu\nu}$$

and

$$[L_{\alpha\beta} L_{\gamma\delta}] = X^\mu{}_\alpha X^\nu{}_\beta X^\rho{}_\gamma X^\sigma{}_\delta [L_{\mu\nu} L_{\rho\sigma}].$$

That is,

$$[L_{\mathbf{ij}} L_{\mathbf{kl}}] = (g_{\mathbf{ik}} L_{\mathbf{jl}} + g_{\mathbf{jl}} L_{\mathbf{ik}} - g_{\mathbf{il}} L_{\mathbf{jk}} - g_{\mathbf{jk}} L_{\mathbf{il}}),$$
$$[L_{\mathbf{ij}} L_{\mathbf{kA}}] = (g_{\mathbf{ik}} L_{\mathbf{jA}} + g_{\mathbf{jA}} L_{\mathbf{ik}} - g_{\mathbf{iA}} L_{\mathbf{jk}} - g_{\mathbf{jk}} L_{\mathbf{iA}}),$$
$$[L_{\mathbf{ij}} L_{\mathbf{AB}}] = (g_{\mathbf{iA}} L_{\mathbf{jB}} + g_{\mathbf{jB}} L_{\mathbf{iA}} - g_{\mathbf{iB}} L_{\mathbf{jA}} - g_{\mathbf{jA}} L_{\mathbf{iB}}),$$
$$[L_{\mathbf{iA}} L_{\mathbf{jB}}] = (g_{\mathbf{ij}} L_{\mathbf{AB}} + g_{\mathbf{AB}} L_{\mathbf{ij}} - g_{\mathbf{iB}} L_{\mathbf{Aj}} - g_{\mathbf{Aj}} L_{\mathbf{iB}}),$$
$$[L_{\mathbf{iA}} L_{\mathbf{BC}}] = (g_{\mathbf{iB}} L_{\mathbf{AC}} + g_{\mathbf{AC}} L_{\mathbf{iB}} - g_{\mathbf{iC}} L_{\mathbf{AB}} - g_{\mathbf{AB}} L_{\mathbf{iC}}),$$
$$[L_{\mathbf{AB}} L_{\mathbf{CD}}] = (g_{\mathbf{AC}} L_{\mathbf{BD}} + g_{\mathbf{BD}} L_{\mathbf{AC}} - g_{\mathbf{AD}} L_{\mathbf{BC}} - g_{\mathbf{BC}} L_{\mathbf{AD}}).$$

Now define the "translation" operator

$$\pi_\mathbf{i} = \alpha^\mathbf{A} L_{\mathbf{iA}}$$

where the $\alpha^\mathbf{A}$ are some conveniently chosen space–time functions so that they vanish in the flat limit. In terms of $\pi_\mathbf{i}$ the above commutators are

$$[L_{\mathbf{ij}} L_{\mathbf{kl}}] = (g_{\mathbf{ik}} L_{\mathbf{jl}} - g_{\mathbf{jl}} L_{\mathbf{ik}} - g_{\mathbf{il}} L_{\mathbf{jk}} - g_{\mathbf{jk}} L_{\mathbf{il}}),$$
$$[L_{\mathbf{ij}} \pi_\mathbf{k}] = (g_{\mathbf{ik}} \pi_\mathbf{j} - g_{\mathbf{jk}} \pi_\mathbf{i}) + \alpha^\mathbf{A} (g_{\mathbf{jA}} L_{\mathbf{ik}} - g_{\mathbf{iA}} L_{\mathbf{jk}}),$$
$$\alpha^\mathbf{A} \alpha^\mathbf{B} [L_{\mathbf{ij}} L_{\mathbf{AB}}] = \alpha^\mathbf{A} (g_{\mathbf{iA}} \pi_\mathbf{j} - g_{\mathbf{jA}} \pi_\mathbf{i}) + \alpha^\mathbf{B} (g_{\mathbf{jB}} \pi_\mathbf{i} - g_{\mathbf{iB}} \pi_\mathbf{j}) = 0,$$
$$[\pi_\mathbf{i} \pi_\mathbf{j}] = (g_{\mathbf{AB}} \alpha^\mathbf{A} \alpha^\mathbf{B} L_{\mathbf{ij}} - g_{\mathbf{iB}} \alpha^\mathbf{B} \pi_\mathbf{j} - g_{\mathbf{Aj}} \alpha^\mathbf{A} \pi_\mathbf{i}),$$
$$[\pi_\mathbf{i} L_{\mathbf{BC}}] = \alpha^\mathbf{A} (g_{\mathbf{iB}} L_{\mathbf{AC}} + g_{\mathbf{AC}} L_{\mathbf{iB}} - g_{\mathbf{iC}} L_{\mathbf{AB}} - g_{\mathbf{AB}} L_{\mathbf{iC}}),$$
$$[L_{\mathbf{AB}} L_{\mathbf{CD}}] = (g_{\mathbf{AC}} L_{\mathbf{BD}} + g_{\mathbf{BD}} L_{\mathbf{AC}} - g_{\mathbf{AD}} L_{\mathbf{BC}} - g_{\mathbf{BC}} L_{\mathbf{AD}}).$$

Projecting these commutators on $R4$ and taking the flat limit, we obtain the group contraction[11]

$$[L_{\mathbf{ij}} \pi_\mathbf{k}]\big|_{R4,\mathrm{flat}} = (g_{\mathbf{ik}} \pi_\mathbf{j} - g_{\mathbf{jk}} \pi_\mathbf{i})\big|_{R4},$$
$$[\pi_\mathbf{i} \pi_\mathbf{j}]\big|_{R4,\mathrm{flat}} = 0,$$
$$[\pi_\mathbf{i} L_{\mathbf{BC}}]\big|_{R4,\mathrm{flat}} = 0,$$

where we used $g_{\mathbf{iA}}\big|_{R4} = 0$. We notice that in the flat limit $\pi_\mathbf{k}$ behaves like a translation operator of the Poincaré

group. Consequently, the π_k are the translation operators in $R4$. They are given by the second equation (4.5), which together with the first equation give the Killing vectors of $R4$. In general we will be dealing with the $L_{i\mathbf{A}}$ in the group representations so that we do not need to specify the functions $\alpha^{\mathbf{A}}$.

The third equation (4.5) correspond to a degree of freedom in the choice of the complete set of Gaussian coordinates. This freedom of coordinates is eliminated when we define once for all the orthogonal coordinates $x^{\mathbf{A}}$ to coincide with some of the Cartesian coordinates.

Finally, if Killing's equations in $R4$ have no solution apart from the trivial one, we have

$$\xi^i|_{R4} = x^i{}_\mu U^\mu|_{R4} \equiv 0,$$

which together with (4.4) gives

$$\xi^\alpha|_{R4} = \epsilon^{\alpha\beta} X^\mu{}_\beta X_\mu|_{R4} = 0,$$

so that in this case the projection of $L(p,r,s)$ on $R4$ gives only the identity transformation. Therefore, for a given class of space–times the class group $L(p,r,s)$ satisfy the conditions for generalization of the de Sitter model. In particular, it applies to the flat space–time case giving the Lorentz group $L(4,3,1)$ (in this special case translations have to be added separately). Another example is the de Sitter group $L(5,4,1)$. In this case (as in any constant curvature space–time), it is important to notice that the conditions (4.4) are trivially satisfied so that $L(5,4,1)$ is identical to $L(5,4,1)|_{\text{de Sitter}}$. This is not the general case where distinct space–time embedded in $M(p,r,s)$ have distinct solutions for (4.4) and consequently distinct groups $L(p,r,s)|_{R4}$.

Thus, assuming that the isometric local elementary systems in general relativity are defined by the unitary representations of the various groups $L(p,r,s)$, the elementary systems on the space–time $R4$ are defined by the unitary representations of the group $L(p,r,s)|_{R4}$ defined by (4.4) and (4.5). Since for $L(p,r,s)$ we do not have a previously given space–time, we refer to the elementary systems defined by this group as "abstract objects" in the sense that they can only attain space–time meaning when restricted to a space–time.

5. ISOSPINORS

An elementary system is described by fields which are defined in the space of the unitary irreducible representations of the adopted groups of symmetries. Taking this group as being $L(p,r,s)$, these fields can be obtained from the spinor representation of the Clifford algebra defined on $M(p,r,s)$. If $p=2\nu$ or $p=2\nu+1$, these spinors have 2^ν components (half the number of components can be considered in certain cases). These spinors transform according to a representation of the group of automorphisms of the Clifford algebra. Denoting the generators of this algebra by e_μ, then the subset of the algebra generated by

$$L_{\mu\nu} = \tfrac{1}{2} e_{[\mu} e_{\nu]}, \tag{5.1}$$

is isomorphic to the Lie algebra of $L(p,r,s)$. Choosing one of the many possible Weyl representations of the Clifford algebra[12] and denoting by $M_{\mu\nu}$ the matrices representing $L_{\mu\nu}$, the infinitesimal transformations of the spinor group S are given by

$$S = 1 + \tfrac{1}{2}\epsilon^{\mu\nu} M_{\mu\nu}. \tag{5.2}$$

With the conditions (4.4) the group $L(p,r,s)|_{R4}$ gives the isometries of the space–time $R4$. Under the same conditions the matrices (5.2) generate a spinor representation of this group of isometries, denoted by $S|_{R4}$ and called the isospinor group of $R4$. The spinors which transform according to $S|_{R4}$ are called isospinors.[10]

Since S is a representation of $L(p,r,s)$, the elementary systems obtained by the unitary representations of S are described by the spinor fields of the representation space. Similarly, the representations of $S|_{R4}$, which can be obtained from the representations of S, give the space–time elementary systems which are described by the isospinors of the representation space.

6. FIELD EQUATIONS

Since the spinors constructed in the last sections are defined on the fibers of the embedding bundles they are only locally defined. Furthermore, they must satisfy some field equations, which are defined on these fibers but subjected to physical considerations, defined on the space–time. We have a situation in which a set of field variables is defined in the spaces $M(p,r,s)$ but only those which are "space–time defined" are to be considered as having physical meaning. Let $\psi^{(\alpha)}(x^\alpha)$ be any field variable defined on the Gaussian system, where (α) stands for any collection of indices. In particular, $\psi^{(\alpha)}$ may be the components of the spinors constructed on $M(p,r,s)$.

A function defined in $M(p,r,s)$ is said to be space–time defined if it depends only on the space–time coordinates. If the function f is defined in Gaussian coordinates, then clearly $f(x^i)$ is space–time defined. On the other hand, if f is defined in the Cartesian system, $f(X^\mu)$ is space–time defined only if the coordinates X^μ correspond to a point of the space–time. In general, the projection $f(x^\alpha)|_{R4}$ of a function f defined on $M(p,r,s)$ on the space–time is space–time defined.

The sought field equations are defined on $M(p,r,s)$ but must yield space–time defined field equations.

Given a set of space–time defined field variables there are two cases to consider depending whether the Lagrangian function is or is not space–time defined.

In the first case we obtain field equations which are space–time defined, independently of the choice of a particular space–time. In the second case we get field equations which are not necessarily space–time defined but that can be projected on the space–times afterwards.

Consider the space–time defined Lagrangian

$$L = L(\psi^{(\alpha)}(x^i), \psi^{(\alpha)}(x^i)_{,j}) \tag{6.1}$$

and the action integral $A = \int L d^p x$, where $d^p x$ is the p-dimensional volume element defined in the Gaussian systems. We can write $d^p x = d^t x\, d^4 x$ where $d^t x$ is the part of the volume element corresponding to the subspace orthogonal to the space–time. Let δA be a varia-

tion of A such that $\delta\psi^{(\alpha)}(x^1)$ vanishes on two three-dimensional neighbouring surfaces Σ_1 and Σ_2 in the space–time:

$$\delta A = \int \left(\frac{\partial L}{\partial \psi^{(\alpha)}} \, \partial\psi^{(\alpha)} + \frac{\partial L}{\partial \psi^{(\alpha)}{}_{,i}} \, \partial\psi^{(\alpha)}{}_{,i} \right) d^p x.$$

Defining

$$\pi^i{}_{(\alpha)} = \frac{\partial L}{\partial \psi^{(\alpha)}{}_{,i}},$$

$$\delta A = \int \left[\left(\frac{\partial L}{\partial \psi^{(\alpha)}} - \pi^i{}_{(\alpha),i} \right) \delta\psi^{(\alpha)} + (\pi^i{}_{(\alpha)} \delta\psi^{(\alpha)}{}_{,i}) \right] d^4x \, d^t x.$$

Using the Gauss theorem in the second term of the integral and assuming $\delta A = 0$,

$$\int \left(\frac{\partial L}{\partial \psi^{(\alpha)}} - \pi_{(\alpha)}{}^i{}_{,i} \right) \delta\psi^{(\alpha)} \, d^p x + \int \left(\int_{\Sigma_1}^{\Sigma_2} \pi_{(\alpha)}{}^i \delta\psi^{(\alpha)} \, d\Sigma_i \right) d^t x = 0.$$

Since $\delta\psi^{(\alpha)}$ vanishes on Σ_1, Σ_2 the last integral is zero. The first integral gives the space–time defined field equations

$$\frac{\partial L}{\partial \psi^{(\alpha)}} - \pi_{(\alpha)}{}^i{}_{,i} = 0. \tag{6.2}$$

In the case $p = 6$ these equations coincide with some of the equations obtained by Fronsdal.[13]

Consider now a situation where the Lagrangian is not space–time defined. This may occur for example when the field variables are subjected to operations which destroy the space–time character. The result is the same as before, but the field equations have to be projected on the space–time

$$\left(\frac{\partial L}{\partial \psi^{(\alpha)}} \right)_{R4} - \pi_{(\alpha)}{}^i{}_{,i\ R4} = 0. \tag{6.3}$$

Consider the following example. The Lagrangian

$$L = -\tfrac{1}{2}[\tilde{\psi} e^\alpha e^\beta (x_\alpha \psi_{,\beta} - x_\beta \psi_{,\alpha}) + \tilde{\psi} m \psi] + \tfrac{1}{2}[(x_\alpha \tilde{\psi}_{,\beta} - x_\beta \tilde{\psi}_{,\alpha}) e^\alpha e^\beta \psi - \tilde{\psi} m \psi], \tag{6.4}$$

where $e^\alpha = x^\alpha{}_\mu e^\mu$, e^μ are the matrices of a Weyl representation of the Clifford algebra defined on $M(p, r, s)$, and ψ are the spinors of a spinor representation of the same algebra. m is a scalar function defined in the space–time, such that it reduces to a constant in the flat limit. $\tilde{\psi} = \psi^\dagger \mu$ where μ is the Hermitian matrix proportional to the product of all anti-Hermitian generators of the algebra.[14] The operator

$$J_{\alpha\beta} = x_\alpha \frac{\partial}{\partial x^\beta} - x_\beta \frac{\partial}{\partial x^\alpha},$$

which appears on the above Lagrangian, when applied to a space–time defined field variable does not necessarily give a space–time defined variable. For example, $J_{AB}\psi(x^1) = 0$ but $J_{1A}\psi(x^1) = x_A(\partial\psi/\partial x^1)$. Consequently, the Lagrangian (6.4) is not space–time defined. Considering ψ as a space–time defined spinor function, Eq. (6.3) gives

$$\begin{aligned} &\tilde{\psi}(J_{ij} e^i e^j - m)_{|R4} = 0, \\ &(e^i e^j J_{ij} + m)\psi_{|R4} = 0. \end{aligned} \tag{6.5}$$

The spinor field which satisfies these equations transform according to $S_{\cdot R4}$ and therefore is an isospinor field. Equations (6.5) generalize the equations proposed by Dirac for the de Sitter space–time.[15]

In the flat limit the isospinor field ψ coincide with Dirac's spinors and Eqs. (6.5) give the equations for spin 1/2 particles. This fact suggests that the elementary systems defined by $L(p, r, s)$ which satisfy Eqs. (6.5) in $R4$ may be labelled spin 1/2 elementary systems. However, this is only a suggestion since in general relativity the meaning of the word spin may differ from the usual concept in special relativity as it is clear from the analysis of de Sitter space–time.[9]

7. UNITARY REPRESENTATIONS OF $L(p, r, s)$

To obtain the elementary systems in the scheme proposed in the previous sections we need to calculate the unitary irreducible representations of each group $L(p, r, s)$, or equivalently, the representations of the corresponding spinor groups S, and classify them. Once a specific space–time $R4$ is chosen and the conditions (4.4) applied on the representations of $L(p, r, s)$, we obtain the representations of $L(p, r, s)_{|R4}$, or of $S_{|R4}$ and the elementary systems of $R4$.

Since these representations involve lengthy calculations for each of the 22 groups $L(p, r, s)$, only the outline of the method of representation is given here. Specific calculations for some interesting cases will be given elsewhere.

We may start by writing down all commutators of the Lie algebra of $L(p, r, s)$ given by (4.6), where the $L_{\mu\nu}$ are given by (5.1).

Next we consider the reduction of $L(p, r, s)$ to its maximal compact subgroups $O(n)$ and their decompositions into $O(3)$ factors denoted $O_i(3)$. For each of these $O_i(3)$ factor groups we determine the well-known unitary representations

$$\begin{aligned} &\langle m_i \ M_Z^{(i)} \ m_i \rangle = m_i, \\ &\langle l_i m_i \ M_+^{(i)} \ l_i m_{i+1} \rangle = [(l_i + m_i + 1)(l_i - m_i)]^{1/2}, \\ &\langle l_i m_i \ M_-^{(i)} \ l_i m_{i-1} \rangle = [(l_i - m_i + 1)(l_i - m_i)]^{1/2}, \end{aligned}$$

where

$$\begin{aligned} &l_i = 0, \tfrac{1}{2}, 1, \cdots, \\ &m_i = l_i, l_i - 1, \ldots, -l_i + 1, -l_i, \end{aligned}$$

$i = 1, 2, \ldots, k$ where k is the number of $O(3)$ subgroups in $O(n)$. $M_+^{(i)}$, $M_-^{(i)}$, $M_Z^{(i)}$ are the operators of the Lie algebra of $O_i(3)$ written in the usual Cartan basis.

Once the above matrix elements are determined we can proceed with the determination of the matrix elements of the remaining Lie algebra operators $L_{\mu\nu}$, calculating the matrix elements of the commutators

$$[L_{\mu\nu}, M_+^{(i)}], [L_{\mu\nu}, M_-^{(i)}], [L_{\mu\nu}, M_Z^{(i)}],$$

in terms of n arbitrary matrix functions of l_i. Some recurrence relations between these functions arise from the matrix elements of the commutators between the $L_{\mu\nu}$'s not appearing in $M_+^{(i)}$, $M_-^{(i)}$, and $M_Z^{(i)}$.

The final step consists of the determination of the Casimir operators and their eigenvalues. As the groups

$L(p, r, s)$ are all semisimple the number of Casimir operators is equal to the rank ν of the group.

The resulting structure of elementary systems is labelled by l_i, m_i and the eigenvalues of the Casimir operators. These quantum numbers in general have not the same meaning of the flat space–time case and for different $L(p, r, s)$ there is a different variety of quantum numbers.

8. PARTICLES AND INTERNAL SYMMETRIES

In order to verify if the elementary systems defined by $L(p, r, s)$, or any other proposed group, have anything to do with the physics of elementary particles it becomes necessary, in the first place, to compare the resulting set of quantum numbers with the observational data. We may either choose to calculate all the representations of the 22 groups, a rather laborious task, or choose a certain space–time $R4$ according to its physical reality and find the corresponding class group $L(p, r, s)$. Thus, for example, if we decide that the de Sitter space–time is a physically interesting model the group to be considered is $L(5, 4, 1)$. In this particular example the calculations of the group representations are simpler than in the other cases. The spinor fields constructed on $M(5, 4, 1)$ are automatically isometric covariant and the field equations are also automatically space–time defined. Consequently, the elementary systems constructed with $L(5, 4, 1)$ may be claimed to have physical meaning. In the general situation this simplity does not occur. While the elementary systems constructed with $L(p, r, s)$ are regarded as abstract objects, it may be claimed that the physical space of the elementary particles is the chosen space–time. Thus in order to obtain the elementary particles from the elementary systems we would need to project these on the space–time. Only then could we deal with the problem of interpretation of the quantum numbers.

From the point of view of fitting the theory with some current theories of elementary particles some of the space–times of general relativity may prove to be more interesting than others. Thus, for example, if we want to comply with the $SU(3)$ model, the de Sitter group is not as interesting as $L(8, 6, 2)$ which contain the Lie algebra $O(6) \sim SU(4) \supset SU(3)$. $L(8, 6, 2)$ is the smallest group in an even-dimensional embedding space which contains $O(6)$. Since eight is the largest number of dimensions needed to embed space–times with a surface orthogonal Killing vector field,[16] the study of the representations of $L(8, 6, 2)$ seems to be interesting as regards the search for a $SU(3)$ subgroup.

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Realizations of the central extension of the inhomogeneous symplectic algebra as time dependent invariance algebras of nonrelativistic quantum systems

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We interpret the one-element central extension of the Lie algebra of the group of real inhomogeneous linear canonical transformations of phase space as a time dependent invariance algebra in the Schrödinger picture. By limiting to a two-dimensional space quantum system, we exhibit all the nonconjugate Hamiltonians contained in the symplectic algebra which, in the Heisenberg picture, plays the role of dynamical algebra and contains several known degeneracy and spectrum generating algebras.

INTRODUCTION

In quantum mechanics the Schrödinger picture is usually a description in which the states evolve in the Hilbert space as time goes on while the operators representing the observables stay fixed. The dynamics of a quantum system is then governed by a time evolution operator and the states satisfy the Schrödinger equation $i(d/dt)\psi_t = H\psi_t$, where H is the Hamiltonian operator of the system.

However, it is also possible to introduce explicit time dependent operators $S(t)$ in the Schrödinger picture. Under the action of such operators the transformed states $\hat{\psi}_t = S(t)\psi_t$ satisfy the Schrödinger equation with the new Hamiltonian $\hat{H} = S(t)HS^{-1}(t) + i[\partial S(t)/\partial t]S^{-1}(t)$. Hence, starting with a good time independent Hamiltonian H, in general we obtain an explicit time dependent one $\hat{H}$. (Conversely such transformations can be used to make time independent an explicit time dependent Hamiltonian.) But it is also possible to select the transformations which keep invariant the Hamiltonian, i. e., such that $\hat{H} = H$; then we are led to consider the time dependent operators satisfying

$$[H, S(t)] = i\frac{\partial S(t)}{\partial t}. \tag{1}$$

Numerous interesting properties have been deduced from the study of this relation.[1a] In this paper we shall need the following ones:

—For a given Hamiltonian the set of all the operators satisfying (1) is a Lie algebra $\mathcal{S}_t$ (not necessarily a finite-dimensional one).

—An operator $S(t)$ satisfying (1) corresponds in the Heisenberg picture to a time independent operator S given by

$$S = \exp(iHt)S(t)\exp(-iHt) = S(0). \tag{2}$$

Consequently the operators S generate a Lie algebra $\mathcal{S}_0$ isomorphic to $\mathcal{S}_t$, i. e., from a mathematical point of view, $\mathcal{S}_t$ is the same algebra as $\mathcal{S}_0$ but depending on t as a real parameter.

—Conversely to every algebra of time independent operators which do not commute with a given Hamiltonian (in the Heisenberg picture) there corresponds an explicit time dependent invariance algebra in the Schrödinger picture.

Then the above properties permit us to give an answer to the two following questions:

(a) Consider a Hamiltonian possessing some time dependent invariance algebra $\mathcal{A}$, the generators of which being written as functions of some fundamental observables $\{w\}$. Is it possible then to embody this invariance algebra into a largest one, the added generators being expressed in terms of the same fundamental observables $\{w\}$?

(b) A quantum mechanical system being given characterized partly by some noncommuting observables generating a Lie algebra $\mathcal{A}$, what could be the Hamiltonians of the system if they are going to act on $\mathcal{A}$ by their adjoint representation, namely $ad(H)$. $\mathcal{A} \subseteq \mathcal{A}$, hence admiting $\mathcal{A}$ as a time dependent invariance algebra?

Technically a solution is obtained by considering the derivation algebra $\mathcal{D}(\mathcal{A})$ of what we call the "germ" $\mathcal{A}$ and by constructing the semidirect sum $\mathcal{A} \square \mathcal{D}(\mathcal{A})$, i. e., the split extension of $\mathcal{D}(\mathcal{A})$ by $\mathcal{A}$, this construction has been described in Ref. 1(a). Indeed let $\mathcal{E}(\Omega)$ be the enveloping algebra of the Lie algebra Ω generated by the fundamental observables $\{w\}$. Then problem (a) amounts to extracting from $\mathcal{A} \square \mathcal{D}(\mathcal{A})$ the largest subalgebra Z isomorphic to an algebra in $\mathcal{E}(\Omega)$, and all the one-dimensional subalgebras of Z are solutions of the problem (b).

Now we are interested in applying the above general considerations to a quantum system of N (interacting) particles of different masses $m(\mu)$ $(\mu = 1, 2, \ldots, N)$, without spin. Every particle is characterized by the components of its position vector $\mathbf{q}(\mu)$ and of the canonically conjugate momentum $\mathbf{p}(\mu)$ which generate the Heisenberg algebra $H_3(\mu)$, $[q_j(\mu), p_k(\mu)] = i\delta_{jk}$ $(j, k = 1, 2, 3)$. The q's and p's are the fundamental observables and generate the Lie algebra $\Omega = \oplus_{\mu=1}^{N} H_3(\mu)$.

TABLE I. Miscellaneous realizations of the $\mathcal{Sp}(6,\mathbb{R})$ algebra.

$\mathcal{Sp}(6,\mathbb{R})_A$	$\mathcal{Sp}(6,\mathbb{R})_{CM}$	$\mathcal{Sp}(6,\mathbb{R})_R$
$T^A_{jk}=\sum_{\mu=1}^{N}\frac{p_j(\mu)p_k(\mu)}{m(\mu)}$	$T^{CM}_{jk}=\frac{P_jP_k}{M}$	$T^R_{jk}=\sum_{\mu,\nu}\frac{[m(\mu)+m(\nu)]^2}{2Mm(\mu)m(\nu)}p_j(\mu,\nu)p_k(\mu,\nu)$
$S^A_{jk}=\sum_{\mu=1}^{N}m(\mu)q_j(\mu)q_k(\mu)$	$S^{CM}_{jk}=\frac{K_jK_k}{M}$	$S^R_{jk}=\sum_{\mu,\nu}\frac{m(\mu)m(\nu)}{2M}q_j(\mu,\nu)q_k(\mu,\nu)$
$R^A_{jk}=(1/2)\sum_{\mu=1}^{N}\{p_j(\mu),q_k(\mu)\}_+$	$R^{CM}_{jk}=\frac{\{K_k,P_j\}_+}{2M}$	$R^R_{jk}=\sum_{\mu,\nu}\frac{m(\mu)+m(\nu)}{2M}\{q_k(\mu,\nu),p_j(\mu,\nu)\}_+$

In Ref. 1(a) problem (a) has been treated in the case of a free system of particles possessing either the derived extended Galilei algebra $\tilde{\mathcal{G}}'$ or the center of mass Heisenberg algebra $\mathcal{H}_3$ alone as a germ. We recall that $\tilde{\mathcal{G}}'\approx\mathcal{H}_3\square\mathcal{SO}(3)$, i. e., besides the Heisenberg algebra generated by

$$M=\sum_{\mu=1}^{N}m(\mu),\quad P_j=\sum_{\mu=1}^{N}p_j(\mu),\quad K_j=\sum_{\mu=1}^{N}m(\mu)q_j(\mu) \tag{3}$$

with

$$[K_j,P_k]=i\delta_{jk}M, \tag{4}$$

the derived extended Galilei algebra contains the $\mathcal{SO}(3)$ algebra generated by the total angular momentum J of the system

$$J_j=\sum_{\mu=1}^{N}(q(\mu)\wedge p(\mu))_j. \tag{5}$$

We have then shown that $\tilde{\mathcal{G}}'$ can be enlarged up to the so-called extended Schrödinger algebra $\tilde{\mathcal{Sch}}=\tilde{\mathcal{G}}'\square\mathcal{Sl}(2,\mathbb{R})$, which is known as the Lie algebra of the one-parameter central extension of the group of transformations of the Newtonian space–time which keep invariant the Schrödinger equation.

By removing the rotational invariance, i. e., by restricting the germ to the Heisenberg algebra, one obtains a larger derivation algebra so that the Heisenberg algebra can be embedded into the central extension of the inhomogeneous symplectic algebra denoted $\mathcal{A}_s$ in Ref. 1(a): $\mathcal{A}_s=\mathcal{T}\mathcal{Sp}(6,\mathbb{R})\approx\mathcal{H}_3\square\mathcal{Sp}(6,\mathbb{R})$.

In Ref. 1(b) we have also treated problem (b) starting with the germ $\tilde{\mathcal{G}}'$; in this case the problem is algebraically simple since we have to consider the one-dimensional subalgebras of $\mathcal{Sl}(2,\mathbb{R})$ only. There are three classes of Hamiltonians representative elements, which are respectively the Hamiltonians of an isolated system of interacting particles and of a system subject to external isotropic harmonic or "antiharmonic" fields.

In this paper we want to treat problem (b) by considering the Heisenberg algebra as a germ and consequently looking for Hamiltonians contained in $\mathcal{Sp}(6,\mathbb{R})$. But quickly the Lie algebra technics appear too cumbersome if we deal with a three-dimensional space. Then in the largest part of the paper we restrict ourselves to the study of two-dimensional space systems without an appreciable loss of information.

The paper is organized as follows

—First we present the quantum mechanical part which is divided into six sections

I. Miscellaneous realizations of the $\mathcal{Sp}(6,\mathbb{R})$ algebra.
II. Selected classes of Hamiltonians.
III. The Heisenberg algebra in the Schrödinger picture.
IV. Possible chains of invariance algebras contained in the symplectic algebra.
V. The Symplectic algebra in the Schrödinger picture.
VI. The mutual interaction problem.

—Then the Lie algebra technical part is treated in four Appendices

A. Symmetric decompositions of the $\mathcal{Sp}(2n,\mathbb{R})$ algebra.
B. The isomorphy between $\mathcal{Sp}(4,\mathbb{R})$ and $\mathcal{SO}(3,2)$. Related basis and Casimir operators.
C. Daughters, grandchildren and one-dimensional nonconjugate subalgebras of $\mathcal{Sp}(4,\mathbb{R})\approx\mathcal{SO}(3,2)$.
D. Automorphisms induced by the general element of $\mathcal{Sp}(4,\mathbb{R})$.

I. MISCELLANEOUS REALIZATIONS OF THE $\mathcal{Sp}(6,\mathbb{R})$ ALGEBRA

In Ref. 1(a) we have given a realization of the $\mathcal{Sp}(6,\mathbb{R})$ algebra related to the absolute motion of the system. In this realization, denoted $\mathcal{Sp}(6,\mathbb{R})_A$, all the generators are expressed as sums of individual particle generators (acting in their respective Hilbert spaces), i. e., we are dealing with a reducible representation of $\mathcal{Sp}(6,\mathbb{R})$. Up to the mutual interaction term the possible total Hamiltonians can be written in terms of the $\mathcal{Sp}(6,\mathbb{R})_A$ generators. But there exists another realization of $\mathcal{Sp}(6,\mathbb{R})$ related to the motion of the center of mass, denoted $\mathcal{Sp}(6,\mathbb{R})_{CM}$ the generators of which are expressed in terms of $\mathbf{K},\mathbf{P},M$. The actions of $\mathcal{Sp}(6,\mathbb{R})_A$ and $\mathcal{Sp}(6,\mathbb{R})_{CM}$ on the Heisenberg algebra are identical; then

$$\mathcal{H}_3\square\mathcal{Sp}(6,\mathbb{R})_A\approx\mathcal{H}_3\square\mathcal{Sp}(6,\mathbb{R})_{CM}.$$

It is then easy to see that by substracting from each generator of $\mathcal{Sp}(6,\mathbb{R})_A$ the corresponding generator of $\mathcal{Sp}(6,\mathbb{R})_{CM}$ a third representation of $\mathcal{Sp}(6,\mathbb{R})$ is obtained which does not act on $\mathcal{H}_3$. We denote by $\mathcal{Sp}(6,\mathbb{R})_R$ this realization which is related to the internal or relative motion of the constituent particles of the system. Its generators can be written in terms of the relative canonical coordinates:

$$\mathbf{q}(\mu,\nu)=\mathbf{q}(\mu)-\mathbf{q}(\nu) \quad \text{and} \quad \mathbf{p}(\mu,\nu)=\frac{m(\nu)\mathbf{p}(\mu)-m(\mu)\mathbf{p}(\nu)}{m(\mu)+m(\nu)}. \tag{6}$$

The coexistence of these three realizations of the $\mathcal{Sp}(6,\mathbb{R})$ algebra just reflects the well-known decomposition of the absolute motion of a system into the relative motion and the motion of the center of mass

$$\mathcal{Sp}(6,\mathbb{R})_A=\{X_\alpha^A=X_\alpha^{CM}+X_\alpha^R \backslash X_\alpha^{CM}\in\mathcal{Sp}(6,\mathbb{R})_{CM}, X_\alpha^R\in\mathcal{Sp}(6,\mathbb{R})_R\}$$

Table I gives the expressions of the $\mathcal{Sp}(6,\mathbb{R})$ generators in the three above described realizations, in the particular basis defined in Appendix A [Eq. (A8)].

These three realizations do not commute but are such that for every subalgebra $\mathcal{A}\subseteq\mathcal{Sp}(6,\mathbb{R})$ we have

$$[\mathcal{A}_A,\mathcal{A}_{CM}]\subseteq\mathcal{A}_{CM},\quad [\mathcal{A}_A,\mathcal{A}_R]\subseteq\mathcal{A}_R,\quad [\mathcal{A}_{CM},\mathcal{A}_R]=0. \tag{7}$$

More precisely the actions of $\mathrm{Ad}(\mathcal{A}_A)$ on $\mathcal{A}_{CM}$ and $\mathcal{A}_R$ are "identical," which can be expressed by the relation

$$\mathrm{Ad}(X)\cdot f=f\cdot\mathrm{Ad}(X),$$

f being the canonical linear mapping $f:\mathcal{A}_{CM}\to\mathcal{A}_R$ defined by

$$f(X^{CM})=X^R \quad \text{with } X\in\{T_{jk},R_{jk},S_{jk}\}.$$

Let us remark that the Garthenhaus–Schwartz transformation[2] induced by the unitary (for finite λ) operator $U_\lambda=\exp(-i(\lambda/2)\sum_{j=1}^3 R_{jj}^{CM})$ relates all the generators T_{jk}^A of $\mathcal{Sp}(6,\mathbb{R})_A$ to the corresponding ones in $\mathcal{Sp}(6,\mathbb{R})_{CM}$, but keeps invariant the R_{jk}^A generators and is singular when applied to the S_{jk}^A's; we have

$$U_\lambda T_{jk}^A U_\lambda^{-1}=T_{jk}^A+(e^{-\lambda}-1)T_{jk}^{CM}\underset{\lambda\to+\infty}{\to}T_{jk}^R,$$

$$U_\lambda R_{jk}^A U_\lambda^{-1}=R_{jk}^A,$$

$$U_\lambda S_{jk}^A U_\lambda^{-1}=S_{jk}^A+(e^{\lambda}-1)S_{jk}^{CM}\underset{\lambda\to+\infty}{\to}+\infty.$$

Some other general comments deal with the Casimir operators of invariance algebras. Owing to the semidirect sum structure of every subalgebra $\mathcal{H}_3\square\mathcal{A}_A\subseteq\mathcal{H}_3\square\mathcal{Sp}(6,\mathbb{R})_A$ the invariants are on the one hand the center M of the Heisenberg algebra and on the other hand the Casimir operators of the corresponding $\mathcal{A}_{CM}$ algebra, which by construction of $\mathcal{A}_{CM}$ also belong to the enveloping algebra of $\mathcal{H}_3\square\mathcal{A}_A$.

Obviously the Casimir operators do not depend upon time and are identical in both Heisenberg and Schrödinger pictures, which confirms the unicity of $\mathcal{S}_t$ and $\mathcal{S}_0$, i. e., the role of t as a parameter in the nonrelativistic quantum mechanics. Moreover, the relations (7) are sufficient to assert that the explicit time dependences in the Schrödinger picture are the same for corresponding generators in the three realizations because of the identical action of H belonging to $\mathcal{Sp}(6,\mathbb{R})_A$ on the generators of $\mathcal{Sp}(6,\mathbb{R})_A$, $\mathcal{Sp}(6,\mathbb{R})_{CM}$, and $\mathcal{Sp}(6,\mathbb{R})_R$.

Finally we want to emphasize on the existence of relations in the enveloping algebra of the $\mathcal{Sp}(6,\mathbb{R})$ algebra in some particular cases. For instance, if we consider either the center of mass motion of any system or the absolute motion of one particle or the relative motion of a two-body system there exist numerous relations in the enveloping algebra; in particular, we have

$$\{r_{jk},r_{kj}\}_+=\{s_{jk},t_{jk}\}_+=\tfrac{1}{2}\delta_{jk}+\mathbb{1}.$$

So, in the above three cases the second order Casimir operator given by Eq. (B4) reduces to a number $C_2=\frac{21}{4}$. This is an example of a general property of quantum (and classical) mechanical realizations as demonstrated in Ref. 3: "No semisimple Lie algebra of rank n can be realized with less than n degrees of freedom and if just n degrees of freedom are used then the invariants are multiples of the identity." We recall that $\mathcal{Sp}(6,\mathbb{R})$ is of rank 3.

II. THE SELECTED CLASSES OF HAMILTONIANS

Here we want to study the Hamiltonians as inducing outer automorphisms of the Heisenberg algebra, i. e., acting as outer derivation on it. Then they are compatible with the partial characterization of the system by the canonical quantities of its center of mass.

From this definition all the desired Hamiltonians are contained in the general element of $\mathcal{Sp}(6,\mathbb{R})_A$ which can be written

$$X=\sum_{j,k}\rho^{jk}R_{jk}+\sum_j(\tau^{jj}T_{jj}+\sigma^{jj}S_{jj})+\tfrac{1}{2}\sum_{j\neq k}(\tau^{jk}T_{jk}+\sigma^{jk}S_{jk})$$
$$\text{(with the parameters } \rho^{jk},\tau^{jk},\sigma^{jk}\in\mathbb{R}). \tag{8}$$

But if there are two Hamiltonians H_1 and H_2 conjugated by an inner automorphism of $\mathcal{Sp}(6,\mathbb{R})_A$, i. e., if there exists an element Y belonging to $\mathcal{Sp}(6,\mathbb{R})$ such that $\exp(iY)H_1\exp(-iY)=H_2$, then $\exp(iY)$ transforms the eigenstates of H_1 into the eigenstates of H_2. Therefore, it is interesting to classify the Hamiltonians into conjugacy classes which amounts to looking for the one-dimensional subalgebras of $\mathcal{Sp}(6,\mathbb{R})$ up to a conjugation [or what comes to the same to looking for the orbits of the group $Sp(6,\mathbb{R})$ on the projective space of $\mathcal{Sp}(6,\mathbb{R})$].

Now for mathematical convenience and to be more concise we restrict ourselves to the study of two-dimensional space systems. We therefore consider $\mathcal{H}_2\square\mathcal{Sp}(4,\mathbb{R})$ as the total invariance algebra, and we introduce a "physical" basis of the $\mathcal{Sp}(4,\mathbb{R})$ algebra given by the following ten generators expressed in terms of the generators R_{jk}, S_{jk}, T_{jk} defined in the Appendix A [Eq. (A3)], where we take $n=2$; we set

$J=R_{21}-R_{12}$, the orbital angular momentum operator,

$T = \frac{1}{2}(T_{11} + T_{22})$, the kinetic energy operator of a free system,

$D = -(R_{11} + R_{22})$, the dilation generator,

$C = \frac{1}{2}(S_{11} + S_{22})$, the expansion generator, (9)

$Q = \frac{1}{2}(S_{11} - S_{22})$, $Q_{12} = S_{12}$: the mass-quadrupole momentum operators and their "derivatives":

$\dot{Q} = R_{22} - R_{11}$, $\dot{Q}_{12} = -(R_{12} + R_{21})$; $\ddot{Q} = T_{11} - T_{22}$, $\ddot{Q}_{12} = 2T_{12}$.

The technical aspect of the classification and the results are given in Appendix C where, in every class of nonconjugate one-dimensional subalgebras, we tried to give the more characteristic Hamiltonian as representative element.

There exist three nonconjugate compact subalgebras isomorphic to $\mathcal{S}O(2)$. One of the corresponding classes may be represented by $T + C$ conjugate of the Hamiltonian $T + \omega C$ of a system of particles in an external harmonic field

$$\exp(-i\alpha D)(T + \omega C)\exp(i\alpha D) \sim T + C \quad \text{with } \alpha = \tfrac{1}{2}\log\omega.$$

Another class contains J which governs a system having a magnetic momentum in a static magnetic field.

Finally one finds a one-parameter family of $\mathcal{S}O(2)$ algebras such that to every value of the parameter $\vartheta > 0$ there corresponds a unique $\mathcal{S}O(2)$ algebra up to a conjugation; representative elements can be written $T + C + \vartheta J$. The motion of a charged system of spin zero in the plane perpendicular to a constant uniform magnetic field **B** is governed by the symmetric gauge Hamiltonian

$$H = \frac{1}{2m}\sum_{\mu=1}^{N}\left(\mathbf{p}(\mu) - \frac{e}{2c}\mathbf{B} \quad \mathbf{q}(\mu)\right)^2,$$

which in the "physical" basis becomes

$$H = T + \beta^2 C + \beta J \quad \text{with } \beta = e|B|/2mc. \tag{10}$$

It is seen to be conjugate of $T + C + J$. For one particle one has the Hamiltonian of the Landau electron.

All the other classes of the family $\vartheta \neq 1$ have in common an interesting representative element which is the Hamiltonian of a system of particles in an external anisotropic harmonic field, namely,

$$H = \tfrac{1}{2}(T_{11} + \sigma_{11}S_{11} + T_{22} + \sigma_{22}S_{22}) \quad \text{with } \sigma_{11}, \sigma_{22} > 0,\ \sigma_{11} \neq \sigma_{22}.$$

Indeed, one can check that

$$\exp[i\tfrac{1}{2}\pi(T_{12} + S_{12})]\exp\left[-i\left(\sum_{j=1}^{2}\alpha_j R_{jj}\right)\right] H \exp\left[i\left(\sum_{j=1}^{2}\alpha_j R_{jj}\right)\right]$$
$$\times\exp[-i\tfrac{1}{2}\pi(T_{12} + S_{12})] \sim T + C + \frac{\vartheta_1 - \vartheta_2}{\vartheta_1 + \vartheta_2}J$$
$$\text{with } \alpha_j = \tfrac{1}{2}\log\sigma_{jj} \text{ and } \vartheta_j = \frac{\sigma_{jj}^2 + 1}{\sigma_{jj} + 1}.$$

In all cases starting from a representative element, the whole corresponding class is generated by using the technics described in Appendix D. Then interesting connections between Hamiltonians may appear; for instance, the Hamiltonian of the Landau electron conjugate of $T + C + J$ is also conjugate of $T_{11} + S_{11}$ the one-dimensional harmonic oscillator Hamiltonian as it has been emphasized in Ref. 4.

All the remaining one-dimensional subalgebras are noncompact and among them one identifies:

—the Hamiltonian of a system in an external "anti-harmonic" field: $T - C$, the spectral analysis of which is done in Ref. 5.

—the Hamiltonian of a free or isolated system given by T.

Finally one finds harmonic anisotropic oscillator Hamiltonians containing damping terms, that is, of the form

$$H = T_{11} + T_{22} + \sigma_{11}S_{11} + \sigma_{22}S_{22} + \rho_{11}R_{11} + \rho_{22}R_{22},$$

which correspond to several nonconjugate one-dimensional subalgebras of $\mathcal{S}p(4, \mathbb{R})$ according to the values of the two invariants $\xi_j = 4\sigma_{jj} - \rho_{jj}^2$ $(j = 1, 2)$ of the algebras $\mathcal{S}O(2,1)_j \approx \{T_{jj}, S_{jj}, R_{jj}\}$ [note that $\mathcal{J}_2 = 2(\xi_2 + \xi_1)$]:

$\xi_1 = \xi_2 < 0$, H is conjugate of $T - C$

$\xi_1 < 0,\ \xi_2 < 0,\ \xi_1 \neq \xi_2$, $H \sim T - C + \vartheta(Q - \frac{1}{2}\ddot{Q})$

with $\vartheta = (1 - \exp[2(\xi_1 - \xi_2)])/(1 + \exp[2(\xi_1 - \xi_2)])$,

$\xi_1 < 0,\ \xi_2 = 0$, $H \sim T - \frac{1}{2}[\ddot{Q} + \vartheta(D + \dot{Q})]$

with $\vartheta = \sqrt{-\xi_1}$,

$\xi_1 < 0,\ \xi_2 > 0$:
$\xi_2 > |\xi_1|$, $H \sim T + C + J$,
$\xi_2 = |\xi_1|$, $H \sim T + Q$,
$\xi_2 < |\xi_1|$, $H \sim T - C + Q - \frac{1}{2}\ddot{Q}$,

$\xi_1 = 0,\ \xi_2 > 0$, $H \sim T + C + \frac{1}{2}(\dot{Q} - D)$,

$\xi_1 = \xi_2 = 0$, $H \sim T$,

$\xi_1 > 0,\ \xi_2 > 0$:
$\xi_2 \neq \xi_1$, $H \sim [(\vartheta_1 - \vartheta_2)/(\vartheta_1 + \vartheta_2)]J + T + C$ with $\vartheta_j = (\xi_j^2 + 1)/(\xi_j + 1)$,
$\xi_2 = \xi_1$, $H \sim T + C$.

III. THE HEISENBERG ALGEBRA IN THE SCHRÖDINGER PICTURE

In the Schrödinger picture the Heisenberg algebra takes an explicit time dependence governed by the action on it of the chosen Hamiltonian following the relation

$$H_2^t = \exp(-iHt)H_2^0\exp(iHt). \tag{11}$$

Obviously all the possible representations of H_2^t are obtained if we take for H the general element X of $\mathcal{S}p(4, \mathbb{R})$ given by Eq. (8) with $j, k = 1, 2$. We have then to exhibit the action of X on H_2^0; but it must be noticed that the center of an algebra is kept invariant under the action of any automorphism[1(c)] so that the generator M is not concerned by the transformation (11) and we have only to determine the time dependence of the P and K generators. Following the technics described in Appendix D, the explicit time dependence of **P** and **K** is established by constructing the 4×4 square matrix $e^{\tilde{\Phi}t}$ such that

$$\begin{bmatrix} P_1(t) \\ P_2(t) \\ K_1(t) \\ K_2(t) \end{bmatrix} = e^{\tilde{\Phi}t}\begin{bmatrix} P_1(0) \\ P_2(0) \\ K_1(0) \\ K_2(0) \end{bmatrix}, \tag{12}$$

where $\tilde{\Phi}$ is the coadjoint representation of X in the algebra $H_2 \square X$:

TABLE II. One-dimensional nonconjugate subalgebras of $Sp(4,\mathbb{R})$ and their embedding in miscellaneous (in particular maximal) subalgebras.

$\mathcal{J}_2$	$\mathcal{J}_4$	Representative generators: $SO(3,2)$ basis	Representative generators: "Physical" basis	$W(2,1)$	$SO(2,2)$	$SO(3,1)$	$H_1 \square Sp(2,2)$	$U(2)$	$U(1,1)$	$SO(3)$	$SO(2,1)_I$	$SO(2,1)_{II}$	$SO(2,1)_{III}$
0	0	$M_{12}+M_{20}$	$T-C+Q_{12}+(1/2)Q_{12}$	X	X	X	X				X		
		$M_{00'}+M_{10}$	T	X	X		X		X			X	
		$\sqrt{2}(M_{12}-M_{30})-(M_{00'}+M_{10'}$	$T+(1/2)(\dot{Q}+\dot{Q})+Q_{12}$	X									
		$M_{12}+M_{00'}+M_{10}+M_{20'}$	$T-(1/2)\ddot{Q}\cong T-(1/2)\ddot{Q}_{12}$	X	X		X						X
+	0	M_{12}	J	X	X	X		X	X	X	X		
		$M_{00'}$	$T+C$		X			X	X			X	
		$M_{12}-M_{00'}+M_{30}$	$T+(1/2)J$	X					X				
+	−	$2M_{12}+M_{20'}-M_{10}$	$T-C+(3/2)\ddot{Q}+Q$		X								
		$2M_{00'}+M_{10}-M_{20'}$	$T+C+(1/2)(\dot{Q}-D)$		X								
		$M_{12}+\vartheta M_{00'}$ $(\vartheta>0)$	$T+C+(1/\vartheta)J$		X		$\vartheta=1$	X	X				$\vartheta=1$
−	0	M_{30}	$T+D\cong T-C$	X	X	X	X		X		X	X	
		$M_{12}+M_{20}-M_{30'}$	$T+(1/2)\ddot{Q}-J-C-Q$	X									
−	−	$M_{12}+M_{00'}+(1+\vartheta)M_{10}$ $+(1-\vartheta)M_{20'}$ $(\vartheta>0)$	$T-(1/2)[\ddot{Q}+\vartheta(D+\dot{Q})]$		X		X						
			$T-C+\vartheta(Q-\frac{1}{2}\ddot{Q})$	X	X		X						$\vartheta=1$
0	−	$M_{12}+M_{00'}+M_{20'}-M_{10}$	$T+Q$		X		X						
−	+	$M_{12}-\vartheta M_{30}$ $(\vartheta>1)$	$T-C-(1/\vartheta)J$	X		X			X				
0	+	$M_{12}-M_{30}$	$T-C-J\cong T+D-J$	X		X			X				
+	+	$M_{12}-\vartheta M_{30}$ $(0<\vartheta<1)$	$T+D-(1/\vartheta)J$	X		X			X				

$$\tilde{\Phi}=\begin{bmatrix} \rho_{11} & \rho_{21} & 2\sigma_{11} & \sigma_{12} \\ \rho_{12} & \rho_{22} & \sigma_{12} & 2\sigma_{22} \\ -2\tau_{11} & -\tau_{12} & -\rho_{11} & -\rho_{12} \\ -\tau_{12} & -2\tau_{22} & -\rho_{21} & -\rho_{22} \end{bmatrix}. \tag{13}$$

It is possible to show that $e^{\tilde{\Phi}t}$ depends on the invariants $\mathcal{J}_2$ and $\mathcal{J}_4$ defined in Appendix C which partly characterize X as a subalgebra of $Sp(4,\mathbb{R})$ through the characteristic roots λ' of $\tilde{\Phi}$:

$$\lambda_1'=-\lambda_2'=\tfrac{1}{2}(-\mathcal{J}_2+\sqrt{-\mathcal{J}_4})^{1/2},\quad \lambda_3'=-\lambda_4'=\tfrac{1}{2}(-\mathcal{J}_2-\sqrt{-\mathcal{J}_4})^{1/2}, \tag{14}$$

we have

$$e^{\tilde{\Phi}t}=\frac{1}{\lambda_1'^2-\lambda_3'^2}\left[\tilde{\Phi}^3\left(\frac{\sinh\lambda_1't}{\lambda_1'}-\frac{\sinh\lambda_3't}{\lambda_3'}\right)+\tilde{\Phi}^2(\cosh\lambda_1't-\cosh\lambda_3't)\right.$$
$$\left.+\tilde{\Phi}\left(\lambda_1'^2\frac{\sinh\lambda_3't}{\lambda_3'}-\lambda_3'^2\frac{\sinh\lambda_1't}{\lambda_1'}\right)+\mathbb{1}(\lambda_1'^2\cosh\lambda_3't-\lambda_3'^2\cosh\lambda_1't)\right]. \tag{15}$$

In the particular case $\mathcal{J}_4=0$ the formula (15) is no longer available and we must use the following one:

$$e^{\tilde{\Phi}t}\big|_{\mathcal{J}_4=0}=(1/2\lambda'^2)[\tilde{\Phi}^3(\cosh\lambda't-\sinh\lambda't/\lambda')+\tilde{\Phi}^2\lambda'\sinh\lambda't$$
$$+\tilde{\Phi}(3\lambda'\sinh\lambda't-\lambda'^2\cosh\lambda't)+\mathbb{1}(2\lambda'^2\cosh\lambda't$$
$$-\lambda'^3\sinh\lambda't)], \tag{16}$$

where $\lambda'=\frac{1}{2}\sqrt{-\mathcal{J}_2}$.

The Hamiltonians $T+C$ and $T-C$ belong to the above case, and Eq. (16) leads to the explicit time dependence which has been given in Ref. 1(b) [Eq. (11a), where α stands for λ']. Again another relation corresponds to $\mathcal{J}_2=\mathcal{J}_4=0$:

$$e^{\tilde{\Phi}t}\big|_{\mathcal{J}_2=\mathcal{J}_4=0}=\mathbb{1}+\tilde{\Phi}t+(\tilde{\Phi}^2/2!)t^2+(\tilde{\Phi}^3/3!)t^3; \tag{17}$$

and for the Hamiltonian T of a free system Eq. (17) furnishes the well-known Galilean form of K and P, i.e.,

$$\mathbf{P}(t)=\mathbf{P}(0),\quad \mathbf{K}(t)=\mathbf{K}(0)-t\mathbf{P}(0).$$

IV. POSSIBLE CHAINS OF INVARIANCE ALGEBRAS CONTAINED IN THE SYMPLECTIC ALGEBRA

The one-dimensional nonconjugate subalgebras of $Sp(4,\mathbb{R})$ being taken as Hamiltonians, it is interesting to look for the various chains of subalgebras included between the H's and the whole $Sp(4,\mathbb{R})$ algebra, all these subalgebras being able to play the role of explicit time dependent invariance algebras. However, we do not give the full lattice of the nonconjugate subalgebras of $Sp(4,\mathbb{R})$ because of the great number of the two- and three-dimensional subalgebras it contains.

In Fig. 3 in Appendix C we give the top of the lattice, i.e., the daughters and grandchildren of $Sp(4,\mathbb{R})$. Moreover, we have completed the chains which contain a three dimensional semisimple Lie algebra, i.e., either $SO(3)$ or one of the three nonconjugate $SO(2,1)$ algebras labelled I, II, and III. Let us note that some particular realizations of these semisimple Lie algebras are well known and are used in physical models; for instance:

— $SO(3)\approx SU(2)$ corresponds to the restriction to a two-dimensional space of the algebra used in the so-called Elliott $SU(3)$ nuclear model.[6] It is also the degeneracy algebra of the harmonic oscillator Hamiltonian $\approx SO(2)$. Let us note that $U_2=SO(2)\oplus SU(2)$ is maximal compact in $Sp(4,\mathbb{R})$.

—$\mathcal{S}O(2,1)_{\rm I} \approx \mathcal{S}l(2,\mathbb{R})$ generated by $\{J, \dot{Q}, \dot{Q}_{12}\}$ is the reduction in a two-dimensional space of the $\mathcal{S}l(3,\mathbb{R})$ algebra introduced in Ref. 7 to study the E_2 transitions in nuclear rotational bands.

—$\mathcal{S}O(2,1)_{\rm II} \approx \mathcal{S}\mathcal{U}(1,1)$, a basis of which is furnished by $\{T, C, D\}$, is the spectrum generating algebra of the harmonic oscillator Hamiltonian $T+C$.

—$\mathcal{S}O(2,1)_{\rm III} \approx \mathcal{S}p(2,\mathbb{R})$ is the spectrum generating algebra of the free Landau electron. A basis for $\mathcal{S}p(2,\mathbb{R})$ is obtained by adding to H_L the two following generators:

$$A = \beta^2 Q_{12} + \beta\dot{Q} - \tfrac{1}{2}\ddot{Q}_{12}, \quad B = \beta^2 Q - \beta\dot{Q}_{12} - \tfrac{1}{2}\ddot{Q}.$$

Moreover, in Table II the embedding of the one-dimensional nonconjugate subalgebras (i. e., of the miscellaneous Hamiltonians) into the maximal subalgebras and into the four above-mentioned semisimple subalgebras is given. For instance we remark that:

—The Galilean Hamiltonian T belongs to $\mathcal{S}O(2,1) \oplus \mathcal{S}O(2) \subset_{\max} \mathcal{S}p(4,\mathbb{R})$, which by acting on the Heisenberg algebra corresponds to the chain

$$\tilde{\mathcal{G}}_2 \subset \widetilde{\mathcal{S}\mathrm{ch}_2} \subset \widetilde{\mathcal{G}\mathcal{S}p}(4,\mathbb{R}).$$

—The Landau electron Hamiltonian H_L is contained in

$$\mathcal{S}p(2,\mathbb{R}) \subset \mathcal{S}p(2,\mathbb{R}) \oplus \mathcal{S}p(2,\mathbb{R}) \underset{\max}{\subset} \mathcal{S}p(4,\mathbb{R})$$

which corresponds to the chain

$$H_2 \square \mathcal{S}p(2,\mathbb{R}) \subset H_2 \square \mathcal{S}O(2,2) \subset \widetilde{\mathcal{G}\mathcal{S}p}(4,\mathbb{R}).$$

Let us now give some properties of the Casimir operators. In the same conditions as in Sec. I, i. e., in the case of a system of one particle or in the relative motion of a two-body system or in the center of mass motion of any system, the Casimir operators C_2 and C_4 of $\mathcal{S}p(4,\mathbb{R})$ defined in Appendix B [Eq. (B8)] reduce to the following numbers:

$$C_2 = -\tfrac{5}{4}, \quad C_4 = 0.$$

For the $\mathcal{S}O(3,1)$ and $\mathcal{S}O(2,2)$ subalgebras which are also of rank two the Casimir operators C_2 and $\hat{C}_2$ defined in Appendix B [Eq. (B5)] become

$$C_2 = -\tfrac{3}{4}, \quad \hat{C}_2 = 0.$$

This is due to the fact that in the three cases the corresponding realizations are irreducible unitary representations of the discrete principal series of the algebras.

Obviously the situation is more complex in what concerns the three-dimensional semisimple subalgebras of rank one to which the theorem of Ref. 3 does not apply. The Casimir of $\mathcal{S}O(2,1)_{\rm III}$ always reduce to a number

$$C_2 = H_L^2 - \tfrac{1}{4}(A^2 + B^2) = -\tfrac{3}{4},$$

but, in the three other cases the Casimir operators express in terms of an extra generator, we have:

—For $\mathcal{S}O(2,1)_{\rm I}$: $C_2 = J^2 - \dot{Q}^2 - \dot{Q}_{12}^2 = -(D^2+1)$, where D generates the $\mathbb{R}$ algebra in $\mathcal{S}O(2,1)_{\rm I} \oplus \mathbb{R}^{d_1}$.

—For $\mathcal{S}O(2,1)_{\rm II}$: $C_2 = \frac{1}{2}\{T, C\}_+ - \frac{1}{4}D^2 = J^2 - \frac{1}{4}$, where J is the generator of the $\mathcal{S}O(2)$ algebra in $\mathcal{S}O(2,1)_{\rm II} \oplus \mathcal{S}O(2)_J$.

—For $\mathcal{S}O(3)$: $C_2 = J^2 + (2Q + \ddot{Q})^2 + (2Q_{12} + \ddot{Q}_{12})^2 = (T+C)^2 + 1$, where $T+C$ generates $\mathcal{S}O(2)$ in $\mathcal{S}O(3) \oplus \mathcal{S}O(2) \approx \mathcal{U}(2)$.

Hence in these three cases, the Casimir operators eigenvalues depend on the eigenvalues of another simultaneously diagonalizable operator and consequently some constraints are imposed on the available representation of the semisimple algebras. This fact is well known in the case of the three-dimensional harmonic oscillator problem for which the family of "triangular" $\mathcal{S}\mathcal{U}(3)$ representation is realized only.

V. THE SYMPLECTIC ALGEBRA IN THE SCHRÖDINGER PICTURE

As in the case of the Heisenberg algebra the explicit time dependence of the symplectic algebra depends on the chosen Hamiltonian. We can still treat the general case by taking for Hamiltonian the general element X of $\mathcal{S}p(4,\mathbb{R})$, and we can use the results established in Appendix D which are basis independent; in particular, the column vector W can be as well constructed in the physical basis. Therefore, the explicit time dependence of the generators of the $\mathcal{S}p(4,\mathbb{R})$ algebra in the Schrödinger picture is given by

$$W(t) = \exp(-iXt)W(0) \exp(iXt) = \exp(\tilde{\Delta}t)W(0), \tag{18}$$

where $\exp(\tilde{\Delta}t)$ is deduced from $\exp(\tilde{\Delta})$ with $\tilde{\Delta}t$ taking the place of $\tilde{\Delta}$ in Eqs. (D9), (D11), (D17), (D18), (D19) of Appendix D; note that by doing this all the characteristic roots λ are also multiplied by t. For instance, the relation (D9) becomes

$$\begin{aligned} e^{\tilde{\Delta}t} = (\mathbb{1} + \tilde{\Delta}t) & \prod_{j=1,3,5,7} \frac{\tilde{\Delta}^2 - \lambda_j^2 \mathbb{1}}{\lambda_j^2} \\ & + \sum_{j=1,3,5,7} \left[\frac{\tilde{\Delta}^2}{\lambda_j^3} (\tilde{\Delta} \sinh\lambda_j t + \lambda_j \mathbb{1} \cosh\lambda_j t) \right. \\ & \left. \times \prod_{k \neq j} \left(\frac{\tilde{\Delta}^2 - \lambda_k^2 \mathbb{1}}{\lambda_j^2 - \lambda_k^2} \right) \right]. \end{aligned} \tag{19}$$

More explicitly we can treat as an example the explicit time dependence generated by the rotational symmetric Hamiltonian $H = T + \beta C + \gamma D$ ($\beta, \gamma \in \mathbb{R}$) which corresponds to $\mathcal{G}_2 = 4(\beta - \gamma^2)$ and $\mathcal{G}_4 = 0$; the analog of Eq. (D11) for $\tilde{\Delta}t$ must be used and leads to the following explicit time dependence of the "physical" generators (where $\lambda = \sqrt{-\mathcal{G}_2} \neq 0$):

$$C(t) = \left(\cosh\lambda t + 2\frac{\gamma}{\lambda}\sinh\lambda t\right) C_0 + \frac{1}{\lambda}\sinh\lambda t D_0 + \frac{2}{\lambda^2}(\cosh\lambda t - 1)H,$$

$$\begin{aligned} D(t) = & \left(\cosh\lambda t - 2\frac{\gamma}{\lambda}\sinh\lambda t\right) D_0 - \frac{4\beta}{\lambda}\sinh\lambda t C_0 \\ & + 2\left(\frac{1}{\lambda}\sinh\lambda t - \frac{2\gamma}{\lambda^2}(\cosh\lambda t - 1)\right) H, \end{aligned}$$

$$\begin{aligned} Q(t) = & \left[\left(\frac{2\beta}{\lambda^2} + 1\right)\cosh\lambda t + \frac{2\gamma}{\lambda}\sinh\lambda t - \frac{2\beta}{\lambda^2}\right] Q_0 \\ & + \left(\frac{2\gamma}{\lambda^2}(\cosh\lambda t - 1) + \frac{1}{\lambda}\sinh\lambda t\right)\dot{Q}_0 + \frac{1}{\lambda}(\cosh\lambda t - 1)\ddot{Q}_0, \end{aligned}$$

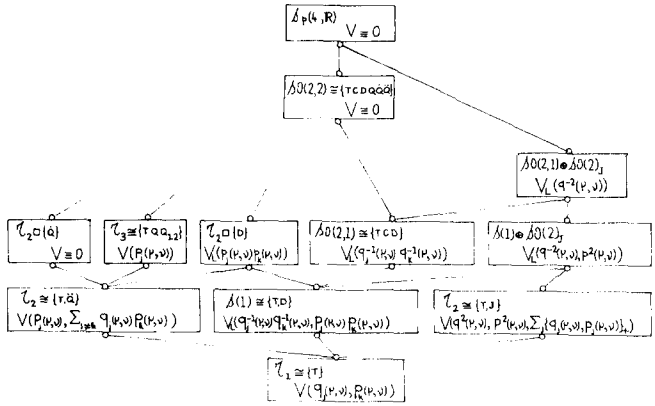

FIG. 1. Mutual interactions compatible with the Hamiltonian T of an isolated system and the chosen invariance algebra among the possible one's between $\{T\}$ and $\mathcal{S}p(4,\mathbb{R})$.

$$\ddot{Q}(t) = \left[\left(1-4\frac{\gamma^2}{\lambda^2}\right)\cosh\lambda t + 4\frac{\gamma^2}{\lambda^2}\right]\dot{Q}_0 + \left(\frac{2\gamma}{\lambda^2}(1-\cosh\lambda t) + \frac{1}{\lambda}\sinh\lambda t\right)\ddot{Q}_0 - 2\frac{\beta}{\lambda}\left(2\frac{\gamma}{\lambda}(\cosh\lambda t - 1) + \sinh\lambda t\right)Q_0, \tag{20}$$

$$\dddot{Q}(t) = \left[\left(\frac{2\beta}{\lambda^2}+1\right)\cosh\lambda t - 2\frac{\gamma}{\lambda}\sinh\lambda t - 2\frac{\beta}{\lambda^2}\right]\ddot{Q}_0 + 2\frac{\beta}{\lambda}\left(2\frac{\beta}{\lambda}(\cosh\lambda t - 1) - \sinh\lambda t\right)Q_0 + 4\frac{\beta^2}{\lambda^2}(\cosh\lambda t - 1)Q_0.$$

We do not write $Q_{12}(t)$, $\dot{Q}_{12}(t)$, and $\ddot{Q}_{12}(t)$ since their expressions are deduced from the expressions $Q(t)$, $\dot{Q}(t)$, and $\ddot{Q}(t)$, respectively, in which one has to read $Q_{12}(0)$, $\dot{Q}_{12}(0)$, and $\ddot{Q}_{12}(0)$ in place of $Q(0)$, $\dot{Q}(0)$, and $\ddot{Q}(0)$, respectively. This is due to the fact that $\{Q, \dot{Q}, \ddot{Q}\}$ and $\{Q_{12}, \dot{Q}_{12}, \ddot{Q}_{12}\}$ are two isomorphic invariant subspaces under the action of H.

The angular momentum J does not take any explicit time dependence owing to the rotational invariance of the Hamiltonian $[H, J] = 0$. $\{H, C, D\}$ being also an invariant subspace under the action of H, the expressions of $C(t)$ and $D(t)$ are identical to the corresponding ones given in Ref. 1(b) [Eq. (15a)] (in which 2α stands for λ), where the $\mathcal{S}O(2,1)_{II}$ algebra generated by $\{H, C, D\}$ has been considered only.

When the parameters β and γ are such that $\mathcal{J}_2 = 0$ the time dependence of the generators becomes a polynomial one given by the analogous of Eq. (D18). But $\tilde{\Delta}^3 = 0$, so that the generators are second order polynomials in t:

$$\begin{aligned} C(t) &= (1+2\gamma t)C_0 + tD_0 + t^2 H, \\ D(t) &= (1-2\gamma t)D_0 - 4\gamma^2 t C_0 + 2t(1-\gamma t)H, \\ Q(t) &= (1+\gamma t)^2 Q_0 + t(1+\gamma t)\dot{Q}_0 + \tfrac{1}{2}t^2\ddot{Q}_0, \\ \dot{Q}(t) &= (1-2\gamma^2 t^2)\dot{Q}_0 + t(1-\gamma t)\ddot{Q}_0 - 2\gamma^2 t(1+\gamma t)Q_0, \\ \ddot{Q}(t) &= (1-\gamma t)^2\ddot{Q}_0 + 2\gamma^4 t^2 Q_0 - 2\gamma^2 t(1-\gamma t)\dot{Q}_0. \end{aligned} \tag{21}$$

Now if we take $\gamma = 0$ in the above expressions we obtain the time dependence generated by the free Hamiltonian $H \equiv T$, already given in Ref. 1(a) [Eqs. (19) and (21)] in the three space-dimensional case.

VI. THE MUTUAL INTERACTION PROBLEM

Up to now we have shown that the general element X of $\mathcal{S}p(4,\mathbb{R})$ can be associated with Hamiltonians describing a collection of particles submitted to miscellaneous external fields except in the case where X reduces to T. But it is also possible to introduce in X some mutual interaction V. At the one-dimensional $\mathcal{S}p(4,\mathbb{R})$ subalgebra level we have just to ensure that V does not modify the action on the Heisenberg algebra of the Hamiltonian. So V must not act on $\mathcal{H}_2$, i.e., $[V, \mathcal{H}_2] = 0$. This condition is satisfied as long as V depends on the relative coordinates defined in Eq. (6) only.

The situation becomes more complicated when the Hamiltonian is included in an $\mathcal{S}p(4,\mathbb{R})$ subalgebra $\mathcal{A}$ because of the commutation relation it must verify. Hence V is submitted to some constraints which differ according to the "kinds" of commutation relations which appear in $\mathcal{A}$. By degrees we find:

—The commutation relations of the form $[H, X_\alpha] = C_\alpha^\beta X_\beta$ (in a basis where H is one generator: $H \cup \{X_\alpha\} = \mathcal{A} \subset \mathcal{S}p(4,\mathbb{R})$) imply $[V, X_\alpha] = 0$ only.

—The commutation relations of the form $[H, X_\alpha] = cH + C_\alpha^\beta X_\beta$ to be conserved require the X acts as a dilatation on V, i.e., $[X_\alpha, V] = cV$.

—The more stringent situation comes from the rising of H on the right-hand side of commutation relations which do not involve H $[X_\alpha, X_\beta] = cH + C_{\alpha\beta}{}^\gamma X_\gamma$. We are then in a Poincaré-like situation: Either several generators must contain interaction terms or there is no possible interaction, i.e., $V \equiv 0$. But our approach does not permit the coexistence of several Hamiltonians. So the Dirac solution cannot be retained[8] and we are left with $V \equiv 0$.

Therefore, given one Hamiltonian, it belongs to several $\mathcal{S}p(4,\mathbb{R})$ subalgebras, and the choice of one of them as invariance algebra depends on the mutual interaction terms we want to keep in H.

It is worth noticing that in all cases the $\mathcal{S}p(4,\mathbb{R})$ algebra does not suffer any mutual interaction.

To illustrate the above discussion, the constraints imposed on the possible mutual interactions associated with a free system of particles by enlarging the invariance algebra from $\mathcal{H}_2$ up to $\widetilde{\mathcal{J}}\mathcal{S}p(4,\mathbb{R})$ are exhibited in Fig. 1. The chains of algebras are stopped when V disappears or when it cannot contain any dependence on the $\mathbf{q}(\mu,\nu)$. Moreover, only two-body terms are given but three- and four-body terms are possible as well.[9] We denote by $V(x, y\cdots)$ the fact that V only depends on $x, y\cdots$ and $V_L(x, y\cdots)$ denotes any linear function of $x, y\cdots$ with coefficients which commute with D, i.e., which depends on terms of the type $q_j(\mu,\nu)p_k(\mu,\nu)$ only.

The essential feature is the fast melting of V as the invariance algebra increases.

CONCLUSION

In this paper we began to study the properties of the one-element central extension of the inhomogeneous symplectic algebra from the quantum mechanical "point of view" of explicit time dependent invariance algebra

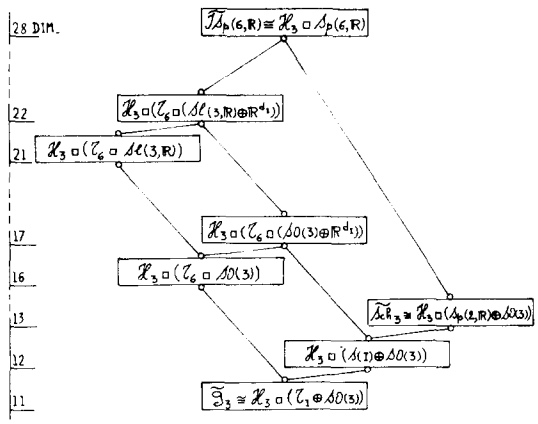

FIG. 2. Chains of nonconjugate $\widetilde{\mathcal{G}Sp}(6, \mathbb{R})$ subalgebras containing the extended Galilean algebra.

in the Schrödinger picture. This Lie algebra approach corresponds to the existence of an unique unitary ray representation of the group of real inhomogeneous linear canonical transformations of phase space the role of which in elementary (Galilean) quantum mechanics is comparable to that of the Poincaré group in relativistic physics."[10] The same algebra was also considered in Ref. 11 as a "limitable" dynamical algebra, i. e., as an algebra which contains the geometrical subalgebra $\tilde{\mathcal{G}}'$ and possesses an integrable representation describing the interacting system. The interaction part in the Hamiltonian is such that it can be switched off by a limiting procedure, giving rise to a representation of the dynamical algebra of a free particle. In Ref. 11 a representation was constructed using Nelson extensions which describes spinless one-particle systems with second-order polynomials in q, p as Hamiltonians.

The algebra $\widetilde{\mathcal{G}Sp}(6, \mathbb{R})$ is the central extension of the derivation algebra of the Heisenberg algebra up to a nonphysical dilation but, by following a more general procedure described in Ref. 1(a), it was introduced as the maximal subalgebra of the split extension $H \square D(H)$ mapped via an injective homomorphism into the enveloping algebra $\mathcal{E}(\Omega)$ of the fundamental observables $\{\mathbf{q}(\mu), \mathbf{p}(\mu), m(\mu)\}$ characterizing the individual constituents of the quantum mechanical system. In fact we have shown in Sec. I that there are two distinct injective homomorphisms: One of them leads to the $Sp(6, \mathbb{R})_A$ realization related to the absolute motion of the system; the other one corresponds to the center of mass motion and can be considered as an injective homomorphism into $\mathcal{E}(\mathbf{K}, \mathbf{P}, M) \subset \mathcal{E}(\Omega)$.

In Secs. II and IV we tried to exhibit the largest number of known Hamiltonians associated with one-dimensional $Sp(4, \mathbb{R})$ subalgebras, and the related known degeneracy (symmetry) algebras and spectrum generating algebras contained in $Sp(4, \mathbb{R})$. In particular we give a complete classification of the harmonic oscillator Hamiltonians with linear damping terms.

Working with two-dimensional space systems greatly lightens the algebraic part without a too big loss of information; however, it seems interesting to give (Fig. 2) the chains of nonconjugate subalgebras of $\widetilde{\mathcal{G}Sp}(6, \mathbb{R})$ which contain the Galilean algebra $\mathcal{G}_3$.

Section VI deals with the problem of introducing a mutual interaction term in the Hamiltonians. It is worth noticing that a given invariance algebra does not characterize the possible interaction term in general, but both chosen Hamiltonian and invariance algebra strongly limit the dependence on the relative coordinates of the individual constituents of the system which can be introduced in the mutual interaction term. Moreover, no Hamiltonians containing relative interactions can possess the whole $\widetilde{\mathcal{G}Sp}(6, \mathbb{R})$ as invariance algebra.

Finally in Secs. III and V we give the explicit time dependence of $\widetilde{\mathcal{G}Sp}(4, \mathbb{R})$ in the Schrödinger picture justifying the introduction of this algebra as a time dependent invariance algebra. We emphasize this concept of explicit-time dependent algebra in the Schrödinger picture which is intimately related to the various notions of dynamical algebras including symmetry or degeneracy algebras and spectrum generating algebras[12] in the Heisenberg picture, and allowed us to get the right nonrelativistic interpretation of the Wigner—Inonü contraction—extension procedure of the de Sitter algebras.[13]

ACKNOWLEDGMENTS

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APPENDIX A: SYMMETRIC DECOMPOSITIONS OF THE $Sp(2n, \mathbb{R})$ ALGEBRA

It is well known that the $Sp(2n, \mathbb{R})$ algebra admits the direct vector space decomposition

$$Sp(2n, \mathbb{R}) = \mathfrak{A}_r \oplus \mathcal{G}l(n, \mathbb{R}) \oplus \mathfrak{A}_r^{\star}. \tag{A1}$$

where $\mathfrak{A}_r$ and $\mathfrak{A}_r^{\star}$ are two r-dimensional $[r = \frac{1}{2}n(n+1)]$ Abelian algebras related by an involutive inner automorphism O of $Sp(2n, \mathbb{R})$ such that

$$O \cdot \mathfrak{A}_r = \mathfrak{A}_r^{\star} \quad \text{and} \quad O \cdot \mathfrak{A}_r^{\star} = \mathfrak{A}_r.$$

Moreover,

$$[\mathfrak{A}_r, \mathfrak{A}_r^{\star}] = \mathcal{G}l(n, \mathbb{R}) \quad \text{and} \quad [\mathcal{G}l(n, \mathbb{R}), \mathfrak{A}_r] \subset \mathfrak{A}_r.$$

Then the above relations imply

$$O \cdot \mathcal{G}l(n, \mathbb{R}) \subset \mathcal{G}l(n, \mathbb{R}) \quad \text{and} \quad [\mathcal{G}l(n, \mathbb{R}), \mathfrak{A}_r^{\star}] \subset \mathfrak{A}_r^{\star}.$$

Therefore the decomposition given in (A1) makes two conjugate semidirect sums appear,

$$\mathfrak{A}_r \square \mathcal{G}l(n, \mathbb{R}) \quad \text{and} \quad \mathfrak{A}_r^{\star} \square \mathcal{G}l(n, \mathbb{R}),$$

and the above properties can be summarized in the explicit notation

$$Sp(2n, \mathbb{R}) \approx \begin{pmatrix} \mathfrak{A}_r \\ \mathfrak{A}_r^{\star} \end{pmatrix} \boxdot \mathcal{G}l(n, \mathbb{R}). \tag{A2}$$

A basis reflecting the decomposition is given by the following set of $2r + n^2 = n(2n+1)$ generators $\{T_{jk} = T_{kj}, S_{jk} = S_{kj}, R_{jk}\}$ satisfying the commutation relations

$$\begin{aligned} &[R_{jk}, R_{lm}] = i(\delta_{kl} R_{jm} - \delta_{jm} R_{lk}), && \text{the } \mathcal{G}l(n, \mathbb{R}) \text{ algebra,} \\ &[S_{jk}, S_{lm}] = [T_{jk}, T_{lm}] = 0, && \text{the } \mathfrak{A}_r \text{ and } \mathfrak{A}_r^{\star} \text{ algebras,} \\ &[R_{jk}, T_{lm}] = i(\delta_{kl} T_{jm} + \delta_{km} T_{jl}), && \end{aligned} \tag{A3}$$

$$[R_{jk}, S_{lm}] = -i(\delta_{jl}S_{km} + \delta_{jm}S_{kl}),$$

$$[S_{jk}, T_{lm}] = i(\delta_{jl}R_{mk} + \delta_{jm}R_{lk} + \delta_{kl}R_{mj} + \delta_{km}R_{lj}),$$

where $j, k, l, m = 1, 2, \ldots, n$.

Let us also note that $\mathcal{G}l(n, \mathbb{R}) \approx \mathcal{S}l(n, \mathbb{R}) \oplus \mathbb{R}^{d_1}$, where the dilatations $\mathbb{R}^{d_1}$ are generated by $\sum_{j=1}^{n} R_{jj}$ and that the involutive inner automorphism $\mathcal{O}$ can be associated with one of the group elements $\exp[i\vartheta \sum_{j=1}^{n} (T_{jj} + S_{jj})]$, ϑ taking the values $\pm\pi/4$, $\pm 3\pi/4$. Moreover, the set $\{\sum_{j=1}^{n} R_{jj}, \sum_{j=1}^{n} S_{jj}, \sum_{j=1}^{n} T_{jj}\}$ generates an $\mathcal{S}p(2, \mathbb{R})$ algebra.

But there exists another symmetric vector space decomposition of the $\mathcal{S}p(2n, \mathbb{R})$ algebra given by

$$\mathcal{S}p(2n, \mathbb{R}) = \mathcal{H}_{n-1} \oplus \mathcal{C}\mathcal{S}p(2(n-1), \mathbb{R}) \oplus \mathcal{H}^{\star}_{n-1}, \tag{A4}$$

where $\mathcal{H}_{n-1}$ denotes the $(2n-1)$-dimensional solvable Heisenberg algebra

$$[\mathfrak{A}^{(q)}_{n-1}, \mathfrak{A}^{(p)}_{n-1}] = \mathbb{R}^{(m)}, \quad \text{the center of } \mathcal{H}_{n-1}, \tag{A5}$$

and

$$\mathcal{C}\mathcal{S}p(2(n-1), \mathbb{R}) \approx \mathcal{S}p(2(n-1), \mathbb{R}) \oplus \mathbb{R}^{d_2} \tag{A6}$$

(the upperscripts q, p, m and d_1, d_2 are just introduced to differentiate the diverse $\mathfrak{A}$ and $\mathbb{R}$ algebras).

Therefore, (A4) appears as a canonical decomposition of the $\mathcal{S}p(2n, \mathbb{R})$ algebra. Again an involutive inner automorphism $\mathcal{O}'$ of $\mathcal{S}p(2n, \mathbb{R})$ is such that $\mathcal{O}' \cdot \mathcal{H}_{n-1} = \mathcal{H}^{\star}_{n-1}$, and we have the following properties:

$$[\mathcal{S}p(2(n-1), \mathbb{R}), \mathcal{H}_{n-1}] \subset \mathcal{H}_{n-1}, \quad [\mathcal{S}p(2(n-1), \mathbb{R}), \mathcal{H}^{\star}_{n-1}] \subset \mathcal{H}^{\star}_{n-1},$$

$$[\mathcal{H}_{n-1}/\mathbb{R}^{(m)}, \mathbb{R}^{(m)\star}] = \mathcal{H}^{\star}_{n-1}/\mathbb{R}^{(m)\star}, [\mathcal{H}^{\star}_{n-1}/\mathbb{R}^{(m)\star}, \mathbb{R}^{(m)}] = \mathcal{H}_{n-1}/\mathbb{R}^{(m)},$$

$$[\mathcal{H}_{n-1}/\mathbb{R}^{(m)}, \mathcal{H}^{\star}_{n-1}/\mathbb{R}^{(m)\star}] = \mathcal{S}p(2(n-1), \mathbb{R});$$

moreover, $\{\mathbb{R}^{(m)}, \mathbb{R}^{(m)\star}, \mathbb{R}^{d_2}\}$ generate an $\mathcal{S}p(2, \mathbb{R})$ algebra.

Likewise there are two conjugate semidirect sums

$$\mathcal{H}_{n-1} \square\, \mathcal{C}\mathcal{S}p(2(n-1), \mathbb{R}) \quad \text{and} \quad \mathcal{H}^{\star}_{n-1} \square\, \mathcal{C}\mathcal{S}p(2(n-1), \mathbb{R}),$$

and so we can write the second symmetric decomposition under the form

$$\mathcal{S}p(2n, \mathbb{R}) \approx \begin{bmatrix} \mathcal{H}_{n-1} \\ \mathcal{H}^{\star}_{n-1} \end{bmatrix} \boxdot\, \mathcal{C}\mathcal{S}p(2(n-1), \mathbb{R}). \tag{A7}$$

From the relations (A3) it is easy to deduce that $\mathcal{S}p(2(n-1), \mathbb{R})$ is generated, for instance, by $\{T_{jk}, R_{jk}, S_{jk}\}$ with $j, k = 1, 2, \ldots, n-1$, the dilatation generator of $\mathbb{R}^{d_2}$ being R_{nn}. The Heisenberg algebra $\mathcal{H}_{n-1}$ (respectively $\mathcal{H}^{\star}_{n-1}$) being given by

$$\mathfrak{A}^{(q)}_{n-1} \approx \{R_{nj}\}(\{S_{jn}\}), \quad \mathfrak{A}^{(p)}_{n-1} \approx \{T_{nj}\}(\{R_{jn}\}),$$

$$\mathbb{R}^{(m)} = T_{nn}, \quad \mathbb{R}^{(m)\star} = S_{nn}$$

Then the involutive automorphism $\mathcal{O}'$ corresponds to the group elements $\exp[i\vartheta(T_{nn} + S_{nn})]$ with $\vartheta = \pm\pi/4$, $\pm 3\pi/4$.

It should be mentioned that many structural properties can be deduced from the existence of both above symmetric decompositions; in particular, the following nonexceptional maximal subalgebras of $\mathcal{S}p(2n, \mathbb{R})$ can be extracted:

$$\mathfrak{A}_r \square\, \mathcal{G}l(n, \mathbb{R}), \quad \mathcal{H}_{n-1} \square\, \mathcal{C}\mathcal{S}p(2(n-1), \mathbb{R}),$$

$$\mathcal{S}p(2k, \mathbb{R}) \square\, \mathcal{S}p(2(n-k), \mathbb{R}), \quad \mathcal{S}p(2, \mathbb{R}) \square\, \mathcal{S}O(n), \tag{A8}$$

where $\mathcal{S}O(n) \subset \mathcal{S}l(n, \mathbb{R})$. Curiously only the maximal compact algebra $\mathcal{U}(n)$ does not appear.

APPENDIX B: THE ISOMORPHY BETWEEN $\mathcal{S}p(4, \mathbb{R})$ AND $\mathcal{S}O(3,2)$. RELATED BASIS AND CASIMIR OPERATORS

The first kind of symmetric decomposition described in the Appendix A also give a canonical decomposition of the $\mathcal{S}O(p, q)$ algebra indeed

$$\mathcal{S}O(p, q) = \begin{bmatrix} \mathfrak{A}_{p+q-2} \\ \star \\ \mathfrak{A}_{p+q-2} \end{bmatrix} \boxdot\, \mathcal{C}\mathcal{S}O(p-1, q-1), \tag{B1}$$

where $\mathcal{C}\mathcal{S}O(p, q) \approx \mathcal{S}O(p, q) \oplus \mathbb{R}^{d}$. It is then interesting to remark that (B1) and (A2) coincide for $p = 3$, $q = 2$, and $n = 2$ since

$$\mathcal{G}l(2, \mathbb{R}) \approx \mathcal{S}l(2, \mathbb{R}) \oplus \mathbb{R} \approx \mathcal{S}O(2, 1) \oplus \mathbb{R} \approx \mathcal{C}\mathcal{S}O(2, 1)$$

so that we obtain the well-known isomorphy between $\mathcal{S}p(4, \mathbb{R})$ and $\mathcal{S}O(3, 2)$.

An usual $\mathcal{S}O(3, 2)$ basis is given by the ten skew-symmetric M_{jk} with $j, k = 0, 0', 1, 2, 3$ satisfying the following commutation relations:

$$[M_{jk}, M_{lm}] = i(g_{jm}M_{kl} + g_{kl}M_{jm} - g_{jl}M_{km} - g_{km}M_{jl}) \tag{B2}$$

with $g_{00} = g_{0'0'} = -g_{11} = -g_{22} = -g_{33} = 1$, and we choose the following relations between the above basis and the $\mathcal{S}p(4, \mathbb{R})$ basis satisfying (A3):

$$\begin{aligned}
&T_{11} + T_{22} = 2(M_{0'0} + M_{30}), \quad T_{22} - T_{11} = 2(M_{32} + M_{0'2}), \\
&T_{12} = M_{13} + M_{10'}, \\
&S_{11} + S_{22} = 2(M_{0'0} - M_{30}), \quad S_{22} - S_{11} = 2(M_{32} - M_{0'2}), \\
&S_{12} = M_{13} - M_{10'}, \\
&R_{11} = M_{30'} - M_{20}, \quad R_{22} = M_{30'} + M_{20}, \quad R_{12} = M_{01} + M_{12}, \\
&R_{21} = M_{01} - M_{12}.
\end{aligned} \tag{B3}$$

The quadratic Casimir operator of the $\mathcal{S}p(2n, \mathbb{R})$ algebra is given by

$$C_2 = \sum_{j=1}^{n} (\{S_{jj}, T_{jj}\}_+ - 2R^2_{jj}) + 2 \sum_{j<k=2}^{n} (\{S_{jk}, T_{jk}\}_+ - \{R_{jk}, R_{kj}\}_+). \tag{B4}$$

But in the $\mathcal{S}p(4, \mathbb{R})$ case it is more convenient to use the isomorphy with $\mathcal{S}O(3, 2)$, and so we gain the nice properties of the $\mathcal{S}O(p, q)$ Casimir operators for $p + q$ odd, which are expressed in terms of the Casimir operators of the contained $\mathcal{S}O(p', q')$ algebras such that $p' + q' = p + q - 1$. In $\mathcal{S}O(3, 2)$ there are two conjugate $\mathcal{S}O(3, 1)$ algebras

$$\mathcal{S}O(3, 1)^{\mathrm{II}} \approx \{M_{jk} | j, k = 0', 1, 2, 3\}$$

and

$$\mathcal{S}O(3, 1)^{\mathrm{IV}} \approx \{M_{jk} | j, k = 0, 1, 2, 3\},$$

and three conjugate $\mathcal{S}O(2, 2)$ algebras labelled I, III, V and generated respectively by the M_{jk} such that $j, k \in (0, 0', 1, 2)$, $(0, 0', 2, 3)$, $(0, 0', 3, 1)$. All these algebras possess two quadratic Casimir operators denoted by C_2

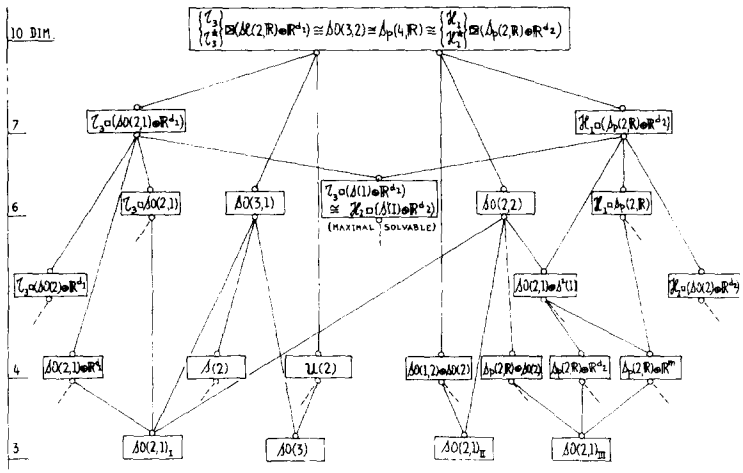

FIG. 3. Daughters, grandchildren, and nonconjugate three-dimensional simple subalgebras of $\mathcal{S}p(4,\mathbb{R}) \cong \mathcal{S}O(3,2)$.

and $\hat{C}_2$ and given by

$$C_2 = \tfrac{1}{2}\eta^{(jk)(lm)} M_{jk} M_{lm}, \quad \hat{C}_2 = \tfrac{1}{2}\eta^{(jk)(lm)} M_{jk} M^{\star}_{lm}, \tag{B5}$$

where $\eta^{(jk)(lm)}$ is the element of the Killing form associated with the pair of generators M_{jk}, M_{kl} belonging to $\mathcal{S}O(3,1)$ [$\mathcal{S}O(2,2)$] and defined by

$$\eta^{(jk)(lm)} = \mathrm{tr}(\mathrm{Ad}M_{jk}\,\mathrm{Ad}M_{lm}), \tag{B6}$$

the symbol Ad being defined by Eq. (D1), and

$$M^{\star}_{lm} = \tfrac{1}{4}\eta_{(pq)(lm)} \epsilon^{pqrs} M_{rs}, \tag{B7}$$

ϵ^{pqrs} being the Levi-Civita alternating symbol defined for the standard ordered sets of indices above given and characterizing the various $\mathcal{S}O(3,1)$ and $\mathcal{S}O(2,2)$ algebras.

Then the Casimir operators of $\mathcal{S}p(4,\mathbb{R}) \approx \mathcal{S}O(3,2)$ can be written

$$C_2 = \tfrac{1}{3}\sum_K C_2^{(K)}, \quad \text{where } K \in \{\mathrm{I}, \mathrm{II}, \mathrm{III}, \mathrm{IV}, \mathrm{V}\},$$
$$C_4 = \sum_K (-1)^K (\hat{C}_2^{(K)})^2. \tag{B8}$$

APPENDIX C. DAUGHTERS' GRANDCHILDREN, AND AND ONE-DIMENSIONAL NONCONJUGATE SUBALGEBRAS OF $\mathcal{S}p(4,\mathbb{R}) \approx \mathcal{S}O(3,2)$

The maximal nonconjugate subalgebras (daughters) of $\mathcal{S}p(4,\mathbb{R})$ have been classified as the stabilizers of the three kinds of vectors and of the three kinds of two-plane of the pseudo-Euclidean space $E(3,2)$ on which $\mathcal{S}O(3,2)$ has a natural action. This can be done either by making use of the representation

$$M_{jk} = i(g_{jl}\xi^l \partial_k - g_{kl}\xi^l \partial_j), \tag{C1}$$

which acts on the vectors $\xi \in E(3,2)$, or by introducing the algebra $\mathfrak{A}_{3+2} \square \mathcal{S}O(3,2)$ where $\mathcal{S}O(3,2)$ acts on the generators V_l of the Abelian algebra according to

$$[M_{jk}, V_l] = i(g_{kl}V_j - g_{jl}V_k). \tag{C2}$$

Then we find

Maximal subalgebras (daughters)	Corresponding invariant subspaces of $E(3,2)$
$\mathfrak{A}_{2+1} \square C\mathcal{S}O(2,1) \approx \mathcal{W}_{2,1}$ (Weyl)	"lightlike" vectors such as $\xi^0 + \xi^3$
$\mathcal{S}p(2,\mathbb{R}) \oplus \mathcal{S}p(2,\mathbb{R}) \approx \mathcal{S}O(2,2)$	"spacelike" vectors s.a. ξ^3
$\mathcal{S}O(3,1)$	"timelike" vectors s.a. ξ^0
$H_1 \square C\mathcal{S}p(2,\mathbb{R})$	"lightlike" two-plane s.a. $(\xi^0 + \xi^1, \xi^{0'} + \xi^2)$
$\mathcal{S}O(3) \oplus \mathcal{S}O(2) \approx \mathcal{U}(2)$	"timelike" two-plane s.a. $(\xi^0, \xi^{0'})$
$\mathcal{S}p(2,\mathbb{R}) \oplus \mathcal{S}O(2) \approx \mathcal{U}(1,1)$	"spacelike" two-plane s.a. (ξ^1, ξ^2)

Hence $\mathcal{S}p(4,\mathbb{R})$ contains the exceptional maximal subalgebra $\mathcal{S}O(3,1)$ besides the expected ones given in (A8).

We have also classified the grandchildren (maximal nonconjugate subalgebras of the daughters) by using powerful theorems developed in Ref. 14. The results are given in Fig. 3, where the chains crossing the three-dimensional simple nonconjugate Lie algebras have been completed.

The one-dimensional subalgebras have been obtained according to the following property: Every one-dimensional subalgebra stabilizes at least one vector belonging to the $E(3,2)$ space. So the problem reduces only to classifying the one-dimensional subalgebras of the stabilizers of the three kinds of vectors in $E(3,2)$, and then to take into account for the "new" conjugations coming from the embedding into the $\mathcal{S}O(3,2)$ algebra.

The one-dimensional subalgebras of $\mathcal{S}O(3,1)$ are well known.[15] Those of the Weyl algebra $\mathcal{W}_{2,1}$ have been obtained from the knowledge of the one-dimensional Poincaré subalgebras in presence of one more dilation generator. Finally the one-dimensional $\mathcal{S}O(2,2)$ subalgebras have been constructed by coupling the one-dimensional ones coming from both members of the direct sum $\mathcal{S}p(2,\mathbb{R}) \oplus \mathcal{S}p(2,\mathbb{R}) \approx \mathcal{S}O(2,2)$. It should be mentioned that $\mathcal{S}O(3,1)$ does not bring any extra algebra besides those furnished by $\mathcal{W}_{2,1}$ and $\mathcal{S}O(2,2)$; this must be related to the exceptional origin of the $\mathcal{S}O(3,1)$ algebra into $\mathcal{S}p(4,\mathbb{R})$.

The results are summarized in Table II in which the embeddings of the nonconjugate one-dimensional subalgebras into the daughters and into the three-dimensional simple subalgebras of $\mathcal{S}p(4, \mathbb{R})$ are pointed out. Obviously the continuous invariants $\mathcal{J}_2$ and $\mathcal{J}_4$ are not sufficient to classify the one-dimensional subalgebras and let many degeneracies subsist. Let us recall that the invariants $\mathcal{J}_2$ and $\mathcal{J}_4$ are formally obtained from the Casimir operators C_2 and C_4 given in Eq. (B8) by substituting the coefficients μ^{jk} of the general element $\frac{1}{2}\mu^{jk}M_{jk}$ of $\mathcal{S}p(4, \mathbb{R})$ to the corresponding generators M_{jk}.

APPENDIX D: AUTOMORPHISMS INDUCED BY THE GENERAL ELEMENT OF $\mathcal{S}p(4, \mathbb{R})$

Each element x in a Lie algebra $\mathcal{A}$ gives rise to a linear operator Adx acting in $\mathcal{A}$, defined for all y in $\mathcal{A}$ by

$$(\mathrm{Ad}x)y = [x, y]. \tag{D1}$$

Adx is an inner derivation of $\mathcal{A}$, the mapping Ad is a linear mapping from the Lie algebra $\mathcal{A}$ into the space of linear operators on $\mathcal{A}$; moreover, it is a (not faithful in general) representation called the adjoint representation of $\mathcal{A}$.

Let us denote (α, β^γ) the structure constants of the Lie algebra defined by

$$[x_\alpha, x_\beta] = (\alpha, \beta^\gamma)x_\gamma; \tag{D2}$$

then the element x_α is given by a matrix Δ_α in the adjoint representation the components of which are

$$(\Delta_\alpha)^\gamma_\beta = (\alpha, \beta^\gamma). \tag{D3}$$

Now it is important to note that

$$(\exp x)y[\exp(-x)] = (\exp \mathrm{Ad}x)y \tag{D4}$$

is not only a shorthand notation of the Baker—Hausdorff formula

$$(\exp x)y[\exp(-x)] = y + [x, y] + (1/2!)[x, [x, y]] + \cdots,$$

but also permits us to obtain the conjugate elements of all the generators of $\mathcal{A}$ under the action of the automorphism induced by the general element of $\mathcal{A}$. To see this, let us return to the specific case of $\mathcal{S}p(4, \mathbb{R})$, the general element of which can be written in the $\mathcal{S}O(3, 2)$ basis defined in Eq. (B2)

$$X = \tfrac{1}{2}\mu^{jk}M_{jk} \quad (\mu^{jk} = -\mu^{kj} \in \mathbb{R}). \tag{D5}$$

Then

$$\mathrm{Ad}X = (i/2)\mu^{jk}\Delta_{(jk)} = i\Delta, \tag{D6}$$

where Δ is a 10×10 square matrix. But to our purpose we prefer to use the coadjoint representation which acts on the dual vector space of the Lie algebra and is just the transpose of the adjoint representation

$$\mathrm{Coad}X = \widetilde{\mathrm{Ad}X} = i\tilde{\Delta}. \tag{D7}$$

Let us denote by W a column vector the ten components of which are the generators M_{jk}; then we obtain the conjugate elements of every generator, and therefore of any element of $\mathcal{S}p(4, \mathbb{R})$, under the action of the general element X by considering

$$[\exp(-iX)]W(\exp iX) = [\exp \mathrm{Ad}(-iX)]W = (\exp\tilde{\Delta})W. \tag{D8}$$

So we have to compute the exponential function of the 10×10 matrix $\tilde{\Delta}$. As a consequence of the Cayley—Hamilton theorem $\exp\tilde{\Delta}$ is expressed in terms of the nine first powers of $\tilde{\Delta}$ and, by using the Lagrange Sylvester interpolation polynomial,[16] can be written as follows:

$$\exp\tilde{\Delta} = (\mathbb{I} + \tilde{\Delta}) \prod_{j=1,3,5,7} \left(\frac{\tilde{\Delta}^2 - \lambda_j^2\mathbb{I}}{\lambda_j^2}\right) + \sum_{j=1,3,5,7} \left\{\frac{\tilde{\Delta}^2}{2\lambda_j^3}\left[\prod_{k\neq j}\left(\frac{\tilde{\Delta}^2 - \lambda_k^2\mathbb{I}}{\lambda_j^2 - \lambda_k^2}\right)\right][e^{\lambda_j}(\tilde{\Delta} + \lambda_j\mathbb{I}) - e^{-\lambda_j}(\tilde{\Delta} - \lambda_j\mathbb{I})]\right\}, \tag{D9}$$

where the λ's are the nonzero roots of the characteristic polynomial of $\tilde{\Delta}$ which are function of the invariants $\mathcal{J}_2$ and $\mathcal{J}_4$ defined in Appendix C, we have

$$\begin{aligned}
&\lambda_1 = -\lambda_2 = (-\mathcal{J}_2 + \sqrt{-\mathcal{J}_4})^{1/2},\\
&\lambda_3 = -\lambda_4 = (-\mathcal{J}_2 - \sqrt{-\mathcal{J}_4})^{1/2},\\
&\lambda_5 = -\lambda_6 = \frac{1}{\sqrt{2}}[-\mathcal{J}_2 + (\mathcal{J}_2{}^2 - \mathcal{J}_4)^{1/2}]^{1/2},\\
&\lambda_7 = -\lambda_8 = \frac{1}{\sqrt{2}}[-\mathcal{J}_2 - (\mathcal{J}_2{}^2 - \mathcal{J}_4)^{1/2}]^{1/2}.
\end{aligned} \tag{D10}$$

But in the particular case where $\mathcal{J}_4$ vanishes $\lambda_1 = \lambda_3 = \lambda_7$ and $\lambda_5 = 0$, the relation (D9) is no longer available and we must use the following one:

$$\begin{aligned}
\exp\tilde{\Delta}\big|_{\mathcal{J}_4=0} = {}& \left[\mathbb{I} + \tilde{\Delta} + \left(\frac{1}{2!} + \frac{3}{\lambda_1^2}\right)\tilde{\Delta}^2 + \left(\frac{1}{3!} + \frac{3}{\lambda_1^2}\right)\tilde{\Delta}^3\right]\frac{(\tilde{\Delta}^2 - \lambda_1^2\mathbb{I})^2}{-\lambda_1^6}\\
&+ \left[\mathbb{I} + \left(1 - \frac{11}{2\lambda_1}\right)(\tilde{\Delta} - \lambda_1\mathbb{I}) + \frac{1}{2}\left(1 + \frac{35 - 11\lambda_1}{\lambda_1^2}\right)\right.\\
&\times \left.(\tilde{\Delta} - \lambda_1\mathbb{I})^2\right]\frac{\tilde{\Delta}^4}{8\lambda_1^7}e^{\lambda_1}(\tilde{\Delta} + \lambda_1\mathbb{I})^3 - \left[\mathbb{I} + \left(1 + \frac{11}{2\lambda_1}\right)\right.\\
&\times (\tilde{\Delta} + \lambda_1\mathbb{I}) + \frac{1}{2}\left(1 + \frac{35 + 11\lambda_1}{\lambda_1^2}\right)(\tilde{\Delta} + \lambda_1\mathbb{I})^2\Big]\\
&\times \frac{\tilde{\Delta}^4}{8\lambda_1^7}e^{-\lambda_1}(\tilde{\Delta} - \lambda_1\mathbb{I})^3.
\end{aligned} \tag{D11}$$

Obviously the relations (D9), (D11) can be reduced to every $\mathcal{S}p(4, \mathbb{R})$ subalgebra; in particular, it is interesting to give the reductions to the $\mathcal{S}O(2, 2)$ and $\mathcal{S}O(3, 1)$ subalgebras which possess nice properties. Let us introduce the vector $W^\star$, analogous of the vector W, but constructed from the $M^\star$'s defined by Eq. (B7) and the matrix $\tilde{\Delta}^\star$ defined by

$$\tilde{\Delta}^\star W = -\tilde{\Delta}W^\star. \tag{D12}$$

Then, for any $\mathcal{S}O(2, 2)$ or $\mathcal{S}O(3, 1)$ subalgebra associated respectively with an index K odd (even), we have

$$\mathrm{tr}(\tilde{\Delta}_K)^2 = -4\mathcal{J}_2^{(K)}, \quad \mathrm{tr}(\tilde{\Delta}_K^\star\tilde{\Delta}_K) = (-)^{K+1}4\hat{\mathcal{J}}_2^{(K)} \tag{D13}$$

and

$$(\tilde{\Delta}_K)^2 = (-)^{K+1}(\tilde{\Delta}_K^\star)^2. \tag{D14}$$

The useful property is that $\tilde{\Delta}_K$, $(\tilde{\Delta}_K)^2$, $\tilde{\Delta}_K^\star$, and $(\tilde{\Delta}_K^\star)^2$ furnish a basis for the powers of $\tilde{\Delta}_K$; indeed

$$(\tilde{\Delta}_K)^3 = -\mathcal{J}_2^{(K)}\tilde{\Delta}_K + \hat{\mathcal{J}}_2^{(K)}\tilde{\Delta}_K^\star,$$
$$\tilde{\Delta}_K^\star(\tilde{\Delta}_K)^2 = -\mathcal{J}_2^{(K)}\tilde{\Delta}_K^\star + (-)^{K+1}\hat{\mathcal{J}}_2^{(K)}\tilde{\Delta}_K. \tag{D15}$$

Finally the coefficients of the exponential terms with λ_5 and λ_7 vanish in (D9) and the other parts can be managed so that $\exp\tilde{\Delta}_K$ is given by a relation formally identical to (D9) with two λ's only which are the characteristic roots of $\tilde{\Delta}_K$:

$$\lambda_1^{(K)} = [-\mathcal{J}_2^{(K)} + (-)^{K(K+2)+1}\hat{\mathcal{J}}_2^{(K)}]^{1/2} = -\lambda_2^{(K)},$$
$$\lambda_3^{(K)} = [-\mathcal{J}_2^{(K)} - (-)^{K(K+2)+1}\hat{\mathcal{J}}_2^{(K)}]^{1/2} = -\lambda_4^{(K)}. \tag{D16}$$

Now by taking into account the relations (D15), the particular case $\hat{\mathcal{J}}_2^{(K)} = 0$ can be deduced which also corresponds to the reduction to $\mathcal{S}O(2,2)$ or $\mathcal{S}O(3,1)$ of the relation (D9). Then we obtain a formula formally identical to the one which can be directly computed starting from a $\mathcal{S}O(2,1)$ algebra, we have

$$\exp\tilde{\Delta}_K\big|_{\hat{\mathcal{J}}_2^{(K)}=0} = \frac{(\tilde{\Delta}_K)^2 + \mathcal{J}_2^{(K)}}{\mathcal{J}_2^{(K)}} - \frac{\tilde{\Delta}_K}{2\mathcal{J}_2^{(K)}}[e^{\lambda}(\tilde{\Delta}_K + \lambda\mathbb{1}) + e^{-\lambda}(\tilde{\Delta}_K - \lambda\mathbb{1})],$$
$$\text{where } \lambda = (-\mathcal{J}_2^{(K)})^{1/2}. \tag{D17}$$

The last particular case corresponds to $\mathcal{J}_2 = \mathcal{J}_4 = 0$; then there is only one null root of multiplicity nine and we obtain

$$\exp\tilde{\Delta}\big|_{\mathcal{J}_2=\mathcal{J}_4=0} = \mathbb{1} + \sum_{m=1}^{9}\frac{\tilde{\Delta}_m}{m!}. \tag{D18}$$

whereas for the $\mathcal{S}O(2,2)$ and $\mathcal{S}O(3,1)$ subalgebras, if $\mathcal{J}_2^{(K)} = \hat{\mathcal{J}}_2^{(K)} = 0$, again we obtain a formula analogous to the $\mathcal{S}O(2,1)$ case due to the relations (D15), we have

$$\exp\tilde{\Delta}_K\big|_{\mathcal{J}_2^{(K)}=\hat{\mathcal{J}}_2^{(K)}=0} = \mathbb{1} + \tilde{\Delta}_K + \frac{\tilde{\Delta}_K^2}{2!}. \tag{D19}$$

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Erratum: Four examples of the inverse method as a canonical transformation [J. Math. Phys. 16, 96 (1975)]

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In our initial computations, a condition was checked which is necessary, but not sufficient, for the maps to be canonical. Since then, following Zakharov and Manakov [Theor. Math. Phys. 19, 332 (1974)] we have checked the invariance of the Poisson brackets and have found errors, primarily normalization errors, in the Toda Lattice column of Table I. Because of these errors, as well as several minor errors and misprints in the other columns, it seems best to publish a corrected table.

TABLE I. The main results.

	Toda lattice	Nonlin. Schröd.	Sine—Gordon	Korteweg—deVries
1. Nonlinear dynamics	$\ddot{Q}_n = \exp(Q_{n-1} - Q_n) - \exp(Q_n - Q_{n+1})$	$\dot{u} = iu_{xx} + i\mathfrak{K}u^2u^*$	$\dot{u}_x = \sin(u)$ $\begin{vmatrix} v = u_x \\ \dot{v} = \sin(u) \end{vmatrix}$	$\dot{u} = 6uu_x - u_{xxx}$
2. Hamiltonians	$H = \sum_{n=-\infty}^{\infty} \frac{P_n^2}{2} + [\exp(\Delta_n) - (1+\Delta_n)]$	$H = i\int_{-\infty}^{\infty}[P_xQ_x - (\mathfrak{K}/2)P^2Q^2]\,dx$	$H = \int_{-\infty}^{\infty}[\cos(\int_{-\infty}^{x} v(x')\,dx') - 1]\,dx$	$H = \int_{-\infty}^{\infty}[u^3 + u_x^2/2]\,dx^2$
	$\dot{Q}_n = \frac{\partial H}{\partial P_n} = P_n$	$\dot{Q} = \frac{\delta H}{\delta P} = -iQ_{xx} - i\mathfrak{K}PQ^2$	$\dot{v} = \frac{\partial}{\partial x}\frac{\delta H}{\delta v}$	$\dot{u} = \frac{\partial}{\partial x}\frac{\delta H}{\delta u}$
3. Canonical eq. from H	$\dot{P}_n = -\frac{\partial H}{\partial Q_n} = e^{\Delta_n} - e^{\Delta_{n+1}}$, $\Delta_n \equiv Q_{n-1} - Q_n$	$\dot{P} = -\frac{\delta H}{\delta Q} = iP_{xx} + i\mathfrak{K}P^2Q$	$= \frac{\partial}{\partial x}\int_{-\infty}^{x} dx' \sin\left(\int_{-\infty}^{x'} v(x'')\,dx''\right)$	$= \frac{\partial}{\partial x}[3u^2 - u_{xx}]$
4. Hamiltonian —"action angle"	$K = \sum_{j=1}^{N} \frac{1}{2}[\zeta_j^{-2} - \zeta_j^2] + \ln(\zeta_j^2)$ $+ \int_0^{\pi} 2\sin(\phi)p(\phi)\,d\phi$	$K = -\frac{2i}{3\mathfrak{K}}\sum_{j=1}^{N}(p_j^{*3} - p_j^3)$ $+ \int_{-\infty}^{\infty} 4\xi^2 p(\xi)\,d\xi$	$K = -2i\sum_{j=1}^{N} e^{(\varphi_j/4)}$ $-\frac{1}{2}\int_0^{\infty}\frac{1}{\xi}p(\xi)\,d\xi$	$K \equiv -\frac{32}{5}\sum_{j=1}^{N} p_j^{5/2}$ $+ \int_{-\infty}^{\infty} 8\xi^3 p(\xi)\,d\xi$
5. Canonical eq. "action angle" "$\dot{p} \equiv 0$"	$\dot{q}_j = \frac{\partial K}{\partial p_j} = (\zeta_j - \zeta_j^{-1})$ $\dot{q}(\varphi) = \frac{\delta K}{\delta p} = 2\sin(\varphi)$	$\dot{q}_j = \frac{\partial K}{\partial p_j} = \frac{2i}{\mathfrak{K}}p_j^2$ $\dot{q}(\xi) = \frac{\delta K}{\delta p} = 4\xi^2$	$\dot{q}_j = \frac{\partial K}{\partial p_j} = -\frac{i}{2}e^{(\varphi_j/4)}$ $\dot{q}(\xi) = \frac{\delta K}{\delta p} = -\frac{1}{2\xi}$	$\dot{q}_j = \frac{\partial K}{\partial p_j} = -16p_j^{3/2}$ $\dot{q}(\xi) = \frac{\delta H}{\delta p} = 8\xi^3$
6. Canonical maps	$p(\phi) = (1/\pi)\sin(\phi)\ln\{1 + \lvert b\rvert^2\}$ $q(\phi) = \arg b(e^{i\phi})$ $p_j = -(\zeta_j + \zeta_j^{-1})$ $q_j = \ln[-c_j^2\zeta_j a'(\zeta_j)]$	$p(\xi) = (-2i/\mathfrak{K}\pi)\ln\{1 - \lvert b\rvert^2\}$ $q(\xi) = \arg b(\xi)$ $p_j = 2i\zeta_j$ $q_j = -(2/\mathfrak{K})\ln c_j$	$p(\xi) = -(2/\pi\xi)\ln\{1 - \lvert b\rvert^2\}$ $q(\xi) = \arg b(\xi)$ $p_j = -4\ln\xi_j$ $q_j = \ln c_j$	$p(\xi) = (\xi/\pi)\ln\{1 + \lvert b\rvert^2\}$ $q(\xi) = \arg b(\xi)$ $p_j = -\zeta_j^2$ $q_j = 2\ln[ic_j a'(\zeta_j)]$

