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New integral equations for the transition operators of many-body systems*

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A new set of coupled integral equations for the transition operators of a nonrelativistic quantum-mechanical n-body system is presented. These equations are a generalization to the many-body system of a special case of a set suggested for the three-body problem by Kouri, Baer, and Levin. The Kouri-Baer-Levin formalism effectively couples together the Lippmann-Schwinger integral equations for the transition operators for all open channels thus simultaneously imposing all asymptotic boundary conditions. The effect of our specialization of these equations is to make the kernel of the integral equations connected so that the resulting equations appear to be a suitable basis for many-body calculations.

One can reduce the problem of determining the properties of a nonrelativistic, quantum-mechanical n-body system to the evaluation of the elements of the transition operator[1]

$$X_{\alpha\beta} = V_\alpha + V_\alpha G V_\beta \tag{1a}$$

$$G = (E - H)^{-1} \tag{1b}$$

$$H = H_\alpha + V_\alpha = H_\beta + V_\beta = \ldots , \tag{1c}$$

where the subscript α identifies the different ways of partitioning the n (distinguishable) particles into two clusters and V_α is the interaction potential operating between the two clusters of particles of partition α. H is the Hamiltonian operator of the system and E is the energy of the system. By appropriately specifying the asymptotic boundary conditions imposed on the system Green's function G, one can identify the transition operator $X_{\alpha\beta}$ with the T-matrix operator or the K-matrix operator. (To cause X to be the K-matrix operator one does not require G be the principal value of $(E - H)^{-1}$, but instead requires that G have the same asymptotic behavior as the principal values of $(E - H_\alpha)^{-1}$, $(E - H_\beta)^{-1}, \ldots$, etc.)

One can seek to evaluate the transition operator by a direct evaluation of the system Green's function operator[2] or by solving an integral equation for X. To get an integral equation for X one merely substitutes into Eq. (1a) the integral equation for G in terms of the partition Green's function operator G_β:

$$G = G_\beta + G V_\beta G_\beta = G_\beta + G_\beta V_\beta G , \tag{2a}$$

$$G_\beta = (E - H_\beta)^{-1} , \tag{2b}$$

$$X_{\alpha\beta} = V_\alpha + V_\alpha(1 + G V_\beta) G_\beta V_\beta$$
$$= V_\alpha + X_{\alpha\beta} G_\beta V_\beta . \tag{3}$$

The inadequacy of these Lippmann-Schwinger-type integral equations for calculating the transition operators is well known.[3] There are two shortcomings: (a) Equation (3) fails to incorporate the full asymptotic boundary conditions of the problem within itself since it contains only one of the partition Green's function operators. What is needed is some procedure that would make use of all of the partition Green's function operators in calculating each transition operator element. (b) Equation (3) is not susceptible to solution by conventional methods because the kernel $G_\beta V_\beta$ is not in the Hilbert-Schmidt class. That is to say, an iteration series expansion of Eq. (3) will contain in all orders terms whose graphs are disconnected.

Faddeev[3] has shown how these difficulties may be overcome for the three-body problem. His method depends on the possibility of making a one to one correspondence between the cluster interaction potentials V_α and the two-body interaction potentials for a three body system. The method is not readily generalized to more complex systems.

Recently Kouri, Baer, and Levin[4] have suggested a new way of deriving a set of coupled integral equations for the transition operators. These integral equations contain a set of arbitrary coefficients. We show here how these coefficients may be selected so as to overcome both shortcomings mentioned above. The resulting set of integral equations would appear to be a suitable basis for calculating the transition operators for many-body systems.

The Kouri-Levin approach is to use for the system Green's function in Eq. (1a) the following representation:

$$G = \sum_\gamma W_{\alpha\gamma} G_\gamma (1 + V_\gamma G) , \tag{4a}$$

$$\sum_\gamma W_{\alpha\gamma} = 1 . \tag{4b}$$

The result is

$$X_{\alpha\beta} = V_\alpha + V_\alpha \sum_\gamma W_{\alpha\gamma} G_\gamma (V_\beta - V_\gamma) + V_\alpha \sum_\gamma W_{\alpha\gamma} G_\gamma X_{\gamma\beta}$$

$$= V_\alpha \sum_\gamma W_{\alpha\gamma} G_\gamma G_\beta^{-1} + V_\alpha \sum_\gamma W_{\alpha\gamma} G_\gamma X_{\gamma\beta} \ . \quad (5)$$

In our discussion we will use a slightly different version of the formalism which results from using

$$G = \sum_\gamma (1 + G V_\gamma) G_\gamma W_{\gamma\beta} \ , \quad (6a)$$

$$\sum_\gamma W_{\gamma\beta} = 1 \quad (6b)$$

in Eq. (1a). The result then is

$$X_{\alpha\beta} = V_\alpha + \sum_\gamma X_{\alpha\gamma} G_\gamma W_{\gamma\beta} V_\beta \ . \quad (7)$$

This equation is similar to one given by Baer and Kouri.[4] Except for constraint (6b) the coefficients $W_{\gamma\beta}$ are arbitrary. Equation (7) then is a set of coupled integral equations for $X_{\alpha 1}, X_{\alpha 2}, X_{\alpha 3}, \ldots$ which for suitable choice of the $W_{\gamma\beta}$'s will involve *all* the partition Green's function operators G_α and *all* the partition residual interaction potentials V_α. The complete set of asymptotic boundary condition constraints are brought into play by means of the G_α's.

Can coefficients $W_{\gamma\beta}$ be chosen so that the kernel of integral equation (7) does not give rise to infinite sets of disconnected diagrams? The formal solution of Eq. (7) is

$$X_{\alpha\beta} = V_\alpha \sum_\gamma [(1 - K)^{-1}]_{\gamma\beta}$$

$$= V_\alpha + \sum_\gamma V_\alpha K_{\gamma\beta} + \sum_\gamma \sum_{\gamma'} V_\alpha K_{\gamma\gamma'} K_{\gamma'\beta}$$

$$+ \sum_\gamma \sum_{\gamma'} \sum_{\gamma''} V_\alpha K_{\gamma\gamma'} K_{\gamma'\gamma''} K_{\gamma''\beta} + \cdots \ , \quad (8a)$$

$$K_{\alpha\beta} = G_\alpha W_{\alpha\beta} V_\beta \ . \quad (8b)$$

Thus the kernel is $K_{\alpha\beta} = G_\alpha W_{\alpha\beta} V_\beta$. The interaction V_γ will contain the two-body interaction operating between particle a and particle b only if particles a and b are assigned to different clusters in partition γ. To avoid the appearance of a set of terms containing nothing but ladder diagrams of various orders connecting particles a and b we must make sure that no term in the interaction expansion of $X_{\alpha\beta}$ can be of high order without including the partition in which particles a and b constitute one cluster by themselves and all the other particles are necessarily included in the other cluster. Similarly, to prevent an infinite series of diagrams which are disconnected by virtue of a particular group of particles having only mutual interactions, we need to make sure that no diagram can be of high order without including the factor corresponding to the partition where this group is one of the two clusters of the partition.

The restrictions desired will be operative if the kernels $G_\alpha W_{\alpha\beta} V_\beta$ always appear in a given sequential order and if every possible partition is included in the sequence. This can be achieved by choosing

$$W_{\alpha,\alpha+1} = 1, \quad \alpha = 1, 2, \ldots, N-1, \quad (9)$$

$$W_{N,1} = 1,$$

$$\text{all other } W_{\alpha\beta} = 0 \ ,$$

where N is the total number of partitions possible for the n-particle system. With this choice there will be no diagram of order N or greater which is disconnected.

In the above analysis it is assumed that the particles are distinguishable. If the particles are indistinguishable, then one must make appropriately symmetrized sums of transition amplitudes calculated on the assumption of distinguishability.[5]

The new integral equation for the many-body transition operator which we propose is just Eq. (7) or Eq. (5) with the W coefficients given by Eq. (9). By virtue of coupling together all the transition operator elements $X_{\alpha 1}, X_{\alpha 2}, \ldots$ and employing all the partition Green's function operators $G_1, G_2, \ldots$ in one set of coupled integral equations, we are assured that all the asymptotic boundary condition constraints play a role in the calculation of the transition operator elements. Our choice of the W coefficients prevents any N-or-greater order iterate of the integral equation from containing any term associated with a disconnected diagram.

Other treatments[6] of the many-body problem eliminate the disconnected diagrams by procedures which replace the two-body interaction potentials contained in the $V_1, V_2, \ldots$ by transition amplitudes that result from the solution of the (lower order) many-body problems for all the clusters that appear in the partitions of the original many-body system. In these treatments only the free particle Green's function operator G_0 appears in the integral equations. In our treatment the same result is achieved by using the partition Green's function operators $G_1, G_2, \ldots$ in the integral equations and not eliminating the two-body interaction potentials. The evaluation of the partition Green's function operator G_α, of course, requires the de-

termination of the internal motion eigenstates of the two clusters that comprise partition α. So in our method, as well as in the other treatments, one must use the solutions of all lower order many-body problems to generate a solution of a given many-body problem.

It is expected that calculations based on Eq. (7) will be facilitated by replacing the partition cluster interaction V_α by a reduced interaction $V_\alpha - U_\alpha$ where U_α is an interaction potential that depends only on the relative displacement of the centers of mass of the two partition-α clusters. The resulting transition operator elements will then be used in matrix elements with distorted-wave relative motion wave functions instead of plane-wave relative motion wave functions.

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