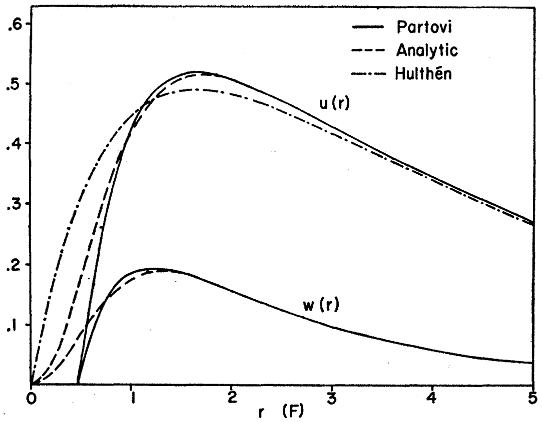

FIG. 1. S and D states of the deuteron for the numerical wave function obtained from the Hamada-Johnston potential and the analytic wave function with the parameters of Table I. Wave functions are normalized as $\int_0^\infty [u^2(r)+w^2(r)]dr=1$. The parameters for the Hulthén S-state wave function are $N^2=0.765$ F^{-1}, $\beta=1.26$ F, corresponding to a normalization $\int_0^\infty u_H{}^2(r)dr=0.93$.

0.7% for the D state. This error is largest for $r\lesssim 2.5$ F and decreases very rapidly as the wave functions approach their asymptotic values. Near the origin the abrupt character of the hard-core wave functions is replaced by the smooth behavior of the analytic wave functions.[9] However there is a question of how well one ought to fit the core region since its form reflects our inability to specify the wave function in this region from experimental data. Only in very high energy scattering could one hope to detect differences in the two types of core behavior. The important feature of the present analytic wave function is that it does very well in the region where all numerical wave functions agree on the basis of scattering data up to ~300 MeV. Furthermore, refinement in the fit, without loss in simplicity of form, can easily be obtained by adding more poles and sum rules to Eq. (6).

The parameters given in Table I give a deuteron effective range $\rho(-\epsilon,-\epsilon)=1.749$ F, ($N=0.8896$ F$^{-1/2}$), a quadrupole moment, $Q=0.282$ F^2, an asymptotic D to S ratio, $\rho=0.0269$, and a percentage D state of 7%, all in agreement with the experimental data.[10]

The author is indebted to Professor L. Durand, III for calling attention to this problem, and to Dr. B. M. Casper for supplying several numerical wave functions.

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[10] M. J. Moravcsik, *The Two Nucleon Interaction* (Clarendon Press, Oxford, England, 1963).

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Comprehensive Formalism for Nuclear Reaction Problems. I. Derivation of Existing Reaction Theories*

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An attempt is made to reduce the confusion arising from the existence of many different theories of resonance reactions. The method is to set up a formalism which is sufficiently general so that individual theories may be obtained by appropriate specialization. Such a formalism is obtained by suitably generalizing that devised by Bloch for a smaller range of theories. The formalism facilitates comparison of the structure of the various theories. Also, as we shall show in a subsequent paper, it gives a neat and systematic framework for study of the line-broadening problem.

I. INTRODUCTION

THERE now exist a multitude of theories of nuclear reactions, expressed in different formalisms and designed for various objectives. In this situation, it is useful to have a formal framework such that any particular theory can be derived by appropriate specialization. This facilitates comparison of different theories, and creates order out of chaos. Such a framework was given by Bloch[1] several years ago, and he showed how it could be specialized to the theories then available. The number of theories has since doubled, and it is again desirable to systematize the field in this manner. It turns out that the method

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* Supported in part by the U. S. Air Force Office of Scientific Research.

[1] C. Bloch, Nucl. Phys. 4, 503 (1957).

of Bloch is sufficiently powerful to cope with the new influx. Our main objective in the present paper is to demonstrate this.

The basic problem in nuclear reaction theory is to find the most useful expression for the scattering matrix. Since resonances are a common feature of observed nuclear reactions, such an expression should contain both "resonance" and "background" terms. There are many different ways of introducing resonances into the theory. Essentially one must fabricate a set of discrete states, and then express the actual wave function (and the scattering matrix) in terms of these. There are two main methods available, and existing theories can accordingly be classified into two groups.

A. Theories Using the Artifice of Imposed Boundary Conditions at the Channel Radii

Such theories inevitably involve a dependence of all parameters (widths, resonance energies) on the radii and on the boundary condition parameters; to compensate for this, the compound states are solutions of the total Hamiltonian, and the theories include re-arrangement and antisymmetry effects without difficulty.

(a) Kapur and Peierls[2] use the boundary condition of outgoing waves, so that all states and parameters are complex and energy-dependent.

(b) Wigner and Eisenbud[3] (*R*-matrix theory) use boundary conditions which are real and energy-independent, and all parameters have these same features.

(c) Brown and de Dominicis[4] use the theory of Kapur and Peierls to discuss the separation of "background" and "resonance" contributions to elastic scattering. They set up the average $\bar{S}$ of the elastic scattering amplitude S over an energy region containing many compound states. (An optical potential is defined to reproduce this quantity.) The scattering amplitude S in an energy region is then a sum of two parts; one is the "resonance" term corresponding to levels in the region (the "local levels"); the other is the "background," equal (apart from end effects) to $\bar{S}$ minus the averaged resonance term. Since the local levels depend on channel radii, this division into "resonance" and "background" also depends on these radii.

(d) Sano, Yoshida, and Terasawa[5] made a similar division, but the treatment is more general in that the entire scattering matrix is averaged, and reproduced by an optical potential matrix (implying coupled-channel effects).

B. Theories Using the Artifice of a Modified Hamiltonian

These theories avoid the introduction of channel radii, but contain implicit energy dependences and complex parameters. When the Hamiltonian is modified with projection operators (as in the first two of the three cases below), it is not easy to antisymmetrize or to take rearrangements into account.

(a) Feshbach[6] introduces the modified Hamiltonian QHQ, where H is the normal Hamiltonian and Q projects on to closed channels. Q changes discontinuously with energy[7] at each threshold, and so do the eigenstates of QHQ. In the energy region between two consecutive thresholds, Q and the states are fixed. Those states whose energies fall inside the region are real and discrete. Resonances arise through the coupling of these states to the continuum by $H\text{-}QHQ$. The calculations of Lemmer and Shakin[8] are based on this method, and explicitly evaluate the eigenstates of QHQ.

(b) Rodberg[9] and MacDonald[10] consider the modified Hamiltonian H_M which is the sum of the Hamiltonian of the target and incident particle in a potential U. When the effects of the coupling $(H-H_M)$ are included, the unbound states of H_M are taken to modify the "background" scattering matrix due to the real potential U, while the bound states give rise to resonances. This division is somewhat arbitrary, especially for states of H_M near zero energy, but at least the states do not change when thresholds are crossed. In general, U is chosen to reduce the above modification to the background to a minimum, but this is not a necessary choice. Garside and MacDonald[11] have shown that it is convenient to modify (increase) U to bind any single-particle states just above zero energy, thereby making them appear in the theory in resonances rather than in the background. The channel-coupling calculations of Hill and Buck[12] fit into the present scheme, in the sense that their channel-coupling potential is just $(H-H_M)$. However, they solve the coupled differential equations directly, and so avoid explicitly introducing "resonances" and "backgrounds." In the simple case of one open and one closed channel, the Feshbach method (a) above coincides with the present one.

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[2] P. L. Kapur and R. E. Peierls, Proc. Roy. Soc. (London) **A166**, 277 (1938).

[3] E. P. Wigner and L. Eisenbud, Phys. Rev. **72**, 29 (1947).

[4] G. E. Brown and C. T. de Dominicis, Proc. Phys. Soc. (London) **A72**, 70 (1958).

[5] M. Sano, S. Yoshida, and T. Terasawa, Nucl. Phys. **6**, 20 (1958).

[6] H. Feshbach, Ann. Phys. (N.Y.) **5**, 357 (1958); **19**, 287 (1962).

[7] Feshbach has pointed out that, when interest is restricted to an energy range containing a limited number of thresholds, P may be made independent of energy by letting it project on all of the relevant channels. The penalty for this is that QHQ omits such a large part of H that its eigenstates are unlikely to have any relation to the observed resonances.

[8] R. Lemmer and C. Shakin, Ann. Phys. (N.Y.) **27**, 13 (1964).

[9] L. Rodberg, Phys. Rev. **124**, 210 (1961).

[10] W. M. MacDonald, Nucl. Phys. **54**, 393 (1964); **56**, 636 (1964); **56**, 647 (1964).

[11] L. Garside and W. M. MacDonald, Phys. Rev. **138**, B582 (1965).

[12] A. D. Hill and B. Buck (to be published).

(c) Herzenberg, Kwok, and Mandl[13] also consider a modified Hamiltonian to set up a complete set of states which are to be associated with resonances. Their method is quite different to the last two. They multiply the total potential energy of the system by a variable parameter μ, and find the eigenvalues, μ_n, of μ such that the corresponding wave functions, Φ_n, satisfy the outgoing boundary condition at given total energy E. All wave functions Φ_n have energy E. Both μ_n and Φ_n are complex and energy dependent. The Φ_n form, in a sense, a complete orthonormal set, and the scattering matrix can be expanded as a sum over levels n. Instead of the usual resonance denominators, there are denominators (μ_n-1). As E varies, a resonance appears in the scattering matrix if E passes through an energy range where, for one of the n, $\mathrm{Re}[\mu_n(E)]=1$.

In the next section, Bloch's method is described, and in subsequent sections, it is specialized to the various theories above. In order to extend to theories of class B, it is necessary to generalize the Bloch theory by introducing Green's functions for the modified Hamiltonian. In a future paper, the extended method is applied to the line-broadening problem, and to the study of doorway states.

2. BLOCH METHOD FOR THE ONE-BODY PROBLEM

Any nuclear reaction theory has to take account of the fact that, when open channels are present, the momentum is not a Hermitian operator, and neither are functions of it such as H or $(H-E)^{-1}$, where H is the Hamiltonian.

A. Mathematical Preliminaries

Consider the one-body problem, for simplicity, and work in spherical coordinates (r,Ω). The Hermiticity of H is related to the validity of certain vital mathematical operations in the theory, viz., the commuting of differentiation and summation. Take two states $X\equiv\chi(r)Y(\Omega)$ and $\Phi\equiv\phi(r)Y(\Omega)$, where $Y(\Omega)$ is a spherical harmonic, and the operator $A=(1/r)(d^2/dr^2)r$. All matrix elements, e.g.,

$$\langle X|A|\Phi\rangle\equiv\int_0^{(a+\delta)} r^2dr\,\chi^*(r)\frac{1}{r}\frac{d^2}{dr^2}r\phi(r)\,, \tag{1}$$

are defined with upper limit $(a+\delta)$, where $\delta\to 0_+$ after integration. Suppose that ϕ can be expanded in an infinite series which converges uniformly in $0\leqslant r<a$:

$$\phi(r)=\sum_\lambda a_\lambda u_\lambda(r)\,.$$

The uniform convergence means that the series can be differentiated, i.e., $(d/dr)\sum_\lambda=\sum_\lambda(d/dr)$, for $0\leqslant r<a$. Integration by parts gives

$$\int dr(r\chi)^*\frac{d^2}{dr^2}(r\phi)=\int dr(r\phi)\frac{d^2}{dr^2}(r\chi)^* +\left[(r\chi)^*\frac{d}{dr}(r\phi)-(r\phi)\frac{d}{dr}(r\chi)^*\right]_{r=a}. \tag{2}$$

This equation also holds with ϕ replaced by u_λ. Summing the equation thus obtained with coefficients a_λ, and using the uniform convergence of ϕ to perform term-by-term integration, i.e., $\int dr\sum_\lambda=\sum_\lambda\int dr$, we get

$$\int dr(r\chi)^*\left[\frac{d^2}{dr^2}(r\phi)-\sum_\lambda a_\lambda\frac{d^2}{dr^2}(ru_\lambda)\right] =\left[(r\chi)^*\left\{\frac{d}{dr}(r\phi)-\sum_\lambda a_\lambda\frac{d}{dr}(ru_\lambda)\right\}\right]_{r=a}; \tag{3}$$

thus

$$\langle X|A|\phi\rangle\neq\sum_\lambda\langle X|A|\lambda\rangle\langle\lambda|\phi\rangle.$$

Since ϕ is uniformly convergent for $r<a$, d^2/dr^2 and $\sum_\lambda$ commute everywhere except for $r=a$, and it is the contribution from $r=a$ that gives rise to the right-hand side of (3). A finite contribution from a vanishingly small region implies a delta function in the integrand. We see that the right-hand side is canceled if d^2/dr^2 is replaced by the combination $[(d^2/dr^2)-\delta(r-a)(d/dr)]$. This combination is also Hermitian, as is clear from (2). Thus, with d^2/dr^2, the additions needed to allow commutivity with $\sum_\lambda$ and for Hermiticity are the same. This is not always so. $[(1/r)(d/dr)r]$ is not Hermitian [its conjugate is $-(1/r)(d/dr)r+\delta(r-a)$], but

$$\langle\chi|\frac{1}{r}\frac{d}{dr}r|\phi\rangle=\sum_\lambda a_\lambda\langle\chi|\frac{1}{r}\frac{d}{dr}r|u_\lambda\rangle.$$

The same is true of any complex function or r. Thus Hermiticity is not necessary to guarantee commutivity, but it is sufficient[14] (provided always that term-by-term integration is correct, and that the operator differentiates only to the right):

$$\begin{aligned}\langle X|A|\Phi\rangle&=\langle\Phi|A|X\rangle^*\\&=\sum_\lambda\langle\Phi|\lambda\rangle^*\langle\lambda|A|X\rangle^*\\&=\sum_\lambda\langle X|A|\lambda\rangle\langle\lambda|\Phi\rangle.\end{aligned}$$

A less stringent sufficient condition is clearly that the Hermitian conjugate A^+ operate only to the right. This then includes $[(1/r)(d/dr)r]$, and all complex functions of r. We will call the operators that commute with

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[13] A. Herzenberg, K. L. Kwok, and F. Mandl, Proc. Phys. Soc. (London) 84, 477 (1964).

[14] It is easy to find examples to show that it is not necessary. When integrals are over all space, and we expand a free-state $|\psi\rangle$ in plane waves $|\mathbf{k}\rangle$, ∇^2 is not Hermitian: $\langle\mathbf{k}|\nabla^2|\psi\rangle\neq\langle\psi|\nabla^2|\mathbf{k}\rangle^*$, but nevertheless the relation $\langle\mathbf{k}|\nabla^2|\psi\rangle\int d\mathbf{k}'\langle\mathbf{k}|k'^2\psi(\mathbf{k}')|\mathbf{k}'\rangle=k^2\psi(\mathbf{k})$ is used in the transformation to momentum space. In such cases, the necessary condition of uniform convergence is weaker than the Hermiticity requirement.

$\sum_\lambda$ "realizable operators." If A is realizable[15] in the representation $|\lambda\rangle$, then

$$\langle X|A|\Phi\rangle=\langle X|A)(|\Phi\rangle,$$
$$\langle X|AB|\Phi\rangle=\langle X|A)(B|\Phi\rangle,$$

where the notation means

$$\langle\cdots P)(Q\cdots\rangle\equiv\textstyle\sum_\lambda\langle\cdots P|\lambda\rangle\langle\lambda|Q\cdots\rangle.$$

B. Application to Reaction Theory

It is easy to see that the operator H cannot be commuted with a summation over a complete set of states of H defined inside $r=a$. For instance, if $\phi=\sum_\lambda a_\lambda\psi_\lambda$, $H\phi=E\phi$, $H\psi_\lambda=E_\lambda\psi_\lambda$, then operating on the expansion with H, and taking the scalar product with ψ_λ gives $E=E_\lambda$ for any λ, which is absurd. The same result applies to any function of H. Errors may occur from passing $(H-E)^{-1}$ through expansions.[16] From the above discussion, a sufficient means to avoid this pitfall is to make H "realizable" by a suitable addition, viz. $[H+\mathcal{L}(b)]$, where

$$\mathcal{L}(b)=\frac{\hbar^2}{2m}\delta(r-a)\left(\frac{d}{dr}-\frac{(b-1)}{a}\right). \tag{4}$$

Here, b can be any prescribed real or complex number. If a wave function $\psi(r)$ satisfies $\mathcal{L}(b)\psi(r)=0$, this means that

$$\left[\frac{d}{dr}\psi-\frac{(b-1)}{a}\right]_{r=a}=0$$

or

$$\left[\frac{r}{(r\psi)}\frac{d}{dr}(r\psi)\right]_{r=a}=b; \tag{5}$$

i.e., b is the logarithmic derivative of the radial wave function.

The Schrödinger equation may be written as

$$[H+\mathcal{L}(b)-E]\psi=\mathcal{L}(b)\psi,$$

with solution [for $\psi(r)$ in terms of $\psi(a)$ and $(d\psi/dr)_{r=a}$]

$$\psi=[H+\mathcal{L}(b)-E]^{-1}\mathcal{L}(b)\psi. \tag{6}$$

We now assume that, if an operator like $H+\mathcal{L}(b)$ is realizable, then any function of it like $[H+\mathcal{L}(b)-E]^{-1}$ is also. Thus we may insert the unit operator. Suppose that the states $|\lambda\rangle$ form a complete orthogonal set inside $r=a$ and satisfy a boundary condition at $r=a$. In general, this condition is complex and the orthogonality relation has the form

$$\langle\tilde\lambda|\mu\rangle\equiv\int\tilde\psi_\lambda{}^*(\mathbf{r})\psi_\mu(\mathbf{r})d\mathbf{r}=\delta_{\lambda\mu},$$

where

$$\psi_\lambda(\mathbf{r})\equiv\langle\mathbf{r}|\lambda\rangle,\quad \tilde\psi_\lambda(\mathbf{r})\equiv\langle\mathbf{r}|\tilde\lambda\rangle$$

and $\langle\mathbf{r}|\tilde\lambda\rangle$ is the complex conjugate of the time-reversed state:

$$\langle\mathbf{r}|\tilde\lambda\rangle=\langle\mathbf{r}|K|\lambda\rangle^*,$$

K being the usual time-reversal operator. In terms of radial and angular coordinates for one particle, if $\psi_\lambda(\mathbf{r})=u_\lambda(r)Y(\Omega)$ then $\tilde\psi_\lambda(\mathbf{r})=u_\lambda{}^*(r)Y(\Omega)$. The completeness relation is

$$\sum_\lambda\tilde\psi_\lambda{}^*(\mathbf{r})\psi_\lambda(\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')$$

or

$$\sum_\lambda|\lambda\rangle\langle\tilde\lambda|=1.$$

Thus Eq. (6) may be written as

$$\psi=\sum_{\lambda,\mu}|\mu\rangle\langle\tilde\mu|[H+\mathcal{L}(b)-E]^{-1}|\lambda\rangle\langle\tilde\lambda|\mathcal{L}(b)\psi\rangle. \tag{6$'$}$$

The last matrix element is, from (4),

$$\langle\tilde\lambda|\mathcal{L}(b)\psi\rangle=\frac{\hbar^2}{2m}u_\lambda(a)\left[r\frac{d}{dr}(ru)-b(ru)\right]_{r=a}. \tag{7}$$

The matrix elements of $(H+\mathcal{L}-E)$ satisfy

$$\begin{aligned}\langle\tilde\mu|H+\mathcal{L}-E|\lambda\rangle&=\langle\lambda|H+\mathcal{L}^*-E|\tilde\mu\rangle^*\\&=\langle(H+\mathcal{L}^*-E)\tilde\mu|\lambda\rangle\\&=\langle\tilde\lambda|H+\mathcal{L}-E|\mu\rangle.\end{aligned}$$

These relations follow from the Hermiticity of

$$H+\tfrac{1}{2}(\mathcal{L}+\mathcal{L}^*)\quad\text{and}\quad i(\mathcal{L}-\mathcal{L}^*)$$

and the reality of the angular integration.

C. Kapur-Peierls Theory

Kapur and Peierls[2] defined their complete set by the boundary condition of outgoing waves, i.e., if the outgoing wave solution in the channel is $u(r)=r^{-1}O(r)$

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[15] In formal quantum-mechanical terms, the position is this: Consider $A|\Phi\rangle$. There exists at least one representation in which A is "realized," i.e., $A=\sum_{p,q}|p\rangle\langle p|A|q\rangle\langle q|$ (since A is defined in some such representation). There also exists a representation in which $|\Phi\rangle$ is realized (i.e., expandable) i.e., $|\Phi\rangle=\sum_\alpha|\alpha\rangle\langle\alpha|\Phi\rangle$. The condition that $A|\Phi\rangle$ can be written in matrix form, i.e., $A|\Phi\rangle=\sum_{p,q}|p\rangle\langle p|A|q\rangle\langle q|\Phi\rangle$, is clearly that there exists a common representation $|p\rangle$ in which both A and $|\Phi\rangle$ are realized. In the type of problem we are considering, most representations other than that of energy eigenfunctions are in this category; for instance, the space coordinate or momentum representation. The energy-eigenfunction representation $|\lambda\rangle$ is exceptional in that certain operators are not realized in it, i.e., $A\neq\sum_{\lambda,\mu}|\lambda\rangle\langle\lambda|A|\mu\rangle\langle\mu|$. The wave functions Φ are realized, however, i.e., $|\Phi\rangle=\sum_\lambda|\lambda\rangle\langle\lambda|\Phi\rangle$ (unless the states $|\lambda\rangle$ are defined with the boundary condition that they vanish at $r=a$).

It is important that the property of being realizable is not an absolute property of the operator, but is a property of the operator and the representation. An operator can be realizable in one representation, but not in another.

For some operators, one must establish a more basic property, viz., their existence; for example, inverse operators, like $(H-E)^{-1}$. We shall not discuss this problem, but note that existence is independent of representation, in contrast to realizability (since the determinant of an operator is independent of representation).

[16] W. Tobocman and M. A. Nagarajan, Phys. Rev. 138, B1351 (1965). If the ϕ_n are defined by boundary conditions at $r_\alpha=R_\alpha'$, then Eq. (21) in this reference becomes invalid when $R_\alpha=R_\alpha'$.

where $O(r)\propto e^{ikr}$ as $r\rightarrow\infty$, then the wave functions satisfy

$$\mathcal{L}(b)\psi_\lambda=0,$$

where

$$b=\left[\frac{r}{O}\frac{d}{dr}O\right]_{r=a}.$$

This choice of b is the most important in practice: we denote the corresponding $\mathcal{L}(b)$ simply by $\mathcal{L}$. The important consequence of this particular choice is that $\mathcal{L}\psi$ contains no outgoing wave, but only the (known) ingoing wave. Thus (6′) is truly a solution. If the incoming wave part of $ru(r)$ is $I(r)$, with $I(r)\propto e^{-ikr}$ as $r\rightarrow\infty$, and if I and O satisfy the relations

$$I=O^*=\tilde{O},$$
$$I\frac{d}{dr}O-O\frac{d}{dr}I=2ik, \tag{8}$$

then (7) becomes

$$\langle\tilde{\lambda}|\mathcal{L}\psi\rangle=\left\langle\tilde{\lambda}\middle|\mathcal{L}\frac{I}{r}Y\right\rangle=-\frac{\hbar^2}{2m}\left(\frac{ru_\lambda}{O}\right)_{r=a}(2ik)$$
$$=-\frac{2ika}{O(a)}\left(\frac{\hbar^2}{2ma}\right)^{1/2}\gamma_\lambda, \tag{9}$$

where we have introduced reduced width amplitudes by the definition

$$\gamma_\lambda=\left(\frac{\hbar^2a}{2m}\right)^{1/2}u_\lambda(a). \tag{10}$$

Equating expression (6′) to $(1/r)(I-SO)Y(\Omega)$ at $r=a$, the scattering amplitude S emerges as

$$S=\frac{I(a)}{O(a)}+\frac{2ika}{[O(a)]^2}\sum_\lambda\frac{\gamma_\lambda{}^2}{E_\lambda-E}. \tag{11}$$

An instructive alternative derivation of S is as follows: Using the fact that $\psi(r)=(1/r)(I-SO)$, and the definition of $\mathcal{L}$, one may derive a number of alternative formal expressions for S:

$$S=\frac{i}{\hbar v}\langle\mathcal{O}|\mathcal{L}^*|\psi\rangle \tag{12a}$$

$$=\frac{i}{\hbar v}\langle\mathcal{O}-\tilde{\psi}|\mathcal{L}|\mathcal{I}\rangle, \tag{12b}$$

where v is velocity $(\hbar k/m)$, and $\mathcal{I}$, $\mathcal{O}$ are the complete in- and outgoing-wave solutions:

$$\mathcal{I}(r,\Omega)=\frac{I(r)}{r}Y(\Omega),\quad \mathcal{O}(r,\Omega)=\frac{O(r)}{r}Y(\Omega).$$

Using the fact that

$$\langle\mathcal{O}|\mathcal{L}^*|\mathcal{O}\rangle=-\langle\mathcal{I}|\mathcal{L}|\mathcal{I}\rangle=i\hbar v,$$

the further forms of S may be found:

$$i\hbar v(S-\mathcal{S})=-\langle\mathcal{O}|\mathcal{L}^*|\psi+\mathcal{S}\mathcal{O}\rangle, \tag{12c}$$

and

$$i\hbar v(S-\mathcal{S})=-\langle\tilde{f}-\tilde{\psi}|\mathcal{L}|f\rangle, \tag{12d}$$

where $\mathcal{S}$ is any assigned number and $f=\mathcal{I}-\mathcal{S}\mathcal{O}$.

The rederivation of Kapur-Peierls is best made from (12a). However, we must be careful. We cannot make a dispersion sum directly out of

$$\mathcal{L}^*|\psi\rangle=\mathcal{L}^*(H+\mathcal{L}-E)^{-1}\mathcal{L}|\mathcal{I}\rangle,$$

since $\mathcal{L}^*$ is not realizable.

However, $(H+\mathcal{L}^*)$ and $(\mathcal{L}-\mathcal{L}^*)$ are realizable, so

$$\begin{aligned}\mathcal{L}^*|\psi\rangle&=(H+\mathcal{L}^*-E)|\psi\rangle\\&=(H+\mathcal{L}-E)|\psi\rangle+(\mathcal{L}^*-\mathcal{L})|\psi\rangle\\&=\mathcal{L}|\mathcal{I}\rangle+(\mathcal{L}^*-\mathcal{L})(H+\mathcal{L}-E)^{-1}\mathcal{L}|\mathcal{I}\rangle,\end{aligned}$$

whence

$$\begin{aligned}\langle\mathcal{O}|\mathcal{L}^*|\psi\rangle&=\langle\mathcal{O}|\mathcal{L}|\mathcal{I}\rangle-\langle\mathcal{O}|(\mathcal{L}^*-\mathcal{L})(H+\mathcal{L}-E)^{-1}\\&\qquad\times(\mathcal{L}^*-\mathcal{L})|\mathcal{I}\rangle\\&=\langle\mathcal{O}|\mathcal{L}|\mathcal{I}\rangle-\langle\mathcal{L}^*\mathcal{O}|(H+\mathcal{L}-E)^{-1}\mathcal{L}|\mathcal{I}\rangle.\end{aligned} \tag{13}$$

Now

$$\begin{aligned}\langle\mathcal{O}|\mathcal{L}^*-\mathcal{L}|\lambda\rangle&=\langle\tilde{\lambda}|\mathcal{L}^*-\mathcal{L}|\mathcal{I}\rangle\\&=-\langle\tilde{\lambda}|\mathcal{L}|\mathcal{I}\rangle=-\langle\mathcal{L}^*\mathcal{O}|\lambda\rangle,\end{aligned} \tag{14}$$

so

$$\langle\mathcal{O}|\mathcal{L}^*|\psi\rangle=\langle\mathcal{O}|\mathcal{L}|\mathcal{I}\rangle-\sum_\lambda\frac{\langle\tilde{\lambda}|\mathcal{L}|\mathcal{I}\rangle^2}{E_\lambda-E}. \tag{15}$$

Using (9) and (12a) we find this to be the same as (11).

D. Brown–de Dominicis Theory

The essential feature that distinguishes this form of S from the Kapur-Peierls one is the elimination of $\mathcal{L}$ in favor of the potential V.

It is most convenient to start from (12d) with $\mathcal{S}=1$, the point being that the combination $J=\mathcal{I}-\mathcal{O}$ is regular at $r=0$, and this is necessary for the Hermiticity property of matrix elements that is to be used. We write

$$\begin{aligned}\langle\tilde{J}-\tilde{\psi}|\mathcal{L}|J\rangle=\langle\tilde{J}|\mathcal{L}|\mathcal{I}\rangle-\langle\tilde{\psi}|H+\mathcal{L}-E|J\rangle\\+\langle\tilde{\psi}|H-E|J\rangle.\end{aligned}$$

Since

$$\begin{aligned}\langle\tilde{\psi}|H+\mathcal{L}-E|J\rangle&=\langle\tilde{J}|H+\mathcal{L}-E|\psi\rangle\\&=\langle\tilde{J}|\mathcal{L}|\mathcal{I}\rangle,\end{aligned}$$

the first two terms cancel, and

$$\begin{aligned}i\hbar v(S-1)&=-\langle\tilde{\psi}|H-E|J\rangle\\&=-\langle(H-E)\tilde{J}|\psi\rangle\\&=-\langle\tilde{J}|V|\psi\rangle,\end{aligned}$$

where we have used $(H-E-V)J=0$.

The solution ψ may be written:

$$\begin{aligned} |\psi\rangle &= (H+\mathcal{L}-E)^{-1}\mathcal{L}|\psi\rangle \\ &= (H+\mathcal{L}-E)^{-1}\mathcal{L}|J\rangle \\ &= [1-(H+\mathcal{L}-E)^{-1}(H-E)]|J\rangle. \end{aligned} \tag{16}$$

Thus

$$i\hbar v(S-1) = -\langle\tilde{J}|V-V(H+\mathcal{L}-E)^{-1}V|J\rangle. \tag{17}$$

This is the expression given by Brown and de Dominicis[4]; the term in V is the Born term, and the other term is a dispersion sum if the Kapur-Peierls set is introduced.

It is easy to modify this so that the free-space solution J is replaced by that of a given potential $\mathcal{V}$. If this is ϕ, which is $\mathcal{I}-\mathcal{S}(\mathcal{V})\mathcal{O}$ for $r\geqslant a$, where $S(\mathcal{V})$ is the scattering amplitude for $\mathcal{V}$, then (12d) with $\mathcal{S}=S(\mathcal{V})$ is

$$\begin{aligned} i\hbar v[S-S(\mathcal{V})] &= -\langle\tilde{\phi}-\tilde{\psi}|\mathcal{L}|\phi\rangle \\ &= -\langle\tilde{\psi}|H-E|\phi\rangle \\ &= -\langle(H-E)\tilde{\phi}|\psi\rangle \\ &= -\langle\tilde{\phi}|\Delta|\psi\rangle, \end{aligned} \tag{18}$$

where $\Delta=V-\mathcal{V}$. The solution (16) may be rewritten:

$$|\psi\rangle = [1-(H+\mathcal{L}-E)^{-1}(H-E)]|\phi\rangle, \tag{19}$$

so

$$i\hbar v[S-S(\mathcal{V})] = -\langle\tilde{\phi}|\Delta-\Delta(H+\mathcal{L}-E)^{-1}\Delta|\phi\rangle. \tag{20}$$

E. Relation to Lippmann-Schwinger Theory

Expressions (17) and (12) give a form for the scattering amplitude S which is almost identical to that obtainable from the theory of Lippmann and Schwinger[17]; the same is true of (16) for the wave function. The only difference is that the function $\langle\mathbf{r}'|(H+\mathcal{L}-E)^{-1}|\mathbf{r}\rangle$ replaces the Green's function which incorporates the outgoing-wave boundary condition, viz.,

$$G(\mathbf{r}',\mathbf{r}) = \underset{\epsilon\to 0+}{L}\int\rho(\mathbf{k})d\mathbf{k}\int\rho(\mathbf{k}')d\mathbf{k}'\langle\mathbf{r}'|\mathbf{k}'\rangle \times\langle\mathbf{k}'|(H-i\epsilon-E)^{-1}|\mathbf{k}\rangle\langle\mathbf{k}|\mathbf{r}\rangle,$$

where $\rho(\mathbf{k})$ is the density of the set of continuum states labeled by $\mathbf{k}$:

$$\int\langle\mathbf{r}|\mathbf{k}\rangle\langle\mathbf{k}|\mathbf{r}'\rangle\rho(\mathbf{k})d\mathbf{k} = \delta(\mathbf{r}-\mathbf{r}'),$$

and the limit is taken after integration.

In fact, the two functions are identical in the region $r\leqslant a$. The only difference is that $G(\mathbf{r}',\mathbf{r})$ is defined for all $\mathbf{r}'$, $\mathbf{r}$, whereas the Bloch function is defined for r, $r'\leqslant a$ only. This difference is irrelevant in (17) since the presence of V restricts the ranges of integration; it is irrelevant if (16) is applied to $\langle\mathbf{r}|\psi\rangle$ for $r\leqslant a$. The two functions must be identical for $r\leqslant a$ since they are both Green's functions satisfying the same boundary conditions, *viz.*, $G(\mathbf{r}',\mathbf{r})$ is regular at r, $r'=0$ and becomes an outgoing wave in r (or r') if r (or r') is outside the region of V while r' (or r) is inside. There is only one function satisfying these requirements, viz., $G(\mathbf{r}',\mathbf{r})=\text{const}\times u(r_<)u_0(r_>)$, where $u(r)$, $u_0(r)$ are the solutions of H at energy E such that $u(0)=1$, $u_0(r)\to e^{ikr}/r$ for $r\geqslant a$.

F. Mandl-Kwok-Herzenberg Theory

Instead[13] of developing the last term of (17) with the Kapur-Peierls set, which depends on radius a, one may define a set by

$$\begin{aligned} [T+\mu_n(E)V-E]\phi_n(\mathbf{r},E) &= 0, \\ \mathcal{L}\phi_n(\mathbf{r},E) &= 0. \end{aligned} \tag{21}$$

The eigenvalues $\mu_n(E)$ are the complex multiplicative factors of the potential needed to make the solution at energy E satisfy the outgoing wave boundary condition. The solutions $\phi_n(\mathbf{r},E)$ differ from the Kapur-Peierls ones in that they continue as outgoing waves to $r=\infty$. Thus the choice of radius a in the operator $\mathcal{L}$ is irrelevant, and the theory is independent of this parameter. The orthogonality and completeness relations are

$$\begin{aligned} \langle\tilde{\phi}_n|V|\phi_m\rangle &= \delta_{nm}\langle\tilde{\phi}_n|V|\phi_n\rangle, \\ \sum_n \frac{V|\phi_n\rangle\langle\tilde{\phi}_n|}{\langle\tilde{\phi}_n|V|\phi_n\rangle} &= 1. \end{aligned} \tag{22}$$

Thus the form of $(H+\mathcal{L}-E)^{-1}$ in terms of the set is

$$\begin{aligned} (H+\mathcal{L}-E)^{-1} &= \sum_n (H+\mathcal{L}-E)^{-1}\frac{V|\phi_n\rangle\langle\tilde{\phi}_n|}{\langle\tilde{\phi}_n|V|\phi_n\rangle} \\ &= \sum_n \frac{|\phi_n\rangle\langle\tilde{\phi}_n|}{[1-\mu_n(E)]\langle\tilde{\phi}_n|V|\phi_n\rangle}. \end{aligned} \tag{23}$$

Insertion of this into the last term of (17) gives the form of S derived by Mandl, Kwok, and Herzenberg. The factors in the numerator satisfy the relation

$$\langle\tilde{\phi}_n|V|\mathcal{I}-\mathcal{O}\rangle = [\mu_n(E)]^{-1}\langle\tilde{\phi}_n|\mathcal{L}|\mathcal{I}\rangle.$$

The right-hand side is still independent of the radius a as a consequence of the fact that $\phi_n\propto\mathcal{O}$ for $r>a$.

A more compact and symmetric statement of the above relations is in terms of operator $V^{1/2}$ and functions

$\Phi_n=V^{1/2}\phi_n\langle\tilde{\phi}_n|V|\phi_n\rangle^{-1/2}$, i.e.

$$\begin{aligned} \langle\tilde{\Phi}_n|\Phi_m\rangle &= \delta_{nm}, \\ \sum_n |\Phi_n\rangle\langle\tilde{\Phi}_n| &= 1, \\ V^{1/2}(H+\mathcal{L}-E)^{-1}V^{1/2} &= \sum_n \frac{|\Phi_n\rangle\langle\tilde{\Phi}_n|}{1-\mu_n(E)}. \end{aligned} \tag{24}$$

A straightforward generalization can be made to the case where V is replaced in the Schrödinger equation by $\mu_n(E)V_1+V_2$, where $V=V_1+V_2$.

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[17] B. A. Lippmann and J. Schwinger, Phys. Rev. 79, 469 (1950)

3. GENERALIZATION TO MANY CHANNELS

Label various two-particle channels by c, where this represents αsl, α being the intrinsic states of the pair, s their channel spin, and l their relative angular momentum. (We will not bother to indicate coupling of **s** and **l** to total spin **J** as this only serves to complicate the notation.) Like R-matrix theory, the present theory cannot cope with channels with $\geqslant 3$ particles.

The new form of $\mathcal{L}(b)$ is

$$\mathcal{L}(b)=\sum_c |c\rangle\frac{\hbar^2}{2m_c}\delta(r_c-a_c)\left(\frac{d}{dr_c}-\frac{(b_c-1)}{a_c}\right)\langle c| , \quad (25)$$

where b now stands for the set b_c, m_c is the reduced channel mass and $|c\rangle$ is the channel wave function $|\phi_{\alpha s}Y_l\rangle$ which is a function of intrinsic and angular variables, but not r_c.

A. Kapur-Peierls Theory

As before, the Kapur-Peierls[2] form is $\mathcal{L}(b)\equiv\mathcal{L}$, say, where

$$b_c=\left[\frac{r_c}{O_c}\frac{d}{dr_c}O_c\right]_{r_c=a_c} . \quad (26)$$

Suppose that the wave function in the external region is $\psi^{(c)}$ for incoming waves in channel c:

$$\psi^{(c)}=\mathcal{I}_c-\sum_{c'} S_{c'c}\left(\frac{v_c}{v_{c'}}\right)^{1/2}\mathcal{O}_{c'} , \quad (27)$$

(where v_c are velocities) then $\mathcal{L}\psi$ retains only the term in $\mathcal{I}_c$. The incoming and outgoing wave solutions $\mathcal{I}_c$ and $\mathcal{O}_c$ are as before except that they contain also the channel spin and intrinsic wave functions:

$$\mathcal{I}_c=r_c^{-1}I_c(r_c)\{\phi_{\alpha s}Y_l\} .$$

Evaluating (6) and (27) on the channel surface of the c' channel and equating gives

$$S_{c'c}=\frac{I_c(a_c)}{O_c(a_c)}\delta_{c'c}+i\sum_\lambda\frac{g_{\lambda c}g_{\lambda c'}}{E_\lambda-E} , \quad (28)$$

where

$$g_{\lambda c}=(2k_ca_c)^{1/2}\gamma_{\lambda c}[O_c(a_c)]^{-1} , \quad (29)$$

and the reduced-width amplitudes are defined [cf. Eq. (10)]

$$\gamma_{\lambda c}=\left(\frac{\hbar^2 a_c}{2m_c}\right)^{1/2}\left\langle\frac{1}{r_c^2}\delta(r_c-a_c)\phi_{\alpha s}Y_l\middle|\lambda\right\rangle . \quad (30)$$

The alternative route to this form of $S_{c'c}$ starts from

$$S_{c'c}=\frac{i}{\hbar(v_{c'}v_c)^{1/2}}\langle\mathcal{O}_{c'}|\mathcal{L}^*|\psi^{(c)}\rangle . \quad (31)$$

From (6′), the matrix element is

$$\begin{aligned}\langle\mathcal{O}_{c'}|\mathcal{L}^*|\psi^{(c)}\rangle&=\langle\mathcal{O}_c|\mathcal{L}|\mathcal{I}_c\rangle\delta_{cc'}\\&\quad-\langle\mathcal{O}_{c'}|(\mathcal{L}^*-\mathcal{L})(H+\mathcal{L}-E)^{-1}(\mathcal{L}^*-\mathcal{L})|\mathcal{I}_c\rangle\\&=\langle\mathcal{O}_c|\mathcal{L}|\mathcal{I}_c\rangle\delta_{cc'}-\sum_\lambda\frac{\langle\tilde{\lambda}|\mathcal{L}|\mathcal{I}_{c'}\rangle\langle\tilde{\lambda}|\mathcal{L}|\mathcal{I}_c\rangle}{E_\lambda-E} ,\end{aligned} \quad (32)$$

and this gives the same as (28) when we use the relation

$$\langle\tilde{\lambda}|\mathcal{L}|\mathcal{I}_c\rangle=-\frac{2ik_ca_c}{O_c(a_c)}\left(\frac{\hbar^2}{2m_ca_c}\right)^{1/2}\gamma_{\lambda c}=-i\hbar^{1/2}v_c^{1/2}g_{\lambda c} . \quad (33)$$

B. Brown-de Dominicis Theory

The many-channel generalization of this[4] is almost immediate. In exact parallel to the development in Sec. 2, we find

$$i\hbar(v_cv_{c'})^{1/2}(S_{c'c}-\delta_{c'c})=-\langle(H-E)\tilde{J}_{c'}|\psi^{(c)}\rangle , \quad (34)$$

$$\psi^{(c)}=[1-(H+\mathcal{L}-E)^{-1}(H-E)]|J_c\rangle . \quad (35)$$

Defining channel potentials V_c by

$$(H-E)|J_c\rangle=V_c|J_c\rangle , \quad (36)$$

we find

$$\begin{aligned}&i\hbar(v_cv_{c'})^{1/2}(S_{c'c}-\delta_{c'c})\\&\quad=-\langle\tilde{J}_{c'}|V_{c'}-V_{c'}(H+\mathcal{L}-E)^{-1}V_c|J_c\rangle .\end{aligned} \quad (37)$$

Again the close connection with Lippmann-Schwinger theory[17] is evident. The corresponding equations in terms of solutions $\phi^{(c)}$ of a Hamiltonian H_0 are

$$\begin{aligned}&i\hbar(v_cv_{c'})^{1/2}[S_{c'c}-S_{c'c}(H_0)]\\&\quad=-\langle\tilde{\phi}^{(c')}-\tilde{\psi}^{(c)}|\mathcal{L}|\phi^{(c')}\rangle\\&\quad=-\langle(H-E)\tilde{\phi}^{(c')}|\psi^{(c)}\rangle ,\end{aligned} \quad (38)$$

$$|\psi^{(c)}\rangle=[1-(H+\mathcal{L}-E)^{-1}(H-E)]|\phi^{(c)}\rangle , \quad (39)$$

$$\begin{aligned}&i\hbar(v_cv_{c'})^{1/2}[S_{c'c}-S_{c'c}(H_0)]\\&\quad=-\langle(H-E)\tilde{\phi}^{(c')}|1-(H+\mathcal{L}-E)^{-1}(H-E)|\phi^{(c)}\rangle\\&\quad=-\langle\tilde{\phi}^{(c')}|\Delta_{c'}-\Delta_{c'}(H+\mathcal{L}-E)^{-1}\Delta_c|\phi^{(c)}\rangle .\end{aligned} \quad (40)$$

$\phi^{(c)}$ has incident waves in channel c only, but can have outgoing waves in any channel, i.e., H_0 can include channel coupling. $S_{c'c}(H_0)$ is the scattering matrix for H_0. Δ_c is given by $(H-E)\phi^{(c)}=(H-H_0)\phi^{(c)}=\Delta_c\phi^{(c)}$. The form (40) was derived by Sano, Yoshida, and Terasawa[5] for this general case including channel coupling. They set up the optical-model Hamiltonian H_0 for a set of channels by requiring that $\mathbf{S}(H_0)$ equals the energy average of $\mathbf{S}$ taken over fine-structure levels. This means that the average of the right-hand side of (40) must be zero. In the absence of exchange and rearrangements, this condition can be solved for H_0. This is more conveniently done in the Feshbach formalism to be discussed below.

As in the one-channel case treated in Sec. 2, the Green's function in (39) is identical to the one occurring in the Lippmann-Schwinger[17] solution for $\psi^{(c)}$, except that the former is defined in the internal region only.

C. Herzenberg, Kwok, and Mandl Theory

The generalization in this case[13] is obtained by inserting the appropriate form of $(H+\mathcal{L}-E)^{-1}$ in (37). This form is identical to (19), where the ϕ_n are now multi-channel wave functions satisfying

$$\begin{aligned}[][T+\mu_n(E)V-E]\phi_n&=0,\\ \mathcal{L}\phi_n&=0,\end{aligned}\tag{41}$$

where V is the total potential energy. More generally, if $V=V_1+V_2$, then we may work with $\mu_n(E)V_1+V_2$. However, in order to preserve antisymmetry of the theory, both V_1 and V_2 must be symmetric functions.

4. BLOCH METHOD FOR LINEAR MOMENTUM STATES

This is another easy generalization to make. We will label linear momentum channels by $a\equiv\alpha s\mathbf{k}$, $\mathbf{k}$ being momentum. Let us consider solutions $|\pi^{(a+)}\rangle$ and $|\pi^{(a-)}\rangle$ to the Hamiltonian H_0. These are solutions with a plane wave $|a\rangle$, say, in channel a, and differ in that $|\pi^{(a\pm)}\rangle-|a\rangle$ contains only outgoing (ingoing) waves. Since $\mathcal{L}$ eliminates outgoing waves,

$$\mathcal{L}|\psi^{(a+)}\rangle=\mathcal{L}|\pi^{(a+)}\rangle=\mathcal{L}|a\rangle.\tag{42}$$

From $(H-E)\psi^{(a+)}=0$,

$$\begin{aligned}|\psi^{(a+)}\rangle&=(H+\mathcal{L}-E)^{-1}\mathcal{L}|\pi^{(a+)}\rangle\\ &=[1-(H+\mathcal{L}-E)^{-1}(H-E)]|\pi^{(a+)}\rangle.\end{aligned}\tag{43}$$

The transition amplitude matrix $\mathbf{T}$ has a form very similar to the scattering matrix element of (34):

$$T_{a'a}-T_{a'a}(H_0)=\mathcal{T}_{a'a},\tag{44}$$

where

$$\mathcal{T}_{a'a}=\langle(H-E)\pi^{(a'-)}|\psi^{(a+)}\rangle\tag{45}$$

and $T_{a'a}(H_0)$ is the transition amplitude arising from H_0:

$$T_{a'a}(H_0)=\langle(H_0{}^*-E)a'|\pi^{(a+)}\rangle.\tag{46}$$

A. The Kapur-Peierls Theory

This theory[2] may be developed as in Sec. 3, using the fact that $H+\mathcal{L}$ is associative:

$$\begin{aligned}\mathcal{T}_{a'a}&=\langle(H-E)\pi^{(a'-)}|\psi^{(a+)}\rangle\\ &=\langle(H+\mathcal{L}^*-E)\pi^{(a'-)}|\psi^{(a+)}\rangle-\langle\mathcal{L}^*\pi^{(a'-)}|\psi^{(a+)}\rangle\\ &=\langle\pi^{(a'-)}|H+\mathcal{L}-E|\psi^{(a+)}\rangle-\langle\mathcal{L}^*\pi^{(a'-)}|\psi^{(a+)}\rangle\\ &=\langle\pi^{(a'-)}|\mathcal{L}|\pi^{(a+)}\rangle\\ &\qquad\qquad-\langle\mathcal{L}^*\pi^{(a'-)}|(H+\mathcal{L}-E)^{-1}\mathcal{L}|\pi^{(a+)}\rangle,\end{aligned}$$

whence

$$T_{a'a}=\langle a'|\mathcal{L}|a\rangle-\langle\mathcal{L}^*a'|(H+\mathcal{L}-E)^{-1}\mathcal{L}|a\rangle,\tag{47}$$

where we have used the relations

$$\begin{aligned}\langle a'|\mathcal{L}|a\rangle&=\langle a|\mathcal{L}^*|a'\rangle^*=\langle\mathcal{L}^*a'|a\rangle,\\ \langle(H_0{}^*-E)a'|\pi^{(a+)}\rangle&=\langle\pi^{(a'-)}|(H_0-E)a\rangle.\end{aligned}\tag{48}$$

Introduction of the Kapur-Peierls set (including all angular momentum states) gives

$$T_{a'a}=\langle a'|\mathcal{L}|a\rangle-\sum_\lambda\frac{g_{\lambda a'}g_{\lambda a}}{E_\lambda-E},\tag{49}$$

where

$$g_{\lambda a}=\langle\mathcal{L}^*a|\lambda\rangle=\langle\tilde{\lambda}|\mathcal{L}a\rangle.\tag{50}$$

The first term $\langle a'|\mathcal{L}|a\rangle$ is the hard-sphere scattering and is diagonal in αs.

B. Theories of Rodberg and MacDonald

The form of $\mathcal{T}_{a'a}$ used by these authors[9,10] follows directly from (43) and (45):

$$\begin{aligned}\mathcal{T}_{a'a}&=\langle(H-E)\pi^{(a'-)}|1-(H+\mathcal{L}-E)^{-1}(H-E)|\pi^{(a+)}\rangle\\ &=\langle\pi^{(a'-)}|\Delta_{a'}-\Delta_{a'}(H+\mathcal{L}-E)^{-1}\Delta_a|\pi^{(a+)}\rangle,\end{aligned}\tag{51}$$

where the channel potentials Δ_a are defined by $(H-H_0)\times|\pi^{(a+)}\rangle=\Delta_a|\pi^{(a+)}\rangle$. This is the linear momentum analogue of (40) set up by Sano, Yoshida, and Terasawa.

5. *R*-MATRIX THEORY

Let us consider a set of boundary conditions b_c which are different from the outgoing-wave condition of Kapur-Peierls theory. Denote the new boundary condition operator by $\mathcal{L}^0$, and define $\Delta\mathcal{L}\equiv\mathcal{L}^0-\mathcal{L}$. Bloch[1] has already written down the expression for the scattering matrix in terms of states satisfying arbitrary boundary conditions. We wish to generalize this result by letting the states be eigenstates of a Hamiltonian H^0 which differs from the actual Hamiltonian H. We write the difference $H-H^0\equiv H'$. The division of H in this way is not entirely free, but is constrained by certain conditions to be discussed below. Introduce the definitions

$$\begin{aligned}H'-\Delta\mathcal{L}&\equiv h,\\ (H+\mathcal{L}-E)^{-1}&=\mathcal{G},\\ (H^0+\mathcal{L}^0-E)^{-1}&=\mathcal{G}^0.\end{aligned}\tag{52}$$

Since $\Delta\mathcal{L}$ is associative, then assuming H' to be the same, so is h. It follows that

$$\mathcal{G}=\mathcal{G}^0-\mathcal{G}^0h\mathcal{G},\tag{53}$$

whence

$$\mathcal{G}=(1+\mathcal{G}^0h)^{-1}\mathcal{G}^0.\tag{54}$$

Introduce the complete set of states $|p\rangle$ satisfying

$$\begin{aligned}H^0|p\rangle&=E_p|p\rangle,\\ \mathcal{L}^0|p\rangle&=0;\end{aligned}\tag{55}$$

then

$$\mathcal{G}^0=\sum_p\frac{|p\rangle\langle\tilde{p}|}{E_p-E},\tag{56}$$

and

$$\mathcal{G}=\left(1+\sum_p \frac{|p\rangle\langle\tilde{p}|h}{E_p-E}\right)^{-1}\left(\sum_{p'}\frac{|p'\rangle\langle\tilde{p}'|}{E_{p'}-E}\right). \tag{57}$$

This form can be simplified. Expand

$$\mathcal{G}=\sum_{p,q}|p\rangle A_{pq}\langle\tilde{q}|\,, \tag{58}$$

then

$$A_{pq}=\langle\tilde{p}|\mathcal{G}|q\rangle.$$

Since

$$\begin{aligned}\sum_q \langle\tilde{p}|\mathcal{G}|q\rangle\langle\tilde{q}|\mathcal{G}^{-1}|p'\rangle&\equiv\delta_{pp'}\,,\\ \mathbf{A}&=(\mathbf{B}-\mathbf{E})^{-1},\end{aligned} \tag{59}$$

where

$$\begin{aligned}B_{pq}&=E_p\delta_{pq}+\langle\tilde{p}|h|q\rangle\,,\\ E_{pq}&=E\delta_{pq}.\end{aligned} \tag{60}$$

Thus $\mathcal{G}$ is expressed in terms of states $|p\rangle$ by (58), once the matrix $(\mathbf{B}-\mathbf{E})^{-1}$ is inverted.

The connection with Kapur-Peierls theory is obtained by diagonalizing $\mathbf{B}$. Suppose that this is achieved by the complex orthogonal matrix $\mathbf{T}$:

$$\mathbf{TT}^*=1;\qquad \mathbf{T}^*\mathbf{BT}=\mathbf{D}\,, \tag{61}$$

where $\mathbf{D}$ is diagonal with elements E_λ. Thus

$$\mathbf{A}=\mathbf{T}(\mathbf{D}-\mathbf{E})^{-1}\mathbf{T}^* \tag{62}$$

and

$$\mathcal{G}=\sum_\lambda \frac{|\lambda\rangle\langle\tilde{\lambda}|}{E_\lambda-E}\,, \tag{63}$$

where $|\lambda\rangle=\sum_q T_{\lambda q}|q\rangle$. This form of $\mathcal{G}$ is the familiar one of Kapur-Peierls theory; the matrix $\mathbf{T}$ is clearly just the transformation matrix between the two sets of states.

In the case $H'=0$, the matrix B_{pq} involves surface quantities (reduced width amplitudes) only, and we recognize the level-matrix inversion problem of R-matrix theory[18] with

$$\begin{aligned}\langle\tilde{p}|\Delta\mathcal{L}|q\rangle&=\sum_c \gamma_{pc}\gamma_{qc}\left[b_c-\left(\frac{r_c}{O_c}\frac{d}{dr_c}O_c\right)_{r_c=a_c}\right],\\ &=\sum_c \gamma_{pc}\gamma_{qc}(b_c-S_c-iP_c)\,,\end{aligned} \tag{64}$$

in terms of the usual shift and penetration factors. In the usual R-matrix development, the level matrix inversion is replaced by a channel matrix inversion using the easily proved relations [from (58), (59), (60), (64)]

$$\begin{aligned}\left(\frac{\hbar^2a_c}{2m_c}\right)^{1/2}\left(\frac{\hbar^2a_{c'}}{2m_{c'}}\right)^{1/2}\left\langle\frac{1}{r_c{}^2}\delta(r_c-a_c)c\right|\mathcal{G}\left|\frac{1}{r_{c'}{}^2}\delta(r_{c'}-a_{c'})c'\right\rangle\\ =\sum_{p,q}\gamma_{pc}\gamma_{qc'}A_{pq}\\ =[(\mathbf{1}-\mathbf{RL})^{-1}\mathbf{R}]_{cc'}\,,\end{aligned} \tag{65}$$

where

$$\begin{aligned}R_{cc'}&=\sum_p \frac{\gamma_{pc}\gamma_{pc'}}{E_p-E}\,,\\ L_{cc'}&=\delta_{cc'}(S_c-b_c+iP_c).\end{aligned} \tag{66}$$

Alternatively, (65) can be obtained directly from (57). From (30) and (32), these equations are sufficient to give the S matrix.

A. Constraints on $H=H^0+H'$

This division must be compatible with the basic assumptions embodied in the use of channel surfaces (as manifested in the $\mathcal{L}$ operator), viz., the eigenstates of H^0 in the energy range considered must generally have the same surface properties as those of H. This means that the constituents of all open channel pairs must be unchanged[19] (i.e., $\phi_{\alpha s}$ is unchanged), and also that no breakups into $\geqslant 3$ particles be allowed. The latter requirement means, for instance, that we could not take H^0 to be the free-particle Hamiltonian, (i.e., the kinetic energy). It is interesting that a very similar restriction occurs in Lippmann-Schwinger theory. Faddeev[20] and others have noted that the equation $\Psi=\Phi-(H^0-E-i\epsilon)^{-1}(H'\Psi)$ is not solved by $\Psi=[1+(H^0-E-i\epsilon)^{-1}H']^{-1}\Phi$, when H^0 is the free-particle Hamiltonian; the reason is that the inverse of operator $[1+(H^0-E-i\epsilon)^{-1}H']$ does not exist, since its determinant is infinite. This operator is (apart from the replacement of $-i\epsilon$ by $\mathcal{L}^0$) exactly the combination $(1+\mathcal{G}^0h)$ occurring in our "solution" (54).

Certain choices of H^0 will imply that, for some two-particle channels, the thresholds are changed relative to those of H, i.e., for given energy, some channels that are open for H are closed for H^0 (or vice versa). These choices are permitted provided that (a) H^0 satisfies the previous condition that the internal wave functions of the channel pairs be the same[19]; and (b) that the $\mathcal{L}$ operator includes reference to all such channels. This will be automatic in Kapur-Peierls or R-matrix theory, since, in order to define the complete orthogonal set of states (which contains members with unlimited energy), boundary conditions must be prescribed on all surfaces, irrespective of whether the channels are open or closed in the energy range of interest. This requirement includes channels for $\geqslant 3$ particle breakup. In the usual form of Kapur-Peierls theory, bound channels never occur explicitly since their surface integrals are zero as a result of the actual wave function satisfying the outgoing (decaying) wave boundary condition, i.e., $\mathcal{L}|\psi\rangle=0$ for bound channels c.

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[18] A. M. Lane and R. G. Thomas, Rev. Mod. Phys. **30**, 257 (1958).

[19] Actually, at the cost of more complicated expressions one can relax this condition. The only choices of H^0 which cannot be dealt with are those for which the internal states of the channel wave functions contain appreciable amounts of unbound constituents (since these have no set of orthogonal surface functions).

[20] L. D. Faddeev, Zh. Eksperim. i Teor. Fiz. **39**, 1459 (1960) [English transl.: Soviet Phys.—JETP **12**, 1014 (1961)].

A simple example of an H^0 with different thresholds is that considered by Garside and MacDonald.[11] We have a one-body potential with a resonance just above zero-energy. H^0 is chosen so that the new potential is just deep enough to bind the state (p, say). Suppose that both $\mathcal{L}$ and $\mathcal{L}^0$ are taken as the Kapur-Peierls boundary conditions for their respective problems, so that $\Delta\mathcal{L}\rightarrow 0$ as $H'\rightarrow 0$. Expanding matrix **B** of (60) in powers of its off-diagonal part (assuming this is small relative to the diagonal part), and keeping the leading term only in (59) gives

$$A_{pp}{}^{-1}=E_p-E+\langle\tilde{p}|H'|p\rangle+\langle\tilde{p}|\mathcal{L}-\mathcal{L}^0|p\rangle,$$

$$\frac{A_{pq}}{A_{pp}}=O(H'/D),\quad A_{qr}=O(H'/D^2),$$

where D is the single-particle-level spacing. The resonance width comes from $\langle\tilde{p}|\mathcal{L}|p\rangle$ and has the familiar form $2P\gamma_p{}^2$. It would be interesting to compare the accuracy of this result with that of Garside and MacDonald, who give their result in terms of matrix elements of H' between $|p\rangle$ and the continuum states.

6. FESHBACH'S PROJECTION-OPERATOR THEORY

It is a standard exercise in the use of Sec. 5 to derive Feshbach's results.[6] Define P as the projection operator on open-channel components of any wave function, and $Q\equiv 1-P$. In order that P is a true projector operator satisfying $P-P^2=QP=0$, and is unambiguous, this treatment is restricted[21] to elastic and inelastic scattering without exchange.

The appropriate separation of H is

$$\begin{aligned}&H=H^0+H',\\&H^0=PH_0P+QH_0Q,\\&H'=PHQ+QHP+P(H-H_0)P+Q(H-H_0)Q.\end{aligned}\tag{67}$$

This is a slight generalization of Feshbach's theory in that he effectively takes

$$H^0=PHP+QHQ,\quad H'=PHQ+QHP.$$

Since we are not going to introduce a complete orthogonal set, there is no need to introduce $\mathcal{L}$ operators for bound channels. If integrations in these are taken to infinity, there are no surface correction terms, and H in Hermitian for these channels.

For free channels, choose $\mathcal{L}^0=\mathcal{L}$ so $\Delta\mathcal{L}=0$.

By expanding as a power series in H^0 and using $(H^0)^n=(PH_0P)^n+(QH_0Q)^n$, we find for $\mathcal{G}^0=(H^0+\mathcal{L}-E)^{-1}$:

$$\mathcal{G}^0=\mathcal{G}_P{}^0+\mathcal{G}_Q{}^0,\tag{68}$$

where

$$\begin{aligned}&\mathcal{G}_P{}^0=(PH_0P+\mathcal{L}-E)^{-1},\\&\mathcal{G}_Q{}^0=(QH_0Q-E)^{-1}.\end{aligned}\tag{69}$$

We wish to express $\mathcal{G}$ in terms of these operators which are assumed known and hereby solve the problem. To do this, consider a special case of the above division, *viz.*, $H_0=\bar{H}_0$, $H'=\bar{H}'$ (say) where $P\bar{H}_0P=PHP$, $Q\bar{H}_0Q=QHQ$, $P\bar{H}_0Q=Q\bar{H}_0P=0$, $\bar{H}'=PHQ+QHP$. This is Feshbach's choice. For this case we have, from (54),

$$\mathcal{G}=(1+G^0\bar{H}')^{-1}G^0,\tag{70}$$

where $G^0\equiv(\bar{H}^0+\mathcal{L}-E)^{-1}$. As in the general case, G^0 splits up into $G^0=G_P{}^0+G_Q{}^0$, where

$$\begin{aligned}&G_P{}^0=(PHP+\mathcal{L}-E)^{-1},\\&G_Q{}^0=(QHQ-E)^{-1}.\end{aligned}\tag{71}$$

By operator algebra, (70) can be transformed into

$$\begin{aligned}\mathcal{G}=G_P{}^0+&[1-G_P{}^0(PHQ)]\\&\times[(G_Q{}^0)^{-1}-(QHP)G_P{}^0(PHQ)]^{-1}\\&\qquad\times[1-(QHP)G_P{}^0].\end{aligned}\tag{72a}$$

Clearly, since P and Q occur symmetrically in the original equations, this can also be written as

$$\begin{aligned}\mathcal{G}=G_Q{}^0+&[1-G_Q{}^0(QHP)]\\&\times[(G_P{}^0)^{-1}-(PHQ)G_Q{}^0(QHP)]^{-1}\\&\qquad\times[1-(PHQ)G_Q{}^0].\end{aligned}\tag{72b}$$

Finally, we see that $G_P{}^0$ is related to the earlier $\mathcal{G}_P{}^0$ by

$$G_P{}^0=\mathcal{G}_P{}^0-\mathcal{G}_P{}^0H_P{}'G_P{}^0,\tag{73}$$

where $H_P{}'=P(H-H_0)P$, whence

$$G_P{}^0=(1+\mathcal{G}_P{}^0H_P{}')^{-1}\mathcal{G}_P{}^0.\tag{74}$$

Similarly, $G_Q{}^0$ can be expressed in terms of $\mathcal{G}_Q{}^0$. Thus, from (72a) or (72b), the Green's function $\mathcal{G}$ can be expressed in terms of the known functions $\mathcal{G}_P{}^0$ and $\mathcal{G}_Q{}^0$. Once the Green's function is known, any properties of the system can be deduced. We give two examples.

A. The Optical Potential

From (72b) we find

$$P\mathcal{G}P=P[(G_P{}^0)^{-1}-(PHQ)G_Q{}^0(QHP)]^{-1}P.$$

The scattering matrix **S** is determined by this quantity by (32) or (47). We see that **S** and this open-channel part of $\mathcal{G}$ are reproduced by an effective Hamiltonian:

$$H_{\text{eff}}=PHP-(PHQ)G_Q{}^0(QHP).\tag{75}$$

H_{eff} has the matrix elements only in the open-channel space. The solutions of H_{eff} satisfy the coupled one-

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[21] When rearrangements occur, the various sets of channel wave functions are not orthogonal, and no satisfactory explicit form of P has been found. It is possible to find a form of P (Ref. 6) such that $\langle\psi(P^2-P)\psi\rangle=0$, but this is not sufficient to justify the vital step in the theory, which is $H(P-P^2)|\psi\rangle=0$, since this involves off-diagonal elements of P^2-P. Note that the non-Hermiticity of H for continuum states means that $H(P-P^2)|\psi\rangle$ is not trivially equal to $\sum_\alpha H|\alpha\rangle\langle\alpha|(P-P^2)|\psi\rangle$.

body equations:

$$T_c u_c + \sum_{c'} \mathcal{V}_{cc'} u_{c'} - \epsilon_c u_c = 0\,, \tag{76}$$

where ϵ_c is the channel kinetic energy, T_c is the radial part of the kinetic energy operator, and $\mathcal{V}_{cc'}$ is the optical-potential matrix given by

$$T_c \delta_{cc'} + \mathcal{V}_{cc'} = \langle c | PHP - (PHQ) G_Q{}^0 (QHP) | c' \rangle\,, \tag{77}$$

where the integration is over the coordinates occurring in the channel states $|c\rangle$, $|c'\rangle$ (i.e., the internal and relative angle coordinates). The optical potential which produces only elastic scattering is obtainable from an H_{eff} like (75). The only changes are that P projects onto the elastic channel only and $\mathcal{L}$ must be added to QH_0Q in $\mathcal{G}_Q{}^0$ of (69).

B. Resonances in the Scattering Matrix

From (40), if $\phi^{(c)}$ are solutions of $H^0 = PH_0P + QH_0Q$, then

$$\begin{aligned} i\hbar(v_c v_{c'})^{1/2}&[S_{c'c} - S_{c'c}(H^0)] \\ &= -\langle \tilde{\phi}^{(c')} | H' - H'\mathcal{G}H' | \phi^{(c)} \rangle\,. \end{aligned} \tag{78}$$

The right-hand side of this is best developed using form (72a) for $\mathcal{G}$, whence

$$\begin{aligned} i\hbar(v_c v_{c'})^{1/2}[S_{c'c} - S_{c'c}(H^0)] = -\langle \tilde{\phi}^{(c')} | H_P{}'(1+\mathcal{G}_P{}^0 H_P{}')^{-1} \\ \times |\phi^{(c)}\rangle + \langle \tilde{\phi}^{(c')} | (1+H_P{}'\mathcal{G}_P{}^0)^{-1}(PHQ) \\ \times [(G_Q{}^0)^{-1} - (QHP) G_P{}^0 (PHQ)]^{-1} \\ \times (1+\mathcal{G}_P{}^0 H_P{}')^{-1} | \phi^{(c)} \rangle\,. \end{aligned} \tag{79}$$

Noting that the solution $\eta^{(c)}$ of the special problem $\bar{H}^0 = PHP + QHQ$ is given by

$$|\eta^{(c)}\rangle = (1+\mathcal{G}_P{}^0 H_P{}')^{-1} | \phi^{(c)} \rangle\,, \tag{80}$$

we see that this is equivalent to

$$\begin{aligned} i\hbar(v_c v_{c'})^{1/2}[S_{c'c} - S_{c'c}(\bar{H}^0)] = -\langle \tilde{\eta}^{(c)\prime} | (PHQ) \\ \times [(G_Q{}^0)^{-1} - (QHP) G_P{}^0 (PHQ)]^{-1} (QHP) | \eta^{(c)} \rangle\,, \end{aligned} \tag{81}$$

which we could have written down directly by specializing (78) to $H^0 = \bar{H}^0$. This is Feshbach's formula for the scattering matrix. The central operator gives resonances arising naturally from the eigenstates $|n\rangle$ say, of the closed-channel Hamiltonian QHQ. The states $|n\rangle$ have eigenvalues E_n which are real if they occur below that threshold next above the given energy E. We can express the above operator in terms of resonance energies E_λ and resonance states $|\lambda\rangle$:

$$(PHQ)\mathcal{G}(QHP) = \sum_\lambda \frac{PHQ|\lambda\rangle\langle\lambda|QHP}{E_\lambda - E}\,,$$

where $|\lambda\rangle = \sum_n \langle n|\lambda\rangle |n\rangle$, and the E_λ and $\langle n|\lambda\rangle$ are eigenvalues and eigenvectors of the matrix

$$E_n \delta_{nn'} - \langle n' | QHP(PHP + \mathcal{L} - E)^{-1} PHQ | n \rangle\,.$$

Since this involves energy E, the states $|\lambda\rangle$ and energies E_λ depend on energy. These states and energies are, of course, just those of Kapur-Peierls theory, and the form (81) is just that previously given (28).

In the work of Sano, Yoshida, and Terasawa they derive (78) but develop it by introducing the Kapur-Peierls representation of $\mathcal{G}$.

C. Channel-Coupling Theory of Hill and Buck

In this case,[12] the appropriate division $H = H^0 + H'$ is

$$H^0 = \sum_c |c\rangle\langle c|H|c\rangle\langle c|\,,$$

$$H' = \sum_{c,c' \neq c} |c'\rangle\langle c'|H|c\rangle\langle c|\,,$$

where c and c' include both open and closed channels. This H' is the channel-coupling term. The solutions of H^0 are the uncoupled channel solutions. In the case of one open and one closed channel, this division is the same as the Feshbach one in Sec. 6. When more than two channels occur, this is not so. Further, no choice of projection operator P gives PHP equal to H^0 above

7. THEORIES OF RODBERG AND MACDONALD

These authors[9,10] make a different division of

$$H = H^0 + H'.$$

Suppose that H_0 is a soluble Hamiltonian, and define $\Delta = H - H_0$. H^0 and H' have the form

$$\begin{aligned} H^0 &= H_0 + \Delta P_c\,, \\ H' &= \Delta P_d\,, \end{aligned} \tag{82}$$

where P_c and P_d are orthogonal projection operators $P_c + P_d = 1$, $P_c P_d = P_d P_c = 0$ which commute with H_0. Note the difference of form with that met in Sec. 6. There H^0 and H' contained terms of types PyP, QyQ and PyQ, QyP, PyP, QyQ, respectively, whereas here H^0 has P_dyP_d, P_cyP_c, P_dyP_c and H' has P_cyP_d, P_dyP_d. For this division,

$$\mathcal{G}^0 = (H_0 + \Delta P_c + \mathcal{L} - E)^{-1}. \tag{83}$$

Using (54) with some operator algebra we can express $\mathcal{G}$ in terms of $\mathcal{G}^0$ and H':

$$\begin{aligned} \mathcal{G} &= (1+\mathcal{G}^0 H' P_d)^{-1} \mathcal{G}^0 = \mathcal{G}^0 (1 + H' P_d \mathcal{G}^0)^{-1} \\ &= \mathcal{G}^0 - \mathcal{G}^0 H' (1 + P_d \mathcal{G}^0 H' P_d)^{-1} P_d \mathcal{G}^0. \end{aligned} \tag{84}$$

The scattering matrices for Hamiltonians H^0 and H are given by

$$\begin{aligned} i\hbar(v_c v_{c'})^{1/2}&[S_{c'c}(H^0) - S_{c'c}(H_0)] \\ &= -\langle \tilde{\phi}^{(c')} | (\Delta P_c) - (\Delta P_c)\mathcal{G}^0(\Delta P_c) | \phi^{(c)} \rangle\,, \end{aligned} \tag{85}$$

$$\begin{aligned} i\hbar(v_c v_{c'})^{1/2}&[S_{c'c} - S_{c'c}(H_0)] \\ &= -\langle \tilde{\phi}^{(c')} | \Delta - \Delta\mathcal{G}\Delta | \phi^{(c)} \rangle\,. \end{aligned} \tag{86}$$

The scattering-matrix operator for the Hamiltonian H^0 is $\hat{S}^0$, where

$$\hat{S}^0 = (\Delta P_c) - (\Delta P_c)\mathcal{G}^0(\Delta P_c). \tag{87}$$

For H, it is $\hat{S}$ where

$$\hat{S} = \Delta - \Delta\mathcal{G}\Delta. \tag{88}$$

Defining $\mathcal{J} \equiv \Delta - \Delta P_c \mathcal{G}^0 \Delta$, so that $\hat{S}^0 = \mathcal{J} P_c$, we can write $\hat{S}$ in terms of this:

$$\begin{aligned}\hat{S} - \mathcal{J} &= \Delta(P_c\mathcal{G}^0 - \mathcal{G})\Delta \\ &= -\Delta(P_d\mathcal{G}^0 - \mathcal{G}^0 H'(1+P_d\mathcal{G}^0 H' P_d)^{-1} P_d \mathcal{G}^0)\Delta \\ &= -\Delta(1 - P_c\mathcal{G}^0\Delta)(1+P_d\mathcal{G}^0 H' P_d)^{-1} P_d\mathcal{G}^0\Delta. \end{aligned} \tag{89}$$

Using the definition of $\mathcal{J}$, we can show that

$$P_d\mathcal{G}^0\Delta = \mathcal{G}^0 P_d \mathcal{J},$$

$$(1+P_d\mathcal{G}^0 H' P_d)^{-1} P_d = [(\mathcal{G}^0)^{-1} + P_d\mathcal{J}P_d]^{-1} P_d \mathcal{G}^0,$$

so that

$$\hat{S} = \mathcal{J} - \mathcal{J}P_d[(\mathcal{G}^0)^{-1} + P_d\mathcal{J}P_d]^{-1} P_d\mathcal{J}, \tag{90}$$

which is the relation derived by Rodberg[9] and MacDonald.[10] Note that, because of the presence of operators P_d, $(\mathcal{G}^0)^{-1}$ can be replaced by $(H_0+\mathcal{L}-E)^{-1}$, so that the resonance energies are the eigenvalues of the operator

$$P_d(H_0+\mathcal{L}+\mathcal{J})P_d.$$

As in other theories, these eigenvalues depend on incident energy. In contrast to Feshbach's theory, the original eigenvalues (i.e., those of H_0) do not change when E crosses a threshold.

In this description, we have not had to specify P_c and P_d beyond the fact that they commute with H_0. Also we have not specified H_0. In fact, there is not much freedom in choosing H_0. Like the Feshbach theory, the present theory cannot describe rearrangements or exchange but only direct elastic and inelastic scattering. Since H^0 must preserve the internal wave functions of the target states, it must include the target Hamiltonian H_t, so H_0 must have the form

$$H_0 = H_t + \sum_{c,c'} |c\rangle(T_c\delta_{cc'} + V_{cc'})\langle c'|,$$

where $|c\rangle$ are target states, and $V_{cc'}$ is a one-body potential. The simplest choice of $V_{cc'}$, is the diagonal one: $\epsilon_c + T_c + V_{cc'} = \langle c|H|c\rangle\delta_{cc'}$. In this case, $(H_0+\mathcal{L})$ has solutions of the form $u_{\lambda c}(\mathrm{r})|c\rangle$ satisfying $\mathcal{L}u_{\lambda c}(\mathrm{r}) = 0$ and the uncoupled equations

$$(T_c + V_{cc} - \epsilon_{\lambda c})u_{\lambda c} = 0,$$

where $\epsilon_{\lambda c}$ is the channel energy: $\epsilon_{\lambda c} = E_\lambda - \epsilon_c$.

Now let us discuss P_c and P_d. Since they are assumed to commute with H_0, they must project on states of H_0. In fact, P_c projects on states of H_0 such that $\mathrm{Re}(\epsilon_{\lambda c}) > \epsilon$, where ϵ is a prescribed critical energy. (Since states of the special H_0 are products $u_{\lambda c}|c\rangle$, each state has only one channel c for the criterion to be applied to.) In addition to H_0, H^0 includes $(H-H_0)P_c$ which is that part of the coupling

$$(H-H_0) = \sum_{c',c\neq c'} |c\rangle\langle c|H|c'\rangle\langle c'|,$$

which acts on states of H_0 with channel energy greater than ϵ. Since Rodberg and MacDonald do not use the $\mathcal{L}$ operator and discrete sets of states, there is only one natural choice of ϵ then, viz., $\epsilon = 0$, so that P_c projects on "continuum" states of H_0. By "continuum" here, we do not mean $\mathrm{Re}(E_\lambda)$ is above the lowest threshold, but rather that the channel energy (of the unique channel) is >0. The definition of P_c in terms of the unique channel energy means that H_0 cannot include channel coupling. When channels are coupled, all states with $\mathrm{Re}(E_\lambda)$ above the lowest threshold will be in the continuum.

The solutions of H^0 are of two types:

(i) *discrete*: $u_{\lambda c}^-(r)|c\rangle$, where $(T_c + V_{cc} - \epsilon_{\lambda c})u_{\lambda c} = 0$ and $\mathrm{Re}(\epsilon_{\lambda c}) < 0$;

(ii) *continuum*: $\sum_c u_{\lambda c}^+(r)|c\rangle$, where

$$(T_c + V_{cc} - \epsilon_{\lambda c})u_{\lambda c}^+ = -\sum_{c'\neq c} V_{cc'}u_{\lambda c'}^+$$

and $\mathrm{Re}(\epsilon_{\lambda c})$ for the ground-state channel is >0. For a given $\mathrm{Re}(\epsilon_{\lambda c})$, some channels are closed. These channels contribute their $u_{\lambda c}^+$; for such channels $u_{\lambda c}^+(r) \to 0$ as $r \to \infty$ in spite of the fact that they are superpositions of positive energy states of $(T_c + V_{cc})$. We see that the scattering $\hat{S}^0$ from H^0 involves no reference to the discrete states $u_{\lambda c}^-|c\rangle$; this was already expected from the definition below (88).

If the $\mathcal{L}$ operator is used, there is no natural basis for a choice of ϵ, and we can choose it for convenience. This may be an advantage. For example, when there is a low-lying narrow single-particle resonance in the continuum, it would be better to omit this from the calculation of the background term $\hat{S}^0$, and to introduce it as a resonance. This will happen if ϵ is chosen to be a positive energy above the channel energy of the resonance. Alternatively, H_0 may be allowed to be different from $\langle c|H|c\rangle$ for the channel c in question, and taken to have a deeper potential which just binds the single-particle state. This was the procedure used by MacDonald and Garside.[10] Since one of their basic motivations was to set up a description of the origin of resonances free from the use of channel radii, this was the only course that could be consistently taken. However, from a purely calculational viewpoint, in practice, the alternative method from the $\mathcal{L}$ operator formalism may be equally good or better (see remarks at the end of Sec. 5).

8. DISCUSSION

We have seen how a large number of theories can be extracted from the one basic formalism. Until this point, we have made no value judgements on these theories.

Let us ignore rearrangement processes (which give trouble for theories of type B); then all theories are exact, and so are equivalent if applied exactly. It is only when applied in an approximate manner that some theories may be more useful in that they give a better first approximation.

There are two situations in particular where such approximate theories are useful.

A. Analysis of Resonance Cross-Section Data

Ideally, one would predict the exact cross section from a given assumed Hamiltonian and then vary any parameters in the Hamiltonian until the data were fitted. In practice, this is only possible for the two-body system. For few-nucleon systems, this program can be done only approximately. For systems with several nucleons ($\geqslant 5$) a new feature appears, viz., resonances. From their general features such as widths and spacings, it is certain that these resonances reflect the continuation of the bound-state spectrum into the continuum. Thus, if the lowest threshold could be artificially raised through some resonances, they would become normal bound states like those below in energy. This suggests that one can separate the problem of fitting into two parts. First, one fits the data with a formula containing resonance and background terms, and thereby extracts values of nuclear constants; this eliminates all reference to the reaction problem as such. The second part is a pure structure problem, viz., to predict the constants.

B. Prediction of Cross Section from a Given Model Hamiltonian

Ideally, one solves the Hamiltonian problem exactly at each energy, and thereby predicts the cross section. In practice, however, an exact solution may be impossible and, even if it were possible, the computing requirements may be exorbitant. Thus, in essence, we need precisely the same intermediary between the Hamiltonian and the cross section as in the preceding situation, viz., a resonance formalism, whose *form* is independent of the Hamiltonian, which only affects values of the parameters in the formalism. This means that, given a solution to a structure problem for a number of discrete levels, the formalism enables one to predict the cross section continuously as a function of energy.

In searching for a suitable formalism, we must be warned that the fact that a given theory can yield resonances in a natural fashion is no argument that it is the correct one for fitting an observed level or set of levels. *All* of the theories we have reviewed can be easily specialized to give a one-level formula of the classic Breit-Wigner form. The vital question is: "When an observed isolated resonance is fitted with the Breit-Wigner form, which one gives the most correct identification of the extracted parameters (partial widths, resonance energies and background)?" Equivalently [since all theories are exact when all terms (levels) are included], which theory gives a single-level formula which is least subject to interference from other levels? It is clear that level interference can be strong or weak in any theory, depending on the conditions. In Feshbach's theory,[6] the most directly obtained one-level form is one which is valid when the continuum coupling $(PHQ+QHP)$ is a weak perturbation on $(QHQ+PHP)$, i.e., it serves only to shift and damp the original discrete state but does not mix it appreciably with other states. This situation may be correct for many atomic levels, and for a few special nuclear levels where mixing is rather weak, but it is not true for the generality of nuclear energy levels. More generally, one can derive the one-level formula for resonances which occur at energies obtained by a suitable diagonalization of the coupling, viz., they are eigenstates of

$$QHQ-QHP(PHP+\mathfrak{L}-E)^{-1}PHQ.$$

Unfortunately the resonances now depend on energy E through its occurrence in the second term; and all level parameters are complex[22] and energy dependent. Thus the theory is not so useful in this strong coupling situation.

The R-matrix theory[3] is not subject to any weak-coupling restriction, since its eigenstates are those of the total Hamiltonian. In this sense, it is least committed to any specific model of structure. However, it may also be subject to level interference in certain unsuitable situations. If the interaction radius parameters a_c or the boundary condition parameters b_c are increased without limit then level interference *must* occur ultimately. Increasing the radius must increase the density of states, which means that one observed level arises from a highly special interference of many underlying levels. Increasing b_c means that observed levels appear as a special interference of levels lying between and alternating with the observed ones. Clearly, the radii should be taken as small as possible, $a_c(\text{min})$ (say), in order to minimize level interference (since this minimizes the number of levels). However, if a_c is increased above this value, no significant increase in level density occurs until a certain critical point A_c is reached. This

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[22] Theories of class B can be modified so that they involve the minimum number of real parameters. This is done by developing (81) using states $|\bar{\lambda}\rangle$ which differ from the states $|\lambda\rangle$ below (81) by the omission of the imaginary part of the matrix. The parameters are $E_{\bar{\lambda}}$ and $|\langle\bar{\lambda}|QHP|\eta^{(c)}\rangle|$, and although these level parameters are real they are energy-dependent.

is where the logarithmic derivative changes through an entire cycle (passing once through 0 and ∞) when the energy changes by the order of the level spacing, keeping the logarithmic derivative at a_c (min) *fixed*. If the turning point in the channel is at $a_c = t_c$, then $(A_c - t_c)$ in fermis $\approx 20\ (E/D)$, where channel energy E and level spacing D are in MeV. For slow-neutron resonances with $E/1000 \approx D \approx 1$ eV, this is $\sim 10^4$. Thus small variations in a_c give no trouble for one one-level formula in R-matrix theory. They only change the factorization of width into penetration and reduced width, and the division of background into distant resonances and potential scattering.

The one-level formula has a similar stability for changes in the parameters b_c. The basic approximation in deriving the one-level form is to retain only one term in the R-matrix sum over levels. This will be valid only for energies near the level energy of the retained term. Thus the level shift must be small compared to the level spacing D. Taking the value $\gamma_{\lambda c}^2 \approx (1/20)D$ gives the condition that the variation Δb_c in b_c about the value $b_c = S_c$ is restricted by $\Delta b_c \ll 20$. A more stringent condition is obtained[18] by demanding that the one-level formula be optimized. This gives $b_c - S_c = O(P_c)$.

Since the radii a_c have well-defined minimum values for nuclear reactions we expect the R-matrix theory to be especially appropriate. This is not so for atomic problems where the Coulomb potential prevents any such "natural" choice of radius.

Although in nuclear reactions a wide range of the radii a_c give rise to resonances in one-one correspondence with those observed, one may inquire whether, within this range, one choice is better than another. For example, to eliminate barrier effects and to separate widths into the physically distinct penetration and reduced width factors, a_c should be chosen on the inner side of the barrier. One may also inquire whether reducing a_c still further will give a better expression for the background in the sense that the distant resonances are negligible and the potential scattering term dominates. Thomas[23] and others[24] considered taking a_c into the interacting region on the grounds that interactions in the outer fringe of this region were mainly responsible for the direct reactions and potential scattering. Putting this fringe region outside would expose these effects explicitly instead of hiding them in distant resonances. (Of course, a_c cannot strictly be taken into the inner region when rearrangement channels are present or else the vital channel orthogonality on the surface of the inner region will be lost.) This point of view has been superceded by the one[4] in which, for given a_c, the distant terms are summed by introducing the optical potential matrix which reproduces the scattering and reactions averaged over fine structure. It is assumed that the contribution of distant terms is unchanged by the averaging, so that S takes the form

$$\begin{aligned} S &= S_l + S_d = S_l + \bar{S}_d \\ &= S_l + \bar{S} - \bar{S}_l \\ &= S_l + S_{\mathrm{OP}} - \bar{S}_l , \end{aligned}$$

where l = local and d = distant, and OP = optical potential.

Relative to other theories of class A, the R-matrix form has the merit that its parameters are real and energy independent. For a single isolated level, this is not important since all theories of class A have these properties in this case. For an isolated group of two or more anomalously close levels for which $\Gamma \gtrsim D$, the R-matrix theory retains these features, while, in other theories, the parameters are complex, i.e., there are twice as many real parameters. This undesirable element is an unavoidable feature of any theory which gives the scattering matrix the form of a single sum over levels. Such a matrix can only be unitary over the level group if the complex parameters of the levels are related (by n relations in the single-channel case where n is the number of levels).

The latter alternative applies to theories of resonance reactions based on studies of the analytical properties[25,26] of the scattering matrix **S**. Such theories have the advantage that they are not committed to the viewpoints of class A or class B. This is also true of the general Bloch formalism, as we have shown in this paper, although this formalism does not give resonances of itself but only after specialization to class A or class B. In contrast, the analytical studies give a resonance expansion under very general conditions, the complex resonance energies being the poles of $\mathbf{S}(E)$, and the other resonance parameters being related to these poles by the unitarity conditions. Apart from the evident formal attractions of such theories, their existence does not affect the practical issues that we have just discussed. There is no easy way to calculate the poles of **S**, starting from a given soluble Hamiltonian. What appears to be needed is numerical investigations of the properties of simplified Hamiltonians, and comparison with the various theories.[27] For certain reactions, neither class A or class B viewpoints are natural ones, in which case the calculation of the poles of **S** may be the best way to proceed. For the nuclear case, however, class A seems appropriate and may give the easiest route to the calculated cross sections.

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