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Approximate scattering wave functions for few-particle continua

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An operator identity which allows the wave operator for N particles interacting pairwise to be expanded as products of operators in which fewer than N particles interact is given. This identity is used to derive approximate scattering wave functions for N-particle continua that avoid certain difficulties associated with Faddeev-type expansions. For example, a derivation is given of a scattering wave function used successfully recently to describe the three-particle continuum occurring in the electron impact ionization of the hydrogen atom.

I. INTRODUCTION

The treatment of scattering processes involving more than two particles at high energies often involves approximations in which the exact many-particle transition or Green's operator is expanded in terms of operators in which only two particles at a time interact. The simplest example of this is an expansion of the full Green's operator G_m, involving a total of $m=N(N-1)/2$ pairwise interactions among N particles, in terms of the pairwise potential operators and G_0, the Green's operator for N free, noninteracting particles. Such a Born series is of limited value since it contains disconnected terms and, particularly for Coulomb interactions, it is slowly convergent (if at all). The situation is improved somewhat by Faddeev-type expansions[1] in which certain pair interactions are summed to infinite order. However, these theories still represent the transition operator as sums or differences of individual terms whose interference may lead to spurious structures in the resulting cross sections. This feature is particularly a problem when dealing with Coulomb forces of infinite range, since then the interference effects persist even in high-energy collisions.[2] To eliminate such difficulties in multiple-scattering theories, an approximation scheme is suggested here in which the full N-particle transition operator (or more exactly, the corresponding wave or Møller operator) is expanded not as a sum but as a *product* of operators involving the interaction of fewer numbers of particles. The approximation scheme is based on a simple operator identity.

The expansion of the full wave operator in product form leads to a product form of the resulting approximate scattering wave function. In fact, this investigation was prompted by a recent successful application of a product wave function to the three-body problem of electron impact ionization of the hydrogen atom.[3]

II. THE TRANSITION OPERATOR

The T-matrix element for N-body scattering can be written in two different forms

$$T_{fi}=\langle\Phi_f|V_f|\Psi_i^+\rangle=\langle\Phi_f|V_f(1+G^+V_i)|\Phi_i\rangle,$$

or

$$T_{fi}=\langle\Psi_f^-|V_i|\Phi_i\rangle=\langle\Phi_f|(1+V_fG^-)^\dagger V_i|\Phi_i\rangle. \quad (1)$$

Here $G^\pm=(E-H\pm i\delta)^{-1}$ is the full Green's operator corresponding to the total Hamiltonian H,

$$H|\Psi_f^-\rangle=E_f|\Psi_f^-\rangle;\ H|\Psi_i^+\rangle=E_i|\Psi_i^+\rangle, \quad (2)$$

with $E=E_f=E_i$. The initial and final states are defined by

$$H_i|\Phi_i\rangle=(H-V_i)|\Phi_i\rangle=E_i|\Phi_i\rangle \quad (3a)$$

and

$$H_f|\Phi_f\rangle=(H-V_f)|\Phi_f\rangle=E_f|\Phi_f\rangle. \quad (3b)$$

Since the final state resulting from a collision is often "more complicated" than the initial state, the approximation of the scattering state $|\Psi_f^-\rangle$ will be considered. The same method is readily applied to $|\Psi_i^+\rangle$. More precisely, since

$$|\Psi_f^-\rangle=(1+G^-V_f)|\Phi_f\rangle, \quad (4)$$

an expansion of the operator $(1+G^-V_f)$ will be considered.

The interaction between the kth pair of particles will be designated v_k and the totality of interactions

$$V=\sum_{k=1}^{m}v_k, \quad (5)$$

where $m=N(N-1)/2$ for m particles. We then define Green's operators

$$G_n^-=\left[E-K-\sum_{k=1}^{n}v_k-i\delta\right]^{-1}, \quad (6)$$

in which K is the total kinetic energy operator but only the first n pairwise interactions are taken into account. In this notation $G_m^-\equiv G^-$ is the full Green's operator and G_0^- is the free N-particle Green's operator. Green's operators involving only one specific interaction, say v_k are designated

$$g_k^-=(E-K-v_k-i\delta)^{-1}. \quad (7)$$

If the final state $|\Phi_f\rangle$ is such that H_f contains the first i

interactions, then

$$(1+G^{-}V_f)=\left(1+G_m^{-}\sum_{k=i+1}^{m}v_k\right). \tag{8}$$

The following development rests on the simple identity

$$\left(1+G_m^{-}\sum_{k=i+1}^{m}v_k\right)=(1+G_m^{-}v_m)(1+G_{m-1}^{-}v_{m-1})\cdots(1+G_{i+1}v_{i+1}). \tag{9}$$

This identity is readily established by operating with $(G_m^{-})^{-1}=(E-K-\sum_{k=1}^{m}v_k-i\delta)$ from the left and using the definition (6). The case $i=0$ in (9) is especially interesting since it corresponds to N free particles in the final state. This N-particle breakup case will be discussed further.

For N free particles the final-state wave function is

$$|\Psi_f^{-}\rangle=(1+G^{-}V)|\Phi_f\rangle\equiv\Omega^{-}|\Phi_f\rangle \tag{10}$$

and the expansion (9) can be written, for $i=0$,

$$\Omega^{-}=\prod_{k=1}^{m}\Omega_k^{-}, \tag{11}$$

with

$$\Omega_i^{-}\equiv(1+G_i^{-}v_i). \tag{12}$$

If one also defines two-body wave operators

$$\omega_i^{-}=(1+\mathcal{G}_i^{-}v_i), \tag{13}$$

it can be shown that Ω_i^{-} satisfies the equation

$$\Omega_i^{-}=\omega_i^{-}+\Omega_i^{-}(\Omega_{i-1}^{-}-1)\omega_i^{-}. \tag{14}$$

Then the expansion (11) has a lowest-order term

$$\Omega^{-}\approx\prod_{i=1}^{m}\omega_i^{-}. \tag{15}$$

For example, for $N=3$ this reads explicitly

$$(1+G^{-}V)\approx(1+\mathcal{G}_3^{-}v_3)(1+\mathcal{G}_2^{-}v_2)(1+\mathcal{G}_1^{-}v_1), \tag{16}$$

or

$$|\Psi_f^{-}\rangle\approx\omega_1^{-}\omega_2^{-}\omega_3^{-}|\Phi_f\rangle. \tag{17}$$

From (10), the wave-operator expansion corresponds to an expansion of the wave function Ψ_f^{-}. In the Faddeev approach this expansion is

$$|\Psi_f^{-}\rangle=\sum_{j=1}^{m}|\Psi^{(j)}\rangle+|\Phi_f\rangle \tag{18}$$

and $|\Psi\rangle$, the column vector composed of the elements $|\Psi^{(j)}\rangle$, satisfies the integral equation

$$|\Psi\rangle=(\omega-1)|\Phi_f\rangle+G_0^{-}\mathsf{T}|\Psi\rangle, \tag{19}$$

where

$$T_{ij}=v_i\omega_i^{-},\quad j\neq i,$$
$$T_{ij}=0,\quad j=i,$$

are two-body T operators for interaction v_i. For example, for $N=3$, the first-order term is

$$|\Psi_f^{-}\rangle\approx(\omega_1^{-}+\omega_2^{-}+\omega_3^{-}-2)|\Phi_f\rangle, \tag{20}$$

which is to be contrasted with (17).[4]

In applications in atomic physics the Faddeev approximation (20) has various shortcomings. For example, it was first used by Macek[5] to calculate the electron capture to the continuum (ECC) process where electrons are ionized into states of low momentum with respect to the moving projectile positive ion. Although describing the essential dynamics of this process correctly, due to interference between the various terms in (20), the predicted cross section shows oscillations which appear to be spurious.[2] If the positive-ion projectile is replaced by an electron, it is clear that the cross section for two electrons to emerge with exactly equal momenta must vanish. However, only one term in (20) vanishes, namely, that involving the electron-electron interaction. The remainder does not vanish and yields a spurious finite cross section for two electrons to emerge with equal momenta.[6] In addition, the wave function (20) does not satisfy the correct boundary conditions on the three-body Coulomb problem.[3] A wave function based on the approximation (17) removes all of these difficulties, i.e., it is of product form and therefore does not show interference, if one factor is zero then the whole wave function vanishes and it satisfies the exact boundary condition for an N-body free Coulomb wave function.

The wave function (16) could be evaluated exactly but a particularly transparent and readily calculable form emerges from the further approximation that all two-body interactions occur "on shell." It suffices to consider only three particles. Here $(\mathbf{k}_i,\mathbf{K}_i)$, $i=1,2,3$ will denote the final-state momenta conjugate to each set of Jacobi coordinates describing the internal motion of the three-body system. Consider

$$(\omega_2^{-}\omega_1^{-})|\Phi_f\rangle=\int d\mathbf{k}\,d\mathbf{K}\,\omega_2^{-}|\mathbf{k},\mathbf{K}\rangle\langle\mathbf{k},\mathbf{K}|\omega_1^{-}|\mathbf{k}_1,\mathbf{K}_1\rangle, \tag{21}$$

where $|\mathbf{k}_1\rangle$ is a plane wave describing relative motion of the two particles interacting in ω_1^{-} and $\mathbf{K}_1$ is the momentum of the third particle relative to their center of mass. Then one can write

$$\omega_1^{-}|\mathbf{k}_1,\mathbf{K}_1\rangle=|\psi_{\mathbf{k}_1}^{-},\mathbf{K}_1\rangle$$
$$\equiv|f_{\mathbf{k}_1}^{-},\mathbf{k}_1,\mathbf{K}_1\rangle, \tag{22}$$

where $\psi_{\mathbf{k}_1}^{-}$ is a two-body eigenfunction for potential v_1 alone. In the second line the plane-wave part has been factored out, i.e., $f_{k_1}^{-}$ represents the distortion due to v_1. Similarly, by choosing $\mathbf{k}$ to be a momentum conjugate to the interparticle coordinate in v_2 one has

$$\omega_2^{-}|\mathbf{k},\mathbf{K}\rangle=|f_{\mathbf{k}}^{-},\mathbf{k},\mathbf{K}\rangle. \tag{23}$$

The factor f in (22) is on shell, but that in (23) is off shell. However, if the factor $f_{\mathbf{k}}^{-}$ in (23) is approximated by its on-shell value, i.e., $\mathbf{k}=\mathbf{k}_2$, $\mathbf{K}=\mathbf{K}_2$ in $f_{\mathbf{k}}^{-}$, then

$$(\omega_1^{-}\omega_2^{-})\,|\mathbf{k}_1,\mathbf{K}_1\rangle \approx |f_{\mathbf{k}_1}^{-},f_{\mathbf{k}_2}^{-},\mathbf{k}_1\mathbf{K}_1\rangle . \tag{24}$$

This process can be continued to give

$$\omega_1^{-}\omega_2^{-}\omega_3^{-}\,|\mathbf{k}_1,\mathbf{K}_2\rangle \approx |f_{\mathbf{k}_1}^{-},f_{\mathbf{k}_2}^{-},f_{\mathbf{k}_3}^{-},\mathbf{k}_1\mathbf{K}_1\rangle . \tag{25}$$

When applied to Coulomb potentials, (25) is precisely the wave function used recently[3] to describe with great success the triply differential cross section for electron impact ionization of the hydrogen atom. There the derivation was performed by a method due to Pluvinage.[7] Here the essential approximation is seen to be the assumption that all two-body interactions occur on the energy shell.[4]

There is, however, a fundamental difficulty in applying the foregoing to Coulomb potentials. For short-range potentials the analysis is applicable as it stands. However, for Coulomb potentials the T-matrix elements and wave operators must be suitably renormalized[8-11] or the asymptotic plane waves modified by Coulomb distortion factors.[12,13] The rigorous application of the product expansion of the wave operator for Coulomb potentials remains to be developed. Here, to keep the analysis simple, the expedient approach is adopted of assuming cutoff Coulomb potentials. Taking a limit of infinite cutoff radius after the formal manipulation leading to (25) then introduces a divergent overall phase factor, but this does not affect cross sections calculated from the modulus squared of the matrix element (1). This procedure is also justified by the close agreement of the calculations of Ref. 3 with experiment, even though the expression (25) was used in (1) to calculate scattering due to pure Coulomb interactions.

This method can be extended to approximate an N-body continuum wave function as a product of $N(N-1)/2$ two-body distortion factors and $(N-1)$ three-dimensional plane waves. For charged particles, unlike any approximation based on operator sum expansions, this wave function will give a vanishing cross section when two particles approach in velocity space and has the same limit as the exact wave function when the distances between all particles tends to infinity.

In conclusion, an operator-product expansion has been given of the wave operator for N-body scattering via pairwise potentials. In specific applications involving Coulomb potentials this expansion avoids certain inadequacies of Faddeev operator-sum expansions.

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