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PERTURBATIVE SOLUTION OF INTEGRO–DIFFERENTIAL EQUATION FOR A SYSTEM OF IDENTICAL BOSONS

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We have solved the integro-differential equation for a system of A identical bosons interacting via two body potentials by applying a perturbative method up to the second order. Calculated binding energy has been compared with a solution by projection method. The perturbative solution is found to be fairly reliable for a soft potential and it improves with increasing particle number (A), whereas other numerical methods become very difficult with increasing particle number. Thus perturbation method becomes a useful alternative for large particle number and soft potentials.

1. *Introduction*

Hyperspherical Harmonic Expansion Method (HHEM) is one of the techniques for solving the few body Schrödinger equation in an essentially exact manner. But the complexity of the formalism increases rapidly and the calculation becomes prohibitively extensive (both in memory and computer time requirements) as the number of particle increases. Thus for more than four particles the equations cannot be solved easily without introducing approximations. Moreover the expansion basis of the hyperspherical harmonics is truncated to a finite set for practical purposes and the truncation is determined by convergence of binding energy. For potentials which have a strong short range repulsion, the convergence is very slow and a large number of partial waves are to be included, making the calculation of the matrix elements and in general the numerical solution very difficult.

The difficulty arising out of the convergence requirement has been avoided by an alternative formulation [1-2] resulting in an integro-differential equation (IDE) in two variables for a system of many bosons interacting via two body interactions in which all correlations higher than two body correlations are disregarded. The IDE has since been extended to few nucleon system with realistic potentials. It can be shown [2] that the IDE for three particles is equivalent to the Faddeev equation. The IDE has the same structure for all particle numbers (A) and its explicit complexity does not increase with A. However the kernel function involves a sum over the partial waves and numerical difficulties in calculating this function arise for large A. This makes the numerical solution of the IDE a difficult task. The IDE has been solved [2] by direct integration using the adiabatic approximation (AA), for the three and four nucleon ground state, with several test potentials. A variational solution of the IDE, decoupled by AA, has been solved [3] for $A = 3, 4$.

Both these methods involve very complex computer codes requiring large memory and CPU time. For $A > 4$, the variational method becomes less reliable due to numerical instabilities. An alternative approach, referred to as the projection method, has been applied to expand the unknown solution of IDE, $P_l(z, r)$, for a fixed value of r, in a suitable complete basis of Jacobi polynomials ($P_K^{\alpha,\beta}(z)$), leading to a system of coupled differential equations [4]. However, this approach has the disadvantage that the convergence with respect to the order of the Jacobi polynomial is slow and in a sense the advantage gained by reducing the Schrödinger equation into an IDE is lost. However, one has to remember that although there is no explicit convergence requirement in the IDE, the kernel function involves the sum over K [see Eq. (4) below], whose convergence is again rather slow.

In the present work, we investigate a simple minded perturbation solution of the IDE. In sharp contrast to the other approaches for the solution of the IDE, the perturbation approach is both simple and easy to compute, so that one can solve the IDE for a fairly large number of particles on a small personal computer. We have solved the IDE by this method for $A \leq 14$ with three standard S-projected nucleon-nucleon potentials having varying softness and compared the results with those obtained by the projection method.

In Section 2, we describe the method employed. Calculated ground state binding energy (BE) and comparison with results by EAA (Extreme Adiabatic Approximation) have been presented in Section 3. Finally we draw our conclusion in Section 4.

2. Method

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

$$\left[\frac{\hbar^2}{m}\left\{\frac{\partial^2}{\partial r^2}-\frac{\mathcal{L}(\mathcal{L}+1)}{r^2}+\frac{4}{r^2}\frac{1}{w_l(z)}\frac{\partial}{\partial z}(1-z^2)w_l(z)\frac{\partial}{\partial z}\right\}+E\right]\ P_l(z,r)=$$
$$=V(r_{ij})\pi_l(z,r) \tag{1}$$

where

$$\mathcal{L}=l+(3A-6)/2 \tag{2}$$
$$w_l(z)=(1-z)^{\alpha}(1+z)^{\beta},\quad \alpha=(3A-8)/2,\quad \beta=l+1/2 \tag{3}$$
$$\pi_l(z,r)=P_l(z,r)+\int\limits_{-1}^{+1}f_l(z,z')P_l(z',r)\,\mathrm{d}z'; \tag{4}$$
$$f_l(z,z')=w_l(z')\sum_K(f^2_{Kl}-1)\frac{P_K^{\alpha\beta}(z)P_K^{\alpha\beta}(z')}{h_K^{\alpha\beta}}\ ,$$

l is 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^2_{Kl} is given by

$$f^2_{Kl}=1+\left[2(A-2)\left(-\frac{1}{2}\right)^l P_K^{\alpha\beta}\left(-\frac{1}{2}\right)+\right.$$
$$\left.+\ \frac{1}{2}(A-2)(A-3)\,P_K^{\alpha\beta}(-1)\,\delta_{l,0}\right]\ \frac{1}{P_K^{\alpha\beta}(1)}\ . \tag{5}$$

The variable r is the hyper-radius and z is defined through $r_{ij}=r\sqrt{(1+z)/2}$, r_{ij} being the (ij) pair separation. Subtraction of the hypercentral potential $V_0(r)$ defined by

$$V_0(r)=\frac{1}{h_0^{\alpha\beta}}\int\limits_{-1}^{+1}V(r\sqrt{(1+z)/2})\,w_l(z)\,\mathrm{d}z \tag{6}$$

from both sides of Eq. (1) makes the right side small and is taken as a perturbation term:

$$\left[\frac{\hbar^2}{m}\left\{\frac{\partial^2}{\partial r^2}-\frac{\mathcal{L}(\mathcal{L}+1)}{r^2}+\frac{4}{r^2}\frac{1}{w_l(z)}\frac{\partial}{\partial z}(1-z^2)\,w_l(z)\frac{\partial}{\partial z}\right\}+\right.$$
$$\left.+E-\frac{A(A-1)}{2}V_0(r)\right]P_l(z,r)=\lambda\left[V\left(r\sqrt{(1+z)/2}\right)-V_0(r)\right]\pi_l(z,r)\,. \tag{7}$$

We have introduced a perturbation parameter λ (constant) on the right side to take into account various orders of perturbation. This parameter will be set equal to 1 at the end. We express E and $P_l(z,r)$ in perturbation series as,

$$E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \dots \tag{8}$$

$$P_l(z,r) = P_l^{(0)}(z,r) + \lambda P_l^{(1)}(z,r) + \lambda^2 P_l^{(2)}(z,r) + \dots \tag{9}$$

Substituting Eq. (8) and (9) in Eq. (7) and separating various orders (by equating coefficients of equal power of λ on both sides) we get the zeroth order equation as,

$$\left[\frac{\hbar^2}{m}\left\{\frac{\partial^2}{\partial r^2} - \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + \frac{4}{r^2}\frac{1}{w_l(z)}\frac{\partial}{\partial z}(1-z^2)\,w_l(z)\frac{\partial}{\partial z}\right\} + \right.$$
$$\left. + E^{(0)} - \frac{A(A-1)}{2}V_0(r)\right] P_l^{(0)}(z,r) = 0\,. \tag{10}$$

The first order equation is,

$$\left[\frac{\hbar^2}{m}\left\{\frac{\partial^2}{\partial r^2} - \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + \frac{4}{r^2}\frac{1}{w_l(z)}\frac{\partial}{\partial z}(1-z^2)\,w_l(z)\frac{\partial}{\partial z}\right\} + \right.$$
$$\left. + E^{(0)} - \frac{A(A-1)}{2}V_0(r)\right] P_l^{(1)}(z,r) + E^{(1)}P_l^{(0)}(z,r) =$$
$$= V'(r,z)\sum_{K'} f_{K'l}^2 \frac{P_K^{\alpha\beta}}{h_{K'}^{\alpha\beta}} \int_{-1}^{+1} w_l(z')P_{K'}^{\alpha\beta}(z')P_l^{(0)}(z',r)\,\mathrm{d}z' \tag{11}$$

where, $V'(r,z) = V(r\sqrt{(1+z)/2}) - V_0(r)$.

The second order equation is,

$$\left[\frac{\hbar^2}{m}\left\{\frac{\partial^2}{\partial r^2} - \frac{\mathcal{L}(\mathcal{L}+1)}{r^2} + \frac{4}{r^2}\frac{1}{w_l(z)}\frac{\partial}{\partial z}(1-z^2)w_l(z)\frac{\partial}{\partial z}\right\} + \right.$$
$$\left. + E^{(0)} - \frac{A(A-1)}{2}V_0(r)\right] P_l^{(2)}(z,r) + E^{(1)}P_l^{(1)}(z,r) + E^{(2)}P_l^{(0)}(z,r) =$$
$$= V'(r,z)\sum_{K'} f_{K'l}^2 \frac{P_{K'}^{\alpha\beta}}{h_{K'}^{\alpha\beta}} \int_{-1}^{+1} w_l(z')P_{K'}^{\alpha\beta}(z')P_l^{(1)}(z',r)\,\mathrm{d}z'. \tag{12}$$

The zeroth order equation is separable in r and z:

$$P_l^{(0)} = \Phi_{K\mu}^{(0)}(r)\;\mathcal{Z}(z)$$

where Φ satisfies

$$\left[\frac{\hbar^2}{m}\left\{\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\mathcal{L}(\mathcal{L}+1)}{r^2}\right\} - \frac{4\hbar^2}{m}\frac{K(K+\alpha+\beta+1)}{r^2} - \right.$$
$$\left. - \frac{A(A-1)}{2}V_0(r) + E_{K\mu}^{(0)}\right]\Phi_{K\mu}^{(0)}(r) = 0, \tag{13}$$

The quantum number μ represents different radial excitation modes for a fixed K. The z equation, which corresponds to the hyper-angular motion, is just the Jacobi differential equation such that $\mathcal{Z}(z)$ is the Jacobi polynomial $P_K^{\alpha\beta}$. It satisfies the equation

$$(1-z^2)\frac{\mathrm{d}^2 P_K^{\alpha\beta}(z)}{\mathrm{d}z^2}+[\beta-\alpha-(\alpha+\beta+2)z]\frac{\mathrm{d}P_K^{\alpha\beta}(z)}{\mathrm{d}z}+K(K+\alpha+\beta+1)P_K^{\alpha\beta}(z)=0. \quad (14)$$

The unperturbed ground state energy is obtained by the lowest lying solution of Eq. (13) for which the quantum numbers K and μ are denoted by K_0 and μ_0. It is clear from Eq. (13) that the lowest energy is obtained for $K = K_0 = 0$ and $\mu = \mu_0 = 0$. Therefore the unperturbed ground state radial wave function $\Phi^{(0)}_{K_0\mu_0}(r)$ has no nodes. The unperturbed ground state energy is $E^{(0)} = E^{(0)}_{K_0\mu_0}$.

We expand the n^{th} order wave functions in terms of the complete set of zeroth order wave functions,

$$P_l^{(n)}(z,r)=\sum_{K'\mu'} a^{(n)}_{K'\mu'}P^{(0)}_{K'\mu'}(z,r)=\sum_{K'\mu'} a^{(n)}_{K'\mu'}\Phi^{(0)}_{K'\mu'}P^{\alpha\beta}_{K'}(z); \quad (n=1,2,\ldots) \quad (15)$$

Substituting Eq. (15) with $n = 1$ in Eq. (11), multiplying by $P_K^{\alpha\beta}(z)w_l(z)/h_K^{\alpha\beta}$ and using the orthogonality relation of Jacobi polynomials [5] we get the first order perturbation energy to be

$$E^{(1)}=\frac{f^2_{K_0 l}}{h^{\alpha\beta}_{K_0}}\,\langle\Phi^{(0)}_{K_0\mu_0}(r)|V_{K_0K_0}(r)|\Phi^{(0)}_{K_0\mu_0}(r)\rangle \quad (16)$$

where

$$V_{KK_0}(r)=\int_{-1}^{+1} P_K^{\alpha\beta}(z)\,[V(r)\sqrt{(1+z)/2}-V_0(r)]\,P_K^{\alpha\beta}(z)w_l(z)\,\mathrm{d}z\,. \quad (17)$$

For $K = K_0 = 0$, $V_{KK_0}(r) = 0$ and hence $E^{(1)} = 0$. So there is no first order energy shift for the ground state. The second order energy shift is obtained by substituting Eq. (15) with $n = 2$ in Eq. (12) and using the orthogonality of Jacobi polynomials [5], as

$$E^{(2)}=\sum_{\substack{K'\\ \mu'\\ K'\neq K_0}}\left(\frac{f^2_{K_0 l}}{h^{\alpha\beta}_{K_0}}\right)\left(\frac{f^2_{K' l}}{h^{\alpha\beta}_{K'}}\right)\frac{|\langle\Phi^{(0)}_{K_0\mu_0}(r)|V_{K_0K'}(r)|\Phi^{(0)}_{K'\mu'}(r)\rangle|^2}{(E^{(0)}_{K_0\mu_0}-E^{(0)}_{K'\mu'})}\,. \quad (18)$$

Up to second order the ground state energy is given by $E^{(0)} + E^{(2)}$.

We first solve the unperturbed radial Eq. (13) for various values of K and μ, obtaining $E^{(0)}_{K\mu}$ and $\Phi^{(0)}_{K\mu}(r)$ for each (K, μ). Using these quantities in Eq. (18), $E^{(2)}$ is calculated. The matrix elements of V are obtained by numerical integration. The expansion (15) has been restricted for convenience to the bound state solutions of Eq. (13). For large A and moderate K, the effective hyperradial well of Eq. (13) is deep enough to support a large number of radially excited bound states and so the expansion basis is reasonably complete. Hence one can expect that the perturbation calculation will be better for large A. On the other hand, as A increases, α increases rapidly (for ex. for $A = 14$, $\alpha = 17$), and the weight function $w_l(z)$ become an extremely singular function of z. This makes all the numerical methods very difficult for larger values of A. Since $w_l(z)$ is required only for the calculation of the second-order matrix elements, the problem is less serious for perturbation method. Such integrals can be evaluated with careful numerical techniques without an enormous increase of the computation time.

We have calculated the ground state binding energy of identical boson system containing several particles and interacting via the standard S-projected two body potentials. The perturbation result is compared to a solution of Eq. (1) by a projection method [4], which can be considered as an essentially exact method, provided convergence is achieved with respect to addition of partial waves.

For our calculation, we have chosen three simple test potentials, namely, Baker [6], Volkov [7] and Malfleit-Tjon MT-V [8] potentials. The Baker potential is the softest of the three, there being no repulsive core. The Volkov potential has a mildly repulsive core, whereas the MT-V potential has a very strong repulsion at short interparticle separation. These potentials have been chosen in order that a study of the reliability of the perturbation treatment for various core repulsion can be made.

The chosen potentials are commonly used semi-realistic nuclear potentials. We have taken the mass of the particle to be the nucleon mass. Thus our model becomes a travesty of the several nucleon system. However there are two important differences: the Coulomb interaction active between pairs of protons in a real nucleus has been disregarded. Secondly the components of the space wave function other than the totally symmetric one (which in general, has the largest contribution in the ground state) have also been neglected, that is the spin and isospin of the particles have been disregarded. Hence we get binding energy (BE) much higher than what would be expected for real nuclei. The motivation for the present calculation is to see under what condition the perturbation result is expected to be reliable.

The calculations have been performed on the Hallmark II (based on 80486 processor with an EISA bus) computer. Integration of Eq. (17) was done by Gauss quadrature and that of Eq. (18) by Simpson method, with mesh size 0.05 fm.

3. *Results and comparison to the projection method*

In Table 1 we present the ground state BE up to second order perturbation for various particle numbers and the chosen potentials. The last column contains the BE calculated by the projection method. It can be seen that the perturbation result is close to the projection result for soft potentials, while the difference is appreciable for the harder potentials. This can be understood from the fact that higher partial waves play increasingly more important role as the potential becomes harder. As the two body potential becomes more strongly repulsive at short separation, it prevents the interacting particles to come too close together, thereby invoking higher hyper-angular momentum of the system. On the other hand the zeroth-order perturbation corresponds to the hypercentral approximation which is the same as the first ($K = 0$) partial wave. Thus in the perturbation approach higher partial waves are not adequately represented, thereby making the approximation worse for harder potentials. Moreover the residual part obtained by subtracting the hypercentral part from the full potential can no longer be treated as a small perturbation for potentials with a strong short range repulsion.

In the absence of more accurate results, we are comparing the perturbation results with those by the projection method, although the latter did not fully converge for harder potentials, which require large number of partial waves. Furthermore the calculation of the potential multipole

$$\int_{-1}^{+1} V\left(r\sqrt{\frac{1+z}{2}}\right) P_n^{\alpha\beta}(z) w_l(z) \mathrm{d}z$$

needed in the projection method, is very tricky and involves relatively large errors for large particle number (A) and higher partial waves. This is so because the weight function gradually resembles a δ-function centred at $z = -1$ as A increases (see Eq. (3)).

What is more interesting is the observation from Table 1 that the perturbative approximation becomes progressively better as the particle number (A) increases for both soft and hard potentials, the percentage difference gradually decreasing as A increases. However for the Volkov potential, the relative error apparently decreases, then again increases. This is probably due to the fact that the projection results for large A did not fully converge for relatively harder Volkov potential, as explained earlier. In view of this, the apparent rapid improvement of perturbative result for the hardest potential chosen (MT-V) as A increases is illusive and the actual error is larger.

One can observe from Table 1 that for the MT-V potential, the perturbation result for smaller number of particles differs by a very large amount from the projection value. This is due to the fact that the hypercentral part, $V_0(r)$, is quite small for such potentials and the zeroth order Eq. (13) has only a small number of bound states. Since in our perturbation expansion we have included only the bound states of the unperturbed Hamiltonian for feasibillity of numerical calculation, a

TABLE 1.

Potential	Particle number	Calculated ground state binding energy	
		Perturbation method	Projection method
Baker	7	300.1976	299.3907
	8	451.5261	450.129
	9	636.635	635.444
	10	857.745	856.380
	12	1410.182	1408.525
	14	2114.145	2112.222
Volkov	7	200.1364	190.5221
	8	285.808	276.7622
	9	386.640	379.6151
	10	512.193	499.149
	12	822.088	788.4306
	14	1200.589	1144.8553
MT-V	8	123.7994	249.728
	10	281.0164	405.667
	12	576.432	604.552

Comparsion of calculated ground state energy by perturbation and projection methods.

substantial contribution coming from the continuum states is disregarded whenever the hypercentral potential supports only a few bound states. On the other hand, for large A, the zeroth-order equation has a large number of bound states and the perturbative expansion is more complete. Thus for large particle numbers the perturbative technique becomes a viable alternative.

4. *Conclusion*

We conclude by noting that the perturbation result is fairly reliable for soft potentials, but not so when the two body interaction has a strong short range repulsion. However, the perturbation result gradually improves as the particle number increases. This is of a practical importance because serious numerical difficulties arise with other methods for large A.

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PERTURBATIVNO RJEŠENJE INTEGRO – DIFERENCIJALNE JEDNADŽBE ZA SISTEM IDENTIČNIH BOZONA

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Koristeći perturbativni razvoj do drugog reda riješili smo integro-diferencijalnu jednadžbu za sistem od A identičnih bozona interagirajući ih preko dvočestičnog potencijala. Izračunate energije vezanja uspoređene su s rješenjem dobivenim projektivnom metodom. Nađeno je da je perturbativno rješenje pouzdano za slabe potencijale a poboljšava se povećanjem broja čestica. S druge strane numeričko rješavanje drugim metodama postaje vrlo otežano s porastom broja čestica. Dakle, perturbativna metoda postaje korisna alternativa kod velikog broja čestica i slabih potencijala.