Incremental Approach to Strongly Correlated Many-Body Finite Systems

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The transition and the Green operators of an interacting N body system are obtained from the solutions of the $N - M$ body problem where $M = 1, 2, \ldots, N - 2$. This is achieved via the development of a cumulative, nonperturbative approach that makes use of existing knowledge on the system when the number of interacting particles is reduced. The method is applied to four interacting Coulomb particles where the Green operator is expressed as a sum of Green operators of all three body subsystems that can be combined within the four body system. The calculated four particle continuum spectrum is in a remarkable agreement with recent experimental findings.

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The description of the spectrum of many interacting particles is a problem of a long-standing history in theoretical physics. One of the efficient solution procedures has been to reduce the many-body problem to one for a single particle moving in an effective (nonlocal) field created by all other particles. For computationally tractable solutions approximate expressions for the effective field are employed according to certain recipes such as those provided by the local approximation within the density functional theory [1]. With the advent of many particle spectroscopy, however, it has been possible to probe in great detail the properties of many-body systems that are strongly dependent on the interparticle correlation. For example, the double and triple ionization and ionization/excitation of localized and delocalized electronic systems by an ultraviolet photon [2–4] cannot be described without the explicit use of correlated few-body states. Recently, experiments have pushed the limits to explore in full detail the many-body continuum spectrum of four or more interacting particles [4–10]. For this case, theory is lagging way behind. On the other hand, a system studied intensively in nuclear, atomic, and molecular physics is that consisting of three interacting particles. In 1961 Faddeev proposed coupled linear integral equations with a square integrable kernel to solve the three particle problem [11,12]. Nowadays, we have a wealth of further analytical and numerical methods at hand to deal with three body systems. In view of this situation it seems worthwhile to develop for the four body problem, in particular, and for N body systems in general, a cumulative method that takes advantage of previously accumulated knowledge on the solution of the $N - 1$ particle problem.

The fundamental quantity that describes the microscopic properties of N body quantum systems is the Green operator $G^{(N)}$ which is the resolvent of the total Hamiltonian. It can be deduced from the Lippmann-Schwinger equation $G^{(N)} = G_0 + G_0 U^{(N)} G^{(N)}$ where G_0 is the Green operator of a reference N particle system which is usually chosen as a noninteracting system. An equivalent approach to determine the dynamical behavior of a system is to derive the respective transition operator $T^{(N)}$ which satisfies the integral equation $T^{(N)} = U^{(N)} + U^{(N)} G_0 T^{(N)}$. These integral equations for $G^{(N)}$ and $T^{(N)}$ provide a natural framework for perturbative treatments. However, for $N \geq 3$ the application of the above Lippmann-Schwinger equations (and those for the state vectors) is hampered by mainly two difficulties: (1) as shown in Refs. [13,14] the Lippmann-Schwinger equations for the state vectors do not have a unique solution, and (2) as shown by Faddeev [11,12] the kernel of these integral equations $K = G_0 U^{(N)}$ is not a square integrable operator for $N \geq 3$, i.e., the norm $\|K\| = [\mathrm{Tr}(KK^\dagger)]^{1/2}$ is not square integrable. The kernel K is also not compact.

This study proceeds as follows: (a) We develop a recursive procedure to express the Hamiltonian of N interacting body systems in terms of Hamiltonians of systems with a reduced number of interactions. (b) In the spirit of the Faddeev approach [11,15,16] we derive nonperturbative integral equations with the following properties: (1) they treat all N particles on equal footing, and (2) they relate in a linear manner $G^{(N)}$ and $T^{(N)}$ to $G^{(N-M)}$ and $T^{(N-M)}$ where $M = 1, 2, \ldots, N - 2$. (c) We develop a systematic and mathematically sound scheme for approximations and apply it to deduce the continuum spectrum of four interacting Coulomb particles.

To this end we consider a nonrelativistic system consisting of N interacting particles. We assume the total potential to be of the class $U^{(N)} = \sum_{j>i=1}^{N} v_{ij}$ without any further specification of the individual potentials v_{ij}. The potential $U^{(N)}$ satisfies the recurrence relations

$$U^{(N)} = \frac{1}{N-2} \sum_{j=1}^{N} u_j^{(N-1)}, \tag{1}$$

$$u_j^{(N-1)} = \frac{1}{N-3} \sum_{k=1}^{N-1} u_{jk}^{(N-2)}, \qquad j \neq k, \tag{2}$$

where $u_j^{(N-1)}$ is the total potential of a system of $N - 1$ interacting particles in which the j particle is missing, i.e., in terms of the physical pair potentials v_{mn} one can write $u_j^{(N-1)} = \sum_{m>n=1}^{N} v_{mn}, m \neq j \neq n$. It is straightforward to show that the potential expansions [Eqs. (1)

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and (2)] are reflected in similar relations for the total Hamiltonian. Figure 1 illustrates how, according to Eqs. (1) and (2), the potential of a system of six interacting particles is expressed in terms of potentials of five correlated particles. The latter potentials can be further expressed in terms of four body potentials [cf. Eq. (2)]. This procedure is repeated until a potential with a desired number of interactions is achieved. From Fig. 1 it is clear that this "minimal geometric reduction" scheme [Eqs. (1) and (2)] treats all interactions on equal footing and provides maximal flexibility to reduce systematically the N body potential (Hamiltonian) to sums of $N - M$ potentials (Hamiltonians) with $M = 1, 2, \ldots, N - 2$. This simple geometric observation has wide ranging consequences in that the transition and the Green operators can be expanded in the same way. This can be seen as follows:

According to the decomposition (1), the integral equation for the transition operator can be written as

$$T^{(N)} = \sum_{j=1}^{N} T_j^{(N-1)}, \tag{3}$$

$$T_j^{(N-1)} = \tilde{u}_j^{(N-1)} + T^{(N)} G_0 \tilde{u}_j^{(N-1)}, \qquad j = 1, \ldots, N. \tag{4}$$

Here we introduced the scaled potentials $\tilde{u}_j^{(N-1)} = (u_j^{(N-1)})/(N-2)$. The physical meaning of the operators (4) is illustrated in Fig. 2 for the system depicted in Fig. 1.

The transition operator of the system, when $N - 1$ particles are interacting via the scaled potential $\tilde{u}_j^{(N-1)}$, is $t_j^{(N-1)} = \tilde{u}_j^{(N-1)} + \tilde{u}_j^{(N-1)} G_0 t_j^{(N-1)}$. With this relation Eq. (4) can be reformulated as

$$\begin{aligned} T_j^{(N-1)} &= t_j^{(N-1)} + t_j^{(N-1)} G_0 T^{(N)} - t_j^{(N-1)} G_0 (\tilde{u}_j^{(N-1)} + \tilde{u}_j^{(N-1)} G_0 T^{(N)}) = t_j^{(N-1)} + t_j^{(N-1)} G_0 (T^{(N)} - T_j^{(N-1)}) \\ &= t_j^{(N-1)} + t_j^{(N-1)} G_0 \sum_{k \neq j}^{N} T_k^{(N-1)}. \end{aligned} \tag{5}$$

Equation (5) can be expressed alternatively in a matrix form as

$$\begin{pmatrix} T_1^{(N-1)} \\ T_2^{(N-1)} \\ \vdots \\ T_{N-1}^{(N-1)} \\ T_N^{(N-1)} \end{pmatrix} = \begin{pmatrix} t_1^{(N-1)} \\ t_2^{(N-1)} \\ \vdots \\ t_{N-1}^{(N-1)} \\ t_N^{(N-1)} \end{pmatrix} + [\mathbf{K}^{(N-1)}] \begin{pmatrix} T_1^{(N-1)} \\ T_2^{(N-1)} \\ \vdots \\ T_{N-1}^{(N-1)} \\ T_N^{(N-1)} \end{pmatrix}. \tag{6}$$

The kernel $[\mathbf{K}^{(N-1)}]$ is a matrix operator whose elements consist of $t_j^{(N-1)}; j = 1 \cdots N$. From Eq. (2) it is clear that $t_j^{(N-1)}$ can also be expressed in terms of the transition operators of the $N - 2$ interacting subsystems as $t_j^{(N-1)} = \sum_{k \neq j}^{N-1} T_k^{(N-2)}$. The operators $T_k^{(N-2)}$ are deduced from Eq. (6) with N being replaced by $N - 1$.

From the relation $G^{(N)} = G_0 + G_0 T^{(N)} G_0$ we conclude that the Green operator of the interacting N particle system has the form $G^{(N)} = G_0 + \sum_{j=1}^{N} G_j^{(N-1)}$. The operators $G_j^{(N-1)}$ are related to the Green operators $g_j^{(N-1)}$ of the systems in which only $N - 1$ particles are correlated by virtue of $\tilde{u}_j^{(N-1)}$. This interrelation is given via

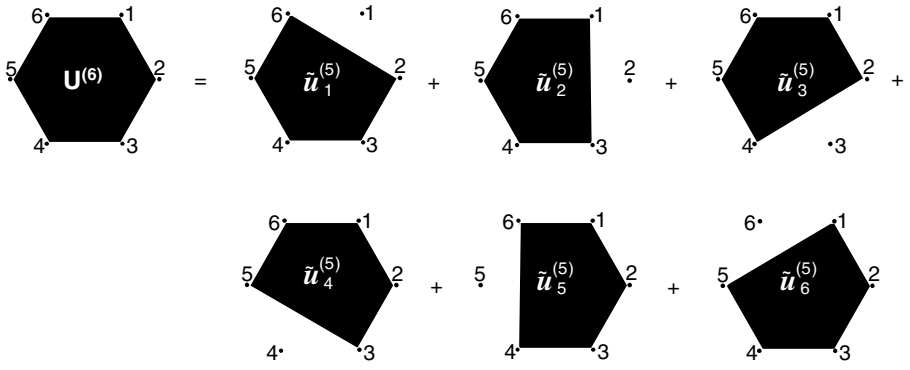

FIG. 1. A pictorial interpretation of the total potential expansion (1) for six interacting particles enumerated and marked by the full dots at the corners of the hexagon. The hexagon indicates the full potential $U^{(6)}$ of the six correlated particles. Each pentagon symbolizes the full five body potential $\tilde{u}_j^{(5)} = (u_j^{(5)})/4$ of those five particles that are at the corners of the pentagon. The particle being not at a corner of a pentagon is free (disconnected).

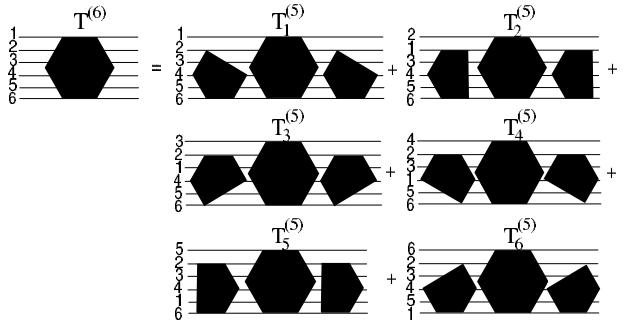

FIG. 2. A diagrammatic representation of Eq. (4) for a system of six correlated particles (cf. Fig. 1). The hexagons and the pentagons (with a specific orientation) label the same potentials as explained in Fig. 1. Each of the pictures stands for a transition operator of the six body system (the particles are labeled by straight lines). For example, the diagram $T_1^{(5)}$ means that the five particles 2, 3, 4, 5, and 6 interact first, propagate, and then all six particles interact with each other. The system then propagates and finally the five particles 2, 3, 4, 5, and 6 interact again.

$$\begin{pmatrix} G_1^{(N-1)} \\ G_2^{(N-1)} \\ \vdots \\ G_{N-1}^{(N-1)} \\ G_N^{(N-1)} \end{pmatrix} = \begin{pmatrix} g_1^{(N-1)} - G_0 \\ g_2^{(N-1)} - G_0 \\ \vdots \\ g_{N-1}^{(N-1)} - G_0 \\ g_N^{(N-1)} - G_0 \end{pmatrix} + [\tilde{\mathbf{K}}^{(N-1)}] \begin{pmatrix} G_1^{(N-1)} \\ G_2^{(N-1)} \\ \vdots \\ G_{N-1}^{(N-1)} \\ G_N^{(N-1)} \end{pmatrix}, \tag{7}$$

where $[\tilde{\mathbf{K}}^{(N-1)}] = G_0[\mathbf{K}^{(N-1)}]G_0^{-1}$. From Eqs. (6) and (7) we conclude that if the Green operator of the interacting $N-1$ body system is known the Green operator of the N particles can then be deduced by solving a set of N linear, coupled integral equations [namely, Eqs. (6) and (7)]. According to the above equations, if only the solution of the $N-M$ problem is known where $M = 1, 2, \ldots, N-2$ we have to perform a hierarchy of calculations starting by obtaining the solution for the $N-M+1$ problem and repeating the procedure to reach the solution of the N body problem. For $N = 3$ the present scheme reduces to the well-established Faddeev equations.

As an example we apply the method to the four body problem. This is particularly instructive, for a substantial body of knowledge on the three particle problem has been accumulated whereas theoretical studies on the four body problem are still scare. Moreover, an impressive amount of experimental data is available [4–8,10] that renders possible a detailed insight into the four body continuum spectrum. Therefore, using the present method, we express the four body Green operator in terms of known, approximate solutions of three body systems. For $N = 4$ the first iteration of Eq. (7) yields

$$G^{(4)} = \sum_{j=1}^{4} g_j^{(3)} - 3G_0\,, \tag{8}$$

where $g_j^{(3)}$ is the Green operator of the interacting three body system (particle j is noninteracting) and can be taken from other numerical or analytical studies. For example, it has been shown recently [17] that, under certain conditions specified in Ref. [17], the Hamiltonian of a general three body system reduces to a sum of three commuting Hamiltonians $h_k^{(2)}$ in which only two particles are interacting (particle k is free). The Green operators $g_j^{(3)}$ in Eq. (8) can therefore be written as $g_j^{(3)} \approx G_0^{-2} \prod_{k \neq j} g_k^{(2)}, k \in \{1, 2, 3, 4\} \ni j$ where $g_k^{(2)}$ is the resolvent of $h_k^{(2)}$. Thus we obtain from Eq. (8) $G^{(4)} = [\sum_{j=1}^{4} G_0^{-2} \prod_{k \neq j} g_k^{(2)}] - 3G_0, j \neq k \in \{1, 2, 3, 4\}$. In many situations it is possible to encompass in the reference Hamiltonian G_0 valuable and easily accessible preknowledge of the system which reduces the number of interactions in the potential (1). For example, we consider here the continuum dynamics of three electrons (or two electrons and a positron) in the Coulomb field of a heavy nucleus. Such a state is achieved following the electron and positron impact double ionization. As a reference we choose G_0 to be the Green operator of the three continuum particles moving independently in the Coulomb nuclear field. What remains in the potential (1) is then the interaction among the continuum particles which is treated according to the present method. Figures 3(a) and 3(b) show the results for the electron and the positron impact double ionization of ground state helium along with the experimental data [5,10] and a full numerical evaluation of the first Born term within a convergent close coupling (CCC) method [18]. The first Born approximation (FBA) corresponds to one term in Eq. (8) where the projectile motion is decoupled from the rest of the system. Thus, the results of the FBA are insensitive to the projectile charge state. The origin of the main peaks in the FBA spectrum has been unraveled in Ref. [10]. Thus we focus here on the novel additional structures predicted by the present theory. From Figs. 3 and 4 the following important implications are inferred: (i) The difference between the positron and the electron impact case indicates that the Born limit is not yet reached. We note that at such a high impact energy and a small momentum transfer as considered in Fig. 3 and 4 the Born limit is usually achieved in single ionization. This emphasizes the fundamental difference between single and double ionization as the latter having much higher ionization threshold and being basically correlation induced. (ii) The Born (and the optical) limit is approached differently depending on the emission angles and energies of the ejected electrons. (iii) In the author's view, the most remarkable prediction

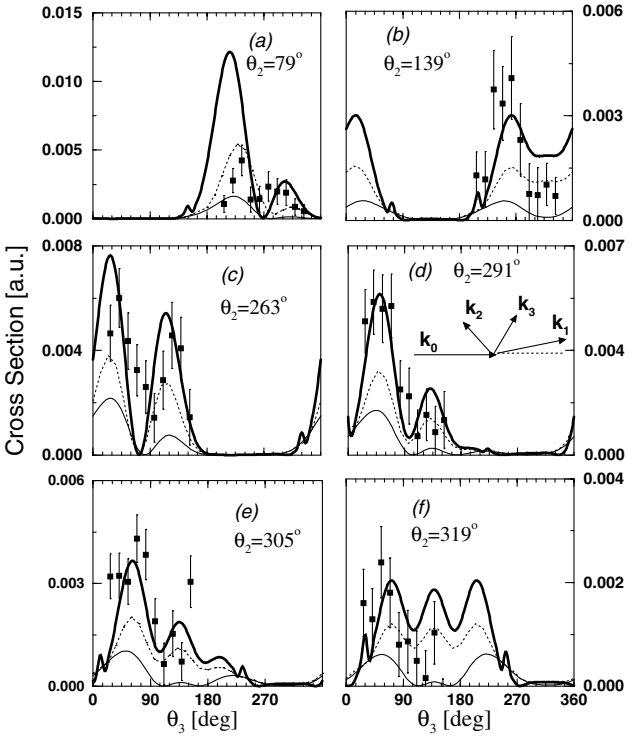

FIG. 3. The fully resolved double ionization cross section of He($1S^e$) following electron (solid lines) or positron (dotted line) impact. The scattering geometry is shown by the inset in (d). $\mathbf{k}_0$ and $\mathbf{k}_1$ are the initial and final state momenta of the projectile while $\mathbf{k}_2$ and $\mathbf{k}_3$ refer to the momenta of the two ejected electrons. The incident energy is 5.6 keV and $k_2^2/2 = k_3^2/2 = 10$ eV. All angles are measured with respect to $\hat{\mathbf{k}}_0$. The projectile is scattered through an angle of 0.45°. The emission angle θ_2 of one of the electrons is fixed at the value indicated on the figures while the cross section is scanned as a function of the emission angle θ_3 of the second electron. The thick solid (dotted) line is the result of the present model for electron (positron impact) whereas the light solid curve is the outcome of the CCC method within the first Born approximation [18]. The data (full square [10]) are on absolute scale.

of the present calculations is the presence of additional subsidiary peaks (in the spectrum shown in Figs. 3 and 4 which are absent in the FBA (CCC) results (cf. also Ref. [10]). An optimistic observer can identify these structures in the experimental data of Figs. 3(b), 3(e), and 3(f). In Fig. 4, however, these peaks are clearly observable. The origins of these peaks are interference effects between the various terms in the sum (8) when evaluating the cross sections. It is most interesting to recall here that the appearance of such interference effects in a Faddeev-type approach to Coulomb scattering problems [19] has been considered hitherto as a drawback and has not been confirmed experimentally [19]. The present study which is in the spirit of the Faddeev theory together with the notable agreement with experiment sheds a new light on Faddeev-type approaches as a useful route to few-body systems with long range correlations. In spite of this exciting result it should be noted that only the first iteration of (7) is used for the calculation of Figs. 3 and 4.

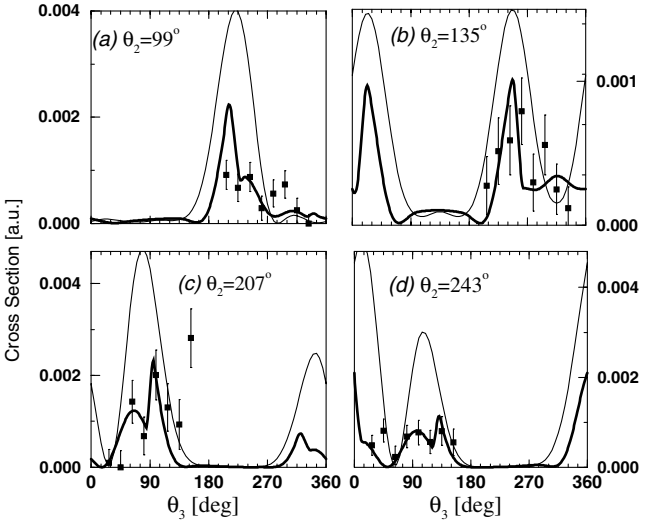

FIG. 4. The same as in Fig. 3 with the same labeling of curves, however the ejection energies are lowered to $k_2^2/2 = k_3^2/2 = 4$ eV. For shape comparison, the experimental data have been normalized by a single factor to the present theory.

The evaluation of higher order terms should remove the remaining discrepancies between theory and experiment. The compactness of the kernel of the integral equation (7) for *Coulomb* potentials is the subject of current research [20].

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