with meson production as well as at a peak energy of 255 Mev when meson production processes were appreciable. Despite the strong energy dependence of the fast-photoneutron angular distributions for carbon and deuterium, they are similar to each other at both values of the peak energy.

4. The upper limit of the probability that a meson produced on one of the nucleons of a deuteron or quasi-deuteron of a carbon nucleus will be reabsorbed by the second nucleon, can be estimated by comparing our results with the data on photoproduction of mesons on deuterium and carbon. In the range of energies at 250 Mev and higher, this probability is <0.1 for deuterium and is apparently appreciably smaller than 0.5 for carbon.

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Outgoing Boundary Condition in Rearrangement Collisions*

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The boundary condition on the solution to the nonrelativistic time-independent Schrödinger equation for arbitrarily complicated rearrangements of spinless particles is carefully examined. For real energies E it is shown that the outgoing boundary condition on the scattered wave φ need not imply that φ is "everywhere outgoing." This and similar considerations make apparent the fact remarked by Foldy and Tobocman, namely that the Lippmann-Schwinger integral equation need not have a unique solution for real energies. The relationship of this result to the added fact that solutions to the Lippmann-Schwinger integral equation are unique for complex energies $E+i\epsilon$, $\epsilon>0$ is discussed, as is also the relationship of the usual operator manipulations to the outgoing boundary condition.

I. INTRODUCTION AND SUMMARY

FOLDY and Tobocman[1] have remarked recently that the Lippmann-Schwinger integral equation[2] need not have a unique solution. This observation, which has been discussed by Epstein,[3] is based on Lippmann's[4] reformulation of the integral equation for rearrangement collisions. Similar reformulations in more specific cases also have been given by Altshuler[5] and Wu.[6]

In this paper we examine carefully the boundary condition on the solution to the nonrelativistic Schrödinger equation $(H-E)\Psi=0$ for an arbitrarily complex collision of a system of n particles. The main conclusions, subject to certain limitations which are amplified in the text, are as follows:

1. The usual condition that the scattered wave φ be "everywhere outgoing" means qualitatively that φ behaves asymptotically like the outgoing Green's function G for the total Hamiltonian, and implies the vanishing of an integral $\mathcal{J}(G,\varphi)=\int dS\nu\cdot\mathbf{W}[G,\varphi]$ [see Eqs. (1.3) and (2.3c) below] integrated over the surface at infinity in the $3n$-dimensional space of all the particles. Conversely, the requirement that $\mathcal{J}$ vanish is a formal statement of the boundary condition since $\mathcal{J}(G,\varphi)$ vanishes for at most one solution to the Schrödinger equation. However the requirement that $\mathcal{J}$ be zero does not necessarily imply that φ behaves asymptotically like G. The Lippmann-Schwinger and other integral equations imply the vanishing of surface integrals similar to but not identical with $\mathcal{J}(G,\varphi)$. These considerations make it apparent that for real energies E the Lippmann-Schwinger integral equation need not have a unique solution.

2. For complex energies $E+i\epsilon$, no boundary conditions are required and the solution to the Lippmann-Schwinger integral equation is unique. Since the surface integral $\mathcal{J}(G,\varphi)$ is automatically zero when $\epsilon>0$, the only possible boundary condition making the solution for real E consistent with the limit $\epsilon\to0$ is $\mathcal{J}(G,\varphi)=0$. In general, results proved by operator techniques will apply to the solution of $(H-E)\Psi=0$ satisfying this boundary condition, but will not apply to an arbitrary solution Ψ of the Lippmann-Schwinger integral equation for real energy E.

To avoid extra elaborations we take the particles to be distinguishable and spinless; the angular momentum of any aggregate[7] in its center-of-mass system is not restricted however, and may be nonvanishing. Dis-

* Supported by the Office of Naval Research.
[1] L. L. Foldy and W. Tobocman, Phys. Rev. **105**, 1099 (1957).
[2] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).
[3] Saul T. Epstein, Phys. Rev. **106**, 598 (1957).
[4] B. A. Lippmann, Phys. Rev. **102**, 264 (1956).
[5] S. Altshuler, Phys. Rev. **91**, 1167 (1953).
[6] Ta-You Wu, Can. J. Phys. **34**, 179 (1956). See also H. E. Moses, Phys. Rev. **91**, 185 (1953).

[7] By "particle" we mean always a spinless "fundamental" particle having no internal degrees of freedom. The somewhat unesthetic term "aggregate" denotes either a single particle or a collection of particles; in the latter event the particles are presumed bound in a specified eigenstate of negative energy (in the rest system of the aggregate).

tinguishability is not a serious limitation, since it is well known[8] that with indistinguishable particles, though the cross sections are given by squares of linear combinations of ordinary and exchange amplitudes, the amplitudes continue to be computed as if the particles were distinguishable. The nontrivial modifications produced by particle spin and some less evident concomitants of particle indistinguishability are left to a future communication. Our procedures have not been extended to relativistic or time-dependent problems, nor to collisions involving particle creation or annihilation.

1. Mathematical Preliminaries

In this section, to make our subsequent discussion less disjointed, we introduce our notation and summarize our mathematical contentions. We are concerned mostly with reactions of the type

$$a+b\rightarrow c+d, \tag{1.1a}$$

where the aggregates c, d are a rearrangement of the particles contained in the aggregates a, b. Our results pertain also to more complex collisions however, e.g., of type

$$a+b\rightarrow c+d+e. \tag{1.1b}$$

Subscripts i and f, designate, respectively initial and final reaction channels. Unbarred symbols refer to the laboratory system; German characters, barred symbols, or symbols with the superscript °, refer to the center-of-mass system.[9] The superscript (+) distinguishes solutions satisfying the boundary condition $\mathfrak{g}(G,\varphi)=0$. For the reaction channels of Eq. (1.1a) the total Hamiltonian in the laboratory system $H=T+V$ is partitioned into

$$H=H_i+V_i=H_f+V_f, \tag{1.2a}$$

$$V=V_a+V_b+V_{ab}=V_c+V_d+V_{cd}, \tag{1.2b}$$

where T represents kinetic energy, V potential energy; V_a is the sum of the interactions between the particles composing the aggregate a; $V_{ab}\equiv V_i$ for the reaction (1.1a) is the interaction between the aggregates a, b. To illustrate, if particles 1, 2 form a, particles 3, 4 form b, $V_a=V_{12}$, $V_{ab}=V_{13}+V_{14}+V_{23}+V_{24}$. The eigenfunctions of a in its own rest system are $u_a(\mathbf{s}_a;E_a)$ satisfying $(T_a+V_a-E_a)u_a=0$; $\mathbf{s}_a$ are the set of internal coordinates of aggregate a.

The coordinates of the n particles comprising the system are $\mathbf{r}_j=r_j\mathbf{n}_j$, $j=1,\cdots,n$, measured relative to a fixed origin in the laboratory system; $\mathbf{r}_a$ is the location in the laboratory system of the center-of-mass of a; $\mathbf{r}_{jk}=\mathbf{r}_k-\mathbf{r}_j$; $\mathbf{r}_{ab}=\mathbf{r}_b-\mathbf{r}_a$. The entire set $\mathbf{r}_1,\cdots,\mathbf{r}_n$ will be symbolized by $\mathbf{r}=r\mathbf{n}$, which can be regarded as a vector in the $3n$-dimensional combined coordinate space with coordinates $\mathbf{r}_1=(x_1,y_1,z_1)$ along unit vectors $\mathbf{i}_1$, $\mathbf{j}_1$, $\mathbf{k}_1$, $\cdots$, coordinates $\mathbf{r}_n=(x_n,y_n,z_n)$ along $\mathbf{i}_n$, $\mathbf{j}_n$, $\mathbf{k}_n$; $r=|\mathbf{r}|=(r_1^2+\cdots+r_n^2)^{\frac{1}{2}}$ is the magnitude of $\mathbf{r}$; in the center-of-mass system the coordinates form a $3(n-1)$-dimensional vector symbolized by the German $\mathfrak{r}=r\mathfrak{n}$. Each direction $\mathbf{n}$ in the laboratory system corresponds to possible formation of a definite class of aggregates. Along most directions $\mathbf{n}$ the separation r_{jk} of each pair of particles becomes infinite as $r\rightarrow\infty$; these are the directions corresponding to complete dissociation of all the aggregates. There also are special directions $\mathbf{n}_t$, corresponding for instance to possible formation of t aggregates a, b, $\cdots$, along which the separations r_{ab} of each pair of aggregates become infinite as $r\rightarrow\infty$, but along which the distances $|\mathbf{r}_{aj}-\mathbf{r}_{ak}|$, $\cdots$, $|\mathbf{r}_{bj}-\mathbf{r}_{bk}|$, $\cdots$, between pairs of particles belonging to the same aggregate remain finite. Directions $\mathfrak{n}$ in the center-of-mass system are classified similarly.

Integration by parts in the many-dimensional $\mathbf{r}$ space yields

$$\int d\mathbf{r}[XTY-YTX]=-\int dS\nu\cdot\mathbf{W}[X,Y], \tag{1.3a}$$

where the integral on the right is over the surface bounding the closed volume of integration on the left; ν is the outward drawn normal to the surface element dS; X and Y are any two functions of $\mathbf{r}$ which are well behaved in the integration volume; $\mathbf{W}\equiv\mathbf{W}_1,\cdots,\mathbf{W}_n$ is a $3n$-dimensional vector; and the components of $\mathbf{W}_j$ (along the same unit vectors $\mathbf{i}_j$, $\mathbf{j}_j$, $\mathbf{k}_j$ as the components of $\mathbf{r}_j$) are defined by

$$\mathbf{W}_j=\frac{\hbar^2}{2M_j}(X\nabla_jY-Y\nabla_jX). \tag{1.3b}$$

We term Eqs. (1.3) Green's theorem.

For complex λ there are unique Green's functions G, G_i, G_f, $G_F{}^{(n)}$ in the laboratory system. The Green's functions are analytic functions of λ, are exponentially decreasing as the space coordinates become infinite, and are defined by

$$(H-\lambda)G(\lambda)=I, \tag{1.4a}$$

$$(H_i-\lambda)G_i=I, \tag{1.4b}$$

$$(H_f-\lambda)G_f=I, \tag{1.4c}$$

$$(T-\lambda)G_F{}^{(n)}=I, \tag{1.4d}$$

with $I=\delta(\mathbf{r}-\mathbf{r}')\equiv\delta(\mathbf{r}_1-\mathbf{r}_1')\cdots\delta(\mathbf{r}_n-\mathbf{r}_n')$ the unit operator in $\mathbf{r}$ space. Each of these Green's functions is symmetric; $G(\mathbf{r};\mathbf{r}';\lambda)=G(\mathbf{r}';\mathbf{r};\lambda)$. Their limits as $\epsilon\rightarrow 0$ with $\lambda=E+i\epsilon$, $\epsilon>0$ are the corresponding outgoing Green's functions $G(E)$, $G_i(E)$, etc. These assertions have a rigorous mathematical basis for the case of a

[8] See, e.g., L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), second edition, Sec. 34.

[9] We apologize for this proliferation, forced by the requirements of the printer and of further theoretical treatment in preparation.

single one-dimensional particle.[10] In more complicated cases for reasonably well-behaved interactions it may be presumed that the Hamiltonian is a self-adjoint operator in Hilbert space, although the precise requirements on the potentials to assure H is self-adjoint are not known.[11] We infer[12] that G fails to exist only at the point eigenvalues of H; elsewhere, although unique, G may not be a single-valued function[10] of λ. The Green's functions satisfy[13]

$$G=G_i-G_iV_iG=G_i-GV_iG_i, \tag{1.5a}$$

$$G=G_f-G_fV_fG=G_f-GV_fG_f, \tag{1.5b}$$

$$G=G_{F^{(n)}}-G_{F^{(n)}}VG=G_{F^{(n)}}-GVG_{F^{(n)}}. \tag{1.5c}$$

Equations (1.5) are consistent with the usual operator formalism in implying integration over the entire range of the suppressed intermediate variables, i.e., since $V(\mathbf{r},\mathbf{r}')=V(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')$ is a point operator

$$(G_FVG)_{\mathbf{r},\mathbf{r}'}=\int d\mathbf{r}''G_F(\mathbf{r};\mathbf{r}'')V(\mathbf{r}'')G(\mathbf{r}'';\mathbf{r}'). \tag{1.6}$$

We claim that the asymptotic limits of $G(E)$, $G_i(E)$, $\cdots$ at large $r\mathbf{n}$, excepting terms which become negligibly small, represent propagation of the particles in the aggregates corresponding to $\mathbf{n}$. Moreover, where the asymptotic limit of G_f for instance is non-negligible, $\nabla_f G_f \sim G_f$ and $|G_f|^2dS$ is finite and independent of r in Eqs. (1.3). It follows that in considering integrals $\mathcal{I}(G,\varphi)$, $\mathcal{I}(G_i,\varphi)$, $\cdots$ we need be concerned only with surface elements dS at infinity along directions $\mathbf{n}$ corresponding to energetically open channels, provided the Green's functions G, G_i, $\cdots$ in question actually permit propagation in these channels. We remark that all interactions V_{ab} are omitted from H_{ab}, so that G_{ab} can propagate only in bound or dissociated states of a, b, but cannot propagate in a true rearrangement of the particles in a and b. The assertions of this paragraph are crucial and can be made plausible,[14] but we are not prepared to prove them rigorously; they are consistent with the behavior of the n-particle system free space Green's function $G_{F^{(n)}}$, which can be written in closed form, as well as with what is known about the behavior of the Green's function in a channel containing two aggregates only.

To avoid mathematical difficulties which in the main are irrelevant to our purpose, we assume explicitly that whenever a channel specified by bound states of the aforementioned t aggregates a, b, $\cdots$ is open, the interaction V_{ab} between each pair of these aggregates decreases more rapidly than r_{ab}^{-1} as their separation $r_{ab}\to\infty$. This assumption rules out open channels containing two charged aggregates a and b, but it seems clear that in such channels our subsequent analysis is modified only by the replacement of plane waves in $\mathbf{r}_{ab}$ by Coulomb functions. In the event that three or more outgoing aggregates actually are charged, the appropriate modification of the theory is not even surmised, since the asymptotic behavior of the Green's functions for three or more interacting charged particles is not known.

II. REAL ENERGIES

1. Specification of Solution

We proceed to specify the solution in the laboratory system. As will be seen a laboratory system formulation is equivalent to and algebraically somewhat simpler than a formulation *ab initio* in the center-of-mass system. The primary motive for our procedure is frankly pedagogic however; the laboratory system offers the most obvious illustration of the fact that the scattered waves satisfying the boundary condition need not be "everywhere outgoing." We stress that all statements in this Section II pertain to real energies only.

The Schrödinger equation in the laboratory system,

$$(H-E)\Psi=0, \tag{2.1a}$$

is supposed to have a solution $\Psi_i^{(+)}$ of the form

$$\Psi_i^{(+)}=\psi_i+\varphi_i. \tag{2.1b}$$

We intend to make precise the boundary condition on φ_i. The incident wave ψ_i is a solution of

$$(H_i-E)\psi_i=0. \tag{2.1c}$$

Equations (2.1) imply that

$$(H-E)\varphi_i=-V_i\psi_i, \tag{2.2a}$$

$$(H_i-E)\varphi_i=-V_i\Psi_i^{(+)}. \tag{2.2b}$$

Multiply Eq. (2.2a) on the left by the outgoing Green's function $G(\mathbf{r};\mathbf{r}';E)$; Eq. (1.4a) (with $\lambda=E$) on the left by $\varphi_i(\mathbf{r})$; subtract; integrate over all $\mathbf{r}$ space; and

[10] See B. Friedman, *Principles and Techniques of Applied Mathematics* (John Wiley and Sons, Inc., New York, 1956), especially Chaps. 3 and 4. The relevance of this mathematical theory to quantum mechanical scattering problems has been discussed by B. Friedman and E. Gerjuoy, [New York University, Washington Square, Mathematics Research Group, Research Report No. CX-4, 1952 (unpublished)]. Other mathematically more difficult references bearing on the one-particle one-dimensional case are: E. C. Titchmarsh, *Eigenfunction Expansions* (Clarendon Press, Oxford, 1946); F. Rellich, New York University, Institute for Mathematics and Mechanics lectures, 1951 (unpublished); E. A. Coddington and N. Levinson, *Theory of Ordinary Differential Equations* (McGraw-Hill Book Company, Inc., New York, 1955), Chap. 9.

[11] T. Kato, [Trans. Am. Math. Soc. **70**, 195 (1951)] has proved the Hamiltonian is self-adjoint when the total potential is a sum of two-body Coulomb potentials. Consequently H is self-adjoint for any system of particles interacting via two-body potentials which decrease no less rapidly than $|\mathbf{r}_j-\mathbf{r}_k|^{-1}$ at infinity and are not more singular than $|\mathbf{r}_j-\mathbf{r}_k|^{-1}$ at $\mathbf{r}_j=\mathbf{r}_k$. See also T. Kato, Comm. Pure Appl. Math. **10**, 151 (1957).

[12] M. H. Stone, *Linear Transformations in Hilbert Space* (American Mathematical Society, New York, 1932), Chap. 4, especially theorems 4.12 and 4.18. See also R. G. Cooke, *Linear Operators* (Macmillan and Company, Ltd. London, 1953), Chaps. 5 and 6.

[13] These relations are derived and discussed briefly in an Appendix to this paper. The relation $G_iV_iG=GV_iG_i$ has been discussed briefly by B. A. Lippmann, Ann. Phys. **1**, 113 (1957).

[14] E. Gerjuoy (to be published).

use Green's theorem.[15] There results

$$\varphi_i(\mathbf{r}')=-\int d\mathbf{r}G(\mathbf{r};\mathbf{r}')V_i(\mathbf{r})\psi_i(\mathbf{r}) + \int_\infty dS\nu\cdot\mathbf{W}[G(\mathbf{r};\mathbf{r}'),\varphi_i(\mathbf{r})] \quad (2.3a)$$

integrated over the surface at infinity in $\mathbf{r}$ space. It is convenient to rewrite Eq. (2.3a) in the conditional form:

$$\varphi_i(\mathbf{r})=-\int d\mathbf{r}'G(\mathbf{r};\mathbf{r}')V_i(\mathbf{r}')\psi_i(\mathbf{r}'), \quad (2.3b)$$

provided[16] that, for all $\mathbf{r}''$,

$$\mathcal{J}(G,\varphi_i)=\int_\infty dS\nu\cdot\mathbf{W}[G(\mathbf{r};\mathbf{r}''),\varphi_i(\mathbf{r})]=0, \quad (2.3c)$$

integrated over the surface at infinity in $\mathbf{r}$ space. In Eq. (2.3b) we have used the fact that G is symmetric. Similarly, multiplying Eq. (2.2b) on the left by the outgoing $G_i(\mathbf{r};\mathbf{r}';E)$, Eq. (1.4b) on the left by $\varphi_i(\mathbf{r})$, we obtain

$$\varphi_i(\mathbf{r})=-\int d\mathbf{r}'G_i(\mathbf{r};\mathbf{r}')V_i(\mathbf{r}')\Psi_i^{(+)}(\mathbf{r}'), \quad (2.4a)$$

provided[16] that, for all $\mathbf{r}''$,

$$\mathcal{J}(G_i,\varphi_i)=\int_\infty dS\nu\cdot\mathbf{W}[G_i(\mathbf{r};\mathbf{r}''),\varphi_i(\mathbf{r})]=0. \quad (2.4b)$$

Equations (2.3b) and (2.4a) combine with Eqs. (2.1) to give the well-known[2,17] formal solution,

$$\Psi_i^{(+)}=\psi_i-GV_i\psi_i, \quad (2.5a)$$

and the integral equation,

$$\Psi_i^{(+)}=\psi_i-G_iV_i\Psi_i^{(+)}. \quad (2.5b)$$

The more customary notation replaces Eqs. (2.5) by

$$\Psi_i^{(+)}=\psi_i-\frac{1}{H-E-i\epsilon}V_i\psi_i, \quad (2.6a)$$

$$\Psi_i^{(+)}=\psi_i-\frac{1}{H_i-E-i\epsilon}V_i\Psi_i^{(+)}. \quad (2.6b)$$

Presumably the asymptotic behavior of the outgoing Green's function $G(E)$ is consistent with intuitive expectation, namely that at large distances in any open channel the aggregates should be moving not toward but away from each other and the origin. The demand that the scattered wave φ_i be "everywhere outgoing" expresses the conviction that at large distances φ_i should behave like G. If φ_i and G behave similarly at infinity, $\mathbf{W}_j[G,\varphi_i]$ will decrease more rapidly than the product φ_iG, since $G\nabla_j\varphi_i$ and $\varphi_i\nabla_jG$ will tend to cancel; as a result, in view of the assertions in Sec. I.1, $\mathcal{J}(G,\varphi_i)$ of Eq. (2.3c) will vanish because each surface element dS makes a negligible contribution to the integral. For these reasons the boundary condition on φ_i is restated precisely as the requirement that Eq. (2.3c) hold, thereby guaranteeing Eqs. (2.3b) and (2.5a). This requirement we say makes φ_i "outgoing" but not necessarily "everywhere outgoing," because Eq. (2.3b) may hold even though φ_i behaves differently from G along some directions $\mathbf{n}$; there may be cancellations between non-negligible contributions from different surface elements in Eq. (2.3c). Correspondingly, Eq. (2.5a) may yield solutions $\Psi_i^{(+)}$ whose scattered parts $\Psi_i^{(+)}-\psi_i$ are not everywhere outgoing.

Equation (2.3a) is an integral equation of a sort for φ_i; the class of solutions Ψ to Eq. (2.1a) yield a class of scattered waves $\varphi\equiv\Psi-\psi_i$ and a corresponding class of functions $f(\mathbf{r})=\mathcal{J}(G,\varphi)$. Conversely, to any given $f(\mathbf{r})$ there corresponds at most one φ (there may be none) in the class $\Psi-\psi_i$, since Eq. (2.3a) then yields the explicit formula $\varphi=-GV_i\psi_i+f$. In particular, there exists always a unique solution to Eq. (2.1a), namely the function $\Psi_i^{(+)}$ defined by Eq. (2.5a), having the property that $\varphi_i=\Psi_i^{(+)}-\psi_i$ satisfies $\mathcal{J}(G,\varphi_i)=0$; whether or not φ_i of Eq. (2.3b) proves to be "everywhere outgoing," it follows from Eq. (1.4a) that φ_i necessarily satisfies Eq. (2.2a) and therefore, making use of Eq. (1.3a), also satisfies the boundary condition (2.3c). With $\Psi_i^{(+)}$ defined by Eq. (2.5a), it can be shown that φ_i of Eq. (2.4a) satisfies $\mathcal{J}(G_i,\varphi_i)=0$; also Eq. (2.5b) can have at most one solution $\Psi\equiv\Psi_i^{(+)}$ for which $\varphi\equiv\Psi-\psi_i$ satisfies $\mathcal{J}(G,\varphi)=0$. On the other hand, the boundary condition $\mathcal{J}(G_i,\varphi)=0$ yields not an explicit formula for φ but an integral equation (2.5b). Consequently we are not able to conclude immediately, as we did conclude for Eq. (2.3c), that the boundary condition (2.4b) will specify the solution uniquely.

We now observe that because H commutes with $\mathbf{p}_R$, i.e., conserves the total momentum in the laboratory system, we know on physical grounds that an incident wave $\psi_i=\bar{\psi}_i\exp(i\mathbf{K}\cdot\mathbf{R})$ must yield a scattered wave $\varphi_i=\bar{\varphi}_i\exp(i\mathbf{K}\cdot\mathbf{R})$, $\bar{\varphi}_i$ independent of $\mathbf{R}$. In other words, the solutions $\Psi_i^{(+)}$ with which we are concerned never have everywhere outgoing scattered parts φ_i in the laboratory system, although Eq. (2.5a) does specify $\Psi_i^{(+)}$ in terms of the laboratory system outgoing Green's function G; in fact there are no channels in which φ_i behaves asymptotically like G. Formulating the scat-

[15] Strictly speaking, with $X=G$ in Eq. (1.3a), we must integrate only over a volume exterior to the singularity of G at $\mathbf{r}=\mathbf{r}'$. By equally strict definition of G however, the contribution to the right side of Eq. (1.3a) from an infinitesimal surface surrounding $\mathbf{r}=\mathbf{r}'$ then equals $Y(\mathbf{r}')$. Thus it can be seen that this more careful procedure is equivalent to integrating over all space and evaluating the surface integral in Eq. (1.3a) at infinity only.

[16] Our subsequent discussion of Eqs. (2.3) is made less awkward by our insistence on integrating over the unprimed variable in Eq. (2.3c). It is obvious from Eq. (2.3a) that adding to the right side of Eq. (2.3b) the surface integral of Eq. (2.3c) evaluated at $\mathbf{r}''=\mathbf{r}$ yields an expression for $\varphi_i(\mathbf{r})$ which is correct whether or not Eq. (2.3c) holds for all $\mathbf{r}''$. In the same way Eq. (2.4a) is made strictly correct by adding to its right side the surface integral of Eq. (2.4b). The same remark pertains to other similar pairs of equations, e.g., Eqs. (2.15).

[17] M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953).

tering problem in the center-of-mass system, we infer, as in the laboratory system, that

$$\bar{\varphi}_i = -\bar{G}V_i\bar{\psi}_i \tag{2.7a}$$

provided[16] that, for all $\mathfrak{r}''$,

$$\int_\infty d\bar{S}_{\mathfrak{v}}^{\circ}\cdot\mathbf{W}^{\circ}[\bar{G}(\mathfrak{r};\mathfrak{r}''),\bar{\varphi}_i(\mathfrak{r})]=0, \tag{2.7b}$$

integrated over the surface at infinity in $\mathfrak{r}$ space. In Eq. (2.7a) integration over the suppressed variables $\mathfrak{r}'$ is implied, consistent with our practice in the laboratory system. The $3(n-1)$-dimensional vector $\mathbf{W}^{\circ}$ of Eq. (2.7b) is defined by

$$\int d\mathfrak{r}[X\bar{T}Y-Y\bar{T}X]=-\int d\bar{S}_{\mathfrak{v}}^{\circ}\cdot\mathbf{W}^{\circ}[X,Y]. \tag{2.8}$$

Using the coordinate set $\mathfrak{r}=\mathfrak{r}_2,\cdots,\mathfrak{r}_n$, with $\mathfrak{r}_j=\mathbf{r}_j-\mathbf{r}_1$, we have

$$\bar{T}=\sum_j\frac{\mathfrak{p}_j^2}{2\mu_j}+\frac{1}{2M_1}\sum_{j\neq k}\mathfrak{p}_j\cdot\mathfrak{p}_k, \tag{2.9a}$$

$$\mathbf{W}^{\circ}{}_j=\frac{\hbar^2}{2\mu_j}(X\boldsymbol{\nabla}^{\circ}{}_jY-Y\boldsymbol{\nabla}^{\circ}{}_jX)+\frac{\hbar^2}{2M_1}\sum_{k\neq j}(X\boldsymbol{\nabla}^{\circ}{}_kY-Y\boldsymbol{\nabla}^{\circ}{}_kX), \tag{2.9b}$$

where $\mathfrak{p}_j=-i\hbar\boldsymbol{\nabla}^{\circ}{}_j$; μ_j is the reduced mass of the pair of particles 1 and j; and[18] $\mathbf{W}^{\circ}{}_j$ are the components of $\mathbf{W}^{\circ}$ along the same unit vectors as the components of $\mathfrak{r}_j$.

Of course the formulation in the laboratory system, after removing the factor $\exp(i\mathbf{K}\cdot\mathbf{R})$, is identical with the formulation in the center-of-mass system. Specifically it can be proved[14] that the validity of Eq. (2.7b) guarantees the validity of Eq. (2.3c) and vice versa, and that integrating over $\mathbf{R}'$ in Eq. (2.3b) yields Eq. (2.7a). Henceforth, unless there is some special point to be made, we shall not distinguish between formulations in the center-of-mass and laboratory systems; the unqualified phrase "everywhere outgoing" shall mean "everywhere outgoing in the center-of-mass system."

2. Integral Equations. Uniqueness of Solution

In this section we first explain how it comes about that expressions like $GV_i\psi_i$ or $G_iV_i\Psi$, involving outgoing Green's functions, do not necessarily behave asymptotically like G or G_i. We then go on to relate this explanation to the fact that the integral equation (2.5b) does not have a unique solution.

The field $G(\mathbf{r};\mathbf{r}')$ produced by a source at $\mathbf{r}'$ is not necessarily outgoing at large $\mathbf{r}$ if $\mathbf{r}'$ becomes infinite along with $\mathbf{r}$. This obvious remark shows that unless the integral of Eq. (2.3b) converges so rapidly that for large r there are negligible contributions from large r', $\varphi_i(\mathbf{r})$ need not behave like the limit of $G(\mathbf{r};\mathbf{r}')$ as $\mathbf{r}$ becomes infinite *and* $\mathbf{r}'$ *is held constant*,[19] i.e., need not be everywhere outgoing in the laboratory system. In actuality, because $V_i(\mathbf{r}')$ is independent of $\mathbf{R}'$, $-GV_i\psi_i$ does not converge rapidly along all directions $\mathbf{n}'$ in $\mathbf{r}'$ space, and consequently $\varphi_i(\mathbf{r})=\bar{\varphi}_i(\mathbf{r})\exp(i\mathbf{K}\cdot\mathbf{R})$ instead of behaving like $G(\mathbf{r};\mathbf{r}')$. With two incident aggregates a, b, we have

$$\psi_i=\exp[i(\mathbf{k}_a\cdot\mathbf{r}_a+\mathbf{k}_b\cdot\mathbf{r}_b)]u_a(\mathbf{s}_a)u_b(\mathbf{s}_b), \tag{2.10a}$$

$$\bar{\psi}_i=\exp[i(M_a\mathbf{k}_b-M_b\mathbf{k}_a)\cdot\mathbf{r}_{ab}/M]u_au_b=\exp(i\mathbf{k}_{ab}\cdot\mathbf{r}_{ab})u_au_b. \tag{2.10b}$$

From Eq. (2.10b) and our having assumed that $V_i=V_{ab}$ decreases faster than r_{ab}^{-1}, it appears that Eq. (2.7a) does make $\bar{\varphi}_i$ behave asymptotically like $\bar{G}$, in other words everywhere outgoing. With three incident aggregates, however, e.g., c, d, e incident in Eq. (1.1b), even in the center-of-mass system the scattered wave $\bar{\varphi}_i'=-\bar{G}V_i'\bar{\psi}_i'$ is not everywhere outgoing. Here

$$\psi_i'=u_cu_du_e\exp[i(\mathbf{k}_c\cdot\mathbf{r}_c+\mathbf{k}_d\cdot\mathbf{r}_d+\mathbf{k}_e\cdot\mathbf{r}_e)]=\bar{\psi}_i'\exp(i\mathbf{K}\cdot\mathbf{R}), \tag{2.11}$$

and $V_i'=V_{cd}+V_{ce}+V_{de}$; hence the integral $\bar{G}V_{cd}\bar{\psi}_i'$ for instance, in which $V_{cd}(\mathbf{r}_{cd}')$ is independent of $\mathbf{r}_{ce}'$, has the wrong asymptotic dependence on $\mathbf{r}_{ce}$. This difficulty with three incident aggregates is related to some complications which arise when the cross section for the reaction (1.1b) is computed.[14] For the purposes of the remainder of this paper we can and do confine our attention to collisions of the type (1.1a).

The arguments of the preceding paragraph show also that unless $-\bar{G}_iV_i\bar{\Psi}$ converges sufficiently rapidly, functions Ψ formally satisfying Eq. (2.5b) need not have everywhere outgoing scattered parts. To understand this comment, note that an arbitrary solution $\Psi(\mathbf{r}')$ of Eq. (2.1a), unlike $\psi_i(\mathbf{r}')$ of Eq. (2.10a), does not decrease exponentially as $\mathbf{r}'$ goes to infinity along directions $\mathbf{n}'$ corresponding to channels other than the incident channel. Furthermore $V_i(\mathbf{r}')$ generally remains finite as $\mathbf{r}'$ approaches infinity along directions $\mathbf{n}'$ corresponding to true rearrangements (not merely breakup) of $i\equiv a, b$. In Eq. (1.1a) for example, at least one pair of particles which are not in the same aggregate of i will be contained in a single aggregate c or d; calling this pair 1 and 2, $V_i(\mathbf{r})$, which includes $V_{12}(\mathbf{r}_{12}')$,

[18] The terms proportional to M_1^{-1} in Eq. (2.9a), well known in atomic spectroscopy [D. S. Hughes and C. Eckart, Phys. Rev. **36**, 694 (1930)], produce the corresponding complicating terms proportional to M_1^{-1} in Eq. (2.9b). By an appropriate change of variables, the quadratic form (2.9a) can be diagonalized and $\mathbf{W}^{\circ}$ of Eq. (2.9b) accordingly simplified. The new diagonalizing coordinates are not readily interpretable physically however.

[19] More precisely, as $\mathbf{r}$ becomes infinite along a direction $\mathbf{n}$ corresponding to formation of t aggregates, $\varphi(\mathbf{r})=-GV_i\psi_i$ need not behave like the corresponding limit of $G(\mathbf{r};\mathbf{r}')$ holding $\mathbf{r}'$ constant unless $r^{\alpha}\varphi(\mathbf{r})$ converges uniformly as a function of r, where $\alpha=(3t-1)/2$.

does not diminish as $\mathbf{r}'$ approaches infinity along directions $\mathbf{n}_{cd}'$ corresponding to formation of c, d. Let us suppose the $f\equiv c, d$ channel is open, and denote by $\Psi_f^{(+)}=\psi_f+\varphi_f$ the solution to Eq. (2.1a) with φ_f everywhere outgoing and ψ_f an incoming plane wave in channel f. Then, replacing $\Psi_i^{(+)}$ in Eq. (2.4a) by $\Psi=\Psi_i^{(+)}+\Psi_f^{(+)}$ causes the integral to be slowly convergent along directions $\mathbf{n}_f'$ and makes $\varphi=-G_iV_i\Psi$ incoming in the f channel.

Although $\varphi=-G_iV_i\Psi$ is incoming in the f channel, we can prove that $\Psi=\Psi_i^{(+)}+\Psi_f^{(+)}$ is an alternative (to $\Psi_i^{(+)}$) solution of Eq. (2.5b); in other words Eq. (2.5b) does not have a unique solution. Our assertions about the asymptotic behavior of the Green's functions mean $\nu\cdot\mathbf{W}[G_i, \varphi_i+\varphi_f]$ is negligible at infinity, where $\varphi_i=-GV_i\psi_i$ and $\varphi_f=-GV_f\psi_f$ each are everywhere outgoing. Moreover, because G_i does not propagate in true rearrangements of i, we have

$$g(G_i,\psi_f)=\int dS\nu\cdot\mathbf{W}[G_i(\mathbf{r};\mathbf{r}''),\psi_f(\mathbf{r})]=0. \quad (2.12)$$

Thus $\varphi=\Psi-\psi_i=\Psi_i^{(+)}+\Psi_f^{(+)}-\psi_i$ satisfies $g(G_i,\varphi)=0$, implying, referring to Eqs. (2.4), that Ψ is a solution of Eq. (2.5b). At this juncture the significant distinction between the boundary conditions (2.3c) and (2.4b) becomes manifest. G propagates in every channel, so that $g(G,\varphi)$ is not zero unless $\varphi\equiv\varphi_i$ is everywhere outgoing; on the other hand, $g(G_i,\varphi)=0$ puts no restrictions on the asymptotic behavior of φ in channels other than the incident channel. We add that by virtue of Eqs. (1.3a) and (1.4b), whenever Ψ solves Eq. (2.5b) $\varphi=-G_iV_i\Psi$ satisfies $(H-E)\varphi=-V_i\Psi$ and $g(G_i,\varphi)=0$, thereby demonstrating that every solution Ψ of Eq. (2.5b) is a solution of Eq. (2.1a) of form (2.1b) and satisfying the boundary condition (2.4b).

With the aid of Green's theorem, Eqs. (1.4) and (2.1a) yield

$$\Psi(\mathbf{r})=\int_\infty dS\nu\cdot\mathbf{W}[G(\mathbf{r};\mathbf{r}''),\Psi(\mathbf{r})]=g(G,\Psi), \quad (2.13a)$$

$$\Psi=-G_iV_i\Psi+\int dS\nu\cdot\mathbf{W}[G_i(\mathbf{r};\mathbf{r}''),\Psi(\mathbf{r})], \quad (2.13b)$$

$$\Psi=-G_fV_f\Psi+\int_\infty dS\nu\cdot\mathbf{W}[G_f(\mathbf{r};\mathbf{r}''),\Psi(\mathbf{r})], \quad (2.13c)$$

where the surface integrals are evaluated at $\mathbf{r}''=\mathbf{r}$, and Ψ is an arbitrary solution of Eq. (2.1a). When $\Psi=\Psi_i^{(+)}$ of Eq. (2.1b), Eqs. (2.3c) and (2.13a) imply that

$$\Psi_i^{(+)}(\mathbf{r})=\int_\infty dS\nu\cdot\mathbf{W}[G(\mathbf{r};\mathbf{r}''),\psi_i(\mathbf{r})]=g(G,\psi_i) \quad (2.14a)$$

evaluated at $\mathbf{r}''=\mathbf{r}$; also Eqs. (2.5b) and (2.13b) imply that

$$\psi_i(\mathbf{r})=g(G_i,\Psi_i^{(+)})=g(G_i,\psi_i). \quad (2.14b)$$

Because φ_i is everywhere outgoing, $g(G_f,\varphi_i)=0$ and Eq. (2.13c) implies

$$\Psi_i^{(+)}=-G_fV_f\Psi_i^{(+)}, \quad (2.15a)$$

provided[16] that, for all $\mathbf{r}''$,

$$g(G_f,\psi_i)=\int_\infty dS\nu\cdot\mathbf{W}[G_f(\mathbf{r};\mathbf{r}''),\psi_i(\mathbf{r})]=0. \quad (2.15b)$$

Equation (2.15b) holds when $f\equiv c, d$ is a true rearrangement of $i\equiv a, b$, under which circumstance G_f does not propagate in the i channel. For final channels corresponding not to rearrangement (or dissociation), but to scattering of a, b with or without excitation, e.g., the elastic channel, $V_f=V_{ab}=V_i$, $G_f=G_{ab}=G_i$, Eq. (2.15b) is inconsistent with Eq. (2.14b), and Eq. (2.15a) is inconsistent with Eq. (2.5b).

Interchanging i and f in Eqs. (2.15) [i.e., we suppose the arrow points to the left in Eq. (1.1a)], we infer that

$$\Psi_f^{(+)}=-G_iV_i\Psi_f^{(+)} \quad (2.16)$$

provided Eq. (2.12) holds. As has been amply argued, Eq. (2.12) is satisfied when $i\equiv a, b$ is a rearrangement of $f\equiv c, d$. This line of reasoning[1] makes it obvious that the inhomogeneous equation (2.5b) generally has no unique solution, since if $\Psi_i^{(+)}$ solves Eq. (2.5b) so does $\Psi=\Psi_i^{(+)}+\Psi_f^{(+)}$. Evidently the right side of Eq. (2.15a) cannot be everywhere outgoing, since it must yield the incoming part ψ_i of $\Psi_i^{(+)}$; equally evidently $-G_fV_f\Psi_i^{(+)}$ does not converge rapidly as $\mathbf{r}'$ approaches infinity along directions $\mathbf{n}'$ corresponding to formation of aggregates a, b. We scarcely need mention that Eq. (2.15a) does not have unique solutions; for given $f\equiv c, d$, the incident wave ψ_i can be furnished in any channel i which is a rearrangement of c, d.

III. COMPLEX ENERGIES

The usual operator techniques typically involve Green's functions for complex energies $\lambda=E+i\epsilon$, e.g., Eqs. (2.6). As we have explained in Sec. I-1, the Green's functions $G(\lambda)$, $G_i(\lambda)$, $\cdots$ are exponentially decreasing at infinity, so that all surface integrals at infinity of the type we have been considering automatically are zero. Hence, for given ψ_i and every $\epsilon>0$, we have $g(G,\varphi_i)=0$, where here $G\equiv G(E+i\epsilon)$ and $\varphi_i\equiv\varphi_i(E+i\epsilon)\equiv\Psi_i^{(+)}(E+i\epsilon)-\psi_i$ equals $-G(E+i\epsilon)V_i\psi_i$ according to Eq. (2.6a). If we believe, as this writer does, that the physical situation is represented by the limit $\epsilon\to 0$ of $\Psi_i^{(+)}(E+i\epsilon)$, and expect to represent the same physical situation by a solution of the Schrödinger equation $(H-E)\Psi=0$ for real energy E, then the boundary conditions specifying the solution at $\epsilon=0$ must be consistent with the behavior of $\varphi_i(E+i\epsilon)$ for very small ϵ. From this point of view, therefore, the only possible boundary condition at real energies $\epsilon=0$, in the class of boundary conditions $g(G,\varphi_i)=f$, is $f=0$, the boundary condition to which we were led in Sec.

II-1 by the qualitative consideration that thes cattered wave should propagate like the outgoing Green's function. The same consistency requirement suggests that other surface integrals which vanish for the correctly specified solution $\Psi_i^{(+)}(E)$ of Eq. (2.5a), for instance $\mathcal{I}(G_f,\psi_i)$ of Eq. (2.15b) when f is a rearrangement of i, are neglected implicitly (though justifiably) in the routine operator manipulations. On the other hand, such surface integrals need not vanish for an arbitrary solution $\Psi(E)$ at real energies. Similarly, because the Green's functions are exponentially decreasing, it usually (not necessarily always) should be legitimate to invert the order of integration of repeated integrals when the energy is complex, and we anticipate that it will be equally legitimate to perform the same operation for the correctly specified solution $\Psi_i^{(+)}(E)$ when $\epsilon=0$; the operation need not be legitimate for an arbitrary solution $\Psi(E)$, however. We note also that the integrals and other expressions which occur need not converge uniformly as $\epsilon\to 0$, meaning that we cannot assume that results proved for finite though arbitrarily small ϵ necessarily hold at $\epsilon=0$. Failure to recognize these implications of the operator manipulations can lead to erroneous conclusions when, as is frequently the case, the results are applied to solutions of the Schrödinger equation for real energy E.

We shall expand and illustrate these remarks by comparing results for the pair of Eqs. (2.6) with the results obtained in previous sections for Eqs. (2.5). The reader is reminded that Eqs. (2.5) were derived for real energies, $G\equiv G(E)$, $G_i\equiv G_i(E)$, while in Eqs. (2.6) $(H-E-i\epsilon)^{-1}\equiv G(E+i\epsilon)$, $(H_i-E-i\epsilon)^{-1}\equiv G_i(E+i\epsilon)$. By routine operator algebra, solutions to either of Eqs. (2.6) are seen to satisfy

$$(H-E-i\epsilon)\Psi_i^{(+)}=-i\epsilon\psi_i, \tag{3.1a}$$

in which ψ_i still satisfies Eq. (2.1c). Since the Green's function $G(\lambda)$ is unique for complex λ, or alternatively since the homogeneous equation $(H-\lambda)\Psi=0$ has no bounded solutions for complex λ, Eq. (3.1a) has a unique solution:

$$\Psi_i^{(+)}=-i\epsilon G(E+i\epsilon)\psi_i\equiv\frac{-i\epsilon}{H-E-i\epsilon}\psi_i, \tag{3.1b}$$

and no boundary conditions are required. Hence, for arbitrarily small $\epsilon>0$ the integral equation (2.6b) has a unique solution $\Psi_i^{(+)}$ given by Eq. (2.6a) or equivalently by Eq. (3.1b). At $\epsilon=0$, on the other hand, the dependence on the incident wave ψ_i disappears from Eq. (3.1a), making the equation homogeneous instead of inhomogeneous; consequently the solution to the Schrödinger equation $(H-E)\Psi=0$ is not unique and requires a boundary condition.

To make the connection between solutions of Eqs. (2.5) and (2.6) more apparent, let us derive Eqs. (2.6) from Eq. (3.1a) by strict mathematical procedures rather than by operator techniques. Using Eqs. (2.1b) and (2.1c) in Eq. (3.1a) yields

$$(H-E-i\epsilon)\varphi_i=-V_i\psi_i, \tag{3.2a}$$

$$(H_i-E-i\epsilon)\varphi_i=-V_i\Psi_i^{(+)}, \tag{3.2b}$$

in complete analogy with Eqs. (2.2); of course $\varphi_i\equiv\varphi_i(E+i\epsilon)$ in Eqs. (3.2). Multiply Eq. (3.2a) on the left by $G(E+i\epsilon)$, Eq. (1.4a) for $\lambda=E+i\epsilon$ by $\varphi_i(E+i\epsilon)$, and use Green's theorem. We integrate not over all $\mathbf{r}$ space, however, but only over a finite volume, say a $3n$-dimensional sphere of radius ρ centered at $\mathbf{r}=\mathbf{r}'$; in this way we avoid the problem that the integral over all space is itself defined as the limit of the sequence of integrals $\rho\to\infty$, which sequence need not converge uniformly as a function of ϵ. Thereby we find that

$$\varphi_i(\mathbf{r}')=-\int_\rho d\mathbf{r}G(\mathbf{r};\mathbf{r}';E+i\epsilon)V_i(\mathbf{r})\psi_i(\mathbf{r})+\int_\rho dS\nu\cdot\mathbf{W}[G(\mathbf{r};\mathbf{r}';E+i\epsilon),\varphi_i(\mathbf{r})], \tag{3.3a}$$

$$\varphi_i(\mathbf{r}')=-\int_\rho d\mathbf{r}G_i(\mathbf{r};\mathbf{r}';E+i\epsilon)V_i(\mathbf{r})\Psi_i^{(+)}(\mathbf{r})+\int_\rho dS\nu\cdot\mathbf{W}[G_i(\mathbf{r};\mathbf{r}';E+i\epsilon),\varphi_i(\mathbf{r})], \tag{3.3b}$$

wherein the first terms on the right are integrated over the interior[15] of the sphere of radius ρ, and the second terms over the surface bounding this sphere; Eqs. (3.3) involve no infinite integrals. Letting $\rho\to\infty$ for constant $\epsilon>0$ causes the surface integrals to vanish and yields Eqs. (2.6); whereas letting ϵ approach *and equal* zero holding ρ constant and then letting $\rho\to\infty$ yields the previously deduced Eqs. (2.3) and (2.4). With sufficiently rapidly decreasing potentials, the sequence of volume integrals $\rho\to\infty$ in Eq. (3.3a) should converge uniformly as a function of ϵ in the center-of-mass system (not in the laboratory system). Consequently, recalling that we could have formulated the scattering problem *ab initio* in the center-of-mass system (in which event all quantities in Eq. (3.3a) would be replaced by their corresponding center-of-mass quantities, e.g. $G(\mathbf{r};\mathbf{r}')$ by $\bar{G}(\mathbf{r};\mathbf{r}')$, $\mathbf{W}$ by $\mathbf{W}^\circ$, etc.), we are entitled to assume that $\lim\bar{\varphi}_i(E+i\epsilon)$ as $\epsilon\to 0$, which limit we term $\bar{\varphi}_i''(E)$, is found by first letting $\rho\to\infty$ in Eq. (3.3a) and then putting $\epsilon=0$ under the integral sign, in other words that $\bar{\varphi}_i''(E)=-\bar{G}(E)V_i\bar{\psi}_i$ integrated over all space. The consistency requirement implies immediately that we must use the boundary condition (2.7b), or equivalently (2.3c). Equation (3.3a) is an integral equation for $\bar{\varphi}_i(\mathbf{r};E+i\epsilon)$; although it has a unique solution $\bar{\varphi}_i(E+i\epsilon)=-\bar{G}(E+i\epsilon)V_i\bar{\psi}_i$ for every $\epsilon>0$ and although $\bar{\varphi}_i(E+i\epsilon)$ converges uniformly, there is no reason to suppose that the equation which is the limit of Eq. (3.3a) as $\epsilon\to 0$ has a unique solution. Similar comments pertain to Eqs. (2.4) and

(3.3b); in particular, although for every $\epsilon>0$ the Lippmann-Schwinger integral equation (2.6b) has a unique solution, it is not necessarily true that there is a unique solution to Eq. (2.5b), the limit as $\epsilon\to 0$ of the sequence of integral equations (2.6b).

Suppose $\Psi(E+i\epsilon)$ is any solution of Eq. (2.6b). We shall demonstrate explicitly, as we already know from Eq. (3.1b), that Ψ necessarily is identical with $\Psi_i^{(+)}$ of Eq. (2.6a). Using Eq. (2.6b) to eliminate ψ_i in Eq. (2.6a), we find that

$$\Psi_i^{(+)}=\Psi+G_iV_i\Psi-GV_i\{\Psi+G_iV_i\Psi\}, \tag{3.4a}$$

or

$$\Psi_i^{(+)}=\Psi+\{G_i-G-GV_iG_i\}V_i\Psi, \tag{3.4b}$$

implying, according to Eq. (1.5a), that $\Psi(E+i\epsilon)=\Psi_i^{(+)}(E+i\epsilon)$. Putting $\epsilon=0$, we might conclude that the solution to Eq. (2.5b) is unique and identical with $\Psi_i^{(+)}$ of Eq. (2.5a), in contradiction to the results of Sec. II. The apparent inconsistency arises because in going from Eq. (3.4a) to (3.4b) we have inverted the order of a repeated integral, which operation is not permissible when $\epsilon=0$. Specifically, we have assumed that

$$GV_i\{G_iV_i\Psi\}=\{GV_iG_i\}V_i\Psi, \tag{3.5a}$$

i.e.,

$$\int d\mathbf{r}'G(\mathbf{r};\mathbf{r}')V_i(\mathbf{r}')\left\{\int d\mathbf{r}''G_i(\mathbf{r}';\mathbf{r}'')V_i(\mathbf{r}'')\Psi(\mathbf{r}'')\right\}$$

$$=\int d\mathbf{r}''\left\{\int d\mathbf{r}'G(\mathbf{r};\mathbf{r}')V_i(\mathbf{r}')G_i(\mathbf{r}';\mathbf{r}'')\right\}$$

$$\times V_i(\mathbf{r}'')\Psi(\mathbf{r}''). \tag{3.5b}$$

For real E, however, with Ψ an arbitrary solution of Eq. (2.5b), we can define $\varphi\equiv-G_iV_i\Psi$, use Green's theorem, and note that $\mathcal{J}(G_i,\varphi)=0$ [see added remark preceding Eqs. (2.13)]; we then have

$$\{GV_iG_i\}V_i\Psi$$

$$=\{G_i-G\}V_i\Psi=-\{G_i-G\}(H_i-E)\varphi(\mathbf{r}'')$$

$$=-\{[H_i(\mathbf{r}'')-E][G_i(\mathbf{r};\mathbf{r}'')-G(\mathbf{r};\mathbf{r}'')]\}\varphi(\mathbf{r}'')$$

$$+\int_\infty dS''\mathbf{v}''\cdot\mathbf{W}[G_i-G,\ \varphi(\mathbf{r}'')]$$

$$=-\int d\mathbf{r}''V_i(\mathbf{r}'')G(\mathbf{r}'';\mathbf{r})\varphi(\mathbf{r}'')-\mathcal{J}(G,\varphi). \tag{3.6a}$$

In Eq. (3.6a) braces imply integration as in Eqs. (3.5), but brackets do not; the dependence on the coordinates is indicated only where necessary for clarity and is consistent with Eqs. (3.5); we have used

$$(H_i-E)(G_i-G)=V_iG$$

from Eqs. (1.4). Equation (3.6a) means that

$$GV_i\{G_iV_i\Psi\}=\{GV_iG_i\}V_i\Psi$$

$$+\int_\infty dS\mathbf{v}\cdot\mathbf{W}[G(\mathbf{r};\mathbf{r}''),\ \varphi(\mathbf{r})], \tag{3.6b}$$

instead of Eqs. (3.5), the surface integral being evaluated at $\mathbf{r}''=\mathbf{r}$. Returning to Eqs. (3.4) we see that for real E, inverting the order of integration is not justified and hence $\Psi\neq\Psi_i^{(+)}$ unless $\mathcal{J}(G,\varphi)=0$, in complete agreement with Sec. II.

As a final example, we rewrite Eq. (2.17a) in the form

$$(H_f-E-i\epsilon)\Psi_i^{(+)}=-i\epsilon\psi_i-V_f\Psi_i^{(+)}, \tag{3.7a}$$

from which we infer[3,4] that

$$\Psi_i^{(+)}=-i\epsilon G_f(E+i\epsilon)\psi_i-G_f(E+i\epsilon)V_f\Psi_i^{(+)}$$

$$=\frac{-i\epsilon}{H_f-E-i\epsilon}\psi_i-\frac{1}{H_f-E-i\epsilon}V_f\Psi_i^{(+)}. \tag{3.7b}$$

In Eq. (3.7b) the inhomogeneous term disappears at $\epsilon=0$, from which we seemingly obtain the integral equation (2.15a) conditions on the surface integral of Eq. (2.13c). Using Green's theorem and integrating over a sphere of radius ρ as in Eqs. (3.3), we find, however, that letting $\epsilon\to 0$ and then letting $\rho\to\infty$ yields precisely Eq. (2.13c). Alternatively, substituting Eq. (1.5b) for G in Eq. (2.6b) and using Eq. (2.6a) to eliminate $GV_i\psi_i$ yields

$$\Psi_i^{(+)}=\psi_i-G_fV_i\psi_i+G_fV_fGV_i\psi_i \tag{3.8a}$$

$$=\psi_i-G_f(V_i-V_f)\psi_i-G_fV_f\Psi_i^{(+)}. \tag{3.8b}$$

But $G_f(V_i-V_f)\psi_i=G_f(H_f-H_i)\psi_i=G_f(H_f-E)\psi_i$ so that, in Eq. (3.8b),

$$\psi_i-G_f(V_i-V_f)\psi_i$$

$$=\psi_i-\frac{1}{H_f-E-i\epsilon}(H_f-E)\psi_i=\frac{-i\epsilon}{H_f-E-i\epsilon}\psi_i. \tag{3.9}$$

Thus Eq. (3.8b) is equivalent to Eq. (3.7b), as it should be since for $\epsilon>0$ the solution $\Psi_i^{(+)}(E+i\epsilon)$ is unique. From Eq. (3.9) we might infer that for real energies $\psi_i-G_f(V_i-V_f)\psi_i=0$, and therewith from Eq. (3.8b) once more conclude that the integral equation (2.15a) holds without auxiliary conditions. Actually for real energies, using Green's theorem, we have

$$\psi_i-G_f(H_f-E)\psi_i=\mathcal{J}(G_f,\psi_i). \tag{3.10a}$$

Furthermore, in obtaining Eq. (3.8a) we have assumed that $\{G_fV_fG\}V_i\psi_i=G_fV_f\{GV_i\psi_i\}$ whereas, by manipulations similar to Eq. (3.6a), for real E we obtain

$$\{G_fV_fG\}V_i\psi_i=G_fV_f\{GV_i\psi_i\}+\mathcal{J}(G_f,\varphi_i), \tag{3.10b}$$

with $\varphi_i=-GV_i\psi_i$. As we know, $\mathcal{J}(G_f,\psi_i)=\mathcal{J}(G_f,\varphi_i)=0$ when the f channel is a rearrangement of i and when

φ_i is everywhere outgoing, providing a good illustration of our assertion that the operator manipulations neglect implicitly (though for complex energies justifiably) the same surface integrals which we neglected explicitly in Chap. II. Without assumptions about $\mathcal{I}(G_f,\psi_i)$ and $\mathcal{I}(G_f,\varphi_i)$, and using Eq. (3.10b) to go from Eq. (3.8a) to (3.8b), we again arrive at Eq. (2.13c).

Sections II and III amplify and extend results obtained by Foldy and Tobocman[1] and other authors.[3-6] Comparison with Lippmann's purely operational treatment is recommended.

APPENDIX

Equations (1.5) usually are derived by operator techniques. We wish to deduce them by more rigorous procedures, so as to understand their applicability at real energies. We prove first that the Green's functions are symmetric. From Eq. (1.4a), we have

$$[H(\mathbf{r})-\lambda]G(\mathbf{r};\mathbf{r}';\lambda)=\delta(\mathbf{r}-\mathbf{r}'), \tag{A.1a}$$

$$[H(\mathbf{r})-\lambda]G(\mathbf{r};\mathbf{r}'';\lambda)=\delta(\mathbf{r}-\mathbf{r}''). \tag{A.1b}$$

Multiply Eq. (A.1a) by $G(\mathbf{r};\mathbf{r}'';\lambda)$, Eq. (A.1b) by $G(\mathbf{r};\mathbf{r}';\lambda)$, integrate, and use Green's theorem. Then

$$G(\mathbf{r}';\mathbf{r}'';\lambda)-G(\mathbf{r}'';\mathbf{r}';\lambda)$$

$$=-\int_\infty dS\nu\cdot\mathbf{W}[G(\mathbf{r};\mathbf{r}'';\lambda),G(\mathbf{r};\mathbf{r}';\lambda)]. \tag{A.2}$$

The right side of Eq. (A.2) vanishes for all complex λ, so that for all $\epsilon>0$, $G(\mathbf{r}';\mathbf{r}'';E+i\epsilon)=G(\mathbf{r}'';\mathbf{r}';E+i\epsilon)$. Taking the limit of this symmetry relation as $\epsilon\to 0$ and recalling that the outgoing Green's function $G(E)$ is by definition the limit of $G(E+i\epsilon)$ as $\epsilon\to 0$, we infer that $G(E)$ is symmetric for real E. Knowing this, we can start from Eqs. (A.1) with $\lambda=E$, again use Green's theorem, and thereby conclude that the right side of Eq. (A.2) is zero at $\epsilon=0$ for all $\mathbf{r}'$, $\mathbf{r}''$.

In the same way, from Eqs. (1.4a) and (1.4b) we find

$$G_i(\mathbf{r}';\mathbf{r}'';\lambda)-G(\mathbf{r}'';\mathbf{r}';\lambda)$$

$$=\int d\tau G_i(\mathbf{r};\mathbf{r}'';\lambda)V_i(\mathbf{r})G(\mathbf{r};\mathbf{r}';\lambda)$$

$$-\int_\infty dS\nu\cdot\mathbf{W}[G_i(\mathbf{r};\mathbf{r}'';\lambda),G(\mathbf{r};\mathbf{r}';\lambda)]. \tag{A.3}$$

Again for all complex λ the surface integral vanishes. Thus, since the Green's functions are symmetric, rewriting the right side of Eq. (A.3) to be consistent with the notation (1.6) for the $\mathbf{r}''$, $\mathbf{r}'$ element, and interchanging $\mathbf{r}''$ and $\mathbf{r}'$ in G_i on the left side of Eq. (A.3), yields the first equality of (1.5a); interchanging $\mathbf{r}'$ and $\mathbf{r}''$ in G on the left side of Eq. (A.3) and rewriting the right side to be consistent with the notation for the $\mathbf{r}'$, $\mathbf{r}''$ element yields the second equality of (1.5a). This proves Eq. (1.5a) for all complex λ. Taking the limit as $\epsilon\to 0$, we shall conclude that Eq. (1.5a) holds at $\epsilon=0$ provided the integral G_iV_iG converges uniformly as a function of ϵ; G_iV_iG should converge uniformly for sufficiently rapidly decreasing potentials. Starting with Eqs. (1.4), at real energies we infer that if Eq. (1.5a) holds, then $\mathcal{I}(G,G_i)$ vanishes at real energies and conversely; i.e., the validity of Eqs. (1.5) for real E is tied to our assertions in Sec. I.1 concerning the ways in which the Green's functions propagate.