
VARIATIONAL SOLUTION OF THE SCHRÖDINGER EQUATION FOR LIGHT NUCLEI WITHOUT SYMMETRIZATION OF TRIAL FUNCTIONS

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It is shown that the problem of derivation of the antisymmetric wave function (WF) of a system of identical particles can be reduced to that for a system without a predefined permutation symmetry, which considerably simplifies numerical calculations. This approach is used to calculate the binding energies of nuclei with $A = 3 \div 6$, and the results are compared with the literature data.

1. Introduction

In the variational methods of solution of few-body quantum-mechanical problems, the WF for a system of identical particles is approximated by trial functions which possess a necessary permutation symmetry and, in turn, are obtained by a “compulsory symmetrization” of some trial function [2]. Within this approach, an arbitrary matrix element (ME) of the Hamiltonian of a multiparticle system on functions with a permutation symmetry is represented as a sum of MEs on functions without permutation symmetry, where these functions are subjected to the action of the particle permutation operators. In general, the number of terms in this sum is equal to the permutation symmetry group order which is equal to $N!$ for a system of identical particles. This fact puts serious restrictions on the number of particles in systems under investigation, namely $N \leq 10$, and even $N < 8$ in the calculations with the use of personal computers.

In this paper, we present the method that allows us to abandon a “compulsory symmetrization” of trial functions for a system with the interparticle interaction potential that does not include spin (and isospin) operators.

2. Standard Calculation Scheme for Light Nuclei

Within the standard approach to the calculation of many-nucleon systems, the following actions are performed at each step of the expansion of the basis:

1. Choice of non-linear variational parameters, that is, the choice of a trial spatial function without any permutation symmetry.
2. Construction of a trial antisymmetric spin-isospin function.
3. Calculation of ME of the Hamiltonian on antisymmetric functions.
4. Calculation of a variation in the binding energy.
5. Steps 1–4 are performed as many times as necessary until a certain threshold of the binding energy variation is exceeded or a fixed number of times.
6. Adding the best function to the basis and the transition to the next iteration.

Let us consider step 3 in more details. The antisymmetric function of the i -th iteration has a form

$$\Phi_i = \frac{D_f}{g} \sum_{\mu_f} \chi^{[f]\mu_f}(\sigma, \tau) \sum_{P \in \pi_N} \Gamma_{\mu_f, \mu_f}^{[f]*}(P) \hat{P} \times \\ \times \phi(A_i, \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N),$$

where $\phi(A_i, \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is the trial spatial function obtained at step 1, $\chi^{[f]\mu_f}(\sigma, \tau)$ is the spin-isospin function, D_f is the dimension of the irreducible representation (IR) $[f]$, g is the order of the group π_N , $[f]_{\mu_f}$, $[\hat{f}]_{\mu_{\hat{f}}}$ are the joined Young tableaux, and A_i are non-linear parameters.

A ME of the Hamiltonian between two such functions for a given interaction type has the form

$$\langle \Phi_i | \hat{H} | \Phi_j \rangle = \sum_{P_1, P_2} \langle \phi(A_i, \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) | \hat{H} | \times \times | \hat{P}_2 \hat{P}_1^{-1} \phi(A_j, \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \rangle \Gamma_{\mu'_{f_1}, \mu'_{f_2}}^{[f]}(P_1^{-1} P_2). \quad (1)$$

In the calculation of (1), we use the relation $\hat{H} \hat{P} = \hat{P} \hat{H}$ (see below), and other simple properties of the bases and matrices of IR of groups [1].

From (1), it can be seen that we need to calculate $N!$ different MEs of the Hamiltonian on spatial functions. In addition, we should perform this calculation with all basis functions obtained in the preceding iterations and carry out variations of the non-linear parameters, which will lead to the multiple repetition of these calculations. Thus, to obtain each next approximation, we need to calculate $N!mT$ MEs, where m is the basis dimension at a given step of calculations and T is the number of variations of non-linear parameters. Correspondingly, the total number of MEs during the calculation of M basis functions is

$$N_M = \frac{M(M+1)}{2} N!T. \quad (2)$$

Thus, the volume of calculations required for the approximate solution of the Schrödinger equation is proportional at least to the factorial of the number of particles in the system, and this fact puts serious restrictions on the increase of N .

3. Theoretical Prerequisites for the Use of Non-symmetrized Basis Functions

Consider a system of N identical particles with a pairwise interaction and a potential depending on particle spatial coordinates only. In this case, the Hamiltonian of the system

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{i=1}^N \Delta_i + \sum_{j>i=1}^N V(\mathbf{r}_{ij}) \quad (3)$$

commutes, as known, with all permutation operations of the spatial coordinates of particles of the system [3]:

$$\hat{H} \hat{P} = \hat{P} \hat{H}, \forall \hat{P} \in \pi_N. \quad (4)$$

Here, π_N is the permutation group of N particles.

Next for the sake of definiteness, we assume that the system under study consists of nucleons. Let

$$\Psi = \sum_{\mu_f} \chi^{[\hat{f}]\mu_{\hat{f}}}(\sigma, \tau) Y^{[f]\mu_f}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \frac{D_f}{g} \times \times \sum_{\mu_f} \chi^{[\hat{f}]\mu_{\hat{f}}}(\sigma, \tau) \sum_{P \in \pi_N} \Gamma_{\mu_f, \mu'_f}^{[f]*}(P) \hat{P} y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \quad (5)$$

be the exact antisymmetric WF of any steady state of the system, where $Y^{[f]\mu_f}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is the spatial part of the WF with the permutation symmetry $[f]_{\mu_f}$, $\chi^{[\hat{f}]\mu_{\hat{f}}}(\sigma, \tau)$ is the spin-isospin part of the WF with the permutation symmetry conjugated to $[f]_{\mu_f}$, $y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is the spatial part of the WF without any requirements as for its permutation symmetry.

As Ψ is the exact WF, it should obey the Schrödinger equation

$$\hat{H} \Psi = E \Psi. \quad (6)$$

Let us calculate the left-hand and right-hand sides of (6), taking into account (4) and (5). We get

$$\hat{H} \Psi = \frac{D_f}{g} \sum_{\mu_f} \chi^{[\hat{f}]\mu_{\hat{f}}}(\sigma, \tau) \sum_{P \in \pi_N} \Gamma_{\mu_f, \mu'_f}^{[f]*}(P) \hat{P} \times \times \hat{H} y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$$

$$E \Psi = \frac{D_f}{g} \sum_{\mu_f} \chi^{[\hat{f}]\mu_{\hat{f}}}(\sigma, \tau) \sum_{P \in \pi_N} \Gamma_{\mu_f, \mu'_f}^{[f]*}(P) \hat{P} \times \times E y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N).$$

Thus,

$$\frac{D_f}{g} \sum_{\mu_f} \chi^{[\hat{f}]\mu_{\hat{f}}}(\sigma, \tau) \sum_{P \in \pi_N} \Gamma_{\mu_f, \mu'_f}^{[f]*}(P) \hat{P} \times \times [\hat{H} y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) - E y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)] = 0. \quad (7)$$

Equation (7) can be valid in two cases where

1. $y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is an eigenfunction of Hamiltonian (3) with the same energy, that is,

$$\hat{H} y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N). \quad (8)$$

2. The expansion of the function $\hat{H}y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) - Ey(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ in functions that are transformed by IRs of the group π_N does not contain basis functions of the IR $[f]$.

Let us prove that statement 2 is false under condition $\Psi \neq 0$.

It follows from relation (4) that Hamiltonian (3) is transformed as the IR $[N]$, i.e., it is symmetric with respect to all permutations of the spatial coordinates of all particles. Therefore, upon the action on the function $y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$, it cannot change its permutation symmetry. This yields that the permutation symmetry of the function $\hat{H}y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) - Ey(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ is the same as that of the function $y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$. Thus, condition 2 would lead to $\Psi = 0$, which is not true.

We have shown that the function $y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ from (5) is the eigenfunction of Hamiltonian (3) and is not obliged to possess any predefined permutation symmetry. But, from this function, we can obtain a correct antisymmetric WF for a system of several identical particles.

4. Calculation of a Wave Function with the Use of Non-symmetrized Bases

The main idea of the method consists in the calculation of the function $y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ by solving Eq. (8) with the following transition to the WF Ψ of the system with the use of an analog of formula (5) or any other means, but not a direct calculation Ψ from (6), which is carried out in the traditional calculation scheme.

While solving (6) by this method, it is necessary to remember the following facts:

1. While solving Eq. (8), especially for $A > 4$, it is very difficult to achieve such an accuracy of calculations of the functions $y_i(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$, at which the correspondence between the spectra of Eqs. (6) and (8) will be clearly seen. However, we succeeded (see Section 6) to attain a very good agreement of the results

Table 1. Spectra of Eqs. (6) and (8) (in MeV)

Antisymmetric	Non-symmetric
-63.709576	-116.684317
-36.718315	-72.426629
...	-67.890336
	-67.520421
	-67.445331
	-67.227146
	-67.139407
	-62.157451
	...

of calculations according to the proposed scheme with the results of other authors.

2. Because an additional restriction is imposed on WF Ψ with respect to $y(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$ (antisymmetry), the spectrum of Eq. (6) will be embedded in the spectrum of Eq. (8). In other words, if $\{y_i(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)\}_{i=1,2,\dots,K}$ is the discrete spectrum of Eq. (8), some WFs Ψ_i obtained with the use of formulas of type (5) may turn out to be zero.

In a simple way, this fact can be exemplified by the functions Ψ_0 and $y_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$.

It is known that the WF of the ground state of a system of non-identical particles has no nodes, that is, $y_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) > 0$ [3], and thus it can only belong to a spatial basis function of the IR $[N]$. While trying to build the basis function of any other IR from $y_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$, we obtain zero. For the systems of nucleons, this results in that the energies of the ground states of Eqs. (6) and (8) can be the same only for $A \leq 4$. For $A > 4$, the ground state of Eq. (6) corresponds to a certain excited state of Eq. (8).

Let us show this numerically using, as an example, the calculation of a six-nucleon system with the potential $K2$. Table 1 shows the approximate values of the lowest energy levels for non-symmetrized and antisymmetrized solutions.

From Table 1, it can be seen that the difference between the zero level of the antisymmetrized solution (-63.71 MeV) and the zero level of the non-symmetrized solution (-116.68 MeV) is much bigger than the deviation of the former from the excited states (-72.43, -67.89, ...). This shows that the zero level of the antisymmetrized state corresponds to some excited level of the non-symmetrized solution (most likely, beginning from the second excited level).

5. Calculation Scheme

The solution was carried out according to the following scheme:

1. Problem (8) was solved by expansion in a Gaussian basis of the following type [2]:

$$f_{KLM} = \eta_{KLM}(\mathbf{u}, \mathbf{x}) e^{-\frac{1}{2} \bar{\mathbf{x}} \mathbf{A} \mathbf{x}},$$

where

$$\eta_{KLM}(\mathbf{u}, \mathbf{x}) = v^{2K+L} Y_{LM}(\hat{\mathbf{v}}), \mathbf{v} = \sum_{j=1}^{N-1} u_j \mathbf{x}_j = \tilde{\mathbf{u}} \mathbf{x},$$

$$\mathbf{A} = \tilde{\mathbf{G}}_i \mathbf{A}_0 \mathbf{G}_i,$$

\mathbf{A}_0, \mathbf{u} , and i are variational parameters, \mathbf{x} are the Jacobi coordinates, and \mathbf{G}_i is the transform matrix of the Jacobi vectors under the action of a permutation with a number $i \in [1, 2, \dots, N!]$ acting on the coordinates of nucleons.

The calculation of MEs was carried out, as in [2], with the use of the integral transformation

$$f_{KLM} = \frac{1}{B_{KL}} \int d\hat{t} Y_{LM}(\hat{t}) \times \left[\frac{d^{2K+L}}{d\alpha^{2K+L}} g(\alpha, \mathbf{t}; \mathbf{u}, \mathbf{x}, \mathbf{A}) \right]_{\alpha=0, t=1},$$

where

$$g(\alpha, \mathbf{t}; \mathbf{u}, \mathbf{x}, \mathbf{A}) = e^{-\frac{1}{2}\bar{\mathbf{x}}\mathbf{A}\mathbf{x} + \alpha\mathbf{v}\cdot\mathbf{t}},$$

$$B_{nl} = \frac{4\pi(2n+l)!}{2^n n! (2n+2l+1)!}.$$

To optimize the non-linear parameters, we applied a stochastic method described in work [4]. At each calculation step, the optimization was aimed at the maximum decrease of the energy of a certain level p ($p \in [0, \dots, p_{\max}]$). Moreover, p was changed at each step. This approach allowed us to obtain good approximations to first $p_{\max} + 1$ levels. For different numbers of nucleons, we chose the numbers of levels $p_{\max} = 0, 0, 2, 3$ for $N = 3, 4, 5, 6$, respectively. In other respects, the algorithms of solution of the problem were the same for different N , apart from the ground state parameters.

- The transition $y \rightarrow \Psi$ was carried out not according to (5), but by the direct solution of (6) with the use of non-linear parameters obtained at the preceding step. That is, we carried out the full solution of problem (6) according to the standard scheme (see Section 2), apart from the variation of non-linear parameters.

Thus, the solution of the Schrödinger equation according to the above-presented scheme requires the calculation of $\frac{M(M+1)}{2}(T+N!)$ MEs, which is much less than the number of MEs in the standard calculation scheme (2).

6. Calculation Results

Here, we present the solutions for the problem for several nucleons with $A = 3 \div 6$ with the use of nucleon-nucleon potentials given in [5]. In addition, as in [5], we use

$$V(r) = \frac{1}{2}(V_s(r) + V_t(r)).$$

It can be seen that all potentials (and especially potential 2) result in the binding of the five-nucleon system and a significant rebinding of the six-nucleon system. This is related to the fact that, due to restrictions on the interaction type (independence of spin and isospin), this method cannot take into account the main property of the nucleon-nucleon interaction, namely, the dependence of the potential on the state of interacting particles.

Table 2. Model potentials

N	Potential	Parameters
1	Volkov [6]	$V(r) = 144.86e^{-(r/0.82)^2} - 83.34e^{-(r/1.6)^2}$
2	Brink-Boeker [7]	$V(r) = 389.5e^{-(r/0.7)^2} - 140.6e^{-(r/1.4)^2}$
3	Eikemeier-Hackenbroich [8]	$V_t(r) = 600e^{-5.5r^2} - 70e^{-0.5r^2} - 27.6e^{-0.38r^2},$ $V_s(r) = 880e^{-5.4r^2} - 70e^{-0.64r^2} - 21e^{-0.48r^2}$
4	K2 [5]	$V(r) = 37.32e^{-r^2} - 44.68e^{-(r/2)^2}$

Table 3. Binding energies (in MeV) of nuclei for the model potentials of Table 2 ($\hbar^2/M = 41.471 \text{ MeV}\cdot\text{fm}^2$)

Nucleus	$(L, S)J^\pi$	Potential	E_b , MeV		K^1
			This work	Other works	
T	$(0, \frac{1}{2})\frac{1}{2}^+$	1	8.46	8.465 [5] 8.46 [2]	30
		2	11.65	11.645 [5]	
		3	7.04	7.047 [5]	
		4	8.40	8.397 [5]	
		exp.		8.481	
^4He	$(0, 0)0^+$	1	30.40.	30.42 [2]	50
		2	38.30		
		3	28.69		
		4	29.08		
		exp.		28.295	
$A = 5$	$(1, \frac{1}{2})\frac{3}{2}^-$	1	42.99	43.00 [2]	120
		2	55.87		
		3	39.08		
		4	41.18		
		exp.		-	
^6He	$(0, 0)0^+$	1	66.22	66.25 [2]	250
		2	84.16		
		3	59.80		
		4	63.71		
		exp.		29.271	

However, we have also developed a modification of this method that does not suffer from this disadvantage and now undergoes a numerical testing.

7. Conclusions

The results obtained in this work show that the problem of determination of the antisymmetric wave function of a system of identical particles can be reduced to a simpler, concerning a calculational aspect, procedure of determination of the function without any predefined permutation symmetry. This approach allows us to considerably simplify the calculation of MEs of the Hamiltonian and to get additional computational resources that can be used for increasing the accuracy of calculations.

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ВАРІАЦІЙНЕ РОЗВ'ЯЗАННЯ РІВНЯННЯ ШРЕДІНГЕРА ДЛЯ ЛЕГКИХ ЯДЕР БЕЗ СИМЕТРИЗАЦІЇ ПРОБНИХ ФУНКЦІЙ

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Резюме

Описано спосіб, який дозволяє звести задачу знаходження антисиметричної хвильової функції (ХФ) системи тотожних частинок до більш простої (в обчислювальному плані) задачі знаходження функції системи, що не має будь-якої наперед заданої переставної симетрії. Наведено результати обчислень енергій зв'язку ядер з $A = 3 \div 6$, що були розраховані запропонованим методом, і порівняно їх з відомими літературними даними.