Coupled-reaction-channel calculation of a model n-d scattering problem above the breakup threshold

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An s-wave local-potential model of n-d scattering at collision energies above the breakup threshold is solved using a pseudochannel extension of the coupled-reaction-channel method. Results obtained for both quartet and doublet scattering agree within a few percent with the benchmark solutions of Friar *et al.*, Phys. Rev. C **42**, 1838 (1990), for the same model .

Three-particle collisions above the breakup threshold continue to represent a computational challenge for the practitioner. In principle, such problems are solvable within the Faddeev approach [1]. However, numerical handling [2] of the moving logarithmic singularities in the momentum-space integral-equation version of the Faddeev-Alt-Grassberger–Sandhas (AGS) approach can be difficult, or, at least, computationally awkward. On the other hand, due to the nature of the breakup boundary conditions [3], numerical solution of the (differential) Faddeev equations seem to require an excessively large computational domain in coordinate space [4–5]. Clearly, simpler (if approximate) methods are of some interest. One obstacle in investigating such methods in the past had been the lack of results for well-defined model problems with breakup channel. Until quite recently, the standard test problem had been the separable-potential three-particle model which is numerically solvable with sufficient reliability. Thanks to the recent work of Payne *et al.* [5], essentially exact results are now available for an s-wave local-potential model of $n+d$ scattering (the so-called Malfliet-Tjon I-III model), as well. These benchmark results have all been obtained within the Faddeev formalism using five distinct solution techniques; agreement between them being within 1% [5].

In this article we solve the same benchmark problem with a non-Faddeev method, namely, the coupled-reaction-channel method (CRC) [6] extended to include pseudoreaction channels to simulate the breakup channel. This method had earlier been tested on the separable-potential model [7,8], and found to yield the elastic transition amplitudes quite accurately. In this article, we demonstate that these results are not due to the relative simplicity of separable potentials, but the use of L^2 two-particle pseudostates in the CRC expansion is an effective means of treating breakup effects also for the (benchmark) local-potential model of Ref. [5].

Since the derivation and various aspects of the pseudochannel extension of the CRC have been discussed in some detail previously [7,8], we give here only the working equations. Following the standard three-particle notation [9], we take $(\alpha\beta\gamma)$ to stand for the cyclic permutations of particle labels (123), and refer to the partition $(\alpha)(\beta\gamma)$ as the αth rearrangement. Let s (=0, or 1) and i (=0, or 1) denote, respectively, the spin and isospin of a two-nucleon subsytem. The spin-isospin states for the αth rearrangement will be written as $\mid sSiI \rangle_\alpha$, where s (i) is the spin (isospin) of the pair α ($\equiv \beta\gamma$), and S ($=\frac{1}{2}$, or $\frac{3}{2}$) the total spin, and I ($=\frac{1}{2}$) the total isospin. The pair interaction V_α between particles β and γ is assumed to operate only on s-wave states, and to have the form

$$V_\alpha = \sum_{sSiI} |sSiI\rangle_\alpha \, V_{\alpha si\,\alpha} \langle sSiI| \, . \tag{1}$$

With restriction to s waves, the Pauli principle requires $s+i=1$. The pair potentials $V_{\alpha,10}$ (spin-triplet) and $V_{\alpha,01}$ (spin-singlet) are taken from Ref. [5].

The two-particle s-wave pseudostates are generated by diagonalizing the two-particle s-wave Hamiltonian $h_{\alpha si}$ in a subspace spanned by a suitable orthonormal basis $\{|u_{\alpha siv}\rangle\}_{v=1}^{N_{si}^{\max}}$. For a given spin-isospin state of the two-nucleon subsytem, this yields $N_{si}^{\max}$ pseudostates $|\phi_{\alpha siv}\rangle$ with energies $\epsilon_{\alpha siv}$. For the spin-triplet case the lowest state ($v=1$) corresponds to the deuteron bound state. In the present calculations, the same basis has been used for both the spin-triplet and spin-singlet cases. We took $N^{\max}$=15 and employed as basis functions a set of associated Laguerre polynomials (in radial distance) whose form and parameters are given in Ref. [7]. The energies of the first six states obtained from this diagonalization are shown in Table I. Restricting our attention to zero total orbital angular momentum, the asymptotic

TABLE I. The energies ϵ_{siv} of the lowest 6 pseudostates for the spin-triplet and spin-singlet pair potentials. Energies are in fm^{-2}.

v	Spin triplet	Spin singlet
1	−0.05377	0.00853
2	0.03096	0.05255
3	0.11669	0.14358
4	0.25807	0.29000
5	0.46847	0.50705
6	0.77014	0.81854

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states for the αth rearrangement will be denoted as $|cq\rangle_\alpha$ ($\equiv |\phi_{siv}q\rangle_\alpha \otimes |sSiI\rangle_\alpha$), where q is the relative momentum of the particle α, and c is the channel index standing collectively for (siv). Of these channel states, only the one with $s=1$, $i=0$, $v=1$ represents a physical channel, while all the rest are pseudochannels included to simulate the breakup channel.

For the present s-wave local-potential model, the (antisymmetrized) effective transition operators of the CRC method satisfy

$$\mathcal{T}^{SI}_{c'c}(q',q) = \mathcal{V}^{SI}_{c'c}(q',q) + \sum_{c''} \int q''^2 dq'' \frac{\mathcal{V}^{SI}_{c'c''}(q',q'')\mathcal{T}^{SI}_{c''c}(q'',q)}{E+i0-\epsilon_{c''}-3q''^2/4} , \tag{2}$$

where the nucleon mass has been set to unity. The pseudostate indices v, v', and v'' that are implicit in channel indices c, c', and c'' run, for a given spin-isospin state (si), from 1 to N_{si}. In the present work, we set $N_{10} = N_{01} = N$, but, of course, a different number of pseudostates could be used for the triplet and singlet potentials. Typically, $N=10$ gives satisfactory results. Note that $\mathcal{T}_{101,101}$ (designated as $\equiv \mathcal{T}_{el}$) is the only physical transition amplitude corresponding to the antisymmetrized combination of elastic and rearrangement scattering.

The effective interaction matrix V in Eq. (2) is given as

$$\mathcal{V}^{SI}_{c'c}(q',q) = {}_1\langle c'q'|(H-E)(1+P_{123}+P_{132}) - (H_0+V_1-E)|cq\rangle_1 , \tag{3}$$

where H is the total Hamiltonian, H_0 the kinetic-energy operator. To affect the antisymmetrization, rearrangement 1 has been chosen as the reference partition, and P_{123} and P_{132} denote the cyclic permutation operators. Using permutation properties, $\mathcal{V}^{SI}_{c'c}$ can be decomposed, in an obvous matrix notation, as

$$\boldsymbol{\mathcal{V}}^{SI} = \boldsymbol{\mathcal{U}}^{SI} + \boldsymbol{\mathcal{W}}^{SI} - \boldsymbol{\mathcal{Y}}^{SI} + \boldsymbol{\mathcal{Z}}^{SI} , \tag{4}$$

where

$$\mathcal{U}^{SI}_{c'c}(q',q) = 2\,{}_1\langle c'q'|P_{123}\,V_1|cq\rangle_1 , \tag{5}$$

$$\mathcal{W}^{SI}_{c'c}(q',q) = 2\,{}_1\langle c'q'|V_1 P_{123}|cq\rangle_1 , \tag{6}$$

$$\mathcal{Y}^{SI}_{c'c}(q',q) = 2\,{}_1\langle c'q'|(H_0-E)P_{123}|cq\rangle_1 , \tag{7}$$

$$\mathcal{Z}^{SI}_{c'c}(q',q) = 4\,{}_1\langle c'q'|P_{132}V_1P_{123}|cq\rangle_1 . \tag{8}$$

The explicit expressions for $\mathcal{U}$, $\mathcal{W}$, and $\mathcal{Y}$ are

$$\mathcal{U}^{SI}_{c'c}(q,q') = \Lambda^{SI}_{s'i',si}\int_{-1}^{+1} dx\,\phi_{s'i'v'}(p')\chi_{siv}(p) , \tag{9}$$

$$\mathcal{W}^{SI}_{c'c}(q,q') = \Lambda^{SI}_{s'i',si}\int_{-1}^{+1} dx\,\chi_{s'i'v'}(p')\phi_{siv}(p) , \tag{10}$$

$$\mathcal{Y}^{SI}_{c'c}(q,q') = \Lambda^{SI}_{s'i',si}\int_{-1}^{+1} dx\,\phi_{s'i'v'}(p') \times (E-q^2-q'^2-qq'x)\chi_{siv}(p) , \tag{11}$$

where $\Lambda^{SI}_{s'i',si}$ ($\equiv_2 \langle s'Si'I|sSiI\rangle_1$) are the spin-isospin recoupling coefficients,

$$|\chi_{siv}\rangle = V_{1si}|\phi_{siv}\rangle , \tag{12}$$

and

$$p = (q^2/4+q'^2+qq'x)^{1/2} ,$$
$$p' = (q'^2/4+q^2+qq'x)^{1/2} . \tag{13}$$

Integrals over x have been computed using a composite 64-point Gauss-Legendre quadrature. Similar integrals also come up within the separable-expansion approach to Faddeev-AGS equations [9], but with singular integrands in which the position of the singularities changes with q and q'. The spin-recoupling coefficients needed are

$$\Lambda^{1/2,1/2}_{01,01} = \Lambda^{1/2,1/2}_{10,10} = 0.25 ,$$

$$\Lambda^{1/2,1/2}_{01,10} = \Lambda^{1/2,1/2}_{10,01} = -0.75 ,$$

$$\Lambda^{3/2,1/2}_{10,10} = -0.5 .$$

Calculation of the $\mathcal{Z}$ terms involves a triple integral. Considerable simplification can be realized if the two-particle interaction in Eq. (8) is approximated by a rank-K separable expansion, viz.,

$$V^K_{1si} = \sum_{k=1}^{K}\sum_{k'=1}^{K} V_{1si}|\xi_{sik}\rangle(\mathbf{V}^{-1}_{1si})_{kk'}\langle\xi_{sik'}|V_{1si} , \tag{14}$$

where $\{|\xi_{sik}\rangle\}$ is a suitable set of expansion functions, and

$$(\mathbf{V}_{1si})_{kk'} = \langle\xi_{sik}|V_{1si}|\xi_{sik'}\rangle . \tag{15}$$

Note that this expansion is not an essential part of the CRC method, but is introduced solely for computational convenience . The expansion bases $\{|\chi_{sik}\rangle\}$ and K can be chosen independently of the pseudostate basis, i.e., how large K is does not affect the number of coupled equations in (2). For further computational convenience, however, we took $N = K$ and used the pseudostate basis also as the basis for the separable expansion (14). Then, the $\mathcal{Z}$ matrix can be expressed in terms of the $\mathcal{U}$ and $\mathcal{W}$ matrices:

$$\mathcal{Z}^{SI}_{c'c}(q',q) = \sum_{s''i''}\sum_{v''v'''}\int q''^2 dq''\,\mathcal{U}^{SI}_{c'c''}(q',q'') \times (\mathbf{V}^{-1}_{1s''i''})_{v''v'''}\,\mathcal{W}^{SI}_{s''i''v''',c}(q'',q) \tag{16}$$

The coupled set of transition operator equations (2) contain only fixed-point singularities, which are first reg-

TABLE II. Spin-quartet results.

	CRC calculations			Faddeev calculations		
	$N=5$	$N=10$	$N=15$	Separable expansion	Pade	Coordinate space
			$E_{\rm lab}=3.27$ MeV			
Re(δ)	106.5	106.5	106.5			106.4
η	1.000	1.000	1.000			1.000
			$E_{\rm lab}=4.0$ MeV			
Re(δ)	101.6	101.6	101.5	101.6	101.6	101.5
η	1.000	1.000	1.000	1.000	0.999	1.000
			$E_{\rm lab}=10.0$ MeV			
Re(δ)	78.1	78.2	78.0	78.1		
η	0.994	0.993	0.995	0.992		
			$E_{\rm lab}=14.1$ MeV			
Re(δ)	69.0	69.0	69.0	68.9	69.0	69.0
η	0.979	0.979	0.980	0.978	0.978	0.978
			$E_{\rm lab}=42.0$ MeV			
Re(δ)	37.8	37.8	37.7	37.7	37.7	37.8
η	0.904	0.903	0.904	0.903	0.903	0.906

ularized using a multichannel version of the Kowalski-Noyes method [10]. The resulting set of nonsingular equations is then solved by quadrature discretization. A cutoff $q_{\rm max}$ is introduced for the upper limit of the q integrals, again, for computational convenience. The value $q_{\rm max}=8.0$ fm^{-1} was found to be adequate. The interval $[0, q_{\rm max}]$ is divided into a number of subintervals, and a Gauss-Legendre rule is applied on each subinterval. In an effort to treat the open-channel poles as symmetrically as possible, the number and length of these subintervals depend on the number and location of these singularities. The total number of quadrature points used ranged from 40 for $E_{\rm lab}=4.0$ MeV to 64 for $E_{\rm lab}=42$ MeV. The integral in Eq. (16) is evaluated using the same quadrature mesh.

Using the solutions of (2) in the integral formula for the transition amplitudes, an effective post-type operator $T^{(+)SI}_{c'c}$ with a different off-shell extension can be defined:

$$T^{(+)SI}_{c'c}(q',q)=\mathcal{V}^{(+)SI}_{c'c}(q',q)+\sum_{c''}\int q''^2dq''\,\frac{\mathcal{V}^{(+)SI}_{c'c''}T^{SI}_{c''c}(q',q)}{E+i0-\epsilon_{c''}-3q''^2/4}\,, \tag{17}$$

where $\mathcal{V}^{(+)SI}$ $(=\mathcal{U}^{SI}+\mathcal{Z}^{SI})$ is the post-part of the interaction matrix. Calculation of $\mathcal{T}^{(+)SI}$ provides a partial check on the adequacy of the computational parameters used to solve Eq. (2).

Writing the S matrix for the elastic channel as $e^{-2i\delta}$ with δ $(=\delta_R+i\delta_I)$ being the complex phase shift for elastic scattering, the results are presented in Tables II and III in terms of η $(=e^{-2\delta_I})$ and δ_R (in degrees). The results obtained from Eq. (17) are not listed separately, because they agree with the listed CRC results within the number of significant figures retained in these tables.

TABLE III. Spin-doublet results.

	CRC Calculations			Faddeev Calculations		
	$N=8$	$N=10$	$N=15$	Separable expansion	Pade	Coordinate space
			$E_{\rm lab}=4.0$ MeV			
Re(δ)	145.4	143.2	143.8	143.7	143.7	143.7
η	0.927	0.927	0.926	0.964	0.964	0.964
			$E_{\rm lab}=10.0$ MeV			
Re(δ)	124.0	119.9	119.9	120.3		
η	0.609	0.615	0.618	0.601		
			$E_{\rm lab}=14.1$ MeV			
Re(δ)	104.4	105.5	105.5	105.5	105.5	105.4
η	0.470	0.474	0.474	0.465	0.467	0.463
			$E_{\rm lab}=42.0$ MeV			
Re(δ)		41.2	41.4	41.3	41.3	41.2
η		0.517	0.510	0.502	0.504	0.501

In addition to the three energies ($E_{\rm lab}$ = 4.0, 14.1, and 42.0 MeV) for which benchmark Faddeev solutions are given in Ref. [5], we have also considered two other energies for which essentially exact results are available in the literature: $E_{\rm lab}$= 3.27 MeV [11] and 10.0 MeV [12]. The Faddeev results shown in Tables II and III are due to the Hosei, Bochum, and LA/Iowa groups [5]. The three distinct Faddeev techniques used by these groups are [5]: (i) conversion of the Faddeev-AGS equations into a set of effective two-body equations via the use of separable expansions for the pair potentials [11], (ii) solution of the two-variable Faddeev-AGS integral equations in momentum space via Pade summation [13], and (iii) solution of the partial-differential form (in two variables) of the Faddeev equations. Of these three approaches, the "Faddeev+separable-expansion" approach is the closest in spirit to the present CRC method, namely, both solve effective two-body equations. The important distinction, however, is that the effective interaction in the Faddeev case contains logarithmic singularities, whereas the effective interaction of the CRC approach is nonsingular.

In the quartet case ($S = \frac{3}{2}$), the system is weakly interacting, since the Pauli principle does not allow all three nucleons to interact strongly. Hence, the 5-state CRC calculations already provide excellent results. However, as can be judged from the values of the inelasticity parameter η in Table II, the breakup is not very significant at these energies for the quartet state. The doublet case given in Table III provides a more stringent test. The strongly interacting nature of this case is evident from the the inelasticity values. The 5-state CRC calculation no longer provides adequate results, and even the 8-state calculations are not very accurate. But N=10 and 15 results are quite satisfactory. The agreement of the 15-term CRC calculation with the three sets of Faddeev results is in most cases within 0.1° for δ_R and 2% for η. Note that, even the worst-case deviations, namely, 0.4° for δ_R and 4% for η, are comparable with the the deviations of the Utrecht [14] and Julich/NM [15] calculations from those of the Hosei-Bochum-LA/Iowa groups [5].

As our previous tests on the separable-potential model suggest, the CRC results can be improved by using a larger set of pseudochannels. It is likely that the poor quality of the 5- and 8-state calculations is, at least in part, due to using K=5 or 8 in evaluating $\mathcal{Z}$. It would be more proper to use K=15, irrespective of the value of N.

Also, the case $E_{\rm lab}$=4.0 MeV deserves some comment. With the present set of pseudostates, pseudochannels start to become energetically accessible above $E_{\rm lab}$=4.15 MeV in the triplet channel and $E_{\rm lab}$=3.89 MeV for the singlet channel. That is, the breakup thresholds in our approximate theory are $E_{\rm lab}$=3.89 and 4.15 MeV for the doublet and quartet cases, respectively, while the true threshold is 3.35 MeV. Therefore, our method is not, strictly speaking, applicable in the interval 3.35 MeV$\leq E_{\rm lab} \leq$3.89 MeV for the doublet case, and 3.35 MeV$\leq E_{\rm lab} \leq$4.15 MeV for the quartet case. Between 3.89 and 4.15 MeV for the doublet scattering, our method allows for some breakup scattering via a single open pseudostate in the singlet channel, but ignores breakup probability in the triplet channel. This explains the poor agreement for the doublet η at 4.0 MeV. For the quartet case, this problem does not manifest itself in the results, because the breakup probability at 4 MeV is negligibly small, and the correct prediction of the phase shift is an indication of the successful simulation of the virtual breakup effects. Of course, the breakup threshold of the approximate theory can be lowered by employing a larger and more diffuse basis set to generate the pseudostates.

Our results clearly demonstrate the success of the pseudochannel simulation of the breakup channel as far as the rearrangement amplitudes and the total breakup probability are concerned. Of course, this brings the question as to whether this (approximate) method can give any further information about the transitions into the breakup continuum. In Table IV, the elastic and pseudorearrangement probabilities obtained from 15-state calculations are shown for $E_{\rm lab}$=42 MeV. The relationship of the pseudorearrangement amplitudes to breakup amplitudes is, at present, a moot point. To investigate questions like whether the pseudochannel amplitudes can be considered as certain averages of the breakup amplitudes, or whether the discrete set of pseudochannel amplitudes can be smoothed to give the continuum of breakup amplitudes, a set of benchmark calculations for the breakup amplitudes are needed. Such benchmark results would also give us clues as to why such a method (involving a drastic approximation of breakup boundary conditions) should even produce accurate rearrangement amplitudes. An important concern in this connection is whether or not the breakup continuum of the models considered has some special feature making the L^2 discretization a reasonable approximation.

TABLE IV. Transition probabilities at $E_{\rm lab}$=42 MeV.

Final channel	v	Doublet	Quartet
Triplet	1 (elastic)	0.260	0.818
	2	0.079	0.065
	3	0.147	0.102
	4	0.087	0.013
	5	0.002	0.004
Singlet	1	0.080	
	2	0.122	
	3	0.158	
	4	0.065	
	5	0.003	

TABLE V. Breakup probabilities in the doublet scattering.

$E_{\rm lab}$ (MeV)	Final channel	15-state CRC
10.0	breakup (triplet)	0.144
	breakup (singlet)	0.476
14.1	breakup (triplet)	0.241
	breakup (singlet)	0.535
42.0	breakup (triplet)	0.315
	breakup (singlet)	0.428

Finally, we mention that the division of the total breakup probability for the doublet scattering between the triplet and singlet breakup channels is a natural by-product of our calculations, and it would be of great interest to compare the results shown in Table V with those of the Faddeev calculations. To our knowledge, there are no Faddeev calculations reporting this information , or, more generally, the breakup amplitudes, in a form to serve as benchmarks. This article is, therefore, concluded with a call for much-needed benchmark calculations of the breakup amplitudes for the present *n-d* model.

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