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An Efficient Numerical Algorithm for Calculation of Matrix Elements of Trinucleon System with Realistic Potentials

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A new method of evaluation of matrix elements, involving integration of a very rapidly oscillating function, has been developed. The proposed procedure is accurate, efficient, and fast and has been applied to the calculation of potential matrix elements of the trinucleon system with Reid soft core potential in hyperspherical harmonics expansion method.

INTRODUCTION

One of the important tools for the solution of a few-body Schrödinger equation is the hyperspherical harmonics expansion method (HHEM) [1]. Ever since its development in the early 1970s, the method has extensively been used in molecular, atomic, nuclear, and quark bound state problems [2]. In atomic and molecular problems, the particles interact via a pure Coulomb potential. In a few quark systems the potentials employed have been more involved than the Coulomb potential but still have a structure which is much simpler than typical "realistic nucleon–nucleon (NN) potentials," like Reid soft core (RSC) [3], Reid Hard Core (RHC) [3], Hamada Johnston (HJ) [4], Paris [5], Bonn [6], etc. potentials. Use of such realistic potentials in the HHEM for nuclear problems leads to a very complicated numerical procedure, so much so that no HHEM calculation, even for the trinucleon system, with realistic NN potentials has so far been reported. All the HHEM calculations for few-nucleon systems have so far been restricted to simple S-projected potentials [7]. On the other hand, the Faddeev equation method (FEM) [8] is particularly suited for realistic potentials. For example, the RSC potential depends on the state of the interacting pair of nucleons; in the FEM, the equation for each channel can be written separately and, hence, the appropriate interaction potential for the channel can be included [8]. On the other hand, for the HHEM one has to evaluate the matrix elements of the full interaction potential between appropriately antisymmetrised few-nucleon states [10]. This is why there is an abundance of FEM calculations with realistic potentials for a trinucleon system while no such calculation by HHEM has been reported.

The first step in facing the challenge of HHEM with a realistic NN potential is to evaluate the matrix elements involved. In this communication, we present an elegant numerical algorithm for fast and accurate evaluation of the matrix elements for the realistic RSC potential. We will also critically examine some typical terms of the interaction which may present numerical difficulties and we establish that the present method is applicable to such terms as well. We will finally demonstrate our method with the numerical evaluation of a few typical matrix elements.

METHOD

In HHEM the few-nucleon wave function is expanded into a complete set of hyperspherical harmonics (HH) [1] spanning the angular hyperspace (Ω). Substitution of this expansion into the Schrödinger equation and projection onto a particular HH gives a set of coupled differential eigenvalue equations for the partial waves $u^{\varepsilon TS}_{2K+L}(r)$:

$$\left[-\frac{h^2}{m}\left[\frac{d^2}{dr^2}-\frac{(2K+L+2)^2-1/4}{r^2}\right]-E\right]u^{\varepsilon TS}_{2K+L}(r) + \sum_{K'\varepsilon'T'S'L'} C^{K\varepsilon TSL}_{K'\varepsilon'T'S'L'}(r)\, u^{\varepsilon'T'S'}_{2K'+L'}(r)=0, \qquad (1)$$

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where r is the hyperradial variable and m is the nucleon mass; E is the energy of the system and ε represents a particular symmetry component of the full wave function; T, S, L are respectively the total isospin, spin, and orbital angular momenta of this component, and K represents the grand orbital quantum number.

For the trinucleon system the coupling matrix element $C^{K\varepsilon TSL}_{K'\varepsilon'T'S'L'}(r)$ involves integrals of the form [10]

$$I_{nn'}(r)=\int_{-1}^{1} P_n^{(\alpha,\beta)}(x)\; V(r_{ij})\; P_{n'}^{(\alpha',\beta')}(x)(1-x)^{\gamma}\,(1+x)^{\delta}\,dx, \tag{2}$$

where $V(r_{ij})$ is the interaction potential for the (ij) pair and $\alpha=l_1+\frac{1}{2}$ and $\beta=l_2+\frac{1}{2}$, $P_n^{(\alpha,\beta)}$ is a Jacobi polynomial, $\gamma=(\alpha+\alpha')/2$, $\delta=(\beta+\beta')/2$; $\boldsymbol{l}_1$ and $\boldsymbol{l}_2$ are the orbital angular momenta of the interacting pair and the third particle with respect to the centre of mass of the pair respectively such that $\mathbf{L}=\boldsymbol{l}_1+\boldsymbol{l}_2$. Primed quantites refer to corresponding quantities of the ket vector.

As mentioned earlier, the RSC potential depends on the spin (s), isospin (t), and total angular momenta (j) of the interacting pair, with the restriction $j\leqslant 2$. Whenever only one value of l is allowed by angular momentum selection rule and symmetry of the pair, the potential is purely central, while when more than one l value is allowed for the same (tsj) component, the potential is a sum of central, spin-orbit, and tensor terms. The radial dependence of each of the terms is taken as a sum of Yukawa terms multiplied by powers of r_{ij}^{-1} (up to second power). Thus a typical term of the RSC potential contains a radial dependence of the form

$$V(r_{ij})=V(r\sqrt{(1+x)/2})=V_0\frac{e^{-\mu r\sqrt{(1+x)/2}}}{(1+x)^{\rho/2}}. \tag{3}$$

In Eq. (3) μ is the pion mass parameter ($\mu=0.7\ \mathrm{fm}^{-1}$) and ρ is an integer $\leqslant 3$. Substitution of this form of $V(r_{ij})$ in Eq. (2) shows that the principal value of $I_{nn'}$ exists for

$$l_2+l_2'+3\geqslant\rho. \tag{4}$$

Since each of l_2 and l_2' is an integer $\geqslant 0$ and $\rho\leqslant 3$, condition (4) is always satisfied.

For large values of n and n', the integrand in Eq. (2) involves a large number of oscillations in the interval $[-1,1]$ and a direct numerical evaluation with high precision becomes both slow and tricky. To evaluate $I_{nn'}$ we expand $V(r\sqrt{(1+x)/2})$ in the complete set of Jacobi polynomials $\{P_{n''}^{(\alpha'',\beta'')}\}$ for a fixed value of r,

$$V(r\sqrt{(1+x)/2})=V_0\frac{e^{-\mu r\sqrt{(1+x)/2}}}{(1+x)^{\rho/2}}=\sum_{n''=0}^{\infty} a_{n''}(r)\,P_{n''}^{(\alpha'',\beta'')}(x). \tag{5}$$

The potential multipole $a_{n''}(r)$ is given by

$$a_{n''}(r)=(1/h_{n''}^{\alpha'',\beta''})\int_{-1}^{1} V(r_{ij})\,P_{n''}^{(\alpha'',\beta'')}(x)(1-x)^{\alpha''}\,(1+x)^{\beta''}\,dx, \tag{6}$$

where $h_{n''}^{\alpha'',\beta''}$ is the norm of a Jacobi polynomial. The choices of α'' and β'' are arbitrary and for convenience we take $\alpha''=\beta''=\frac{1}{2}$. Substituting the expansion (5) in Eq. (2) we have

$$I_{nn'}(r)=\sum_{n''=0}^{\infty} a_{n''}(r)\langle n|\,n''\,|n'\rangle, \tag{7}$$

where the geometrical structure coefficients (GSC) $\langle n|\,n''\,|n'\rangle$ is given by

$$\langle n|\,n''\,|n'\rangle=\int_{-1}^{1} P_n^{(\alpha,\beta)}(x)\,P_{n''}^{(\alpha'',\beta'')}(x)\,P_{n'}^{(\alpha',\beta')}(x)\times(1-x)^{\gamma}\,(1+x)^{\delta}\,dx. \tag{8}$$

Evaluation of $I_{nn'}$ using Eq. (7) is not advantageous if the sum over n'' is unrestricted. However, $P_n^{(\alpha,\beta)}$ is a polynomial of degree n and satisfies orthogonality relation [11] in the interval $[-1,1]$, with respect to the weight function $(1-x)^{\alpha}\,(1+x)^{\beta}$; then combining any two of the Jacobi polynomials and using the orthogonality of the third, one can see [9] that $\langle n|\,n''\,|n'\rangle$ vanishes unless n'' satisfies relation

$$n_{\min}\leqslant n''\leqslant n_{\max}, \tag{9}$$

where $n_{\min}$ and $n_{\max}$ can be expressed in terms of l_1, l_2, l_1', l_2', n, and n'. Such a restriction on n'' will fail if by isolating one Jacobi polynomial, together with its appropriate weight factor, the remaining part of the integrand in Eq. (8) is not a polynomial. On the other hand, if n'' is limited by the inequality (9), Eq. (7) is replaced by

$$I_{nn'}(r)=\sum_{n''=n_{\min}}^{n_{\max}} a_{n''}(r)\langle n|\,n''\,|n'\rangle. \tag{10}$$

Since only a finite number of terms contribute, Eq. (10) is particularly convenient for the evaluation of $I_{nn'}(r)$. Furthermore, the GSC $\langle n|\,n''\,|n'\rangle$ does not depend on r and can be calculated once only and stored for all values of r. The GSC in turn can be calculated by using the completeness property [11] of $P_{n''}^{(\alpha'',\beta'')}(x)$ and by setting up a system of linear inhomogeneous equations, for which very fast and accurate computer codes exist [9]. To evaluate $I_{nn'}(r)$, using Eq. (10), we need to calculate the potential multipoles $a_{n''}(r)$. For the potential matrix element, we will

always have $l_2' = l_2$, due to the orthonormality of the spectator part of the wave function. For central and spin orbit potentials $l_1 = l_1'$, while for the tensor terms l_1 and l_1' may differ. Hence we consider two specific cases which are the only two possibilities for the RSC potential:

Case 1. $l_1 = l_1'$, $l_2 = l_2'$. In this case $\alpha = \alpha' = l_1 + \frac{1}{2}$, $\beta = \beta' = l_2 + \frac{1}{2}$, $\alpha'' = \beta'' = \frac{1}{2}$. When one Jacobi polynomial with its appropriate weight factor is isolated from the integrand of Eq. (8), the remaining part of the integrand becomes two Jacobi polynomials multiplied by a polynomial of x. Hence the latter can be expanded in the complete set of the previously isolated Jacobi polynomial and use of the orthogonality relation gives the selection rule

$$|n - n'| \leqslant n'' \leqslant (n + n' + l_1 + l_2). \tag{11}$$

In this case the potential multipole is given by Eq. (6), which, as we have already noted, exists for all terms of the RSC potential.

Case 2. $l_1 \neq l_1'$, $l_2 = l_2'$. In this case $\alpha = l_1 + \frac{1}{2}$, $\alpha' = l_1' + \frac{1}{2}$, $\beta = \beta' = l_2 + \frac{1}{2}$, $\alpha'' = \beta'' = \frac{1}{2}$. Isolating one Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$ or $P_{n'}^{(\alpha',\beta')}(x)$ with its appropriate weight factor $(1-x)^{\alpha}(1+x)^{\beta}$ or $(1-x)^{\alpha'}(1+x)^{\beta'}$, one is left with a factor $(1-x)^{(l_1'-l_1)/2}$ or $(1-x)^{(l_1-l_1')/2}$ in the integrand of Eq. (8). The symmetry of the interacting pair demands that l_1 and l_1' be both even or both odd integers. Hence $|(l_1'-l_1)/2|$ is a positive integer $= \nu$ (say) and the remaining factor is $(1-x)^{\nu}$ or $(1-x)^{-\nu}$. In one of the two cases, the exponent is negative and the expression is not a polynomial, so that n'' is no more restricted to a finite set and the proposed procedure fails. However, in this case we can include the factor $(1-x)^{-\nu}$ with the potential function $V(r\sqrt{(1+x)/2})$ and rewrite Eq. (2) as

$$I_{nn'}(r) = \int_{-1}^{1} P_n^{(\alpha,\beta)}(x)\, V'(r_{ij})\, P_n^{(\alpha,\beta)}(x) \times (1-x)^{\gamma+\nu}(1+x)^{\delta}\, dx, \tag{12}$$

where

$$V'(r_{ij}) = V_0 \frac{e^{-\mu r\sqrt{(1+x)/2}}}{(1+x)^{\rho/2}(1-x)^{\nu}}.$$

Thus

$$I_{nn'}(r) = \sum_{n''=0}^{\infty} a_{n''}(r)\langle n|\, n''\, |n'\rangle,$$

where

$$\langle n|\, n''\, |n'\rangle \equiv \int_{-1}^{1} P_n^{(\alpha,\beta)}(x)\, P_{n''}^{(\alpha'',\beta'')}(x)\, P_{n'}^{(\alpha',\beta')}(x) \times (1-x)^{\gamma+\nu}(1+x)^{\delta}\, dx \tag{13}$$

and

$$a_{n''}(r) = (1/h_{n''}^{\alpha'',\beta''}) \int_{-1}^{1} V'(r_{ij})\, P_{n''}^{(\alpha'',\beta'')}(x) \times (1-x)^{\alpha''}(1+x)^{\beta''}\, dx. \tag{14}$$

In this way we are introducing a possible singularity at the upper limit of the integrand of Eq. (14). But for the RSC potential, l_1, and l_1' are integers $\leqslant 3$; moreover, since l_1 and l_1' are both even or both odd integers, $\nu = 1$. Then, since $\alpha'' = \beta'' = \frac{1}{2}$ and $\rho \leqslant 3$, we see that the principal value of the integral in Eq. (14) exists. In this modified procedure the selection rule for n'' becomes

$$\max(n' - n, 0, n - n' - 2) \leqslant n'' \leqslant (n + n' + (l_1 + l_1')/2 + l_2 + 1). \tag{15}$$

Since, again we get a finite set of allowed n'' values and the potential multipole $a_{n''}(r)$ exists, the modified procedure will be valid.

RESULTS AND DISCUSSION

To illustrate the viability of our procedure, we have calculated typical potential matrix elements by the proposed method and compared it with a direct numerical evaluation of Eq. (2). We used a 32-point Gaussian quadrature for the potential multipole $a_n(r)$ used in the present method. For a direct numerical integration of $I_{nn'}$, it was found necessary to integrate in four subintervals, using 32-point Gaussian quadrature for each of the subintervals, in order to obtain a comparable precision of one part in 10^8.

TABLE I

Results of the Calculation of $I_{nn'}$ for Case I

$V(r_{12})$	l_1	l_2	r (fm)	n	n'	By direct method	By proposed method
$V(^3P_1)$	3	3	2.1	2	2	71.89433129	71.89433204
	3	3	2.1	5	4	−100.68444235	−100.68444263
	3	3	2.1	8	8	203.89916394	203.89916465
$V_T(^3S_1 - {}^3D_1)$	2	2	2.1	2	2	−54.88694387	−54.88694404
	2	2	2.1	7	2	27.93785697	27.93785744
	2	2	2.1	9	9	−315.87100766	−315.87101393
	2	2	5.1	2	2	−3.087294553	−3.087294584
	2	2	5.1	8	5	10.53900643	10.539009623
	2	2	5.1	9	9	−28.06005923	−28.06005981
$V_T(^3P_2 - {}^3F_2)$	3	3	2.1	2	2	9.00314219	9.003142255
	3	3	2.1	8	7	−14.09590289	−14.0959031
	3	3	5.1	2	2	0.72367197	0.72367199
	3	3	5.1	8	7	−2.39060681	−2.39060685

TABLE II

Results of Calculation of $I_{nn'}$ for Case II

$V(r_{12})$	l_1	l_1'	l_2	r (fm)	n	n'	By direct method	By proposed method
$V_T(^3S_1-{}^3D_1)$	0	2	0	2.1	2	5	296.22598207	296.22598408
	0	2	0	2.1	5	10	547.25890677	547.25893564
	0	2	0	5.1	2	5	47.79344825	47.79344831
	0	2	0	5.1	5	10	128.97650551	128.97650622
	0	2	2	2.1	2	5	18.39132987	18.3913325
	0	2	2	2.1	10	9	222.48253039	222.48253188
	0	2	2	5.1	2	5	1.20875072	1.20875068
	0	2	2	5.1	10	9	28.12092451	28.12092567
$V_T(^3P_2-{}^3F_2)$	1	3	1	2.1	2	9	−1.813809774	−1.813809779
	1	3	1	2.1	10	9	−33.8835417	−33.8835405
	1	3	1	5.1	2	9	−0.58806388	−0.5880639
	1	3	1	5.1	10	9	−7.290811	−7.2908109

Table I presents the results for a few chosen central terms of the RSC potential with typical but arbitrarily chosen values of l_1, l_2, n, n', and r. In Table II we present similar results for the second case considered above with the tensor parts of RSC potential. In most cases the agreement is up to eight significant digits or more. The calculations have been performed on an EISA-based AT486 personal computer with double precision. The present procedure is roughly 10 to 12 times faster than direct numerical integration. This shows that the present procedure works accurately in all cases.

The procedure proposed here is thus a valuable tool for numerical evaluation of the matrix elements. The direct integration of the full potential matrix must be done for each value of r and for each potential components separately, whereas the present procedure calls for calculation of the GSC (which is independent of r) once only (and stored), while for each value of r and for each potential component, the potential multipole has to be evaluated numerically. If the HH basis is truncated to N elements, the potential matrix will be a $N \times N$ matrix and one needs $N(N+1)/2$ numerical integrations for direct evaluation of the potential matrix for a given value of r, whereas the present procedure requires about $2N$ integration for the potential multipole for a given r. Hence as N increases this procedure rapidly becomes economical in computation time. Moreover, calculation of the GSC by the linear inhomogeneous equatin method is very fast and accurate so that when these are used together, one has an elegant numerical procedure.

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