Distorted-wave amplitudes, distorted-wave Born approximation, and self-energies in the Fock-Tani theory of rearrangement collisions

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In the Fock-Tani representation for rearrangement collisions, the interaction Hamiltonian decomposes into terms representing interactions within each arrangement channel and channel-changing rearrangement interactions. The two-potential formalism is used to cast transition amplitudes into a distorted-wave form in which in-channel interactions are treated exactly and interchannel transitions in finite order, thus separating initial- and final-state interactions from rearrangements. Self-energies arising from infinite-order summations of selected interchannel transitions are also considered and illustrated by shifts and broadenings of scattering and reaction resonances.

I. INTRODUCTION

The Fock-Tani representation[1-3] for rearrangement collisions in a system of composite particles is obtained by a suitable unitary transformation, starting from the standard Fock representation in terms of annihilation and creation operators for all the constituents. The applications made thus far[4-8] are to problems in the theory of atomic collisions and chemical reaction dynamics, in which the constituents are the electrons and nuclei of the atomic, molecular, and ionic species involved. The generator of the unitary transformation to the new "Fock-Tani" representation is constructed in such a way as to introduce new *elementary particle* (Bose or Fermi) annihilation and creation operators $\hat{a}_{\alpha s}$ and $\hat{a}^{\dagger}_{\alpha s}$ for the various *composite* (atomic, molecular, ionic) species s involved.[1] This approach is closely related to Weinberg's "quasiparticle method"[9] for bound-state scattering theory, to Dyson's "ideal-space" representation[10] for spin waves in the Heisenberg model, and to the canonical transformation method of Bohm and Pines[11] for the theory of plasmons in an electron gas. The reader is referred to the literature[1-3] for details of the derivation and structure of the Fock-Tani representation. Here only the qualitative features will be listed.

The Fock-Tani Hamiltonian $\hat{H}$ decomposes naturally into $\hat{H}=\hat{H}_0+\hat{V}$ where $\hat{H}_0$ describes both free composites and free (unbound) constituents, and $\hat{V}$ describes all possible scattering and reaction processes between the composites and constituents. All internal binding of composites is included in $\hat{H}_0$, as in the quasiparticle method.[9] The explicit expression is

$$\hat{H}_0=\sum_{\alpha,s}\epsilon_{\alpha s}\hat{a}^{\dagger}_{\alpha s}\hat{a}_{\alpha s}+\sum_{k,j}\epsilon_{kj}\hat{\psi}^{\dagger}_{kj}\hat{\psi}_{kj}\ , \tag{1}$$

where

$$\epsilon_{\alpha s}=\int\phi^{*}_{\alpha s}(X_s)H_s(X_s)\phi_{\alpha s}(X_s)dX_s\ , \tag{2}$$

$\phi_{\alpha s}$ being the wave function of a composite of species s in state α, X_s being the configuration variables (space and spin) of all the constituents (electrons, nuclei) of the composite, and $H_s(X_s)$ the Schrödinger Hamiltonian of these constituents, including their interactions. The $\hat{\psi}_{kj}$ and $\hat{\psi}^{\dagger}_{kj}$ are annihilation and creation operators for free constituents, ϵ_{kj} being the energy of a constituent of type j in state $\phi_{kj}(x_j)$:

$$\epsilon_{kj}=\int\phi^{*}_{kj}(x_j)H_j(x_j)\phi_{kj}(x_j)dx_j\ . \tag{3}$$

Here $H_j(x_j)$ is the single-particle Schrödinger Hamiltonian of a constituent of type j. If the ϕ_{kj} are chosen to be eigenstates of H_j (plane waves, if there is no external potential), then ϵ_{kj} is the single-particle energy eigenvalue. Similarly, if the $\phi_{\alpha s}$ are chosen to be eigenstates of H_s then $\epsilon_{\alpha s}$ of Eq. (2) is the energy eigenvalue of a single (isolated) bound composite of species s. However, there are cases where it is desirable to include quasibound resonance states in (1). For these states $\epsilon_{\alpha s}$ is only a (real) expectation value, coupling to the continuum leading naturally, through an appropriate self-energy formalism, to a complex resonance energy including shift and broadening. An example will be discussed in Sec. IV. In applications to scattering and reaction problems the quantum numbers α of a composite state $\phi_{\alpha s}$ usually include both a translational wave vector $\mathbf{k}$ and a set of internal (atomic or molecular) quantum numbers. Similarly, the k quantum number of a free-constituent state ϕ_{kj} usually stands for both the translational wave vector $\mathbf{k}$ and a spin z-component quantum number.

The Fock-Tani interaction Hamiltonian $\hat{V}$ contains terms representing all possible scattering and reaction channels of the system of composites and their constituents. For example, if $\phi_{\alpha s}$ is not a single-composite energy eigenstate but rather a resonance, then there are off-diagonal terms

$$\sum_{\alpha,\beta}{}'\,\hat{a}^{\dagger}_{\alpha}(\alpha\,|\,H\,|\,\beta)\hat{a}_{\beta} \tag{4}$$

with

$$(\alpha\,|\,H\,|\,\beta)=\int\phi^{*}_{\alpha}(X_s)H_s(X_s)\phi_{\beta}(X_s)dX_s\ , \tag{5}$$

as well as terms

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$$\text{const}\times \sum_{k_1,\ldots,k_n} [\hat{\psi}^{\dagger}_{k_1 j_1}\cdots\hat{\psi}^{\dagger}_{k_n j_n}(k_1 j_1\cdots k_n j_n \mid H \mid \alpha)\hat{a}_{\alpha s} + \text{H.c.}] \tag{6}$$

representing decay (formation) of the resonance αs into (from) the continuum. The explicit expression for the decay matrix element is[1,2]

$$(k_1 j_1\cdots k_n j_n \mid H \mid \alpha s) = \int \phi^{*}_{k_1 j_1}(x_1)\cdots\phi^{*}_{k_n j_n}(x_n)(x_1\cdots x_n \mid H \mid \alpha s)\,, \tag{7}$$

$$\begin{aligned}(x_1\cdots x_n \mid H \mid \alpha s) &= H_s(x_1\cdots x_n)\phi_{\alpha_s}(x_1\cdots x_n) \\ &\quad - \int \Delta_s(x_1\cdots x_n, x'_1\cdots x'_n)H_s(x'_1\cdots x'_n) \\ &\quad \times\phi_{\alpha_s}(x'_1\cdots x'_n)dx'_1\cdots dx'_n\,,\end{aligned}$$

where Δ_s is the composite-state kernel

$$\Delta_s(X_s, X'_s) = \sum_{\alpha}\phi_{\alpha s}(X_s)\phi^{*}_{\alpha s}(X'_s)\,, \tag{8}$$

with $X_s=(x_1,\ldots,x_n)$. Using the identity

$$\int \Delta_s(X_s, X'_s)\phi_{\alpha s}(X'_s)dX'_s = \phi_{\alpha s}(X_s) \tag{9}$$

following from orthonormality[12] of the $\phi_{\alpha s}$, one proves easily that (7) vanishes identically if $H_s\phi_{\alpha s}=\epsilon_{\alpha s}\phi_{\alpha s}$ (bound state). Thus these matrix elements are nonzero only for states which really do decay (resonances). In the case of monomolecular decay reactions $A^{*}\rightarrow B+C$ (predissociative decay of a molecule into smaller molecules rather than free constituents), there are also terms

$$\text{const}\times \sum_{\alpha,\beta,\gamma} [\hat{a}^{\dagger}_{\beta B}\hat{a}^{\dagger}_{\gamma C}(\beta b,\gamma C \mid H \mid \alpha A)\hat{a}_{\alpha A} + \text{H.c.}]\,. \tag{10}$$

Descriptions of molecular predissociation in this representation have been given recently.[7,8] More complicated terms in $\hat{V}$ describe bimolecular reactions (terms proportional to $\hat{a}^{\dagger}_{\alpha A}\hat{a}^{\dagger}_{\beta B}\hat{a}_{\delta D}\hat{a}_{\gamma C}$), scattering and reactions between composites and constituents, etc.[1]

In the remaining sections of the paper the treatment of initial- and final-state interactions and self-energy effects in this representation will be described. We will not be concerned here with details of the explicit forms of the matrix elements but rather with the general structure of the theory. In Sec. II the two-potential form of Lippmann-Schwinger collision theory is used to cast T-matrix elements into a distorted-wave (DW) form in which initial- and final-state interactions are treated exactly and rearrangements in finite order. The general formalism is illustrated by explicit examples of higher-order Fock-Tani diagrams for the process $D^{+}+H\rightarrow D+H^{+}$. The resultant DW Born series involves distorted intermediate states of the form $\hat{G}^{+d}\mid\nu)$ where $\mid\nu)$ is an eigenstate of $\hat{H}_0$ (undistorted state) but the distorted Green's operator $\hat{G}^{+d}$ contains initial- and final-state interactions to infinite order. A method of evaluating such states through solution of appropriate inhomogeneous equations is described in Sec. III. In certain physical situations it is important to also treat some rearrangement transitions exactly. This is the case, for example, in determination of shifts and broadenings of scattering and reaction resonances, in which decay and formation reactions of the form of (6) or (10) must be treated to infinite order. In Sec. IV a self-energy formalism for doing this is described. It involves distorted intermediate states which can be determined by the method of Sec. III; expressions for resonance shifts and broadenings are derived in a simple example.

II. TWO-POTENTIAL FORMALISM AND DISTORTED-WAVE AMPLITUDES

Consider a rearrangement collision with initial arrangement channel i and final arrangement channel f. We denote the Fock-Tani representation asymptotic initial and final states by $\mid\alpha_i)$ and $\mid\alpha_f)$, respectively, where α_i (α_f) is a complete set of quantum number labels for a state in arrangement channel i (f). They satisfy

$$\begin{aligned}\hat{H}_0\mid\alpha_i) &= E_i\mid\alpha_i)\,, \\ \hat{H}_0\mid\alpha_f) &= E_f\mid\alpha_f)\,.\end{aligned} \tag{11}$$

The exact transition amplitude (T-matrix element) for the process $\alpha_i\rightarrow\alpha_f$ is given by Lippmann-Schwinger theory as

$$\begin{aligned}T_{\alpha_f\alpha_i} &= (\alpha_f\mid\hat{T}\mid\alpha_i) \\ &= (\alpha_f\mid[\hat{V}+\hat{V}\hat{G}^{+}_0(E)\hat{V} \\ &\qquad +\hat{V}\hat{G}^{+}_0(E)\hat{V}\hat{G}^{+}_0(E)\hat{V}+\cdots]\mid\alpha_i) \\ &= (\alpha_f\mid\hat{V}\mid\alpha^{+}_i) = (\alpha^{-}_f\mid\hat{V}\mid\alpha_i)\,,\end{aligned} \tag{12}$$

where

$$\hat{G}^{+}_0(E) = (E+i\eta-\hat{H}_0)^{-1} \tag{13}$$

with $\eta=0^{+}$, $E=E_i=E_f$. The in state $\mid\alpha^{+}_i)$ (ingoing plane wave, outgoing spherical wave) satisfies the Lippmann-Schwinger equation

$$\begin{aligned}\mid\alpha^{+}_i) &= \mid\alpha_i)+\hat{G}^{+}_0(E)\hat{V}\mid\alpha^{+}_i) \\ &= [\hat{1}+\hat{G}^{+}_0(E)\hat{V}+\hat{G}^{+}_0(E)\hat{V}\hat{G}^{+}_0(E)\hat{V}+\cdots]\mid\alpha_i)\end{aligned} \tag{14}$$

whereas the out state (outgoing plane wave, ingoing spherical wave) satisfies

$$\begin{aligned}(\alpha^{-}_f\mid &= (\alpha_f\mid+(\alpha^{-}_f\mid\hat{V}\hat{G}^{+}_0(E) \\ &= (\alpha_f\mid[\hat{1}+\hat{V}\hat{G}^{+}_0(E)+\hat{V}\hat{G}^{+}_0(E)\hat{V}\hat{G}^{+}_0(E)+\cdots]\end{aligned} \tag{15}$$

or equivalently

$$\mid\alpha^{-}_f) = \mid\alpha_f)+\hat{G}^{-}_0(E)\hat{V}\mid\alpha^{-}_f)\,. \tag{16}$$

One should distinguish carefully between the initial and final *arrangement* channels (generic labeling, only *species* specified), which we denote simply by i and f, and the initial and final *channels* (*specific* labeling, both species and states specified), which we denote by α_i and α_f.

Each term in the Fock-Tani interaction Hamiltonian $\hat{V}$ is of the form

$$\hat{V}_{\alpha_f\alpha_i}=\text{const}\times\hat{\Pi}^{\dagger}(\alpha_f)(\alpha_f\,|\,H\,|\,\alpha_i)\hat{\Pi}(\alpha_i)\ , \tag{17}$$

where $\hat{\Pi}(\alpha_i)$ is a product of annihilation operators for all the particles ("elementary" constituents and bound composites) defining a particular initial channel α_i, $\hat{\Pi}^{\dagger}(\alpha_f)$ is a product of creation operators for the particles defining a particular final channel α_f, and $(\alpha_f\,|\,H\,|\,\alpha_i)$ is a matrix element generated by the Fock-Tani canonical transformation from Fock to Fock-Tani state space.[1-3] It is noteworthy that in Fock-Tani representation rearrangement collisions are described by amplitudes of the form (12) used in standard Lippmann-Schwinger *scattering* theory, i.e., one does not need the more complicated rearrangement collision theory expressions involving different initial-arrangement-channel and final-arrangement-channel decompositions $\hat{H}=\hat{H}_{0i}+\hat{V}_i=\hat{H}_{0f}+\hat{V}_f$. In Fock-Tani representation the *same* decomposition $\hat{H}=\hat{H}_0+\hat{V}$ applies to both scattering and rearrangement processes and to all possible initial and final arrangement channels. Those terms in $\hat{V}$ contributing to a given real or virtual scattering or rearrangement process are selected automatically by the particular creation operators occurring in the initial state $\text{const}\times\hat{\Pi}^{\dagger}(\alpha_i)\,|\,0)$, the final state $\text{const}\times\hat{\Pi}^{\dagger}(\alpha_f)\,|\,0)$, and any intermediate states $\hat{\Pi}^{\dagger}(\alpha)\,|\,0)$.

The sum of all those terms in $\hat{V}$ describing a (first-order) transition from a given initial agreement channel i to a given final arrangement channel f is conveniently denoted by $\hat{V}_{fi}$:

$$\hat{V}_{fi}=\sum_{\alpha_f,\alpha_i}\hat{V}_{\alpha_f\alpha_i}\ , \tag{18}$$

where i and f are held fixed in the summation, but α_i and α_f range over all possible quantum numbers for given i and f. One can, similarly, define $\hat{T}_{\alpha_f\alpha_i}$ and

$$\hat{T}_{fi}=\sum_{\alpha_f,\alpha_i}\hat{T}_{\alpha_f\alpha_i} \tag{19}$$

as the sum of all those terms in the Fock-Tani transition operator $\hat{T}$ connecting given initial and final arrangement channels (generic) or states (specific). It is then clear that the exact transition amplitude (12) can be rewritten as

$$T_{\alpha_f\alpha_i}=(\alpha_f\,|\,\hat{T}\,|\,\alpha_i)=(\alpha_f\,|\,\hat{T}_{fi}\,|\,\alpha_i)\ . \tag{20}$$

The relationship between $\hat{T}_{fi}$ and the various operators $\hat{V}_{\alpha\beta}$ is in general quite complicated. It would be useful, both conceptually and for efficient organization of calculations, to rewrite (20) in a form which divides the various contributions into initial-state, final-state, intermediate-state, and rearrangement interactions. This can be done by separating the interaction Hamiltonian $\hat{V}$ into

$$\hat{V}=\hat{V}_{\text{sc}}+\hat{V}_{\text{re}}\ , \tag{21}$$

where $\hat{V}_{\text{sc}}$ is the (inelastic and elastic) *scattering* part of $\hat{V}$ (diagonal with respect to arrangement channel indices) and $\hat{V}_{\text{re}}$ is the *rearrangement* part of $\hat{V}$ (completely off diagonal with respect to arrangement channel indices):

$$\hat{V}_{\text{sc}}=\sum_j\hat{V}_{jj},\quad \hat{V}_{\text{re}}=\sum_{j,l}{}'\,\hat{V}_{jl}\ . \tag{22}$$

Define the initial- and final-state *distorted waves* by

$$\begin{aligned}|\,\alpha_i^{+d})&=|\,\alpha_i)+\hat{G}_0^{+}(E)\hat{V}_{\text{sc}}\,|\,\alpha_i^{+d})\\&=[\hat{1}+\hat{G}_0^{+}(E)\hat{V}_{\text{sc}}\\&\quad+\hat{G}_0^{+}(E)\hat{V}_{\text{sc}}\hat{G}_0^{+}(E)\hat{V}_{\text{sc}}+\cdots]\,|\,\alpha_i)\ ,\end{aligned} \tag{23}$$

$$\begin{aligned}(\alpha_f^{-d}\,|&=(\alpha_f\,|+(\alpha_f^{-d}\,|\,\hat{V}_{\text{sc}}\hat{G}_0^{+}(E)\\&=(\alpha_f\,|\,[\hat{1}+\hat{V}_{\text{sc}}\hat{G}_0^{+}(E)\\&\quad+\hat{V}_{\text{sc}}\hat{G}_0^{+}(E)\hat{V}_{\text{sc}}\hat{G}_0^{+}(E)+\cdots]\ .\end{aligned}$$

Note that all the terms in this series for $|\,\alpha_i^{+d})$ lie in the same (ith) arrangement channel; hence $|\,\alpha_i^{+d})$ differs from $|\,\alpha_i)$ by inclusion of *all initial-state interactions.* Similarly, $(\alpha_f^{-d}|$ differs from $(\alpha_f|$ by inclusion of *all final-state interactions.* The various intermediate states occurring in these expressions involve sums over translational quantum numbers of the various particles involved, and in the case of composite particles the internal quantum numbers are summed over as well (inelastic scattering). The sums over internal quantum numbers are essential for inclusion of certain initial- and final-state interaction effects. For example, monopole-induced dipole interactions involve coupling between atomic (or molecular) translation and internal excitation arising from induced dipole transitions.

The exact transition amplitude $T_{\alpha_f\alpha_i}$ can be rewritten in terms of the distorted waves $|\,\alpha_i^{+d})$ and $(\alpha_f^{-d}|$ by use of the same algebraic manipulations involved in derivation of standard distorted-wave amplitudes. Using the definitions (23) one has

$$\begin{aligned}T_{\alpha_f\alpha_i}&=(\alpha_f\,|\,\hat{V}\,|\,\alpha_i^{+})\\&=(\alpha_f^{-d}\,|\,\hat{V}\,|\,\alpha_i^{+})-(\alpha_f^{-d}\,|\,\hat{V}_{\text{sc}}\hat{G}_0^{+}(E)\hat{V}\,|\,\alpha_i^{+})\\&=(\alpha_f^{-d}\,|\,\hat{V}\,|\,\alpha_i^{+})-(\alpha_f^{-d}\,|\,\hat{V}_{\text{sc}}\,|\,\alpha_i^{+})+(\alpha_f^{-d}\,|\,\hat{V}_{\text{sc}}\,|\,\alpha_i)\\&=(\alpha_f^{-d}\,|\,\hat{V}_{\text{re}}\,|\,\alpha_i^{+})+(\alpha_f^{-d}\,|\,\hat{V}_{\text{sc}}\,|\,\alpha_i)\\&=(\alpha_f^{-d}\,|\,\hat{V}_{\text{re}}\,|\,\alpha_i^{+})\ .\end{aligned} \tag{24}$$

The penultimate equation is a special case of the general two-potential theory[13] and the final equality follows from the orthogonality of states in arrangement channels i and f. We assume here that we are dealing with a true rearrangement process, $i\neq f$. Note that different arrangement channels are orthogonal in Fock-Tani representation[14] even before passing to the infinite-volume limit.

The expression (24) is asymmetrical, involving a distorted wave $(\alpha_f^{-d}|$ on the left but the full Lippmann-Schwinger state (α_i^{+}) on the right.[15] One can obtain a

symmetrical and more useful expression by rewriting $|\alpha_i^+)$ in terms of the initial distorted-wave state $|\alpha_i^{+d})$. To do this, note from (14) and (23) that

$$\begin{aligned}|\alpha_i^+)-|\alpha_i^{+d}) &= \hat{G}_0^+(E)\hat{V}|\alpha_i^+)-\hat{G}_0^+(E)\hat{V}_{sc}|\alpha_i^{+d}) \\ &= \hat{G}_0^+(E)\hat{V}_{re}|\alpha_i^{+d})+\hat{G}_0^+(E)\hat{V}[|\alpha_i^+)-|\alpha_i^{+d})] . \end{aligned} \quad (25)$$

By iteration one generates the series

$$\begin{aligned}|\alpha_i^+)=[\hat{1}+\hat{G}_0^+(E)\hat{V}_{re}+\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V}_{re} \\ +\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V}_{re}+\cdots]|\alpha_i^{+d}) .\end{aligned} \quad (26)$$

Substitution into (24) yields an *exact distorted-wave representation* of the transition amplitude:

$$T_{\alpha_f\alpha_i}=(\alpha_f^{-d}|\hat{T}_{re}|\alpha_i^{+d}) , \quad (27)$$

where the *rearrangement operator* $\hat{T}_{re}$ is defined as

$$\begin{aligned}\hat{T}_{re} &= \hat{V}_{re}+\hat{V}_{re}\hat{G}_0^+(E)\hat{V}_{re}+\hat{V}_{re}\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V}_{re} \\ &\quad +\hat{V}_{re}\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V}_{re}+\cdots \\ &= \hat{V}_{re}+\hat{V}_{re}\hat{G}_0^+(E)\hat{V}_{re}+\hat{V}_{re}\hat{G}_0^+(E)\hat{T}\hat{G}_0^+(E)\hat{V}_{re} ,\end{aligned} \quad (28)$$

and $\hat{T}$ is the full transition operator

$$\hat{T}=\hat{V}+\hat{V}\hat{G}_0^+(E)\hat{V}+\hat{V}\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V}+\cdots . \quad (29)$$

Note that $\hat{T}_{re}$ is represented by diagrams in which the first vertex on the right and last vertex on the left are rearrangement vertices (from $\hat{V}_{re}$), but all other vertices may be either from $\hat{V}_{sc}$ (scattering) or $\hat{V}_{re}$ (rearrangement).

The expression (27) is exact. In order to obtain explicit results in calculations, one can introduce various approximations, obtaining various distorted-wave Born approximations (DWBA). The crudest one is to replace $\hat{T}_{re}$ by its first term $\hat{V}_{re}$, obtaining a form of first DWBA:

$$T_{\alpha_f\alpha_i}\approx(\alpha_f^{-d}|\hat{V}_{re}|\alpha_i^{+d})=(\alpha_f^{-d}|\hat{V}_{fi}|\alpha_i^{+d}) . \quad (30)$$

There is more physics in this first-order amplitude than in standard first DWBA, in that additional orthogonalization contributions are included via the explicit expression[1-4] for the operator $\hat{V}_{fi}$.

The expansion shown in (27) and (28) of the exact T-matrix element can be rewritten in a form in which the infinite-order summations over $\hat{V}_{sc}$ are absorbed into a distorted Green's operator. To do this, first use the standard identity

$$|\alpha_i^+)=(E+i\eta-\hat{H})^{-1}(E+i\eta-\hat{H}_0)|\alpha_i) \quad (31)$$

and the similar one

$$|\alpha_i^{+d})=(E+i\eta-\hat{H}_0-\hat{V}_{sc})^{-1}(E+i\eta-\hat{H}_0)|\alpha_i) . \quad (32)$$

Then

$$\begin{aligned}|\alpha_i^+) &= (E+i\eta-\hat{H}_0-\hat{V}_{sc}-\hat{V}_{re})^{-1} \\ &\quad \times(E+i\eta-\hat{H}_0-\hat{V}_{sc})|\alpha_i^{+d}) \\ &= [\hat{1}-\hat{G}^{+d}(E)\hat{V}_{re}]^{-1}|\alpha_i^{+d}) ,\end{aligned} \quad (33)$$

with $\hat{G}^{+d}$ the distorted-wave Green's operator

$$\hat{G}^{+d}(E)=(E+i\eta-\hat{H}_0-\hat{V}_{sc})^{-1} . \quad (34)$$

Substitution into (24) yields a DW Born expansion

$$\begin{aligned}T_{\alpha_f\alpha_i}=(\alpha_f^{-d}|\hat{V}_{re}|\alpha_i^{+d})+(\alpha_f^{-d}|\hat{V}_{re}\hat{G}^{+d}(E)\hat{V}_{re}|\alpha_i^{+d}) \\ +(\alpha_f^{-d}|\hat{V}_{re}\hat{G}^{+d}(E)\hat{V}_{re}\hat{G}^{+d}(E)\hat{V}_{re}|\alpha_i^{+d})+\cdots\end{aligned} \quad (35)$$

in which initial-, final-, and intermediate-state interactions are included to infinite order in each term via $|\alpha_i^{+d})$ (initial-state interactions), $(\alpha_f^{-d}|$ (final-state interactions), and $\hat{G}^{+d}$ (intermediate-state interactions), whereas the rearrangement interaction is taken to nth order in the nth term of the series. A method of evaluating the effect of $\hat{G}^{+d}$ on various eigenstates of $\hat{H}_0$ (necessary for explicit evaluation of the various terms in the expansion) will be discussed in Sec. III. The initial and final DW states may be taken as the outgoing- and ingoing-wave solutions of the DW Schrödinger equations

$$\begin{aligned}(\hat{H}_0+\hat{V}_{sc})|\alpha_i^{+d}) &= E|\alpha_i^{+d}) , \\ (\hat{H}_0+\hat{V}_{sc})|\alpha_f^{-d}) &= E|\alpha_f^{-d}) ,\end{aligned} \quad (36)$$

where $E=E_i=E_f$, obtained by multiplication of (32) and the corresponding equation for $|\alpha_f^{-d})$ by $(E\pm i\eta-\hat{H}_0-\hat{V}_{sc})$ and passage to the limit $\eta=0$.

An expansion of the general form (35) has been derived and used previously in a different context (elastic and inelastic electron scattering) by Dewangan, Walters, and Kingston.[16] It is also closely related to the DWBA of Hubbard *et al.*[17] Various other forms of DW Born expansions and DWBA could be obtained by somewhat different decompositions of the Fock-Tani $\hat{V}$, either through restriction of $\hat{V}_{sc}$ through inclusion of only some inchannel interactions, or through extension of $\hat{V}_{sc}$ through inclusion of certain virtual rearrangement terms (for example, virtual dipole transitions to or from the continuum), or both.

In order to make these abstract definitions concrete, consider the reaction

$$D^+(\mathbf{k}_i)+H(-\mathbf{k}_i,1s)\rightarrow D(\mathbf{k}_f,1s)+H^+(-\mathbf{k}_f) . \quad (37)$$

The only diagrams contributing to $|\mathbf{k}_i;-\mathbf{k}_i,1s;+d)$ are those of the form shown in Fig. 1 for j ranging from zero [corresponding to the term $|\mathbf{k}_i;-\mathbf{k}_i,1s)$, the "bare asymptotic state"] to infinity; a similar situation holds for the distorted final state $(\mathbf{k}_f,1s;-\mathbf{k}_f;-d|$. The vertex giving the only contribution to (30) or the first-order (in $\hat{V}_{re}$) contribution to (35) is shown in Fig. 2. In second order there is again only one type of diagram, shown in Fig. 3, in which it is to be understood that the intermediate-state

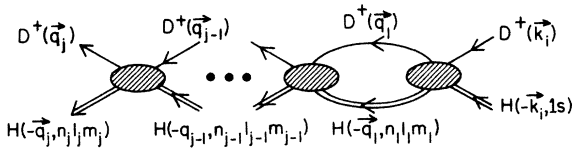


FIG. 1. The general term in the distorted initial state for the reaction $D^+ + H \rightarrow D + H^+$.

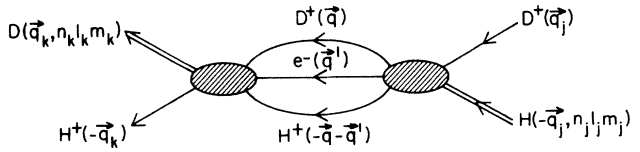


FIG. 3. The general second-order rearrangement contribution for the reaction $D^+ + H \rightarrow D + H^+$.

lines stand for a *distorted* intermediate state, to be obtained by the method of Sec. III. Similarly, the initial and final lines in Figs. 2 and 3 stand for distorted initial and final states to be obtained by solution of (36).

As an example of a situation where one might wish to extend the definition of $\hat{V}_{sc}$ by inclusion of some rearrangement terms, consider the long-range monopole-dipole initial- and final-state interaction effects on the reaction $D^+ + H \rightarrow D + H^+$. In order to include the relevant virtual bound-continuum transitions one can include the vertices of Fig. 4 in the definition of a modified initial-, final-, or intermediate-state interaction Hamiltonian $\hat{V}'_{sc}$, but with the corresponding matrix elements evaluated only in dipole approximation. The same diagrams will also occur in $\hat{V}'_{re}$ (such that $\hat{V} = \hat{V}'_{sc} + \hat{V}'_{re}$), but with the dipole contribution subtracted from the full matrix elements. These dipole contributions need only be included up to second order in evaluating the modified $\hat{G}^{+d}$, equivalent to treating the dipole contributions by second-order perturbation theory when solving the Schrödinger equations (36) and the related inhomogeneous equations of Sec. III. The corresponding modified DW Born expansion is

$$\begin{aligned} T_{\alpha_f \alpha_i} = &(\alpha_f^{-d} | \hat{V}'_{re} | \alpha_i^{+d}) + (\alpha_f^{-d} | \hat{V}'_{sc} | \alpha_i) \\ &+ (\alpha_f^{-d} | \hat{V}'_{re} \hat{G}^{+d}(E) \hat{V}'_{re} | \alpha_i^{+d}) \\ &+ (\alpha_f^{-d} | \hat{V}'_{re} \hat{G}^{+d}(E) \hat{V}'_{re} \hat{G}^{+d}(E) \hat{V}'_{re} | \alpha_i^{+d}) + \cdots , \end{aligned} \tag{38}$$

where $\hat{V}_{sc}$ is replaced by $\hat{V}'_{sc}$ in (34) and (36).

III. DISTORTED INTERMEDIATE STATES

In order to evaluate the various terms in the DW Born series (35) or (38), one needs to evaluate the effect of the DW Green's operator $\hat{G}^{+d}(E)$ on various states. For example, the second DW Born amplitude

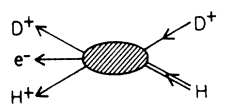
$$(\alpha_f^{-d} | \hat{V}_{re} \hat{G}^{+d}(E) \hat{V}_{re} | \alpha_i^{+d})$$

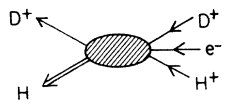
can in principle be evaluated as follows. (a) Determine the DW initial state $|\alpha_i^{+d}\rangle$, expressed as some known linear combination of eigenstates of $\hat{H}_0$, i.e., states of the form $\hat{\Pi}_j^\dagger | 0)$ where each $\hat{\Pi}_j^\dagger$ is a product of creation operators. (b) Operate with $\hat{V}_{re}$, giving a known linear combination of such states. (c) Evaluate $\hat{G}^{+d}(E)\hat{\Pi}_j^\dagger | 0)$ for each such state $\hat{\Pi}_j^\dagger | 0)$, resulting in a known linear combination of such states. (d) Operate with $\hat{V}_{re}$, giving a known linear combination of such states. (e) Determine the DW final state $(\alpha_f^{-d}|$ as a known linear combination of left eigenstates of $\hat{H}_0$, i.e., states of the form $(0 | \hat{\Pi}_j$. (f) Take the inner product of each such state with the result of step (d).

Steps (b), (d), and (f) of this program are in principle trivial, given $\hat{V}_{re}$ as an explicit linear combination of terms of the form (17). Steps (a), (c), and (e) are nontrivial. However, steps (a) and (e) are formulated as eigenvalue problems via (36), and these eigenvalue problems may be treated by standard methods. Step (c) is the most difficult. Indeed, it is often circumvented in standard second-order Born treatments by rather crude approximations, such as the well-known use of closure on intermediate states, with an "average excitation energy" whose precise definition is not clear. However, it is possible to do much better, using a method first advanced by Dalgarno and Lewis[18] and subsequently employed by a number of other workers.[19,20] The distorted intermediate states that have to be evaluated are of the form

$$|\phi_{jE}^{+d}) = \hat{G}^{+d}(E)\hat{\Pi}_j^\dagger | 0) . \tag{39}$$

Then by (34), $|\phi_{jE}^{+})$ satisfies the inhomogeneous equation





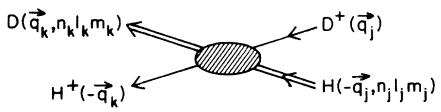
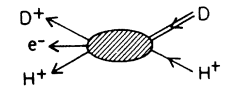


FIG. 2. The general first-order rearrangement contribution for the reaction $D^+ + H \rightarrow D + H^+$.



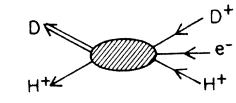


FIG. 4. Additional diagrams to be included to dipole approximation in the definition of $\hat{V}'_{sc}$.

$$(\hat{H}_0+\hat{V}_{sc})\,|\,\phi_{jE}^{+d})=(E+i\eta)\,|\,\phi_{jE}^{+d})-\hat{\Pi}_j^\dagger\,|\,0) \tag{40}$$

which is an inhomogeneous generalization of the DW eigenvalue equation (36), whose solution is expected to be of comparable difficulty[20] to solution of (36).

As an example, consider the second DW Born approximation for the reaction $D^+ + H \rightarrow D + H^+$. The three-line intermediate state of Fig. 3 stands for a distorted state of the form

$$|\,\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}',E,+d)=\hat{G}^{+d}(E)\hat{d}^\dagger_{\mathbf{q}}\hat{e}^\dagger_{\mathbf{q}'}\hat{p}^\dagger_{-\mathbf{q}-\mathbf{q}'}\,|\,0)\ , \tag{41}$$

where $\hat{d}^\dagger$, $\hat{e}^\dagger$, and $\hat{p}^\dagger$ are creation operators for the deuteron, electron, and proton, respectively.[21] This state satisfies an inhomogeneous equation of the form (40), in which the only contributing terms in $\hat{H}_0$ and $\hat{V}_{sc}$ [i.e., those which do not annihilate the states $\hat{d}^\dagger\hat{e}^\dagger\hat{p}^\dagger\,|\,0)$] are[1]

$$\hat{H}_{0d}=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}d}\hat{d}^\dagger_{\mathbf{k}}\hat{d}_{\mathbf{k}}\ ,$$

$$\hat{H}_{0e}=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}e}\hat{e}^\dagger_{\mathbf{k}}\hat{e}_{\mathbf{k}}\ ,$$

$$\hat{H}_{0p}=\sum_{\mathbf{k}}\epsilon_{\mathbf{k}p}\hat{p}^\dagger_{\mathbf{k}}\hat{p}_{\mathbf{k}}\ ,$$

$$\hat{V}_{de}=\tfrac{1}{2}\sum_{\mathbf{k}_1,\ldots,\mathbf{k}_4}\hat{d}^\dagger_{\mathbf{k}_1}\hat{e}^\dagger_{\mathbf{k}_2}(\mathbf{k}_1\mathbf{k}_2\,|\,H_{de}\,|\,\mathbf{k}_3\mathbf{k}_4)\hat{e}_{\mathbf{k}_4}\hat{d}_{\mathbf{k}_3}\ , \tag{42}$$

$$\hat{V}_{dp}=\tfrac{1}{2}\sum_{\mathbf{k}_1,\ldots,\mathbf{k}_4}\hat{d}^\dagger_{\mathbf{k}_1}\hat{p}^\dagger_{\mathbf{k}_2}(\mathbf{k}_1\mathbf{k}_2\,|\,H_{dp}\,|\,\mathbf{k}_3\mathbf{k}_4)\hat{p}_{\mathbf{k}_4}\hat{d}_{\mathbf{k}_3}\ ,$$

$$\hat{V}_{ep}=\tfrac{1}{2}\sum_{\mathbf{k}_1,\ldots,\mathbf{k}_4}\hat{e}^\dagger_{\mathbf{k}_1}\hat{p}^\dagger_{\mathbf{k}_2}(\mathbf{k}_1\mathbf{k}_2\,|\,H_{ep}\,|\,\mathbf{k}_3\mathbf{k}_4)\hat{p}_{\mathbf{k}_4}\hat{e}_{\mathbf{k}_3}\ ,$$

$$\hat{V}_{dep}=\frac{1}{3!}\sum_{\mathbf{k}_1,\ldots,\mathbf{k}_6}\hat{d}^\dagger_{\mathbf{k}_1}\hat{e}^\dagger_{\mathbf{k}_2}\hat{p}^\dagger_{\mathbf{k}_3}(\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\,|\,H_{dep}\,|\,\mathbf{k}_4\mathbf{k}_5\mathbf{k}_6)\times\hat{p}_{\mathbf{k}_6}\hat{e}_{\mathbf{k}_5}\hat{d}_{\mathbf{k}_4}\ .$$

Here $\epsilon_{\mathbf{k}d}$, $\epsilon_{\mathbf{k}e}$, and $\epsilon_{\mathbf{k}p}$ are the same as in the standard Fock Hamiltonian, i.e., they are the kinetic energies of a free deuteron, free electron, and free proton with wave vector $\mathbf{k}$. The same is true of $\hat{V}_{dp}$, i.e., the matrix element has the usual "bare Coulomb" form. On the other hand, the matrix elements in $\hat{V}_{de}$ and $\hat{V}_{ep}$ differ from the bare Coulomb form by subtraction of orthogonalization terms[1,22] involving the bound deuterium and bound hydrogen kernels, analogous to (8). These have the effect of weakening the free d-e and free e-p interactions so that they no longer support bound states[9,22] (these bound states already being included elsewhere, namely, in $\hat{H}_0$), thus greatly improving the convergence[9] of the Born series for d-e and e-p scattering. The three-particle interaction matrix element in the term $\hat{V}_{dep}$ in (42) involves coupling between the d-e and d-p Coulomb interactions and the bound hydrogen kernel, as well as coupling between the e-p and d-p Coulomb interactions and the bound deuterium kernel. It arises physically from the fact that (for example) the "free" electron interacting Coulombically with a deuteron is really moving in a continuum state orthogonal to bound hydrogen, inasmuch as the deuteron-hydrogen interaction appears elsewhere in $\hat{V}$ (as a different arrangement channel term). The explicit form of this matrix element (which we do not require here) can be found from the algebra of the Fock-Tani transformation, for example as represented diagrammatically by Gilbert.[23]

The explicit form of (40) is easy to determine in the present case. It is clear from (41), (42), and (34) that the state (41) can be expanded as

$$|\,\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}',E,+d)=\sum_{\mathbf{k},\mathbf{k}'}f^+_{\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}'}(\mathbf{k}\mathbf{k}',E)\hat{d}^\dagger_{\mathbf{k}}\hat{e}^\dagger_{\mathbf{k}'}\hat{p}^\dagger_{-\mathbf{k}-\mathbf{k}'}\,|\,0)\ , \tag{43}$$

where the amplitude f^+ is to be determined. Substituting (41)–(43) into (40) and equating coefficients of linearly independent states $\hat{d}^\dagger_{\mathbf{k}}\hat{e}^\dagger_{\mathbf{k}'}\hat{p}^\dagger_{-\mathbf{k}-\mathbf{k}'}\,|\,0)$, one finds the following inhomogeneous integral equation for f^+:

$$\begin{aligned}
&(\epsilon_{\mathbf{k}d}+\epsilon_{\mathbf{k}'e}+\epsilon_{-\mathbf{k}-\mathbf{k}',p})f^+_{\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}'}(\mathbf{k}\mathbf{k}',E)\\
&\quad+\tfrac{1}{2}\sum_{\mathbf{l}}(\mathbf{k}\mathbf{k}'\,|\,H_{de}\,|\,\mathbf{k}+\mathbf{l},\mathbf{k}'-\mathbf{l})f^+_{\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}'}(\mathbf{k}+\mathbf{l},\mathbf{k}'-\mathbf{l},E)\\
&\quad+\tfrac{1}{2}\sum_{\mathbf{l}}(\mathbf{k},-\mathbf{k}-\mathbf{k}'\,|\,H_{dp}\,|\,\mathbf{k}+\mathbf{l},-\mathbf{k}-\mathbf{k}'-\mathbf{l})f^+_{\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}'}(\mathbf{k}+\mathbf{l},\mathbf{k}',E)\\
&\quad+\tfrac{1}{2}\sum_{\mathbf{l}}(\mathbf{k}',-\mathbf{k}-\mathbf{k}'\,|\,H_{ep}\,|\,\mathbf{k}'+\mathbf{l},-\mathbf{k}-\mathbf{k}'-\mathbf{l})f^+_{\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}'}(\mathbf{k},\mathbf{k}'+\mathbf{l},E)\\
&\quad+\frac{1}{3!}\sum_{\mathbf{l},\mathbf{l}'}(\mathbf{k},\mathbf{k}',-\mathbf{k}-\mathbf{k}'\,|\,H_{dep}\,|\,\mathbf{k}+\mathbf{l},\mathbf{k}'+\mathbf{l}',-\mathbf{k}-\mathbf{k}'-\mathbf{l}-\mathbf{l}')f^+_{\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}'}(\mathbf{k}+\mathbf{l},\mathbf{k}'+\mathbf{l}',E)\\
&\quad=Ef^+_{\mathbf{q},\mathbf{q}',-\mathbf{q}-\mathbf{q}'}(\mathbf{k}\mathbf{k}',E)-\delta_{\mathbf{k}\mathbf{q}}\delta_{\mathbf{k}'\mathbf{q}'}\ .
\end{aligned} \tag{44}$$

This is to be solved subject to the outgoing-wave boundary condition implied by the term $+i\eta$ in (40).

IV. SELF-ENERGIES AND SCATTERING AND REACTION RESONANCES

We shall consider in this section scattering and reaction resonances arising from a discrete metastable (resonance) state embedded in the scattering continuum. Examples of such states are autoionizing states of atoms and predissociating states of molecules. A general "half-collision" form of Lippmann-Schwinger theory of differential decay cross sections of such states has been given elsewhere.[24] Here we consider the case where the metastable state does not occur as an initial (or final) state, but as an intermediate state, producing resonance behavior in the transition amplitude between initial and final continuum states.

In order to illustrate the ideas without inessential complications, consider first the case of a single discrete resonance wave function $\phi_a(x_1x_2)$ embedded in a continuum of two-particle scattering wave functions $\phi_k^{\pm}(x_1x_2)$. The scattering wave functions are eigenstates of the full two-body Hamiltonian including interactions, but the resonance is not a stationary state, hence not an exact energy eigenstate. However, it has a mean energy $\epsilon_a=(\phi_a \mid H \mid \phi_a)$ which is assumed to be embedded in the continuum in the sense that the equation $E_k=\epsilon_a$ has a solution k, where E_k is the energy eigenvalue of some continuum state $\phi_k^{\pm}$. In Fock-Tani representation the resonance state ϕ_a is represented by

$$|a)=\hat{a}^{\dagger}|0) \tag{45}$$

and the continuum states $\phi_k^{\pm}$ by

$$|(k)^{\pm})=\sum_{k_1,k_2}\phi_k^{\pm}(k_1k_2)\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}|0) \tag{46}$$

in a notation essentially the same as that of the previous sections. The *asymptotic* continuum states (not exact energy eigenstates) are

$$|k_1k_2)=\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}|0) . \tag{47}$$

Initial and final states of this form will be abbreviated herein by $|\psi_i)$ and $|\psi_f)$. The unperturbed Fock-Tani Hamiltonian $\hat{H}_0$ [of which $|a)$ and the $|k_1k_2)$ are eigenstates] and the Fock-Tani interaction Hamiltonian $\hat{V}_{\rm df}$ describing decay and formation of the resonance are of the form

$$\begin{aligned}\hat{H}_0&=\epsilon_a\hat{a}^{\dagger}\hat{a}+\sum_{k_1}\epsilon_{k_1}\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_1}+\sum_{k_2}\epsilon_{k_2}\hat{\psi}_{k_2}^{\dagger}\hat{\psi}_{k_2} ,\\ \hat{V}_{\rm df}&=\sum_{k_1,k_2}[\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}(k_1k_2 \mid H \mid a)\hat{a}+\text{H.c.}] ,\end{aligned} \tag{48}$$

where the 1-particle and 2-particle are assumed to be distinguishable. The resonance is embedded in the continuum in the sense that the equation $\epsilon_{k_1}+\epsilon_{k_2}=\epsilon_a$ is assumed to have solutions[25] for k_1 and k_2. Direct scattering interaction terms

$$\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}(k_1k_2 \mid H \mid k_1'k_2')\hat{\psi}_{k_2'}\hat{\psi}_{k_1'}$$

will also be present in a more realistic model, but are omitted here since we wish to investigate the role of the resonance as an intermediate state in indirect scattering processes of the form $k_1k_2\rightarrow a\rightarrow k_1'k_2'$, $k_1k_2\rightarrow a\rightarrow k_1'k_2'\rightarrow a\rightarrow k_1''k_2''$, etc. The decay-formation interaction $\hat{V}_{\rm df}$ is a simplified form of (6).

The second Born contribution to the exact scattering amplitude T_{fi} is

$$\begin{aligned}T_{fi}^{(2)}&=(\psi_f \mid \hat{V}_{df}\hat{G}_0^{+}(E)\hat{V}_{\rm df} \mid \psi_i)\\ &=\frac{(k_1'k_2' \mid H \mid a)(a \mid H \mid k_1k_2)}{E-\epsilon_a+i\eta} ,\end{aligned} \tag{49}$$

where $\hat{G}_0^{+}$ is the totally unperturbed Green's operator (13), $|\psi_i)=\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}|0)$, and $|\psi_f)=\hat{\psi}_{k_1'}^{\dagger}\hat{\psi}_{k_2'}^{\dagger}|0)$. The approximation (49) diverges at the resonance energy $E=\epsilon_a$, signaling inapplicability of the "bare Born" expansion of which (49) is the first nonzero contribution. More generally, the term of order $2n$ in the Born expansion diverges like $(E-\epsilon_a+i\eta)^{-n}$ at $E=\epsilon_a$ for all $n\geq 1$ due to "pileup" of energy denominators all giving poles at the same point[26] $E=\epsilon_a$. These divergences form a geometric series which can be summed[27] by the usual self-energy formalism of quantum field theory and many-body theory, leading to a complex self-energy of the resonance incorporating both width (finite lifetime) and shift contributions.

An equivalent but more elegant approach avoiding the direct summation of divergences can be based on use of an appropriate distorted-wave Green's operator $\hat{G}^{+d}$ of the form (34) followed by solution of the resultant Dalgarno-Lewis[18–20] equation (40). Here the decay-formation interaction $\hat{V}_{\rm df}$ plays the role of $\hat{V}_{\rm sc}$ in (34), (39), and (40). Thus we define

$$\hat{G}^{+d}(E)=(E+i\eta-\hat{H}_0-\hat{V}_{\rm df})^{-1} . \tag{50}$$

In the case of the simple model (48), $\hat{G}^{+d}$ is the *exact* Green's operator (there is no analog to $\hat{V}_{\rm re}$ of Sec. II) and the *exact* transition amplitude is

$$T_{fi}=(\psi_f \mid \hat{V}_{\rm df}\hat{G}^{+d}(E)\hat{V}_{\rm df} \mid \psi_i) . \tag{51}$$

Indeed, expansion of $\hat{G}^{+d}$ in (51) in powers of $\hat{V}_{\rm df}$ yields the bare Born series

$$T_{fi}=(\psi_f \mid \hat{V}_{\rm df}(\hat{G}_0^{+}+\hat{G}_0^{+}\hat{V}_{\rm df}\hat{G}_0^{+}+\cdots)\hat{V}_{\rm df} \mid \psi_i) . \tag{52}$$

Use of this series is, however, circumvented by solution of the inhomogeneous Dalgarno-Lewis equation

$$(\hat{H}_0+\hat{V}_{\rm df}) \mid \phi_{aE}^{+})=(E+i\eta) \mid \phi_{aE}^{+})-\hat{a}^{\dagger}|0) , \tag{53}$$

yielding the state

$$|\phi_{aE}^{+})=\hat{G}^{+d}(E)\hat{a}^{\dagger}|0) . \tag{54}$$

The transition amplitude (51) is then

$$T_{fi}=(k_1'k_2' \mid H \mid a)(0 \mid \hat{a} \mid \phi_{aE}^{+})(a \mid H \mid k_1k_2) , \tag{55}$$

where we have taken $|\psi_i)=\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}|0)$ and $|\psi_f)=\hat{\psi}_{k_1'}^{\dagger}\hat{\psi}_{k_2'}^{\dagger}|0)$, as in (49). We expect, and will

demonstrate, that the matrix element $(0|\hat{a}|\phi_{aE}^{+})$ is peaked about $E=\epsilon_a+\Delta_a$ and has a half-width γ_a, where Δ_a is the shift and $2\gamma_a$ the decay width of the resonance.

The solution $|\phi_{aE}^{+})$ of Eq. (53) is clearly of the form

$$|\phi_{aE}^{+})=c(E)\hat{a}^{\dagger}|0)+\sum_{k_1,k_2} d_{k_1k_2}(E)\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}|0)\ , \tag{56}$$

where $c(E)$ and $d_{k_1k_2}(E)$ are to be determined. Then

$$T_{fi}=c(E)(k_1'k_2'|H|a)(a|H|k_1k_2)\ . \tag{57}$$

Substituting the above expression for $|\phi_{aE}^{+})$ into (53) and equating coefficients of the linearly independent states $\hat{a}^{\dagger}|0)$ and $\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}|0)$ on both sides, one finds the following coupled equations for the coefficients:

$$\begin{aligned}&\epsilon_a c(E)+\sum_{k_1,k_2}(a|H|k_1k_2)d_{k_1k_2}(E)=(E+i\eta)c(E)-1\ ,\\ &(\epsilon_{k_1}+\epsilon_{k_2})d_{k_1k_2}(E)+c(E)(k_1k_2|H|a)\\ &\qquad=(E+i\eta)d_{k_1k_2}(E)\ .\end{aligned} \tag{58}$$

These equations are very similar to those occurring in Fano's theory[28] of resonances associated with atomic autoionizing states. Aside from notation, they differ in two ways: (a) Eqs. (58) contain an inhomogeneous term (the -1 on the right-hand side of the first equation) whereas Fano's Eqs. (3) are homogeneous; (b) the $i\eta$ in Eqs. (58) implies an outgoing-wave solution, whereas Fano's solution corresponded to a standing wave.

Solution of the second Eq. (58) yields

$$\begin{aligned}d_{k_1k_2}(E)&=\frac{c(E)(k_1k_2|H|a)}{E-\epsilon_{k_1}-\epsilon_{k_2}+i\eta}\\ &=c(E)(k_1k_2|H|a)\\ &\quad\times\left[\mathrm{P}\frac{1}{E-\epsilon_{k_1}-\epsilon_{k_2}}-i\pi\delta(E-\epsilon_{k_1}-\epsilon_{k_2})\right]\end{aligned} \tag{59}$$

use having been made of the standard Dirac identity, where P denotes the principal part in integrations[29] over (k_1k_2) and δ is the Dirac delta function. Substitution into the first Eq. (58) then yields

$$c(E)\left[E-\epsilon_a+i\eta-\mathrm{P}\sum_{k_1,k_2}\frac{|(k_1k_2|H|a)|^2}{E-\epsilon_{k_1}-\epsilon_{k_2}}+i\pi\sum_{k_1,k_2}|(k_1k_2|H|a)|^2\delta(E-\epsilon_{k_1}-\epsilon_{k_2})\right]=1\ . \tag{60}$$

The $i\eta$ in (60) can obviously be dropped[30] so long as $(k_1k_2|H|a)$ does not vanish identically on the hypersurface $\epsilon_{k_1}+\epsilon_{k_2}=E$. Then

$$c(E)=[E-\epsilon_a-\Delta_a(E)+i\gamma_a(E)]^{-1} \tag{61}$$

with

$$\begin{aligned}\Delta_a(E)&=\mathrm{P}\sum_{k_1,k_2}\frac{|(k_1k_2|H|a)|^2}{E-\epsilon_{k_1}-\epsilon_{k_2}}\ ,\\ \gamma_a(E)&=\pi\sum_{k_1,k_2}|(k_1k_2|H|a)|^2\delta(E-\epsilon_{k_1}-\epsilon_{k_2})\ .\end{aligned} \tag{62}$$

Thus finally

$$T_{fi}=\frac{(k_1'k_2'|H|a)(a|H|k_1k_2)}{E-\epsilon_a-\Delta_a(E)+i\gamma_a(E)}\ . \tag{63}$$

In the narrow-line approximation $\Delta_a(E)\approx\Delta_a(\epsilon_a)$ and $\gamma_a(E)\approx\gamma_a(\epsilon_a)$, Eqs. (62) reduce to the standard golden-rule expressions,[31] and (63) yields a Lorentzian line shape.

In a more realistic model than (48), including direct scattering interaction terms

$$\hat{\psi}_{k_1}^{\dagger}\hat{\psi}_{k_2}^{\dagger}(k_1k_2|H|k_1'k_2')\hat{\psi}_{k_2'}\hat{\psi}_{k_1'}$$

and/or more than one resonance, it is not possible to evaluate the exact scattering amplitude T_{fi} in closed form. Nevertheless, in such cases the subset of divergent Born-series contributions resulting from multipole poles $E=\epsilon_a$ can be effectively summed by solution of Dalgarno-Lewis equations of the form (53), yielding complex resonance self-energies $\Delta_a-i\gamma_a$. The corresponding resonant contribution to T_{fi} must then be added to the nonresonant contributions.

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[12]The bound states can be chosen orthonormal by the usual argument. All resonance states are linear combinations (wave packets) of continuum states, and hence orthogonal to the bound states. We assume that the resonances are also orthonormal to each other. This is the case, for example, for Born-Oppenheimer molecular states degenerate with a decay continuum (see Ref. 8).

[13]M. L. Goldberger and K. M. Watson, *Collision Theory* (Wiley, New York, 1964), p. 203, Eq. (103).

[14]This is not the case in standard formulations of rearrangement collision theory. For example, in Schrödinger or standard Fock representation the totally dissociated channel states are complete, hence not orthogonal to partially bound channels. In Fock-Tani representation one makes different arrangement channels truly orthogonal by a suitable extension of the state space (see Refs. 1–3). The distinction is somewhat academic since the volume is infinite in scattering and/or rearrangement problems.

[15]Recall that $(\alpha_f^{-d}|$ involves only the scattering interaction $\hat{V}_{sc}$ whereas $|\alpha_i^{+})$ involves both $\hat{V}_{sc}$ and $\hat{V}_{re}$.

[16]D. P. Dewangan and H. R. J. Walters, J. Phys. B **10**, 637 (1977); A. E. Kingston and H. R. J. Walters, *ibid.* **13**, 4633 (1980).

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[21]The spin degrees of freedom are trivial, so only the momentum indices are indicated.

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[25]In any realistic case these solutions will be degenerate, lying on a $(d-1)$-dimensional hypersurface in the d-dimensional (k_1,k_2) space.

[26]The remaining $n-1$ energy denominators in the term of order $2n$ do not give poles but branch lines coming from the continuum factors $(E-\epsilon_{k_1''}-\epsilon_{k_2''}+i\eta)^{-1}$, etc.

[27]One can give E a large enough positive imaginary part to make the series converge, then analytically continue the sum across the real axis.

[28]U. Fano, Phys. Rev. **124**, 1866 (1961).

[29]Our notation $\sum_{k_1,k_2}$ is symbolic, implying both integration over continuous variables (the limit of infinite system volume having been taken) and summation over discrete variables (such as spin).

[30]Note, however, that the $i\eta$ in (59) was essential for the outgoing-wave boundary condition.

[31]P. A. M. Dirac, *The Principles of Quantum Mechanics*, 3rd ed. (Oxford University, Oxford, 1947), p. 203.