Non-Hermitian Hamiltonians, Decaying States, and Perturbation Theory*

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(Received 13 March 1972)

The conventional time-independent perturbation theory and projection-operator techniques are generalized to systems propagating under the influence of an effective non-Hermitian Hamiltonian, e.g., an optical-model potential. The mathematical complications which can arise due to lack of orthogonality and completeness for the eigenstates of such a Hamiltonian are discussed on an elementary level. Examples of the various techniques involved are taken from considerations of models for exotic atoms and cascade processes.

I. INTRODUCTION

The effective Hamiltonians for many physical problems are not Hermitian. One example is neutron scattering; incident particles are lost from the elastic scattering channel through nuclear excitation. Another example is the effective Hamiltonian for the "eigenstates" of exotic atoms in which a K^-, π^-, $\bar{p}$, or Σ^- particle is bound to a nucleus in an atomic orbit; capture or annihilation reactions become important if the wave function overlaps the nucleus appreciably. In both cases a non-Hermitian "optical potential" arises.

Strictly speaking the "eigenstates" above are not true normalizeable bound states but are, rather, decaying states. An exotic atom is simply one stage of a complicated scattering process in which, for example, a K^- is incident upon an atom, and a pion, several photons, a nucleus, etc. emerge. Formally bound states correspond to poles of the scattering matrix which lie on the real axis of the physical sheet of the complex energy plane. Decaying states correspond to poles on the second sheet below the real axis.[1]

Our recent consideration of a crude model for exotic atoms[2] led us to the conclusion that the non-Hermitian analogs for the familiar perturbation-theory techniques were not available in the literature. Standard textbook treatments apply only to eigenstates of Hermitian Hamiltonians. They cannot be used for decaying states, e.g., exotic atoms. However we have found that methods similar to the standard ones can be used to derive perturbation theory for the non-Hermitian case. Some of these results have also been obtained recently by More[3] using Jost-function methods. We will restrict ourselves to consideration of decaying states that can be thought of as states of two particles bound by a non-Hermitian potential. This is sufficient to include several types of resonant scattering in nuclear physics and auto-ionizing states in atomic physics as well as exotic atoms.

In Sec. II, we review the relationship between open channels and the non-Hermitian optical potential which they generate as an effective interaction in other channels. Section III contains a discussion, from a rather pedestrian point of view, of the orthogonality and completeness properties for the special types of non-Hermitian problems which arise in the use of optical potentials. The formulations of time-independent perturbation theory and of projection-operator theory based on a non-Hermitian Hamiltonian are presented in Secs. IV and V, respectively. In Sec. VI we show that these considerations lead to expressions for exotic-atom x-ray linewidths which are somewhat different from the conventional perturbation-theory expressions.

II. SOURCE OF NON-HERMITICITY

Non-Hermiticity generally enters physical problems via the boundary conditions. The boundary condition for a continuum channel does not require a vanishing wave function but rather, say, an outgoing wave. Consequently the kinetic energy operator is not Hermitian. Also, for another channel coupled to this continuum channel, the effective single-channel Hamiltonian will contain a non-Hermitian potential, the so-called optical potential. In this section we will summarize briefly how this comes about.

The usual Lippman-Schwinger[4] Green's function describing propagation for which the asymptotic

wave function has only outgoing spherical waves is

$$G(E)=\frac{1}{E+i\epsilon-H}. \tag{2.1}$$

Here E is the energy and $\epsilon\to 0^+$ as usual. H is the total Hamiltonian which describes the relative motion in several coupled channels. We assume that at least one of these is a two-body channel.

Because we wish to focus our attention on a particular two-body channel, we define a projection operator P onto this channel. For an arbitrary state $|\Psi\rangle$, $P|\Psi\rangle$ will be that portion of $|\Psi\rangle$ for which the two particles (say a K^- and a nucleus) move relative to one another in some way. The energy E is defined so that $E=0$ is the threshold for this P channel. The complementary projection is $Q\equiv 1-P$. These projection operators satisfy the usual conditions,

$$P^2=P,\quad Q^2=Q,\quad PQ=QP=0, \tag{2.2}$$

$$P^\dagger=P,\quad Q^\dagger=Q. \tag{2.3}$$

For an arbitrary operator A we define

$$A_{PQ}\equiv PAQ,\quad A_{PP}\equiv PAP,\ \text{etc.} \tag{2.4}$$

Thus $H=H_{PP}+H_{PQ}+H_{QP}+H_{QQ}$. H_{PP} contains only the Hamiltonian for the relative motion of the two particles in the P channel. It has no contributions from the other channels. The spectrum of H_{PP} will contain a continuum from $E=0$, and may also contain bound states of the two particles (e.g., K-mesonic atomic states). H_{PQ} and H_{QP} couple the channels, and H_{QQ} is nearly as complicated as H itself.

The projection-operator techniques of Feshbach[5] can be used to consider that portion $G_{PP}(E)$ of the total propagator Eq. (2.1) which describes processes beginning and ending in the P channel.

The standard operator identity

$$A^{-1}=B^{-1}[1+(B-A)A^{-1}] \tag{2.5}$$

gives

$$G(E)=(E+i\epsilon-H_{PP})^{-1}[1+(H-H_{PP})G(E)], \tag{2.6}$$

$$G(E)=(E+i\epsilon-H_{QQ})^{-1}[1+(H-H_{QQ})G(E)]. \tag{2.7}$$

Since $PH_{QQ}=0=H_{QQ}P=QH_{PP}=H_{PP}Q$, Eqs. (2.6) and (2.7), respectively, yield

$$G_{PP}(E)=(E+i\epsilon-H_{PP})^{-1}[1+H_{PQ}G_{QP}(E)], \tag{2.8}$$

and

$$G_{QP}(E)=(E+i\epsilon-H_{QQ})^{-1}H_{QP}G_{PP}(E). \tag{2.9}$$

Substituting Eq. (2.9) into Eq. (2.8) and using the identity (2.5) we find

$$G_{PP}(E)=\frac{1}{E+i\epsilon-\mathcal{H}_P(E)}, \tag{2.10}$$

where the effective P-channel Hamiltonian $\mathcal{H}_P$ contains an energy-dependent optical potential, $\mathcal{V}_P$,[6]

$$\mathcal{H}_P(E)=H_{PP}+\mathcal{V}_P(E), \tag{2.11}$$

$$\mathcal{V}_P(E)=H_{PQ}(E+i\epsilon-H_{QQ})^{-1}H_{QP}. \tag{2.12}$$

III. ORTHOGONALITY AND COMPLETENESS PROPERTIES

The optical potential of Eq. (2.12) is energy dependent and nonlocal. It is usually approximated by a local potential with relatively weak energy dependence. In this section, we study the orthogonality properties and completeness of the eigenstates of a Hamiltonian with an energy-independent optical potential. It is assumed that these results will also be valid for weakly energy-dependent potentials.

Consider a general operator

$$H=H_R+iH_I, \tag{3.1}$$

where H_R and H_I are Hermitian. The eigenstates of H and $H^\dagger$ satisfy

$$H|\phi_n\rangle=E_n|\phi_n\rangle, \tag{3.2a}$$

$$H^\dagger|\tilde{\phi}_n\rangle=\tilde{E}_n|\tilde{\phi}_n\rangle, \tag{3.2b}$$

and

$$\langle\phi_n|H^\dagger=E_n^*\langle\phi_n|, \tag{3.3a}$$

$$\langle\tilde{\phi}_n|H=\tilde{E}_n^*\langle\tilde{\phi}_n|. \tag{3.3b}$$

Now

$$2i\langle\phi_m|H_I|\phi_n\rangle=\langle\phi_m|H-H^\dagger|\phi_n\rangle=(E_n-E_m^*)\langle\phi_m|\phi_n\rangle,$$

so that

$$\mathrm{Im}E_n=\langle\phi_n|H_I|\phi_n\rangle/\langle\phi_n|\phi_n\rangle, \tag{3.4}$$

and

$$\langle\phi_m|\phi_n\rangle=2i\langle\phi_m|H_I|\phi_n\rangle(E_n-E_m^*)^{-1}. \tag{3.5}$$

For the Hermitian case ($H_I=0$) Eqs. (3.4) and (3.5) prove the orthogonality of states for which $E_n\neq E_m$. However, for $H_I\neq 0$ there must be some $n\neq m$ for which the right side of Eq. (3.5) does not vanish (unless we have the trivial case $[H_I,H]=0$). Thus, the eigenstates of a non-Hermitian operator do not form an orthogonal set.

It is true, however, that $\{\tilde{\phi}_n,\phi_n\}$ often form a biorthogonal set. That is

$$\langle\tilde{\phi}_m|\phi_n\rangle=0,\quad n\neq m. \tag{3.6}$$

In order to see this, consider

$$0\equiv\langle\tilde{\phi}_m|H-H|\phi_n\rangle=(E_n-\tilde{E}_m^*)\langle\tilde{\phi}_m|\phi_n\rangle. \tag{3.7}$$

Clearly $\langle\tilde{\phi}_m|\phi_n\rangle=0$ whenever $\tilde{E}_m^*\neq E_n$. However, this set cannot be complete unless there exists some state (we will call it $\tilde{\phi}_n$) for which $\langle\tilde{\phi}_n|\phi_n\rangle$ is nonzero. For this state Eq. (3.7) requires $\tilde{E}_n\equiv E_n^*$.

The existence of such a state $\tilde{\phi}_n$ for each eigenstate ϕ_n of H, is not a general property for arbitrary operators. We refer the interested reader to the discussion of the "residual spectrum" in standard texts on Hilbert-space theory.[7] However, an operator H representing a physically acceptable absorptive Hamiltonian is much less general. It follows from Eq. (3.4) that H_I determines $\mathrm{Im}E_n$ and thus the decay rate for a state ϕ_n. The time-reversed state should grow at the same rate as ϕ_n decays. Therefore the time-reversal operation, $\mathcal{T}$, should change the sign of iH_I, but should not otherwise affect H_R or H_I. Since $\mathcal{T}$ is antiunitary and H_R and H_I are $\mathcal{T}$ invariant,

$$\mathcal{T}H\mathcal{T}^{-1}=H_R-iH_I=H^\dagger. \tag{3.8}$$

The existence of a state $\tilde{\phi}_n$ with $\tilde{E}_n=E_n^*$ is now guaranteed by the existence of a time-reversed state, since

$$H^\dagger\mathcal{T}|\phi_n\rangle=\mathcal{T}H|\phi_n\rangle=\mathcal{T}E_n|\phi_n\rangle=E_n^*\,\mathcal{T}|\phi_n\rangle. \tag{3.9}$$

We therefore choose

$$|\tilde{\phi}_n\rangle\equiv\mathcal{T}|\phi_n\rangle \tag{3.10}$$

at least for the case when E_n is a nondegenerate eigenvalue.

Notice that for the nondegenerate case with only a spatial degree of freedom, the phase of $\tilde{\phi}_n$ can be chosen so that the configuration-space wave function $\tilde{\phi}_n(x)$ is just the complex conjugate of $\phi_n(x)$. This follows from[8]

$$\tilde{\phi}_n(x)\equiv\langle x|\tilde{\phi}_n\rangle=\langle x|\mathcal{T}\phi_n\rangle=\langle\mathcal{T}x|\mathcal{T}\phi_n\rangle=\langle x|\phi_n\rangle^*$$
$$\equiv\phi_n(x)^*.$$

For this case Eq. (3.6) takes the form[9]

$$\int\phi_m(x)\phi_n(x)\,dx=0. \tag{3.11}$$

When degenerate states are classified as eigenstates of Hermitian operators which commute with the Hamiltonian, the state $\tilde{\phi}_n$ cannot be defined so simply as in Eq. (3.10) unless the complete set of commuting operators are all time-reversal invariant. For example, a spin-up state is always orthogonal to a spin-down state whether or not the Hamiltonian is Hermitian. Let A be the Hermitian operator which commutes with H; its eigenstates are defined by

$$A|\alpha\rangle=\alpha|\alpha\rangle.$$

Define the state $|\overline{\alpha}\rangle\equiv\mathcal{T}^{-1}|\alpha\rangle$. The simultaneous eigenstates of H and A we denote by $|\phi_{n,\alpha}\rangle$. If A is odd under time reversal, it is easy to show that $\langle\overline{\alpha}|\alpha\rangle=0$ and $\langle\mathcal{T}(\phi_{n\alpha})|\phi_{n\alpha}\rangle=0$. Therefore Eq. (3.10) is no longer acceptable. In general, therefore, we define

$$|\tilde{\phi}_{n,\alpha}\rangle=\mathcal{T}|\phi_{n,\overline{\alpha}}\rangle, \tag{3.12}$$

where α ranges over all other labels for the state.

We have shown that the existence of a state $\tilde{\phi}_n$ is necessary to have a complete biorthogonal set, but we have certainly not proven the completeness of the set of eigenstates of H. This proof has been given by mathematicians[10] for a somewhat more restricted problem than Eq. (3.8); namely, for a nonrelativistic s-wave particle in a potential of the form $V=V(r)-iW(r)$ with V and W real. The primary conclusions for our purposes are that the set of all normalizeable discrete eigenstates plus the continuum eigenstates is complete, except for isolated potential strengths at which two eigenvalues (and eigenstates) coincide. When this occurs the dimension of the space spanned by the eigenstates is reduced by one. To compensate for this a new function associated with this eigenvalue must be introduced. This "associated function" is the derivative of the corresponding eigenfunction with respect to energy.[11]

It does appear, therefore, that problems due to lack of completeness occur only for isolated potential strengths, and can be circumvented. We will proceed under the assumption that no such problem arises.

The orthogonality property (3.6), coupled with completeness of the eigenstates of H, leads to simple and useful forms for the identity and projection operators. If we normalize the states to

$$\langle\tilde{\phi}_n|\phi_m\rangle=\delta_{n,m}, \tag{3.13}$$

then the identity operator is[12]

$$1=\sum_n|\phi_n\rangle\langle\tilde{\phi}_n|. \tag{3.14}$$

The projection operator onto a subspace R is

$$\mathcal{P}=\sum_{n\in R}|\phi_n\rangle\langle\tilde{\phi}_n|. \tag{3.15}$$

IV. TIME-INDEPENDENT PERTURBATION THEORY

We now develop time-independent discrete-state perturbation theory assuming a non-Hermitian unperturbed Hamiltonian H_0 whose eigenstates $\{\phi_n\}$ and $\{\tilde{\phi}_n\}$ form a complete biorthogonal set with $E_n^{(0)}=\tilde{E}_n^{(0)*}$. Let

$$H=H_0+\lambda H_1 \tag{4.1}$$

and

$$H|\phi\rangle=E|\phi\rangle. \tag{4.2}$$

Expanding in powers of λ,

$$(H_0+\lambda H_1)|(\phi^{(0)}+\lambda\phi^{(1)}+\cdots)\rangle = (E^{(0)}+\lambda E^{(1)}+\cdots)|(\phi^{(0)}+\lambda\phi^{(1)}+\cdots)\rangle . \tag{4.3}$$

Collecting terms gives

$$(E^{(0)}-H_0)|\phi^{(0)}\rangle = 0 , \tag{4.4}$$

$$(E^{(0)}-H_0)|\phi^{(1)}\rangle + (E^{(1)}-H_1)|\phi^{(0)}\rangle = 0 , \tag{4.5}$$

$$(E^{(0)}-H_0)|\phi^{(2)}\rangle + (E^{(1)}-H_1)|\phi^{(1)}\rangle + E^{(2)}|\phi^{(0)}\rangle = 0 . \tag{4.6}$$

Equation (4.4) is the unperturbed problem. Equation (4.5) gives the first-order energy shift if we take the inner product with $|\tilde{\phi}^{(0)}\rangle$. Using Eq. (3.3b),

$$\langle\tilde{\phi}^{(0)}|(E^{(0)}-H_0)|\phi^{(1)}\rangle = (E^{(0)}-\tilde{E}^{(0)*})\langle\tilde{\phi}^{(0)}|\phi^{(1)}\rangle \equiv 0 ,$$

so that, assuming the normalization (3.13)

$$E^{(1)} = \langle\tilde{\phi}^{(0)}|H_1|\phi^{(0)}\rangle . \tag{4.7a}$$

In the special case corresponding to Eq. (3.11), this becomes

$$E^{(1)} = \int \phi^{(0)}(x) H_1 \phi^{(0)}(x)\, dx . \tag{4.7b}$$

This is the result derived recently by More.[3] The first-order correction to the wave function is

$$|\phi^{(1)}\rangle = -(E^{(0)}-H_0)^{-1}(E^{(1)}-H_1)|\phi^{(0)}\rangle . \tag{4.8a}$$

Inserting the identity operator (3.14)

$$|\phi^{(1)}\rangle = \sum_{n\neq i}(E_i^{(0)}-E_n^{(0)})^{-1}\langle\tilde{\phi}_n^{(0)}|H_1|\phi_i^{(0)}\rangle|\phi_n^{(0)}\rangle , \tag{4.8b}$$

where the subscript i has been inserted to indicate the unperturbed eigenstate which ϕ approaches as $\lambda\to 0$. Similarly,

$$E^{(2)} = \sum_{n\neq i}\langle\tilde{\phi}_i^{(0)}|H_1|\phi_n^{(0)}\rangle\langle\tilde{\phi}_n^{(0)}|H_1|\phi_i^{(0)}\rangle(E_i^{(0)}-E_n^{(0)})^{-1} . \tag{4.9}$$

Equations (4.7) – (4.9) differ from the Hermitian counterparts significantly despite their similar form. For example, a real positive perturbation, $H_1(x)\geq 0$ need not produce a positive $E^{(1)}$. This has been verified by considering the soluble model of Ref. 2. Consider for H_0 a spherical box of radius r_A containing a "square well" $V=-iV_I$ for $r<r_N$. If we take

$$\lambda H_1 = \begin{cases} -V_R = \text{const}; & r<r_N \\ 0; & r>r_N , \end{cases} \tag{4.10}$$

then $E=E^{(0)}+c(-V_R)+\cdots$. The exact solution[2] of this problem shows that for the ground state

$$\mathrm{Re}\,c<0 , \quad \mathrm{Im}\,c>0 .$$

The value of c can also be obtained by using Eq. (4.7b); the two values are in agreement.

V. PROJECTION-OPERATOR METHODS

In dealing with problems for which the spectrum and corresponding eigenstates consist of two weakly coupled groups of states, the effect of one on the other can usually be described by the projection-operator techniques introduced for Hermitian problems by Feshbach.[5] The existence of the projection operators (3.15) for the non-Hermitian problem permits a similar derivation here. As in Sec. IV the results will look very similar to those for the Hermitian case, but they are in fact quite different.

Define H as in Eq. (4.1) with H_0 non-Hermitian. We use the eigenstates $\phi_n^{(0)}$ of H_0 to define a projection operator and its complement as in Eq. (3.15):

$$\mathcal{P} = \sum_{n\in R}|\phi_n^{(0)}\rangle\langle\tilde{\phi}_n^{(0)}| , \tag{5.1}$$

$$\mathcal{Q} = 1-\mathcal{P} .$$

They satisfy the same conditions (2.2) as do the projection operators of Sec. II, but they are not Hermitian.

As in Sec. II, the effect of the $\mathcal{Q}$-channel states on the portion $\phi_{\mathcal{P}}\equiv\mathcal{P}\phi$ of the wave function in the $\mathcal{P}$ channel can be expressed as an effective potential in the $\mathcal{P}$ channel given by Eq. (2.12).[13] In the notation of Eq. (2.4)

$$[H_{\mathcal{P}\mathcal{P}}+H_{\mathcal{P}\mathcal{Q}}(E-H_{\mathcal{Q}\mathcal{Q}})^{-1}H_{\mathcal{Q}\mathcal{P}}]\phi_{\mathcal{P}} = E\phi_{\mathcal{P}} . \tag{5.2}$$

The new effective Hamiltonian will also satisfy the condition (3.8) if H does and, if for each $\phi_{n\alpha}$ contained in the set R defining $\mathcal{P}$, $\phi_{n\bar{\alpha}}$ is also in R.

As an illustration of the use of this technique, let us consider once again the model problem of Ref. 2, as stated in the paragraph preceding Eq. (4.10). For sufficiently large V_I the spectrum of H_0 was found to consist of two relatively distinct types of states. "Outer states" are largely confined to the "outer region" ($r_N<r<r_A$) and fall off rapidly in the "inner region" ($r<r_N$). "Inner states" are largely confined to the inner region and fall off rapidly in the outer region. The inner states have $\mathrm{Im}E\sim V_I$ as can be seen from Eq. (3.4), while the outer states have $\mathrm{Im}E\ll V_I$ due to their small penetration into the absorptive inner region. Once this division has been established, then one question of interest is the effect which varying V_R [see Eq. (4.10)] has on the energies of low-lying outer states. Projection-operator techniques can

be used to answer this question, both for this model and for more realistic calculations.

Let $\mathcal{P}$ be the projection operator onto the particular outer state of interest, and $\mathcal{Q}$ be the projection operator onto the inner states of H_0. The effect of the inner states on the outer state, when H_1 is nonzero, is contained in the effective-interaction term obtained by replacing H by $H_0+\lambda H_1$ in Eq. (5.2):

$$\mathcal{V}_{\mathcal{P}}=\lambda^2(H_1)_{\mathcal{P}\mathcal{Q}}[E-(H_0+\lambda H_1)_{\mathcal{Q}\mathcal{Q}}]^{-1}(H_1)_{\mathcal{Q}\mathcal{P}}. \quad (5.3)$$

To determine the effect of $\mathcal{V}_{\mathcal{P}}$ as V_R is increased we require the eigenstates of $(H_0+\lambda H_1)_{\mathcal{Q}\mathcal{Q}}$. That is, we require the V_R dependence of the eigenvalues E_i and corresponding eigenstates Ψ_i which span the same space as the $V_R=0$ inner states ϕ_i:

$$(H_0)_{\mathcal{Q}\mathcal{Q}}|\phi_i\rangle=E_i^{(0)}|\phi_i\rangle, \quad (5.4)$$

$$(H_0+\lambda H_1)_{\mathcal{Q}\mathcal{Q}}|\Psi_i\rangle=E_i|\Psi_i\rangle. \quad (5.5)$$

All such states are well confined to the inner region. We assume therefore that their wave functions change very little as V_R is varied, but that their energies change essentially linearly with V_R. Thus,

$$|\Psi_i\rangle\approx|\phi_i\rangle, \quad E_i=E_i^{(0)}-S_iV_R, \quad (5.6)$$

where S_i is the fraction of the inner state ϕ_i in the inner region.

$$S_i=\langle\tilde{\phi}_i|\theta(r_N-r)|\phi_i\rangle=\frac{\mathrm{Im}E_i^{(0)}}{V_I}\lesssim 1. \quad (5.7)$$

The step function $\theta(x)$ is unity for $x>0$ and zero otherwise. The first-order effect of this term on the energy E_0 of the outer state ϕ_0 is obtained using Eq. (4.7a)[14]:

$$\Delta E_0\approx\sum_i\frac{\langle\tilde{\phi}_0|V_R\theta(r_N-r)|\phi_i\rangle\langle\tilde{\phi}_i|V_R\theta(r_N-r)|\phi_0\rangle}{E_0-E_i+S_iV_R}. \quad (5.8)$$

As V_R is increased, the real part of the denominator in Eq. (5.8) changes sign as the corresponding inner state is "drawn down" into the increasingly more attractive well in the inner region. As this occurs for the various different inner states, the energy contribution ΔE_0 oscillates. A more complete discussion of this phenomenon is contained in Ref. 2. The key to its understanding, however, is the projection-operator theory based on a non-Hermitian Hamiltonian.

VI. *K*-MESONIC ATOMIC CASCADES

As an example of the way in which non-Hermitian Hamiltonians arise in an actual problem, we consider a K-mesonic atom cascade process. Some of the results obtained here refer to any cascade process. Let N and N' denote two nuclei and let $A(nl)$ denote the (n,l) K-mesonic atomic state. Consider a particular process starting from a K^- incident on nucleus N, and terminating with a final state containing the nucleus N', several photons, a hyperon, and a pion,

$$K^-+N\to\cdots\to A(4f)+(n-1)\gamma \to A(3d)+n\gamma\to N'+n\gamma+\Lambda+\pi. \quad (6.1)$$

The total Hamiltonian H consists of the interaction H_γ of the hadronic current with the electromagnetic fields plus the Hamiltonian H_0 for everything else, including the portion of the strong interaction responsible for the ultimate K^- absorption:

$$H=H_0+H_\gamma. \quad (6.2)$$

Let the eigenstate of H which is asymptotically the final state of the process (6.1) be $|\Psi_f(-)\rangle$, and the eigenstate of H_0 which is asymptotically the initial state of (6.1) be $|\Phi_i(+)\rangle$.[15] The amplitude for for the particular process (6.1) may be calculated from the general amplitude

$$T_{fi}=\langle\Psi_f(-)|H_\gamma|\Phi_i(+)\rangle =\langle\Phi_f(-),n\gamma|[H_\gamma+H_\gamma(E-H+i\epsilon)^{-1}H_\gamma]|\Phi_i(+)\rangle, \quad (6.3)$$

where $|\Phi_f(-),n\gamma\rangle$ is the eigenstate of H_0 which goes asymptotically to the final state of the process (6.1). It is the product of the hadronic state $|\Phi_f(-)\rangle$ and the n-photon state which we have abbreviated by $|n\gamma\rangle$, although the momentum and polarization of each photon is actually needed to specify the state. If the propagator $(E-H+i\epsilon)^{-1}$ of Eq. (6.3) were expanded in a power series in H_γ, one would obtain conventional perturbation-theory results and the process (6.1) would be described by the term containing n factors of H_γ. However, this would not contain electromagnetic width effects. We will develop an expansion which keeps both the hadronic and the electromagnetic contributions to the width.

The process (6.1) arises as a special case of Eq. (6.3) for which the photons arise only from the K^-N current. That is, this particular process results from that portion of H_γ which operates in the K^-N subspace of the total hadronic Hilbert space. Letting P_{KN} be the projection operator onto this subspace, we conclude that the amplitude to

be calculated is

$$T_{fi} = \langle \Phi_f(-), n\gamma | P_{KN} H_\gamma P_{KN} (E - H + i\epsilon)^{-1} P_{KN} H_\gamma P_{KN} | \Phi_i(+) \rangle . \tag{6.4}$$

The effective propagator is the projection of the total propagator onto the K^-N subspace. In Sec. II we found that this can be replaced by propagation with a non-Hermitian Hamiltonian. [See Eqs. (2.10), (2.11), and (2.12).]

$$P_{KN}(E - H + i\epsilon)^{-1} P_{KN} = (E - \mathcal{H}_{KN} - H_{\rm em} - V_\gamma + i\epsilon)^{-1} \tag{6.5}$$

In Eq. (6.5) we have explicitly separated the terms in the projected Hamiltonian which refer to the electromagnetic field. The projected interaction Hamiltonian is

$$V_\gamma \equiv P_{KN} H_\gamma P_{KN} , \tag{6.6}$$

and the free-field Hamiltonian for the photons is $H_{\rm em}$. The effective K^-N Hamiltonian $\mathcal{H}_{KN}$ contains an optical potential arising from the coupling to other strong-interaction channels. The transition is now described by

$$T_{fi} = \langle \Phi_f(-) | P_{KN} M_{n\gamma} P_{KN} | \Phi_i(+) \rangle , \tag{6.7}$$

$$M_{n\gamma} = \langle n\gamma | V_\gamma (E - \mathcal{H}_{KN} - H_{\rm em} - V_\gamma + i\epsilon)^{-1} V_\gamma | 0 \rangle . \tag{6.8}$$

The complexities of the final strong decay in the cascade (6.1) will not be treated explicitly, but are contained in the projection of $\langle \Phi_f(-)|$ into the K^-N channel.

The only remaining step in the development of T_{fi} to a form which is recognizable as a sequential decay is the expansion of Eq. (6.8) in powers of V_γ. Since V_γ changes the photon number by 1 each time it operates, and electromagnetic interactions are weak, we need an expansion with n factors of V_γ in the numerator; however, we also wish to keep electromagnetic width effects in the intermediate propagators.

This can be done formally by defining projection operators P_k, $k = 0, 1, 2, \ldots$ onto states of k photons. The interaction V_γ has the special property that $P_k V_\gamma P_{k'}$ is zero unless $k' = k \pm 1$. We require several propagators. The propagator in Eq. (6.8) is

$$G(E) = (E - \mathcal{H}_{KN} - H_{\rm em} - V_\gamma + i\epsilon)^{-1} , \tag{6.9}$$

and the corresponding noninteracting propagator is

$$G^{(0)}(E) = (E - \mathcal{H}_{KN} - H_{\rm em} + i\epsilon)^{-1} . \tag{6.10}$$

The projection of $G^{(0)}(E)$ into the k-photon subspace is

$$G_k^{(0)}(E) \equiv P_k G^{(0)}(E) P_k = [P_k (E - \mathcal{H}_{KN} - H_{\rm em}) P_k + i\epsilon]^{-1} . \tag{6.11}$$

Using the techniques of Sec. II, the projection of G onto the k-photon subspace is seen to be

$$G_k(E) \equiv P_k G(E) P_k = [P_k (E - \mathcal{H}_{KN} - H_{\rm em}) P_k - \Delta_k(k-1) - \Delta_k(k+1) + i\epsilon]^{-1} , \tag{6.12}$$

where

$$\Delta_k(k \pm 1) = P_k V_\gamma P_{k\pm1} G_{k\pm1}^{(0)}(E) P_{k\pm1} V_\gamma P_k . \tag{6.13}$$

These terms $\Delta_k(k \pm 1)$ yield the electromagnetic contributions to the widths and shifts of the K-mesonic atomic states.

The final type of propagator which is needed also operates in the k-photon subspace; it contains width and shift effects corresponding to $k-1$ photon states. It is given by

$$G_{k(k-1)}(E) \equiv [P_k (E - \mathcal{H}_{KN} - H_{\rm em}) P_k - \Delta_k'(k-1) + i\epsilon]^{-1} , \tag{6.14}$$

where

$$\Delta_k'(k-1) = P_k V_\gamma P_{k-1} G_{k-1(k-2)}(E) P_{k-1} V_\gamma P_k \tag{6.15}$$

and

$$\Delta_1'(0) = P_1 V_\gamma P_0 G_0^0(E) P_0 V_\gamma P_1 .$$

Because V_γ is weak, $\Delta_k'(k-1)$ is essentially the same as $\Delta_k(k-1)$. It is convenient to define one last operator,

$$V_{k,k'} \equiv P_k V_\gamma P_{k'} , \quad k' = k \pm 1 . \tag{6.16}$$

We have now defined everything which will be needed to express T_{fi} in a sequential decay form. This form is given in Eqs. (6.25) and (6.26). The reader may at this point wish to skip over the derivation below and proceed directly to Eq. (6.25) and the discussion which follows.

The expansion of $G(E)$ is based on the same operator identity as ordinary perturbation theory:

$$G = G^{(0)} + G V_\gamma G^{(0)} . \tag{6.17}$$

If we use the fact that $G^{(0)}$ does not connect states with different numbers of photons, we find

$$G P_0 = G_0^{(0)} + G P_1 V_{10} G_0^{(0)} ; \tag{6.18}$$

$$G P_1 = G_1^{(0)} + G P_0 V_{01} G_1^{(0)} + G P_2 V_{21} G_1^{(0)} . \tag{6.19}$$

Substituting Eq. (6.18) into Eq. (6.19) gives

$$GP_1(1 - V_{10}G_0^{(0)}V_{01}G_1^{(0)}) = (1 + G_0^{(0)}V_{01} + GP_2V_{21})\,G_1^{(0)}\,. \tag{6.20}$$

Solving Eq. (6.20) gives an expression for GP_1 involving the total propagator G only in the form GP_2:

$$GP_1 = (1 + G_0^{(0)}V_{01})\,G_{1(0)} + GP_2V_{21}G_{1(0)}\,. \tag{6.21}$$

We have used the fact that the propagator $G_{k(k-1)}$ defined in Eq. (6.14) satisfies the identity

$$G_{k(k-1)} = G_k^{(0)}(1 - V_{k,k-1}G_{k-1(k-2)}V_{k-1,k}G_k^{(0)})^{-1}\,,$$

and for the special case of $k=1$,

$$G_{1(0)} = G_1^{(0)}(1 - V_{10}G_0^{(0)}V_{01}G_1^{(0)})^{-1}\,.$$

By iteration of this technique we can obtain formally exact expressions for GP_2 in terms of GP_3 and so on:

$$GP_2 = [1 + (1 + G_0^{(0)}V_{01})\,G_{1(0)}V_{12}]\,G_{2(1)} + GP_3V_{32}G_{2(1)}\,, \tag{6.22}$$

$$\vdots$$

$$GP_k = \big(1 + \{1 + [1 + \cdots (1 + G_0^{(0)}V_{01})\,G_{1(0)}V_{12}]\ldots\} \times G_{k-1(k-2)}V_{k-1,k}\big)\,G_{k(k-1)} + GP_{k+1}V_{k+1,k}G_{k(k-1)}\,. \tag{6.23}$$

In order to calculate $M_{n\gamma}$ [Eq. (6.8)], we need $P_{n-1}GP_1$. From Eq. (6.21) we see that

$$P_{n-1}GP_1 = P_{n-1}GP_2V_{21}G_{1(0)}\,, \tag{6.24}$$

because the first term in Eq. (6.21) has zero projection into the $n-1$ photon space. Now Eq. (6.22) gives $P_{n-1}GP_2$ in terms of $P_{n-1}GP_3$, and so on. Finally, we find the exact formal result

$$P_{n-1}GP_1 = G_{n-1}V_{n-1,n-2}G_{n-2(n-3)}\cdots V_{3,2}G_{2(1)}V_{21}G_{1(0)}\,, \tag{6.25}$$

where G_{n-1} is given by Eq. (6.12), and the remainder of the propagators, by Eq. (6.14). The transition amplitude in terms of the result (6.25) is finally given by

$$T_{fi} = \langle \Phi_f(-), n\gamma\,|\,P_{KN}V_{n,n-1}P_{n-1}GP_1V_{10}P_{KN}|\Phi_i(+)\rangle\,. \tag{6.26}$$

Following the approach of Sec. III, we now expand the propagators in Eq. (6.25) in a complete set of eigenstates of the non-Hermitian Hamiltonian in its denominator. Because the electromagnetic contributions, $\Delta_k(k\pm1)$ in Eq. (6.13) and $\Delta_k'(k-1)$ in Eq. (6.15), are second order in V_γ, they should be small, and may be treated using first-order perturbation theory (Sec. IV) based on the non-Hermitian Hamiltonian $\mathcal{H}_{KN}$ for the K^-N system. The assumption of a particular cascade (6.1) requires each propagator to be replaced by a single term in this expansion. For instance, for propagation in the $5g$ state in the presence of $n-2$ photons, we have

$$G_{n-2(n-3)}(E) = \int \frac{|\Phi_{5g};q_1\cdots q_{n-2}\rangle\langle\tilde{\Phi}_{5g};q_1\cdots q_{n-2}|}{E - E_{5g} - q_1 - \cdots - q_{n-2} - \Delta_{5g}} \times dq_1\cdots dq_{n-2}\,, \tag{6.27}$$

with

$$\Delta_{5g} = \langle\tilde{\Phi}_{5g};q_1\cdots q_{n-2}|\Delta'_{n-2}(n-3)|\Phi_{5g};q_1\cdots q_{n-2}\rangle\,. \tag{6.28}$$

The state $|\Phi_{5g}\rangle$ is an eigenstate of $\mathcal{H}_{KN}$ with eigenvalue E_{5g}, and the photons have momenta q_i, $i=1,\ldots,n-2$. The imaginary part of Δ_{5g} is the total electromagnetic width due to transitions into the $5g$ state.

From this stage on the calculation is conventional, but we wish to stress two points. Even though $\mathrm{Im}E_{nl}$ for each state of the cascade will be small, it cannot be calculated using perturbation theory. This was evident in Sec. V where we saw that the width is small because of the small penetration into the absorptive nuclear region. The small penetration cannot be reproduced in first-order perturbation theory. The second point is that all matrix elements of V_γ will contain the state $\tilde{\Phi}_{nl}$ in the bra vectors rather than Φ_{nl}. Therefore the width for a given transition $(nl \to n'l')$ will be proportional to $|\langle\tilde{\Phi}_{n'l'}|\hat{\epsilon}\cdot\tilde{\mathbf{J}}(q)|\Phi_{nl}\rangle|^2$, where q and $\hat{\epsilon}$ are the momentum and polarization of the emitted photon, and $\tilde{\mathbf{J}}(q)$ is the electromagnetic current operator. It is not likely that this change would have a very large effect on yield calculations,[16] however, because the non-Hermiticity is confined to a relatively small region, and the K-mesonic atomic wave functions are very small in this region.

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*Research supported in part by the National Science Foundation and the U. S. Atomic Energy Commission.

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[12]Expansions similar to this have been assumed by reaction theorists dating back to P. Kapur and R. Peierls, Proc. Roy. Soc. (London) A166, 277 (1938).

[13]This is given here in the standard form. We omit the derivation and refer the reader to Ref. 5. The effective Hamiltonian has the same form as in Eq. (2.11).

[14]The expansion parameter for which this is a first-order contribution is not V_R, which is in fact very large, but rather the square of the overlap between the inner and outer states in the inner region. This is small because the outer states do not penetrate into this region significantly.

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Neutron-Deuteron Elastic Scattering Above the Breakup Threshold*

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Amplitudes for elastic s-wave neutron-deuteron scattering above the breakup threshold are calculated by the method of complex coordinates. The nucleon-nucleon interaction is represented by a local spin- and parity-dependent central Yukawa potential, with parameters chosen to fit low-energy two-nucleon data. Results for inelastic parameters indicate possible errors in a previous phase-shift analysis. Results for the quartet phase shift and quartet and doublet inelastic parameters are consistent with separable potential calculations, but the doublet phase shifts from the two models differ significantly.

I. INTRODUCTION

The three-nucleon scattering problem has received considerable attention in recent years.[1] The use of local nucleon-nucleon potentials has been hampered, however, by the severe numerical problems occasioned by their use in Watson-Faddeev-type integral equations; nonlocal separable potentials or separable nucleon-nucleon t matrices have been used to circumvent these problems. In the energy range below the breakup threshold the Kohn variational principle has provided an efficient technique for finding scattering amplitudes due to local interactions, but a straightforward extension to the breakup region has not so far proved useful.[2] The asymptotic behavior of the wave function necessary to describe three free particles is quite complicated,[3] and this asymptotic behavior must presumably be accurately represented in the trial function if convergence of the Kohn method is to be expected.

In this article we present calculations of s-wave elastic amplitudes in the breakup region, based on the method of complex coordinates[4] reviewed briefly in Sec. II. This method does not require the complicated asymptotic terms representing three free particles, and thus provides what appears to be a useful and productive alternative to the Kohn method. The main result of this paper is to show that for short-range local potentials which are analytic functions of the coordinates (except perhaps at the origin) calculations of elastic scattering can be performed almost as easily above the breakup threshold as below, even if substantial inelastic scattering takes place. The principle of the method also applies to the calculation of break-