Continuum Discretized Coupled-Channels Method as a Truncation of a Connected-Kernel Formulation of Three-Body Problems

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(Received 1 May 1989)

The widely used continuum discretized coupled-channels (CDCC) method for approximate calculations of three-body systems is discussed as a truncation of a Faddeev formulation in angular momentum space. A set of coupled equations is presented for converting a CDCC solution into a full solution of the original Schrödinger equation. A practical iterative procedure for solving the equations is outlined, based on the "distorted Faddeev equations" of Birse and Redish.

PACS numbers: 24.10.−i, 03.80.+r, 11.80.Jy, 34.10.+x

Success of the method of continuum discretized coupled channels (CDCC) in describing direct nuclear reactions involving breakup of colliding nuclei has motivated more general inquiries into its foundations as a numerical procedure for solving many-body scattering problems. When applied to a three-body system this method solves the Schrödinger equation

$$[E-K-V(r)-U(r_p)-U(r_n)]\psi=0 \tag{1}$$

in a restricted model space, as described at length in recent reviews.[1,2] Here the notation refers to the following explicit, *illustrative* problem: A neutron n and a proton p, with coordinates $\mathbf{r}_p$ and $\mathbf{r}_n$, move in the vicinity of an infinitely massive nucleus A, located at the origin. The kinetic-energy operator for the nucleons is K, the interaction potential between then is V, and the interaction potentials between A and the individual nucleons are U_p and U_n. For simplicity we assume that V is a short-ranged central potential. We also assume that incident waves are present only in the deuteron channel. Spins are ignored.

Recent criticisms of the CDCC method consider the possible sensitivity of the results to the choice of model space.[3,4] Discussions of CDCC foundations[5,6] emphasize the importance of complex optical potentials U_p, U_n as a justification for the central approximations. We recall[7] in the present paper that the CDCC method can be derived as a simple truncation of an orderly Faddeev-type formulation. Hence the method is recognized as a practical, physically motivated approximation procedure within the general three-body theory, and this eliminates much of the vagueness of the recent analyses of CDCC. We go on to propose improved procedures and new applications for this approach to three-body analyses.

The CDCC model space is defined primarily by the unusual projection operator P that only selects low angular momenta l associated with the neutron-proton relative coordinate $\mathbf{r}=\mathbf{r}_p-\mathbf{r}_n$, up to a maximum l_m. We will see that the basic properties of the model-space theory are obtained under any finite choice of l_m. Often the parameter l_m is taken to be only 0 or 2. We also define $1-P=Q$. Further properties of the model space appear later when discretization of the P-space continuum is introduced; the resulting finite number of "discretized continuum channels" comprise the standard model space.

Our principal point is that the partial wave functions $P\psi$ and $Q\psi$ not only are orthogonal, but they also meet the essential mathematical requirements for Faddeev components. Namely, the asymptotic two-body channels in distinct partitions of the system are located uniquely either in component $P\psi$ or in $Q\psi$, and the asymptotic boundary conditions for each two-body channel are expressed in finite form in terms of the natural variables of its Faddeev component. Thus, it is obvious that $Q\psi$ has no asymptotic amplitude in the deuteron channel. One can show that $P\psi$ has no asymptotic amplitudes in the two-body rearrangement channels, which have n-A or p-A bound states. In an n-A bound-state channel, for example, ψ reduces to $\phi_n(r_n)\chi_p(r_p)$ for r_p large, where ϕ_n is the n-A bound-state wave function, and χ_p is a proton scattering wave function. It is easy to see that

$$P[\phi_n(r_n)\chi_p(r_p)]\rightarrow O(1/r_p^3)\,, \tag{2}$$

as $r_p\rightarrow\infty$. Hence $\phi_n(r_n)\chi_p(r_p)$ has a negligible asymptotic amplitude in $P\psi$. Similarly this wave function has negligible overlap with p-A bound-state channels.

Because of the properties described above, the boundary conditions for $P\psi$ and $Q\psi$ are expressed in terms of the natural variables of the respective two-body channels contained in the two components. Thus $P\psi$ is expressed in terms of $\mathbf{r}=\mathbf{r}_p-\mathbf{r}_n$ and $\mathbf{R}=(\mathbf{r}_p+\mathbf{r}_n)/2$, the variables

of the deuteron channel, and $Q\psi$ is expressed with $\mathbf{r}_p$ and $\mathbf{r}_n$, the natural variables of the n-A or p-A bound-state channels. Although the asymptotic n-A and p-A channels could be described in $\mathbf{r},\mathbf{R}$ coordinates, this would require contributions from a vast set of l states, which would have negligible relation to the few l states in P space. The further separation of bound p-A or n-A channels from each other is trivial for a short-ranged neutron-proton interaction V, as is seen below. We note that a finite change in l_m does not imply any change in the association of asymptotic two-body partitions with the P and Q parts of the wave function.

Since the rotationally invariant V commutes with P and Q, Eq. (1) reduces to coupled equations for the component wave functions,

$$(E-K-V-PU)P\psi=PUQ\psi\,, \tag{3a}$$

and

$$(E-K-V-QU)Q\psi=QUP\psi\,. \tag{3b}$$

Here we conveniently abbreviate $U=U_p+U_n$. One could conduct a Faddeev-type analysis of the system in configuration space, using these equations, because of the distinct asymptotic behavior of $P\psi$ and $Q\psi$, and because the coupling potentials PUQ and QUP on the right-hand side (RHS) are three-body operators and tend to suppress "disconnected diagrams." It is apparent from the same consideration as in (2) that the operator on the left-hand side (LHS) of (3b) has the asymptotic form

$$(E-K-V-QU)\rightarrow(E-K_p-K_n-U_p-U_n)\,, \tag{4}$$

either for $r_p\rightarrow\infty$ with r_n finite, or vice versa, so that the p-A and n-A channels are asymptotically distinct from each other, as claimed above. More useful coupled equations are given below.

The CDCC approximation is obtained from (3a) by omitting the RHS, so that

$$(E-K-V-PUP)\psi^{\mathrm{CDCC}}=0\,. \tag{5}$$

This step is based on the arguments that the coupling term $PUQ\psi$ tends to be weak, especially for the smooth potentials U_p,U_n in current CDCC applications, (a) because U has small matrix elements between significantly different l states, and (b) because U only links $l\approx l'$ states in the P and Q spaces if $l\approx l'\approx l_m$, a fairly large angular momentum. For such values of angular momenta centrifugal repulsion reduces the wave function at small radii; in general $PUQ\psi$ vanishes rapidly at large radii, giving an overall reduction. In the CDCC approach (5) is solved numerically in $\mathbf{r},\mathbf{R}$ coordinates, using discretization of the P-space continuum. This approach to the three-body system is advantageous when U_p and U_n have appreciable radii, because, once the model space has been chosen, only the one variable $\mathbf{R}$ requires a partial-wave expansion.

The standard Faddeev differential equations for our deuteron-nucleus example are

$$(E-K-V)\psi_d=V(\psi_p+\psi_n)\,, \tag{6a}$$

$$(E-K-U_p)\psi_p=U_p(\psi_d+\psi_n)\,, \tag{6b}$$

$$(E-K-U_n)\psi_n=U_n(\psi_d+\psi_p)\,, \tag{6c}$$

in an obvious notation. These are solved with standard scattering boundary conditions and the constraint $\psi_d+\psi_p+\psi_n=\psi$. In general all three Faddeev components contain admixtures of both the P-space and Q-space components of the model-space approach (although the Q component of ψ_d is negligible if l_m is sufficiently large). We recall that simple truncations[8] of the standard Faddeev equations tend to lose the relations among the three interactions in Eq. (1). In contrast the single model-space equation (5) combines the interactions V and $P(U_p+U_n)P$, a considerable part of the dynamics of the system. We note this result is based on an unsymmetrical approach, which emphasizes particular aspects of the interactions U_p,U_n.

CDCC is sometimes compared with the coupled-reaction-channels (CRC) approach. However, we note that CRC emphasizes coupling among the possible two-body channels of a three-body system, largely without three-body breakup, whereas CDCC emphasizes coupling between breakup and the entrance channel, largely without two-body exit channels.

Additional approximations used in the numerical solution of (5) have been discussed extensively.[1-6] For example, in the customary CDCC procedure[5,6] $P\psi$ is expanded in eigenstates of $K_r+V(r)$ and the spectrum of these eigenstates is discretized. The R-dependent coefficient functions in this expansion (channel functions) are subject to a finite set of coupled differential equations derived from (5). The coupling potentials in these equations, which arise from PUP in (5), are found to have long tails and to depend somewhat on the method of discretization. For example, the potential tail at large R decreases as R^{-4} under one method discussed in Ref. 6 and as R^{-2} under another. Although these tails can seem troublesome, in actual CDCC calculations the standard outgoing-wave boundary condition is imposed on the channel functions at a matching radius R_m that is quite small. This practice[5,6] makes sense because the discretized PUP potential is sufficiently smooth so that a channel function that is outgoing asymptotically does not experience much reflection by the potential tail, and it is still likely to be primarily outgoing at radii as small as $R_m\sim 20$ fm. A numerical test[6] confirms that CDCC results are nearly independent of the method of discretization.

We now return to the more complete theory given by the coupled equations (3a) and (3b) and inquire how it differs from the CDCC approximation. In the complete theory the calculation of $P\psi$ is affected by the coupling term on the RHS of (3a). The principal new effects in-

troduced by this term arise from the rearrangement channels in $Q\psi$. However, we know that if U_p and U_n are realistic nucleon optical potentials, with absorptive imaginary parts, the wave functions in rearrangement channels decay exponentially both in r_p and r_n;[5] they are "closed by absorption" and have no very-high-l components. One expects that the only components of $Q\psi$ that are appreciable will be ones that can be reached directly from the deuteron channel or through a few steps of continuum-continuum coupling. Using realistic nucleon optical potentials, the maximum angular momenta reached in this way are surprisingly small,[9] of the order $l_m \approx 4$. Thus the coupling term may not produce much change of $P\psi$.

There is more scope for new effects if (3a) and (3b) are applied to systems in which U_p and U_n are real. Such systems can have open rearrangement channels, associated with nucleon-A bound states. Since the wave function now has nonzero asymptotic amplitudes in rearrangement channels, $Q\psi$ is not negligible under any finite choice of model space, no matter how large. Coupling to this $Q\psi$ causes $P\psi$ to deviate from ψ^{CDCC}. More specifically, we recognize the RHS of (3a) as a complicated long-ranged effective potential in P space that takes account of the higher-angular-momentum states in Q space. On the other hand, despite the coupling to Q space, ψ^{CDCC} may still be a good approximation to $P\psi$, and hence to ψ, *in a limited region* $R < R_m$. For example, if U_p and U_n are well-behaved, finite-ranged potentials, and if l_m is sufficiently large, then $PUQ\psi$ on the RHS of (3a) is appreciable only at very large R. At sufficiently high energies the presence of $PUQ\psi$ at these large radii causes little reflection of outgoing waves in that region back towards the inner region, $R < R_m$, and it does not much affect the wave function in the inner region. As a corollary it is legitimate to apply the outgoing boundary condition for the channel functions at the radius R_m. These arguments recover CDCC in the region $R < R_m$; nevertheless, the existence of $Q\psi$ still implies that ψ differs from ψ^{CDCC} in the region $R > R_m$. The full ψ has nonzero asymptotic amplitudes in rearrangement channels, and these are missing from ψ^{CDCC}. Thus when rearrangement channels are open, any model-space derivation of ψ is incomplete. It is clear from the above considerations that insensitivity to changes of l_m need not mean that the dynamics are insensitive to rearrangement, as Sawada-Thushima concluded from their model-space calculation with real potentials.[4]

One can approach the exact solution of the complete three-body system by regarding $\psi^{\mathrm{CDCC}} \approx P\psi$ as a first approximation, and taking account of the coupling to $Q\psi$ by iteration. Unfortunately, the Q operators on the LHS of (3b) are inconvenient in $\mathbf{r}_p, \mathbf{r}_n$ coordinates, the natural variables for the rearrangement channels in $Q\psi$. A more satisfactory iteration procedure is obtained from the standard Faddeev equations (6a)–(6c), by a modification that establishes a correspondence with the model-space method.

Birse and Redish pointed out[10] that the insertion of three-body distorting potentials, compact in all their variables, does not change the mathematical properties of the Faddeev equations. We now introduce the model-space interaction $PUP = P(U_p + U_n)P$ as such a "distorting potential," and obtain

$$(E - K - V - PUP)\hat{\psi}_d = V(\hat{\psi}_p + \hat{\psi}_n)\,, \tag{7a}$$

$$(E - K - U_p)\hat{\psi}_p = (U_p - PU_pP)\hat{\psi}_d + U_p\hat{\psi}_n\,, \tag{7b}$$

$$(E - K - U_n)\hat{\psi}_n = (U_n - PU_nP)\hat{\psi}_d + U_n\hat{\psi}_p\,. \tag{7c}$$

The new component functions in (7a)–(7c) are defined by these equations, together with the boundary conditions and equation of constraint given for (6a)–(6c). If (7a)–(7c) are added in the usual manner, the distorting potential cancels and the original three-body Schrödinger equation is recovered.

Addition of only (7b) and (7c) produces the useful equation

$$(E - K - U_p - U_n)(\hat{\psi}_p + \psi_n) = (U - PUP)\hat{\psi}_d\,, \tag{8}$$

which resembles (3b), but without Q operators on the LHS. Thus (8) is a better starting point for iteration. Equation (8) separates in the coordinates $\mathbf{r}_p, \mathbf{r}_n$ if target nucleus recoil is unimportant. The subtraction of PUP on the RHS of (8) considerably weakens the coupling between $\hat{\psi}_p + \hat{\psi}_n$ and $\hat{\psi}_d$.

Since the RHS of (7a) is multiplied by the short-range interaction V, and since $QV(\hat{\psi}_p + \hat{\psi}_n) = VQ(\hat{\psi}_p + \hat{\psi}_n) \approx 0$ within the range of V, (7a) is to a good approximation an equation only in P space, with $\hat{\psi}_d \approx P\hat{\psi}_d$ at all R. CDCC reappears if (7a) is truncated. Under the approximation $\hat{\psi}_d \approx P\hat{\psi}_d$ (8) reduces to

$$(E - K - U_p - U_n)(\hat{\psi}_p + \hat{\psi}_n) \approx QUP\hat{\psi}_d\,. \tag{8a}$$

The important projection operator Q in the RHS of (8a) reduces the magnitude of the source term and displaces it to large radii, $R > R_m$. As a result, the magnitude of $\hat{\psi}_p + \hat{\psi}_n$ extracted from this equation is reduced in the region $R < R_m$, and the RHS of (7a) is reduced. (For $R > R_m$ higher multipoles come into play, and therefore the function $\hat{\psi}_p + \hat{\psi}_n$ increases; indeed, it becomes the source of outgoing waves in the open rearrangement channels.) Although the operators $U_p + U_n$ on the LHS of (8a) mix the P and Q spaces in the solution of this equation, the Q components do not contribute to the RHS of (7a) for a short-ranged V. Thus Eq. (8a) leads to a small coupling term in (7a).

In an iterative approach to (7a) and (8), the CDCC wave function can be inserted in (8) as a zero-order approximation for $\hat{\psi}_d$ on the RHS, and (8) solved as an inhomogeneous differential equation, to produce $\hat{\psi}_p + \hat{\psi}_n$. Insertion of this approximation on the RHS of (7a) produces an improved calculation of $\hat{\psi}_d$, and so on. In this

process, because V is short ranged one only has to worry about the P-space part of $\hat{\psi}_p + \hat{\psi}_n$, as mentioned above. The adiabatic approximation[11] might be used on the RHS of (8) as an alternative starting point for iteration.

One can imagine other ways of solving (8). For example, since the bound states of U_p and U_n have low angular momenta, it can be useful to separate $\hat{\psi}_p + \hat{\psi}_n$ into arrangement channels with bound n-A states and bound p-A states, as mentioned before. To facilitate this one can introduce additional projection operators P_p and P_n that select low angular momenta of the p-A and n-A systems, respectively, and consider

$$[E - K - U_p - P_p U_n P_p]\tilde{\psi}_p = [U_p - P_n U_p P_n]\tilde{\psi}_n + [U_p - P U_p P]\tilde{\psi}_d , \quad (7b')$$

$$[E - K - U_n - P_n U_p P_n]\tilde{\psi}_n = [U_n - P_p U_n P_p]\tilde{\psi}_p + [U_n - P U_n P]\tilde{\psi}_d , \quad (7c')$$

instead of (7b) and (7c). Of course the components $\tilde{\psi}_d, \tilde{\psi}_p, \tilde{\psi}_n$ are inserted in (7a) when it is used with (7b') and (7c'). Addition of (7b') and (7c') again gives (8), which shows that the correspondence between the P,Q operators and $\tilde{\psi}_p + \tilde{\psi}_n$ is maintained. Another way to solve (8) might be to expand in a truncated basis of homogeneous eigensolutions of the LHS of the equation.

For another alternative, we note that the truncated multipole expansion PUP of the interactions U converges rapidly in the bounded region $R < R_m$, as l_m increases. This convergence reduces the RHS of (8) or (8a), so there is less need for iteration of the coupled equations. It may often be practical to choose the parameter l_m large enough so iteration is unnecessary.

A more detailed article is planned. An application of these methods to the standard nD scattering problem would be interesting. It must be noted that the above discussion does not deal with physical complications of U_p and U_n (e.g., energy dependence) due to suppressed internal coordinates of nucleus A.

It has been suggested that our theory resembles that of Osborne and Eyre,[12] who apply iteration to couple the breakup continuum of a three-body system to a coupled-integral-equations calculation of the two-body channels. Not only do we place more emphasis on the three-body continuum, we emphasize a single set of Jacobi coordinates, and we use a mixed representation of the wave function, with eigenfunctions for 1 degree of freedom and position coordinates for the other. CDCC (and our generalization of it) is not entirely a configuration-space calculation.

N.A. is grateful to the National Science Foundation for research support. The authors M.K. and M.Y. are grateful for support by a Grant-in-Aid from the Ministry of Education, Science, and Culture. N.A. acknowledges valuable discussions with Professor E. F. Redish, during a sabbatical visit to the University of Maryland.

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