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Solution of integro-differential equations by projection

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Abstract The integro-differential equation in two variables for a many boson system has been solved by expanding its solution in the complete set of Jacobi polynomials and subsequent projection. This results in a system of coupled differential equations. This has been solved for the triton. The integrals in the potential matrix elements can be done analyticaly for potentials having Gaussian type terms. Calculated binding energy for several simple potentials agree closely with those calculated by other methods.

Keywords. Few body problem; integro-differential equation; hyperspherical harmonics method.

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1. Introduction

Fabre and his collaborators (Fabre 1984, 1986; Fabre and Fieldeldey 1986; Fabre *et al* 1988) have derived an integro-differential equation (IDE) involving two variables for a many-boson system interacting through two body interactions in which all correlations higher than two-body correlations are disregarded. It has been shown by Fabre (Fabre 1986) that the IDE for three bosons in the S state is equivalent to the Feddev equation. The IDE has the same structure for all A(= number of particles) and its explicit complexity does not increase with A. This makes the IDE a powerful tool for an ab initio calculation of a many-body system. However numerical difficulties in calculating the Kernel function develop for large A. This makes the numerical solution of the IDE a difficult task. The IDE has been solved by direct integration using the adiabatic approximation (AA), for the 3 and 4 nucleon ground state, with several test potentials by Fabre *et al* (1988). The results agree closely with those by other methods. A variational solution of the IDE, decoupled by AA, has been solved by Das and Fabre (Das and Fabre 1988) for $A = 3$ and 4. In this report, we present a solution of the IDE by expanding its solution in the complete set of Jacobi polynomials, leading to a system of second order coupled differential equation (CDE). Analytical expressions for the potential matrix elements for Gaussian type potentials have been derived. This makes the calculation easy and fast numerically. However convergence with respect to K-partial waves has to be achieved for solving the CDE. The large system of CDE has been solved by using the AA (Das *et al* 1982a; Ballot *et al* 1982). Most of the numerical difficulties mentioned above can be surmounted by the use of analytic expressions for the integrals.

In the present calculation, we take the IDE for the space totally symmetric S state

of the trinucleon ($A = 3$). This wave function is multiplied by a totally antisymmetric spin-isospin function to make the complete wave function fully antisymmetric under any pair exchange. The percentage probabilities of the space totally symmetric S state ($L = 0$), the mixed symmetry S' state ($L = 0$) and the mixed symmetry D state ($L = 2$) (which are the only possible symmetry components for the trinucleon are about 90%, 20% and 8% respectively (Ballot and Fabre 1980)). Each of these space wave function is multiplied by a spin-isospin wave function of conjugate symmetry, so that the total wave function is fully antisymmetric under any pair exchange. Since the S state has about 90% probability, it is a fairly good approximation to consider only the S state for the trinucleon (Das and Coelho 1982a, b; Das *et al* 1982b). Inclusion of the other two symmetry components increases the complexity of the numerical calculations by at least an order of magnitude, while only marginal improvements result in most of the calculated observables. As a compensation for this approximation, we should use the so called "S projected potentials" for such calculations, which, to some extent, takes into account the effects of the neglected parts of the wave function. Most of such potentials, which are in common use for a few nucleon calculations, are phenomenological in nature, rather than having a theoretical basis like the Yukawa potential. Many of these commonly used potentials are sum of gaussian functions. We demonstrate in the present work that the potential multipoles can be integrated analytically for the gaussian functions. With this and a semi-analytic method for the evaluation of the coupling coefficients make the calculation of the coupling potential matrix very fast, accurate and elegant. Thus the method outlined in this work is useful for fast and accurate numerical solution of the three body problem, although for a restricted class of potentials.

In § 2, we discuss the method employed and present the results of analytic integrations. Calculated ground state binding energy (BE) and convergence behaviour with respect to K values for several test potentials and comparison with the results by other methods have been presented in § 3. Finally we draw our conclusions in § 4.

2. Method

The integro-differential equation (IDE) for a system of A identical bosons (mass m) interacting through two-body potential $V(r_{ij})$ has the form (3) (Fabre 1986)

$$\left[\frac{\hbar^2}{m}\left\{\frac{\partial^2}{\partial r^2} - \frac{\mathscr{L}(\mathscr{L}+1)}{r^2} + \frac{4}{r^2}\frac{1}{w_l(Z)}\frac{\partial}{\partial Z}(1-Z^2)w_l(Z)\frac{\partial}{\partial Z}\right\} + E\right]P_l(Z,r)$$

$$= V\left(r\sqrt{\frac{1+Z}{2}}\right)\pi_l(Z,r) \tag{1}$$

where

$$\mathscr{L} = l + (3A-6)/2 \tag{2}$$

$$w_l(Z) = (1-Z)^{\alpha}(1+Z)^{\beta}, \quad \alpha = (3A-8)/2, \beta = l + \tfrac{1}{2} \tag{3}$$

$$\pi_l(Z,r) = P_l(Z,r) + \int_{-1}^{1} f_l(Z,Z')P_l(Z',r)\mathrm{d}Z' \tag{4}$$

and

$$f_l(Z,Z') = w_l(Z')\sum_K (f_{Kl}^2 - 1)\frac{P_K^{\alpha\beta}(Z)P_K^{\alpha\beta}(Z')}{\mathrm{h}_K^{\alpha\beta}}. \tag{5}$$

l being the total orbital angular momentum (assumed to be contributed solely by the interacting pair) and $h_K^{\alpha\beta}$ is the norm of the Jacobi polynomial $P_K^{\alpha\beta}(Z)$. The quantity f_{Kl}^2 is given by (Fabre 1986).

$$f_{Kl}^2 = 1 + [2(A-2)(-\tfrac{1}{2})^l P_K^{\alpha\beta}(-\tfrac{1}{2}) + (A-2)(A-3)/2 P_K^{\alpha\beta}(-1)\delta_{l,0}]/P_K^{\alpha\beta}(1) \tag{6}$$

The variable r is the hyperradius and Z is defined through $r_{ij} = r\sqrt{1+Z/2}$, r_{ij} being the (ij) pair separation. To solve (1), we expand $P_l(Z,r)$ in the complete set of Jacobi polynomials, for a fixed value of r:

$$P_l(Z,r) = \sum_{K'=0}^{\alpha} S_{K'l}(r) P_{K'}^{\alpha\beta}(Z). \tag{7}$$

Substituting in (1), using the differential equation satisfied by the Jacobi polynomial (Abramowitz and Stegun 1972) $P_{K'}^{\alpha\beta}(Z)$ and projecting on a particular $P_K^{\alpha\beta}(Z)$, we have

$$\left[\frac{-\hbar^2}{m}\frac{d^2}{dr^2} + \frac{\hbar^2}{mr^2}\{\mathscr{L}(\mathscr{L}+1) + 4K(k+\alpha+\beta+1)\} - E\right] S_{Kl}(r) + \sum_{K'}\left\{f_{K'l}^2 \frac{V_{KK'}(r)}{h_K^{\alpha\beta}}\right\} S_{K'l}(r) = 0 \tag{8}$$

where the potential matrix element

$$V_{KK'}(r) = \int_{-1}^{+1} P_K^{\alpha\beta}(Z)\, V\left(r\sqrt{\frac{1+Z}{2}}\right) P_K^{\alpha\beta}(Z) w_l(Z)\, dZ. \tag{9}$$

Equation (8) is a standard coupled differential equation for $S_{Kl}(r)$. However, the coupling term is not symmetric. To symmetrize we multiply (8) by $f_{Kl}(h_K^{\alpha\beta})^{\frac{1}{2}}$ to obtain

$$\left[\frac{-\hbar^2}{m}\frac{d^2}{dr^2} + \frac{\hbar^2}{mr^2}\{\mathscr{L}(\mathscr{L}+1) + 4K(K+\alpha+\beta+1)\} - E\right] U_{Kl}(r) + \sum_{K'} \bar{V}_{KK'}(r) U_{K'l}(r) = 0 \tag{10}$$

where

$$U_{Kl}(r) = f_{Kl}(h_K^{\alpha\beta})^{\frac{1}{2}} S_{Kl}(r) \tag{11}$$

and

$$\bar{V}_{KK'}(r) = f_{Kl}\, V_{KK'}(r) f_{K'l}(h_K^{\alpha\beta} \cdot h_{K'}^{\alpha\beta})^{-\frac{1}{2}}. \tag{12}$$

The coupling potential matrix $\bar{V}_{KK'}(r)$ of (10), is symmetric in r. As expected, (10) is identical with the equation derived by Fabre starting from the potential harmonic expansion (Fabre 1983, 1987).

Evaluation of potential matrix $V_{KK'}(r)$

To evaluate $V_{KK'}(r)$ we again expand $V(r\sqrt{(1+Z)/2})$ in the complete set of Jacobi polynomials

$$V\left(r\sqrt{\frac{1+Z}{2}}\right) = \sum_{K''=0}^{\infty} a_{K''}(r) P_{K''}^{\alpha\beta}(Z). \tag{13}$$

From (13), using the orthogonality relation of Jacobi polynomials, we have

$$a_K(r) = (h_K^{\alpha\beta})^{-1} \int_{-1}^{+1} V\left(r\sqrt{\frac{l+Z}{2}}\right) P_K^{\alpha,\beta}(Z) w_l(Z)\,\mathrm{d}Z. \tag{14}$$

Substituting (13) in (19), one gets

$$V_{KK'}(r) = \sum_{K''=0}^{\infty} a_{K''}(r) C(K, K'', K') \tag{15}$$

where

$$C(K, K'', K') = \int_{-1}^{+1} P_K^{\alpha,\beta}(Z) P_{K'}^{\alpha,\beta}(Z) P_{K''}^{\alpha,\beta}(Z) w_l(Z)\,\mathrm{d}Z \tag{16}$$

are the coupling coefficients, whose evaluation will be discussed in the next subsection.

We calculate the coefficients $a_K(r)$ for two-body interactions which are sum of N Gaussians:

$$V(r_{ij}) = \sum_{n=1}^{N} V_{on} \exp(-(r_{ij}/b_n)^2) \tag{17}$$

where V_{on} and b_n are parameters. For this $a_K(r)$ is given by

$$a_K(r) = (h_K^{\alpha,\beta})^{-1} \sum_{n=1}^{N} V_{on} \exp(-\mathrm{d}_n(r)) \int \exp(-\mathrm{d}_n(r)Z) P_K^{\alpha,\beta}(Z) w_l(Z)\,\mathrm{d}Z \tag{18}$$

where

$$\mathrm{d}_n(r) = \tfrac{1}{2} r^2/b_n^2. \tag{19}$$

For the special case of S state ($l = 0$) of triton $\alpha = \beta = \frac{1}{2}$. In this case the integral of (18) can be done analytically using the standard integrals (Gradshtevo and Ryzhik 1980).

$$\int_0^1 (l - Z^2)^{\nu} \sin bZ\, P_{2n+1}^{\nu,\nu}(Z)\,\mathrm{d}Z = \frac{(-1)^n \sqrt{\pi}\,\Gamma(2n + \gamma + 2) J_{2n+\nu+3/2}(b)}{Z^{\frac{1}{2}-\nu}(2n + l)!\, b^{\nu+\frac{1}{2}}} \tag{20}$$

$$\int_0^1 (l - Z^2)^{\nu} \cos bZ\, P_{2n}^{\nu,\nu}(Z)\,\mathrm{d}Z = \frac{(-1)^n 2^{\nu-\frac{1}{2}} \sqrt{\pi}\,\Gamma(2n + \nu + 1) J_{2n+\nu+\frac{1}{2}}(b)}{(2n)!\, b^{\nu+\frac{1}{2}}} \tag{21}$$

with $b > 0$, Re $\nu > -1$. Using the symmetry property of Jacobi polynomials

$$P_n^{\alpha,\beta}(-Z) = (-1)^n P_n^{\alpha,\beta}(Z). \tag{22}$$

We see that the integrands on left sides of (20) and (21) are symmetric functions of Z and

$$\int_{-1}^{+1} (l - Z^2)^{\nu} \sin bZ\, P_{2n}^{\nu,\nu}(Z)\,\mathrm{d}Z = 0 \tag{23}$$

$$\int_{-1}^{+1} (l - Z^2)^{\nu} \cos bZ\, P_{2n+1}^{\nu,\nu}(Z)\,\mathrm{d}Z = 0. \tag{24}$$

since the integrands in both these integrals are odd functions of Z. Adding $i(=\sqrt{-1})$ times (23) to twice of (21) and putting $b = ia$ and finally using the definition of modified Bessel function (ibid), one gets

$$\mathscr{I}_{2n} = \int_{-1}^{+1} (1-Z^2)^{\nu} e^{-aZ} P_{2n}^{\nu,\nu}(Z)\,dZ = \frac{2^{\nu+\frac{1}{2}}\sqrt{\pi}\,\Gamma(2n+\nu+1) I_{2n+\nu+\frac{1}{2}}(a)}{(2n)!\,a^{\nu+\frac{1}{2}}}. \tag{25}$$

In a similar manner, using (20) and (24) one gets

$$\mathscr{I}_{2n+1} = \frac{-2^{\nu+\frac{1}{2}}\sqrt{\pi}\,\Gamma(2n+\nu+2) I_{2n+\nu+3/2}(a)}{(2n+1)!\,a^{\nu+\frac{1}{2}}} \tag{26}$$

where $I_{\nu}(a)$ is the modified Bessel function. Combining (25) and (26), we have for any integral n,

$$\mathscr{I}_n = (-1)^n \frac{2^{\nu+\frac{1}{2}}\sqrt{\pi}\,\Gamma(n+\nu+1) I_{n+\nu+\frac{1}{2}}(a)}{n!\,a^{\nu+\frac{1}{2}}} \tag{27}$$

Substituting (27) in (18) with $\alpha = \beta = \frac{1}{2}$ (for the S state of triton), we get

$$a_K(r) = (-1)^K 2\sqrt{\pi}\,\Gamma\left(K+\frac{3}{2}\right)(h_K^{\frac{1}{2},\frac{1}{2}} \cdot K!)^{-1} \times \sum_{n=1}^{N} V_{on} I_{K+1}(d_n(r)) \exp(-d_n(r))/d_n(r). \tag{28}$$

Thus a closed analytic expression for the coefficients $a_K(r)$ is obtained.

Calculation of the coupling coefficients, $C(K, K'', K')$

Since $P_n^{\alpha,\beta}(Z)$ is a polynomial in Z of degree n, one can see from (16) that $C(K, K'', K')$ vanishes unless (K, K', K'') satisfy the triangle relation

$$|K - K'| \leqslant K'' \leqslant (K + K'). \tag{29}$$

To calculate the coupling coefficients we follow the method used in reference (De and Das 1987) for the calculation of geometrical structure coefficients of the hyperspherical harmonics method.

We multiply both sides of eq. (16) by $P_K^{\alpha,\beta}(Z')/h_K^{\alpha,\beta}$ and sum over K'' from 0 to α. Then using the completeness relation for Jacobi polynomials (Abramowitz and Stegun 1972).

$$\sum_{K''=0}^{\infty} P_K^{\alpha,\beta}(Z) P_K^{\alpha,\beta}(Z')/h_K^{\alpha,\beta} = \frac{\delta(Z-Z')}{w_l(Z)} \tag{30}$$

and noting that $C(K, K'', K')$ vanishes unless condition (29) is satisfied, we have

$$\sum_{K''=|K-K'|}^{(K+K')} C(K, K'', K') P_K^{\alpha,\beta}(Z')/h_K^{\alpha,\beta} = P_K^{\alpha,\beta}(Z') P_K^{\alpha,\beta}(Z'). \tag{31}$$

Choosing an appropriate number (= number of allowed K'' values) of Z' values in the

interval $[-1, 1]$, eq. (31) becomes a set of linear inhomogeneous equations (LIE) for the unknown coefficients $C(K, K'', K')$, for fixed values of K, K'. Thus all the non-vanishing coupling coefficients for fixed values of K and K' are calculated by solving LIE once only. The coefficients need be calculated once only and stored for all values of r and for various interactions. Obtaining the coefficients by this method is both fast and very accurate (De and Das 1987).

3. Results and comparison with other method

To test this method, we have solved the triton ($A = 3$) ground state for several commonly used test potentials.

All the chosen potentials have the general form of eq. (17), whose parameters are given in table 1. Note that for potentials having separate triplet even and singlet even forms appropriate average value (which is the correct expression for the S state of triton) has been taken. The potentials are arranged in table 1, in decreasing order of "softness" near origin.

Calculations have been performed on a HP 1000 computer, by truncating (7) and (10) to a maximum K value (K_{max}) and choosing uniform r mesh from 0·1 fm to 15·1 fm with a step size of 0·25 fm. Equation (10) has been solved using adiabatic approximation (Das *et al* 1982; Ballot *et al* 1982). Calculated binding energies (BE), both for extreme adiabatic approximation (EAA) and uncoupled adiabatic approximation (UAA), for various illustrative K_{max} values have been presented in table 2, showing the convergence trend. It is seen from table 2, that softer the potential, quicker is the convergence in BE. The trend agrees with calculations by hyperspherical harmonics expansion (HHE) method (Das *et al* 1982a; Ballot *et al* 1972). Comparison of our results with calculations by other methods has been made in table 3. The results agree closely with those calculated by other methods. It is seen in general that our EAA and UAA results are respectively less than and greater than those of reference (Fabre *et al* 1988). Thus the difference between EAA and UAA results is smaller in our calculation than that in reference (Fabre *et al* 1988). However our UAA result is slightly higher than the interpolated value quoted in reference (Fabre *et al* 1988). This appears to be the general trend for all the potentials chosen, when compared with results of other methods.

Table 1. Parameters of chosen test potentials (refer to eq. (17) (from Ballot *et al* 1982).

			V_{on}(MeV)			b_n(fm)		
Potential	Type	N	V_{01}	V_{02}	V_{03}	b_1	b_2	b_3
Baker[13]		1	−51·5	—	—	1·6	—	—
Volkov[14]		2	144·86	−83·34	—	0·82	1·60	—
S4[15]	Singlet	3	880·0	−70·0	−21·0	0·4303	1·25	1·4434
	Triplet	3	600·0	−70·0	−27·6	0·4264	1·4142	1·6222
S3[16]	Singlet	3	1000·0	−166·0	−23·0	0·5774	1·1180	1·5811
	Triplet	3	1000·0	−326·7	−43·0	0·5774	0·9759	1·2910
G2[17]	Singlet	2	2750·0	−261·0	—	0·50	1·10	—
	Triplet	2	2750·0	−355·0	—	0·50	1·10	—

Table 2. Calculated binding energy (in MeV).

	Baker*		Volkov*		S_3		S_4		G_2	
max	EAA	UAA	EAA	UAA	EAA	UAA	EAA	UAA	EAA	UAA
4	9·827	9·796	8·474	8·430	5·183	5·083	6·242	6·184	3·736	3·568
6	9·838	9·812	8·548	8·501	6·331	6·201	6·826	6·763	6·587	6·329
8	9·840	9·813	8·564	8·517	6·641	6·500	7·007	6·938	7·268	6·987
12	9·840	9·814	8·589	8·542	6·885	6·736	7·144	7·071	7·695	7·388

*Baker *et al* 1962; Volkov 1965.

Table 3. Comparison of calculated BE (in MeV).

		IDE		Present Work	
Potential	HHE	EAA	UAA	EAA	UAA
Baker	9·7812			9·840	9·814
Volkov	8·4648	8·67	8·42	8·589	8·542
S4	7·0182	7·372	7·013	7·144	7·071
S3	6·6403	7·235	6·557	6·885	6·736
S2[a]	8·370			7·695	7·388

[a] Note that BE quoted from reference (Ballot *et al* 1972) for G2 potential was obtained by including one single partial wave belonging to $K = 1$ for the mixed symmetry S' state and explains a substantially higher value than the present work.

4. Conclusion

We have presented a method for solving the IDE by expansion and projection on a complete set of Jacobi polynomials. This is equivalent to the HHE method for the three-body system, although much simpler than the latter. Calculated BE agrees closely with previous results. We have demonstrated this method for the triton, but it can easily be generalized to larger values of A, by the use of appropriate recurrence relation of Jacobi polynomials. The numerical difficulties encountered in a direct numerical solution of the IDE are not present in our method, leading to a relatively easy numerical solution. Moreover closed analytical expressions are obtained for integrals needed for the calculation of potential matrix. This together with the semi analytic LIE method for calculating the coupling coefficients make this method fast accurate and elegant. The fact that Rayleigh-Ritz principle, with respect to K_{max} value, applies to our method, is an added advantage.

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