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HYPERSPHERICAL GROUND STATE WAVE FUNCTIONS FOR NUCLEI WITH $A > 4$

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The general formulation of a technically advantageous method to find the ground state solution of the Schrödinger equation in configuration space for systems with the number of particles A greater than 4 is presented. The wave function is expanded in pair-correlated hyperspherical harmonics beyond the lowest-order approximation and then calculated in the Faddeev approach. A recent efficient recursive method to construct antisymmetric A–particle hyperspherical harmonics is used. The accuracy is tested for the bound-state energies of nuclei with $A = 6$ to 12 using the effective V4 potentials. The high quality of the results thus obtained becomes evident from a comparison with other approaches.

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1. Introduction

Few-body nuclei with the number of nucleons A between 5 and 16 are a particularly interesting testground for nuclear theory. They lie in the range between the classical few–nucleon systems ($A \leq 4$) and the smallest nuclei that can be described realistically starting from a mean-field ansatz. Therefore, one hopes that these nuclei could build a link between few–body and many–body physics. At present, quite an effort is made for a better understanding of these intermediate systems. Specific interest is devoted to halo-nuclei, but also the less-exotic nuclei in this mass range are investigated thoroughly. Many theoretical techniques for the calculation of their ground states have been imported from the classical few–body field, where there has

been a considerable progress in the last years. In fact, for the classical few-body systems, several rather different approaches have been developed and proven to lead to precise results. These methods include solutions of the Faddeev–Yakubovsky equation, variational (VMC) and Green function Monte Carlo (GFMC), the hyperspherical harmonic (HH) ansatz, the stochastic variational (SVM), as well as coupled-cluster and resonating-group methods.

For nuclei with $A > 4$, a similar level of precision has not yet been achieved. Here GFMC has led to the most accurate results. Exact bound-state energies with realistic NN interactions have been calculated for $A \leq 9$ [1]. Unfortunately, the wave functions cannot be generated with this method. Recently, a very powerful tool to calculate few-body wave functions has been developed with the SVM ansatz [2,3]. However, this approach is probably most suitable for systems with $A < 8$. For nuclei with $A \geq 8$, rather good results have been obtained in the integro–differential equation approach (IDEA) [4], which uses the HH expansion, and with a variational method, the translational-invariant-configuration-interaction method (TICI) [5,6], which is inspired by the coupled-cluster method.

In this contribution, we summarize the results of a new method [7], which combines the main ideas of the HH expansion, the pair-correlation ansatz and the Faddeev approach to calculate wave functions of few-body systems. Including higher-order HH functions, we make the nontrivial step beyond the IDEA approach. The difficulty in constructing antisymmetric A–particle HH is overcome by the use of a recently developed very efficient recursive method [8], where HH basis functions are constructed, belonging to well defined irreducible representations (irreps) of the orthogonal group of kinematic rotations and the symmetric group.

2. General formulation of the method

It is well known that finding a solution of the Schrödinger equation in terms of the uncorrelated hyperspherical harmonics can be very difficult, because the number of basis functions increases very fast with K, and in order to have a real convergence, one must use a huge number of basis functions [9]. Therefore, a correlation function is advantageous to give the wave function a proper behaviour [10]. Its advantages have been extensively verified for classical few-body systems, reaching a high level of accuracy [11,12]. A general ansatz within the two-body correlation scheme is the Jastrow factor

$$\Psi = \prod_{i<j} f_{ij} \Phi \,, \tag{1}$$

where f_{ij} is a two-body correlation function. However, the use of the Jastrow ansatz leads to $3A - 3$ dimensional integrals. Therefore, it is more convenient to use the so-called pair-correlation ansatz

$$\Psi = \sum_{i<j} \chi_{ij} \Phi, \tag{2}$$

because in this case one can use the Faddeev approach which leads to at most four-body integrals. In the Faddeev approach, the Schrödinger equation is replaced by equivalent equations,

$$(T - E)\Psi_{ij} = -V_{ij}\Psi \,, \tag{3}$$

where $\Psi = \sum_{i<j} \Psi_{ij}$. In order to speed up the convergence, these equations can be further modified [4] to include the contribution of the hypercentral potential explicitly. The hypercentral potential $V_{hc}(\rho)$ is defined as the projection of the two-body interaction on the subspace of the lowest-order hyperspherical state. With the help of $V_{hc}(\rho)$, we can rewrite Eq. (3) as follows

$$\left[T + \frac{A(A-1)}{2} V_{hc}(\rho) - E\right] \Psi_{ij} = -[V_{ij} - V_{hc}(\rho)]\Psi \,. \tag{4}$$

Motivated by the pair-correlation ansatz (2), we shall expand the Faddeev amplitude Ψ_{ij} in the following way,

$$\Psi_{ij} = \sum_{K\nu p} R_{K\nu p}(\rho) H_{K\nu}(\Omega, s_1..s_A, t_1..t_A)\chi_p(z_{ij}) \,, \tag{5}$$

where $H_{K\nu}$ are the antisymmetric hyperspherical-spin-isospin functions, $R_{K\nu p}$ are the hyperradial functions, and $\chi_p(z_{ij})$ is a polynomial of order p, with z_{ij} related to the relative two-body distance through

$$z_{ij} = r_{ij}/\rho \,. \tag{6}$$

Substituting the expansion, Eq. (5), into Eq. (4), after integration over the hypersphere Ω, we get a set of coupled equations for $R_{K\nu p}$. These equations are solved numerically to yield the binding energy and ground-state wave function of the system.

3. *Discussion of the results*

The present method becomes more and more complex as the number of fermions increases. Therefore in this work, we consider only central NN potentials. We present results for 6 and 8 nucleons interacting via the Volkov [13] (VV), the Afnan–Tang [14] (S3), the modified S3 potential [15] (MS3), the Brink–Boeker [16] (B1) and the Malfliet–Tjon [17] potentials (MT–I/III and MT–V). The Coulomb potential is neglected.

Our numerical results are presented in Table 1 for the 6 nucleon system and in Table 2 for the 8 nucleon system.

For ^{6}Li, the calculations include irreps of the kinematical group $\mathcal{O}_5$ with only one line and the irreps [42] and [33] of the permutation group. We compare our values with recent accurate variational results [2] available for some of these central

potentials. One can notice that with the VV potential, one reaches convergence faster than with other potentials. The result for the binding energy starts oscillating around the asymptotic value. It also compares nicely to the variational result of Ref. 2. The other potentials show a tendency to convergence even if $K_{\max}$ is not large enough to establish it. The MT potentials seem to lead to a more rapid convergence than S3 and B1. The differences may be due both to the fact that the limiting value has not yet been reached and to the missing irreps of the permutation group. The two-line irreps of the orthogonal group are of little importance. This has been checked for the 8 particle case, where they give rather small contributions.

TABLE 1. Binding energies of the six-nucleon system ^{6}Li, $(L,S)J^\pi = (0,1)1^+$, *interacting via various* NN *potentials.* $N_{\rm HH}$ *represents the number of hyperspherical harmonic states.*

$K_{\max}$	$N_{\rm HH}$	B1	MT–I/III	MTV	S3	VV
2	1	30.99	30.15	62.45	62.76	66.10
4	4	37.82	34.67	63.27	64.45	66.53
6	12	39.11	35.43	64.10	66.49	66.63
8	31	39.61	35.91	64.55	67.18	66.57
SVM [2]		-	-	66.30	70.65	66.25

TABLE 2. Binding energies of eight–nucleon system ^{8}Be, $(L,S)J^\pi = (0,0)0^+$, *interacting via various* NN *potentials. Also given are results from Ref. 6 with state independent* $TICI_{SI}$ *and state dependent* $TICI_{SD}$ *correlations.*

$K_{\max}$	$N_{\rm HH}$	B1	MT–I/III	MTV	MS3	VV
4	1	56.71	52.82	134.29	31.19	147.42
6	4	65.39	59.31	137.72	38.08	148.70
8	15	70.03	60.64	137.80	42.11	148.49
TICI_{SI}		49.18	46.67	129.25	26.26	
TICI_{SD}		61.30	52.67	130.23	37.30	

The calculations for ^{8}Be include only the irrep (400) of the kinematical group $\mathcal{O}_7$ and irreps with at most 3 rows of the permutation group. Here the comparison is made with the TICI results [6], which, using the variational principle, leads to the highest binding energy to date. In all cases, our results for the binding energy are somewhat larger. They show characteristics similar to the six-body case. Again, one sees that the VV potential result presents small oscillations around the convergent value and that the rather hard core MT potentials seem to give values closer to convergence than B1 or MS3. From the comparison between the TICI results with and without state-dependent correlations, one can infer that for the MT potentials,

state-independent correlations already give rather satisfying results, while state-dependent correlations are more important for B1 and MS3. Since our correlations are state independent, one could expect such a different convergence behaviour as found in Table 2.

4. Conclusions

In this work, we have presented the results of a general method formulated to calculate the wave functions of light systems up to a rather large number of particles. This method combines the main ideas of the HH expansion, the pair-correlation ansatz and the Faddeev approach. The actual application of it is made possible by the use of a very efficient recursive algorithm to construct the antisymmetric A-particle state containing hyperspherical harmonics. We have applied the method to calculate the binding energies of 6- and 8-nucleon systems with central local potentials. The results we have obtained are very encouraging. For some potentials (VV, 6 particles and MTV, 8 particles), we have reached the convergence region with $K_{\max} = 8$ which is the maximum value allowed by our present computer facilities (workstations). The ^{6}Li result for the VV potential is slightly higher than the SVM result. Even if in other cases we have not yet reached the convergence in the HH expansion, our results for the binding energies are close to the TICI results. For the eight–body case, they are higher for all potentials where variational results were available for a comparison.

The method presented here for the solution of the few-body Schrödinger equation can be easily extended to solve the Schrödinger-like equation with a source, necessary for the application of the Lorentz-integral-transform method. Work in this direction is in progress.

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HIPERSFERIČNE VALNE FUNKCIJE OSNOVNOG STANJA JEZGRI S $A > 4$

Predstavlja se opća formulacija tehnički poboljšane metode za nalaženje rješenja osnovnog stanja Schrödingerove jednadžbe u konfiguracijskom prostoru, za sustave s brojem čestica većim od 4. Valna se funkcija razvija po parovno-koreliranim hipersferičnim harmonicima, te računa u Faddeevom pristupu. Primjenjuje se nedavna učinkovita rekurzivna metoda za slaganje antisimetričnih hipersferičnih harmonika za A čestica. Točnost računa se provjerava za energije vezanih osnovnih stanja jezgri s $A = 6$ do 12 primjenom V4 potencijala. Uspjeh dobivenih ishoda računa vidi se usporedbom s drugim pristupima.