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Exact $n-d$ scattering calculation with a separable expansion of the two-body t matrix

Yasuro Koike

Department of Physics, Hosei University, Chiyoda-ku, Tokyo 102, Japan (Received 15 August 1990)

It is demonstrated numerically that a separable expansion of the two-body t matrix gives us an exact method of solving the Faddeev equation with a local potential. The method of a separable expansion adopted is simple and systematic. The result of the three-body calculation on the $n-d$ scattering is stable at least in four significant figures with a lower truncation of the separable series.

It is currently of interest to solve the Faddeev equations in the scattering region exactly. Neutron-deuteron scattering with realistic two-nucleon interactions is especially important because it is expected that the nuclear force can be understood through this study.

The equations can be solved both in momentum space and in configuration space.¹ In the scattering region however, the momentum space equations look simpler. The most widely used technique to solve the Faddeev equations in momentum space for neutron-deuteron scattering up to now has been the direct solution of the two-dimensional integral equations after angular momentum decomposition.²⁻⁴ The merit of this technique is that the exact solution, in principle, can be obtained if the numerical integration is performed carefully, which is not trivial because of the singularities in the kernel. This method, however, usually requires a huge memory as well as a large CPU time, and hence it is a considerable task to solve the equation with this method even in present day vector processors.

A separable two-body t-matrix reduces the twodimensional integral equations to coupled onedimensional integral equations. If the two-body t matrix is expanded into a separable series, it provides another method for solving the Faddeev equations. Several methods have been proposed for the separable expansion of the two-body t matrix. The usefulness of the method depends upon the speed of convergence. It has been demonstrated that some methods are powerful enough to approximate two-body properties with low-rank separable t matrices. $5 - 7$

Separable potentials derived using these methods have been published. One of the most widely used finite-rank two-body separable potentials is the PEST potential, 8 obtained by the Graz group which represent the Paris potential⁹ in a wide energy region reasonably well. The Ernst, Shakin, and Thaler (EST) method of the separable expansion⁵ was used to obtain this potential. The PEST potential has been used successfully in an $n-d$ scattering calculation by the Osaka-Graz group with a refinement of the potential.¹⁰ Since then, versions of the PEST potential have already appeared in literature. Different versions of the PEST potential usually have a different rank. Differences may exist even in the PEST potentials with the same rank because of the freedom of the energy to calculate the form factor. Therefore, it is necessary to make

clear which version of the PEST potential is used in each few-body calculation.

Mathematically, it is impossible to expand the twobody t-matrix of the local potential into a separable form body *t*-matrix of the local potential into a separable form
in the rigorous sense.¹¹ This is because a local potential is noncompact in the two-body Hilbert space while a separable potential is compact. Therefore, it is impossible to have a finite-rank separable two-body t matrix which is a good approximation to the t matrix of the original local potential at all the energies. In a certain region of the energy and momentum, although the region may be large, some finite-rank separable potentials represent the original potential well.

The purpose of the separable expansion of the two-body t matrix, however, is to use it in the few-body equations for the system with more than three particles. In the connected kernel few-body equations, such as Faddeev equations in the three-body case, the kernel itself is compact with a reasonable potential. In other words, the Green's function in the few-body equations is a cutoff factor in the two-body Hilbert space. A proper separable expansion gives a series of three-body results which converges to the exact few-body solutions with the original interactions.

Because it is impossible to have a perfect separable potential as discussed above, we have versions of potentials. Instead, the separable expansion of the two-body t matrix should be used directly to solve the few-body equation. In other words, the convergence check should be done not in the two-body results but in the few-body results. The separable expansion plays the same role as a quadrature for the numerical integration. It is our purpose in this paper to show that a series of the three-body result with a separable expansion of the two-body t matrix converges to a certain number, and hence it is a method to solve the Faddeev equations exactly with local as well as nonlocal potentials. For this purpose, however, the separable expansion should be easy and more or less straightforward. If some complicated procedures are necessary, which is the case of the EST method where a careful choice of the energy is necessary, it is difficult to make the separable expansion directly in the few-body calculation.

We adopt here another method of separable expansion which has been introduced by Adhikari and co-workers.⁷ Contrary to the momentum space base functions in the work of Adhikari and co-workers, we use the Laguerre polynomial in the configuration space as the base function.

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This choice is more reasonable because many two-nucleon potentials are represented in the configuration space. The momentum space form factor is obtained by numerical Fourier transform.

We study the $n-d$ elastic scattering at 10 MeV with the Los Alamos version of the Malfliet-Tjon potential.¹

In the separable expansion method of Adhikari and coworkers, a series of base functions $\phi_1, \phi_2, \ldots, \phi_n$ is needed. We can choose a different series, if necessary, for different $N-N$ states. We define the form factor g_i by

$$
|g_i\rangle = V| \phi_i\rangle \quad (i = 1, 2, \dots, n) \tag{1}
$$

where V is the original potential; i.e., the Malfliet-Tjo potential in this case. We define the rank N separable potential $V^{[N]}$ by

$$
V^{[N]} = \sum_{i,j=1}^{N} |g_i\rangle \lambda_{ij} \langle g_j| \,, \tag{2}
$$

where
$$
\lambda_{ij}
$$
 is the element of the matrix Λ ;
\n
$$
\lambda_{ij} = [\Lambda]_{ij}.
$$
\n(3)

The matrix Λ is defined through its inverse,

$$
[\Lambda^{-1}]_{ij} = \langle \phi_i | V | \phi_j \rangle. \tag{4}
$$

Then the potential $V^{[N]}$ acts just the same as V on ϕ_i ; i.e.,

$$
V^{[N]}|\phi_i\rangle = V|\phi_i\rangle \quad (i \leq N) \tag{5}
$$

The choice of the series of the function $|\phi_i\rangle$, therefore, is essential in this method. We use the Laguerre polynomial in this work, since it is one of the orthogonal polynomials defined in $0 \le r < \infty$. We introduced a factor which is multiplied to the Laguerre polynomial,

$$
F_{\sigma}(r) = \exp[-\sigma r], \qquad (6)
$$

where σ is a cutoff parameter that can be chosen to get a rapid and stable convergence in the three-body calculation. The final result should be independent from the value of σ .

With this factor and Laguerre polynomial L_i , we have a series of base functions by

$$
\phi_j(r) = F_{\sigma}(r)L_{j-1}(\tau r) \quad (j = 1, 2, ...).
$$
 (7)

Here τ is a scaling parameter which we have fixed by

$$
\tau = 1.5 + 2\sigma \tag{8}
$$

As we see from Eq. (4) and the orthogonal condition of the Laguerre polynomial, this choice of τ would make the matrix Λ diagonal under a potential $V(r) \propto e^{-1.5r}/r^2$. It helps to keep the matrix Λ nonsingular. We call this choice of series (7) type A.

There are poles in the two-nucleon t -matrix. A virtual state pole is in the singlet s wave, while the deuteron pole is in the triplet s wave. The approximation of the t matrix is, therefore, better if these poles are well described. Low-rank type-A separable potentials may fail to reproduce these poles.

In the EST method, on the contrary, these poles are reproduced by using the true wave function at corresponding energies. We have introduced another series of base functions by adding the wave function to the type- A base functions in each state. That is,

$$
\phi_1(r) = \chi(r), \n\phi_j(r) = F_{\sigma}(r)L_{j-2}(\tau r) \quad (j = 2, 3, ...).
$$
\n(9)

Here $\chi(r)$ is the deuteron wave function in the triplet s wave, while it is the zero-energy scattering wave function in the singlet s wave. We call this choice of series (9) type $B.$ Type- B separable potentials reproduce the pole in each state.

From these base functions, we easily have form factors defined by Eq. (1) in the configuration space. That is,

$$
g_j(r) = V(r)\phi_j(r) \tag{10}
$$

Then the form factor in the momentum space can be obtained by

$$
g_j(p) = \int r^2 dr j_0(pr) g_j(r) \tag{11}
$$

Here, $j_0(pr)$ is a spherical Bessel function. The integration in Eq. (11) is evaluated numerically.

The momentum space form factor plays an essential role in the kernel of the one-dimensional three-body equations.¹² The present method, contrary to some other separable expansion methods, 6 gives a form factor in one variable; i.e., the momentum. We replaced the numerical form factor by an analytic form factor. This is necessary in order to use the contour deformation technique.

A superposition of the Yamaguchi-type form factor has often been used to have an analytic form factor. Then one has to treat a considerable number of parameters which are obtained by a least-squares fit. The quality of the approximation is sometimes poor.

Instead, we have introduced a procedure based on the Legendre expansion. Since it is an expansion with an orthogonal polynomial, it is straightforward and accurate. A similar treatment has been used before.¹⁰ The present treatment is an improvement. We divide the form factor

TABLE I. Calculated n-d scattering phase shifts δ and the absorption parameters η in ²S_{1/2} at 10 MeV with the Malfliet-Tjon potential. The higher-rank separable potential is used in ¹S₀, while a fixed rank-one potential is used in ³S₁. The cutoff parameter σ is 0.4 fm⁻¹. The phase shift is in degrees.

Rank	Type A		Type B		
	δ	η	δ	η	
	41.41	0.8891	115.39	0.6091	
2	107.40	0.6414	114.01	0.6089	
3	117.23	0.6229	117.96	0.6150	
4	118.31	0.6170	118.36	0.6162	
5	119.07	0.6098	118.46	0.6161	
6	118.09	0.6183	118.34	0.6162	
7	118.28	0.6168	118.35	0.6162	
8	118.33	0.6164	118.35	0.6162	
9	118.34	0.6162	118.35	0.6162	
10	118.35	0.6162	118.35	0.6162	

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Rank	$\sigma = 0.2$		$\sigma = 0.3$		$\sigma = 0.5$	
		n	δ	n	δ	n
	115.39	0.6091	115.39	0.6091	115.39	0.6091
	113.59	0.6086	113.87	0.6088	114.09	0.6090
3	118.31	0.6161	118.21	0.6157	117.48	0.6139
	118.34	0.6161	118.35	0.6162	118.37	0.6162
	118.37	0.6162	118.38	0.6162	118.31	0.6162
6	118.43	0.6162	118.32	0.6162	118.34	0.6162
	118.34	0.6162	118.35	0.6162	118.35	0.6162
8	118.35	0.6162	118.35	0.6162	118.35	0.6162

TABLE II. Same as Table I with a different value of the cutoff parameter. The series of separable potentials is type B.

into two factors,

two factors,
\n
$$
g_j(p) = Y_j(p) R_j(p) \tag{12}
$$

Here, $Y_i(p)$ is a Yamaguchi-type form factor. That is,

$$
Y_j(p) = \frac{\kappa_j}{p^2 + \beta_j^2},\tag{13}
$$

with a fixed value of β_j . Then the parameter κ_j is determined by a requirement that $R_i(0) = 1$. This factor introduces a correct asymptotic and threshold behavior into the analytic form factor $g_i(p)$. All numerical information is contained in $R_i(p)$. Since the threshold and asymptotic behavior of this factor is simple, it is easier to expand.

We expand this factor as follows. We present $R_i(p)$ as

$$
R_j(p) = 1 + \frac{p^2}{p^2 + \gamma_j^2} F_j(p) \tag{14}
$$

Finally, this function $F_i(p)$ is expanded by the Legendre polynomial in a variable t after a standard transform

$$
p^2 = \delta_j^2 \frac{1+t}{1-t} \quad (-1 \le t < 1) \,. \tag{15}
$$

The parameters γ_i and δ_j in Eqs. (14) and (15) can be chosen in order that the Legendre expansion can be truncated faster. The resulting analytic form factor has poles at $p = \pm i\beta_j$, $\pm i\gamma_j$, $\pm i\delta_j$. Due to the construction, the parameter β_i is for long range, while γ_i , and δ_i are for short range. We took $\tilde{\beta}_j = 1.4$ fm ⁻¹, $\gamma_j = 5.0$ fm ⁻¹, and $\delta_j = 2.5$ fm⁻¹. These poles do not cause any problem in the method of contour deformation because they are large enough. We have checked that the quality of the expansion is independent from the choice of these parameters if they are in a reasonable region.

Simpler formulas could be used to expand the form factor in an analytic function. However, the merit of this formula $[Eqs. (12)-(15)]$ is that the analytic form factor obtained is very accurate and smooth in the region of smaller and medium momentum which is very important in the three-body calculation. Typically, the first ten Legendre polynomials are enough to reproduce the form factor in five significant figures or more in the region of $0 \leq p < 5$ $\rm fm$ ⁻¹.

Once the separable potentials in singlet and triplet states are fixed, we solve the resulting one-dimensional coupled equations. We solve the equations repeatedly with the rank of the separable potential increasing to see the convergence of the three-body result. In this work, we calculate the phase shift and the absorption parameter.

As a first example, we solved the equations in the dou-

 ${}^{2}S_{1/2}$ $4S_{3/2}$ $\sigma = 0.3$ $\sigma = 0.4$ Rank δ δ δ η η \overline{p} 0.9922 1 77.16 115.39 0.6091 0.6091 115.39 2 77.09 0.9922 113.35 0.6117 113.66 0.6106 3 77.97 0.9920 120.05 0.6016 0.6015 119.75 4 0.9919 78.08 120.30 0.6012 120.33 0.6013 5 78.08 0.9919 120.36 0.6012 120.45 0.6012 6 78.08 0.9919 120.31 0.6012 120.45 0.6012 7 120.32 0.6012 120.33 0.6012 8 120.33 0.6012 120.34 0.6012 9 120.34 0.6012 120.34 0.6012 10 120.34 0.6012 120.34 0.6012 Our exact 78.08 0.9919 120.34 0.6012

TABLE III. Calculated n-d scattering phase shifts δ and the absorption parameters η with the Malfliet-Tjon potential both in ²S_{1/2} and in ⁴S_{3/2} at 10 MeV. Ranks in the all channels are increased. The type- B series is used.

blet $n-d$ s wave by increasing the rank of the separable potential in the singlet $N-N$ state, keeping the triplet $N-N$ state the rank one of type B . Table I shows the calculated numbers. Two series are shown. One of them is with the type-A series in the singlet state, while the other is with type B. In both cases $\sigma = 0.4$ fm

The convergence shown in type A is typical. The numbers of the successive terms get closer and closer as the rank increases, while the number with rank one is poor.

On the contrary, the rank-one calculation in type B is already a good approximation to the higher-rank calculation. This simply means that the unitary pole approximation is good. The speed of the convergence in the type- B series is faster although the results from both types of series converges to the same number.

Table II shows the series of the type- B calculation with different cutoff parameters. As we have expected, the converged number with higher rank is independent from the cutoff parameter.

The value in these tables is not the final value that we

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want to calculate because the potential in the triplet state is still rank one. As a second example, we repeated the calculation increasing the rank in the triplet potential with a fixed singlet rank-one potential. We also found that the series converges quickly.

In order to calculate the final exact numbers with the original potential, we increase the rank of separable potentials in all relevant channels. Table III shows the series of calculations in the double s state and in the quartet s state of the $n-d$ scattering. Type- B series is used here. The cutoff parameter is 0.4 fm^{-1}. In each state, we found that the series converges to a certain number, which is the result of our exact calculation. The present procedure of the exact method has already been applied at different energies, and compared with solutions from other approaches. ' Our numbers agreed with others.

The calculation was done at the Institute of Nuclear Study, Tokyo University, and at the Hosei University Computer Center.

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