

Ground state properties of doubly closed-shell nuclei with the Potential Harmonic Expansion Method

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Abstract. Ground state properties of doubly closed-shell nuclei are studied using the Potential Harmonic Expansion Method. The method transforms the many-body Schrödinger equation into an infinite set of coupled differential equations. The coupled differential equations are solved using an orthogonal collocation procedure. The resulting eigenvalue equation is solved via the Renormalized Numerov method.

1. Introduction

A considerable number of methods have been employed to study few- and many-body systems. Amongst them are the Faddeev approach for three-body systems [1], Variational Monte-Carlo Methods [2], Integrodifferential Equation Approach (IDEA) [3, 4], Potential Harmonic Expansion Method (PHEM) [5, 6]. The Potential Harmonic Expansion Method, which is used in this work, is based on the expansion of the Faddeev-like amplitude on the potential harmonic basis and takes into account two-body correlations. The substitution of the expansion into the many-body Schrödinger equation, results in an infinite set of one-dimensional Coupled Differential Equations (CDE), which become cumbersome to solve numerically, especially when the number of particles A becomes large, the Jacobi polynomials involved in the construction of the potential harmonic basis, become highly oscillatory. Moreover, the size of the basis set is proportional to the number of particles, and naturally leads to more numerical difficulties in the evaluation of the resulting potential matrix. To address some of these difficulties, Das et al [7] optimized the narrow subinterval in $[-1 : 1]$ which contributes appreciably on the potential matrix as A becomes large. With such an optimization, they investigated a Bose-Einstein Condensate (BEC) containing up to 14000 atoms of ^{87}Rb . This method has been also widely used as well in nuclear physics [8]. The popularity of this method is due to its advantages among which, one mentions: (i) it includes two-body correlations, (ii) is quite simple and fast in contrast to the Diffusion Monte Carlo (DMC) Method which, although it is an exact many-body method, it requires huge computational efforts [9]. The CDE are truncated for numerical purpose without significant loss in the efficiency. Our main concern in this paper, is to calculate ground state energies and root-mean-square radii of doubly closed-shell nuclei. To this end, the CDE are solved subject to appropriate boundary conditions. To check the stability and accuracy of the method employed, for comparison purposes, we first calculate the binding energies of ^3H by solving Differential Faddeev Equations (DFE) and using semi-realistic potentials. Second, we solve the CDE for $A = 3$ and obtain again binding energies of ^3H , using the same potentials.

After the convergence criteria have been established, we employ the method to study ground state properties of considered nuclei where $A > 3$, using the Volkov potential, again for simplicity and for comparison purposes. It is well known that the first term in the potential harmonics is the most dominate and accounts for more than 80% on the total binding energy for ${}^4\text{He}$ [6]. Therefore, in this work, we want to check whether this contribution is proportional to the number of particles A . The convergence of the binding energies in terms of the number of the coupled differential equations is also investigated. This paper is organized as follows: in section 2, we briefly summarize the differential Faddeev equations and the coupled differential equations for the case where the particles are identical, starting from the decomposition of the wave function in terms of Faddeev-like amplitudes. In section 3, we present the results, whereas our conclusions are reported in section 3.

2. Formalism

Consider a system of A particles, each of mass m_i , position vector \mathbf{r}_i interacting via two-body potentials $V(\mathbf{r}_i - \mathbf{r}_j)$. The Schrödinger equation has the form

$$\left[\sum_{i=1}^A \frac{\hbar^2}{m_i} \nabla_i^2 + \sum_{i,j>i}^A V(\mathbf{r}_{ij}) - E \right] \Psi(\mathbf{r}) = 0, \quad (1)$$

where the first term represents the kinetic energy, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, E the energy of the system and $\Psi(\mathbf{r})$ the wave function of the system with $\mathbf{r} \equiv (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$.

2.1. Differential Faddeev Equations

For three-body systems, the wave function $\Psi(\mathbf{r})$ in Eq.(1) can be decomposed in the form

$$\Psi(\mathbf{r}) = \sum_{i=1}^3 \phi_i(x_i, y_i, z_i), \quad (2)$$

where $\phi_i(x_i, y_i)$ are Faddeev amplitudes, with x_i, y_i being Jacobi coordinates and $z_i = \cos(\mathbf{x}_i \cdot \mathbf{y}_i)$. The Hamiltonian of the system reduces to

$$H = H_0 + \sum_{i=1}^3 V_i(x_i), \quad (3)$$

where H_0 is the free Hamiltonian of the three particles, given by [10]

$$H_0 = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \left(\frac{1}{x^2} + \frac{1}{y^2} \right) \frac{\partial}{\partial z} (1 - z^2)^{1/2} \frac{\partial}{\partial z}. \quad (4)$$

Substituting Eqs.(3), (2) into Eq.(1), one obtains a single differential equation for identical particles

$$(H_0 + V - E_{3B})\phi(x, y, z) = -V(I + P^+ + P^-)\phi(x, y, z), \quad (5)$$

where E_{3B} is binding energy and P^\pm are permutation operators. We solve equation (5) to obtain ground state binding energies of ${}^3\text{H}$.

2.2. Coupled Differential Equations

To obtain a infinite set of CDE, we first rewrite Eq.(2) as

$$\Psi(\mathbf{r}) = \sum_{i,j>i}^A \Phi(\mathbf{r}_{ij}, r), \quad (6)$$

where $\Phi(\mathbf{r}_{ij}, r)$ are Faddeev-like amplitudes, with r being the hyperradius. Substituting Eq.(6) into Eq.(1), we obtain the Faddeev-like equations

$$\left[\sum_{i=1}^A \frac{\hbar^2}{m_i} \nabla_i^2 + \sum_{i,j>i}^A V(\mathbf{r}_{ij}) - E \right] \Phi(\mathbf{r}_{ij}, r) = -V(\mathbf{r}_{ij}) \sum_{k,l>k}^{A-1} \Phi(\mathbf{r}_{kl}, r), \quad (7)$$

for the amplitudes. Expanding the Faddeev amplitude in potential harmonic basis, we obtain

$$\Phi(\mathbf{r}_{ij}, r) = r^{(3A-4)/2} \sum_{K=0}^{\infty} \mathcal{P}_{2K}^{0,0}(\Omega_{ij}) u_K(r), \quad (8)$$

where $\mathcal{P}_{2K}^{0,0}(\Omega_{ij})$ are S-state potential harmonics [$\Omega_{ij} \equiv (\omega_{ij}, \theta)$ the set of angular coordinates of \mathbf{r}_{ij}] and $u_K(r)$ the radial part of the wave function. Inserting Eq.(8) into Eq.(7), we obtain an infinite set of CDE [9]

$$\left[-\frac{\hbar^2}{m} \frac{d^2}{dr^2} + \frac{\hbar^2}{m} \frac{\mathcal{L}_{\mathcal{K}}(\mathcal{L}_{\mathcal{K}} + 1)}{r^2} - E \right] u_K(r) + \sum_{K'=0}^{\infty} f_{K'}^2 V_{KK'}(r) u_{K'}(r) = 0, \quad (9)$$

where $\mathcal{L}_{\mathcal{K}} = 2K + \frac{(3A-6)}{2}$, $m = \frac{M}{A}$,

$$f_K^2 = 1 + \frac{2(A-2)P_K^{\alpha,\beta}(-1/2) + [(A-2)(A-3)/2] P_K^{\alpha,\beta}(-1)}{P_K^{\alpha,\beta}(1)}, \quad (10)$$

with α and β being constants, and the potential matrix $V_{KK'}(r)$ is given by

$$V_{KK'}(r) = (N_K^{\alpha,\beta} N_{K'}^{\alpha,\beta})^{-1} \int_{-1}^{+1} P_K^{\alpha,\beta}(z) P_{K'}^{\alpha,\beta}(z) V\left(r\sqrt{(1+z)/2}\right) W(z) dz, \quad (11)$$

with $N_K^{\alpha,\beta}$ as the normalization coefficient of Jacobi polynomials $P_K^{\alpha,\beta}(z)$ and $W(z) = (1-z)^\alpha(1+z)^\beta$. The root-mean-square radii \mathbf{R} are calculated via the following relation [11]

$$\mathbf{R} = \frac{\langle r^2 \rangle^{1/2}}{\sqrt{2A}}, \quad \text{where } \langle r^2 \rangle = \frac{\int_0^\infty |u_K(r)|^2 r^2 dr}{\int_0^\infty |u_K(r)|^2 dr}. \quad (12)$$

3. Results and Discussions

We first solved Eq.(5) using as input the Malfiet-Tjon (MT), Volkov, S_3 and S_4 potentials [4, 12, 13], to obtain ground state energies of ${}^3\text{H}$. Our results, summarized in Table 1, are in good agreement with the literature.

Table 1. Ground state energies of ${}^3\text{H}$ (in MeV) obtained by solving the DFE, using the MTV[12], MTV[14], Volkov, S3 and S4 potentials.

This work				Others
MTV[12]				$E_{3\text{B}}(\text{MeV})$
N_x	N_y	N_z	$E_{3\text{B}}(\text{MeV})$	
14	14	3	-7.7724	-7.73 [15]
18	18	3	-7.7405	-7.68 [17]
20	20	3	-7.7366	-7.7366192[16]
24	24	3	-7.7364	
28	28	3	-7.7364	
MTV[14]	–	–	-8.2578	-8.25 [17]
				-8.34 [15]
Volkov[3]	–	–	-8.4605	-8.47 [17]
S_3 [13]	–	–	-6.6902	-6.695[4]
S_4 [13]	–	–	-7.0598	-7.08[4]

Next we present the results obtained by solving the CDE, Eq.(9) (which are truncated up to K_{max}), using the same inputs. We first calculate the ground state binding energy of ${}^3\text{H}$ as a function of K_{max} using Volkov potential. The results are presented in Table 2, where we see that converged binding energy is -8.4328 MeV for $K_{\text{max}} = 18$, which is comparable with the experimental value -8.45 MeV [18].

Table 2. Convergence of the binding energy of ${}^3\text{H}$ in (MeV) as a function of K_{max} using the Volkov potential.

K_{max}	0	4	6	8	10	14	16	18
$E[\text{MeV}]$	-7.7096	-8.3427	-8.4102	-8.4247	-8.4303	-8.4326	-8.4328	-8.4328

The results obtained using other potentials (i.e the MTV[12], MTV[14], S3 and S4 potentials) are given in Table 3.

In Table 4, we compare the results obtained by the two methods (i.e the Faddeev formalism

Table 3. Ground state binding energies of ${}^3\text{H}$ (in MeV) obtained by solving the CDE, using MTV[12], MTV[14], S3 and S4 potentials.

This work		Others
Potentials	$E(\text{MeV})$	$E(\text{MeV})$
MTV[12]	-7.7325	-7.65 [4]
MTV[14]	-8.2500	-8.25 [15]
S_3	-6.5486	-6.64032[13]
S_4	-7.1526	-7.144[13]

and the PHEM). A good agreement of the two methods is evident. The small differences can be attributed to overall numerical instabilities. It results that for S-projected potentials, the PHEM is in good agreement with the Faddeev formalism, as expected.

Table 4. Comparison between the ${}^3\text{H}$ binding energies obtained by solving FDE and the CDE using, as input the MTV[12], MTV[14], Volkov, S3 and S4 potentials.

Potentials	Faddeev	PHEM	$\Delta E(\text{MeV})$
MTV[14]	-8.2578	-8.2500	0.0078
MTV[12]	-7.7364	-7.7354	0.001
Volkov	-8.4605	-8.4328	0.0277
S3	-6.6902	-6.5486	0.1416
S4	-7.0598	-7.1526	-0.0928

Having established the convergence criteria, we investigated the convergence of the binding energies of the nuclei considered as functions of K_{max} . In Table 5, we present the binding energies of the ${}^4\text{He}$, ${}^8\text{Be}$, ${}^{12}\text{C}$ and ${}^{16}\text{O}$ as functions of K_{max} , using the Volkov potential. From the same table, converged binding energies are obtained up to $K_{\text{max}} = 18$. Our results again are in good agreement with the literature. Evaluating the contribution of the first term ($K_{\text{max}} = 0$) on the total binding energy, from Tables 2 and 5, one obtains that the first term accounts for 91.42% for ${}^3\text{H}$, 94.97% for ${}^4\text{He}$, 97.98% for ${}^8\text{Be}$, 98.84% for ${}^{12}\text{C}$ and 99.24% for ${}^{16}\text{O}$ on the total binding energies. With the Volkov potential, we calculated the root-mean-square radii of

Table 5. Convergence of the binding energies (in MeV) of the doubly closed-shell nuclei ${}^4\text{He}$, ${}^8\text{Be}$, ${}^{12}\text{C}$ and ${}^{16}\text{O}$ in terms of K_{max} obtained with the Volkov potential.

K_{max}	Binding energies in MeV (this work)				Others
	${}^4\text{He}$	${}^8\text{Be}$	${}^{12}\text{C}$	${}^{16}\text{O}$	Binding energies (in MeV)
0	-28.5862	-271.2943	-780.3012	-1559.5220	SIDE[11](-1571) ${}^{16}\text{O}$
2	-29.1157	-272.6871	-782.8049	-1563.2262	HCA[11](-271.1) ${}^8\text{Be}$
4	-29.8599	-275.4594	-786.8792	-1568.2090	HCA[11](-1559) ${}^{16}\text{O}$
6	-30.0504	-276.6124	-788.8436	-1570.6676	HCA[15](-1560) ${}^{16}\text{O}$
8	-30.0895	-276.8460	-789.3045	-1571.3062	SIDE[15](-1571) ${}^{16}\text{O}$
10	-30.0987	-276.8799	-789.3837	-1571.4313	HCA[11](-780) ${}^{12}\text{C}$
12	-30.0984	-276.8832	-789.3946	-1371.4513	SIDE[11](-30.1) ${}^4\text{He}$
14	-30.0986	-276.8842	-789.3958	-1571.4540	
16	-30.0987	-276.8842	-789.3959	-1571.4543	
18	-30.0987	-276.8842	-789.3959	-1571.4543	

the nuclei under investigation. Our results which are compared with the results from [11] are reported in Table 6. For ${}^3\text{H}$, the experiment value is 1.67 fm [18].

Table 6. Root-mean-square radii in (fm) of the ${}^3\text{H}$, ${}^4\text{He}$, ${}^8\text{Be}$, ${}^{12}\text{C}$ and ${}^{16}\text{O}$ nuclei obtained using the Volkov potential.

This work					
Nuclei	${}^3\text{H}$	${}^4\text{He}$	${}^8\text{Be}$	${}^{12}\text{C}$	${}^{16}\text{O}$
$\mathbf{R}[\text{fm}]$	1.7468	1.4833	1.2909	1.2398	1.2077
Ref.[11]					
$\mathbf{R}[\text{fm}]$	-	1.49	1.30	1.25	1.20

In Fig. 1(a) and (b) we plotted the partial waves of ${}^3\text{H}$ and ${}^4\text{He}$ respectively for different terms of the potential harmonics. The figure shows that the first term represents the most important part of the wave function.

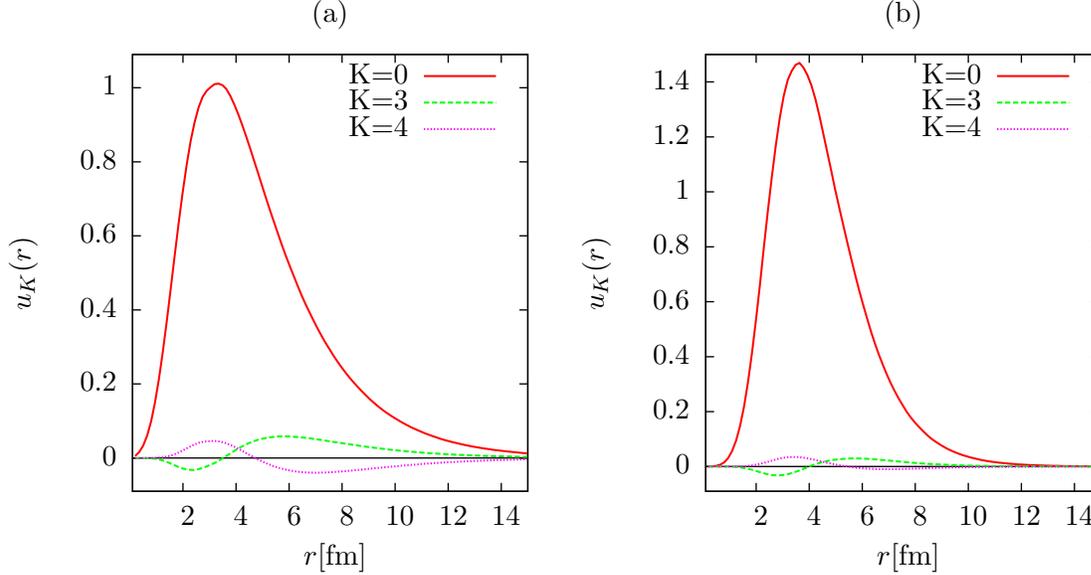


Figure 1. Partial wave functions of ${}^3\text{H}$ and ${}^4\text{He}$.

4. Conclusions

We calculated the ground state energies and root-mean-square radii of nuclear systems in the PHEM framework, and more particularly we looked at the doubly closed-shell nuclei. We focused on the convergence of the binding energies as functions of the truncation K_{max} . From the results obtained we may highlight the following conclusions: (i) the method provides good convergence in the binding energy, (ii) for $A=3$ and for S-projected potentials, the DFE and PHEM give close results as expected, the small differences being attributed to overall numerical instabilities, (iii) using Volkov potential, up to $A = 16$ we are still solve the same number of equations, (iv) as A becomes large, the first term of the potential harmonics is the most dominant and accounts for more that 90% on the total binding energy.

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