BOUND-STATE CALCULATIONS IN THE FRAMEWORK OF A STOCHASTIC VARIATIONAL APPROACH WITH NONSYMMETRIZED BASES

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In the framework of stochastic variational calculations and making no preliminary symmetrization of the wave functions with respect to identical particle coordinate permutations, the possibility of determining the symmetry properties of three- and four-particle energy states with zero angular momentum has been studied. The stochastic variational calculations revealed that the energy spectra obtained for the systems under consideration include the levels with all possible symmetries, provided that it is allowed by the superposition of applied bases. Local and integral schemes for the determination of permutation symmetry using the results of bound-state calculations have been proposed. It is found that the permutation symmetries (the Young tableaux) of energy states below the lowest breakup threshold can be determined with a high precision for a few-particle system. At the same time, the states above this threshold, even if the breakup is prohibited, can be studied only with the use of properly symmetrized bases.

1. Introduction

Advances attained in variational researches of few-particle quantum-mechanical systems of various nature (see works [1–8]) open opportunities for the comparison of different schemes of basis construction and determining the symmetry properties of energy states with the help of precision calculations. Moreover, the issues of whether modern variational approaches possess a capability to reveal various hidden symmetries or a symmetry degeneration of energy spectra by calculations and whether such an approach can be competitive in comparison with the standard scheme, when the symmetry of many-particle problems is determined analytically before calculations, are challenging. Such approaches can be promising both for kinematic symmetries of the prescribed orbital momentum type for spherically symmetric, or partially symmetric, interaction potentials and for prescribed permutation symmetries of systems involving identical particles or particles with similar properties, as well as for the revealing the quasisymmetries originating from the dynamic features of problems.

From the pragmatic viewpoint, it is of importance to answer the questions "Under which conditions can the actual symmetry be determined in the framework of stochastic variational methods (SVMs) that do no apply bases with prescribed symmetries?" and, in addition, "Is this procedure practically expedient?". One more question is "Is it always expedient to find the symmetry first and to carry out calculations afterwards, using a basis with determined symmetry?"

In this work, the problem dealing with the determination of permutation properties of many-particle wave functions with the use of precision schemes of stochastic variational methods has been solved, with some three- and four-particle Coulomb systems serving as examples.

2. Formulation of the Problem with Broken Symmetry in the Framework of SVMs

The application of variational methods for calculating the bound states of quantum-mechanical systems of various nature that contain significant numbers of particles meets, besides all other difficulties, the one associated with the construction of a wave function (WF) characterized by a given symmetry of identical particle coordinates, when the number of terms of the WF grows as $n!$ in the case of n identical particles. Due to the rounding procedure errors, this can result in a decrease of the calculation accuracy for Hamiltonian matrix elements, obtaining ill-conditioned energy matrices that enter the linear algebraic equations for characteristic values, which makes subsequent calculations impossible. At the same time, the application of certain SVM schemes – a procedure that long ago proved itself to be one of the most promising approaches [5] – reveals capabilities for establishing the symmetry properties of energy states, when the latter are obtained from the principle of energy minimum for each bound state.

In the Galerkin variational method, the WFs of bound states are presented in the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_n) = \sum_{i=1}^{N} c_i \phi_i \ , \qquad (1)$$

where c_i is a linear variational parameter that defines the presence probability for a definite configuration ϕ_i (the basis function), and N is the basis dimension. As the basis functions of the system with zero total angular momentum, we will use the Gauss-type basis

$$\phi_i = \exp\left(-\sum_{k<l}^{n} a_{kl}^i \mathbf{r}_{kl}^2\right) \qquad (2)$$

as one of the simplest and universal enough. Here, n is the number of particles, a_{kl}^i are nonlinear variational parameters, and $r_{kl} = |\mathbf{r}_k - \mathbf{r}_l|$ are particle-to-particle distances; knowing the latter is enough for the description of internal states of systems with n particles. The variational problem is reduced to the solution of systems of linear equations for c_i (the discrete algebraic representation for the Schrödinger equation)

$$\sum_{j=1}^{N} \{\langle \hat{S}\phi_i | \hat{H} - E | \hat{S}\phi_j \rangle\} c_j = 0 \ , \quad i = \overline{1, N} \ , \qquad (3)$$

where, in the standard approach, the symmetrization operator $\hat{S}$ is associated with a definite Young tableau with respect to the identical particle permutation for the Hamiltonian $\hat{H}$. By solving the standard linear systems of algebraic equations (3) separately for each given permutation symmetry (the Young tableau), we obtain the energy levels E_α and the corresponding mutually orthogonal wave functions.

The principal and rather cumbersome problem of the variational method is to find the optimal (the lowest) values of energy levels E_α with respect to the nonlinear variational parameters a_{kl}^i. For this purpose, the most universal method is the stochastic variational one, when random samples for the array of nonlinear variational parameters are generated. At the same time, in the SVM, even if the symmetrization with respect to identical particles has not been previously executed, the energy matrix $\langle \phi_i | H | \phi_j \rangle$ contains, in the general case, various blocks which approximately, but efficiently, realize all possible permutation symmetries of the corresponding states. Therefore, we have a possibility to examine the efficiency of such a scheme, when the variational procedure of stochastic optimization can, by itself, both implement a reliable calculation routine for the energy spectrum and reveal the actual permutation symmetry of WFs (this issue was also dealt with in work [9]).

Consider the expression for matrix elements (overlap integrals) $\Lambda_\alpha^{(P)} = \langle \Psi_\alpha | P \Psi_\alpha \rangle$, where P is the permutation operator for identical particle coordinates. The quantity $\Lambda_\alpha^{(P)}$ for the state α over all permutations of particle coordinates can be regarded as a measure of symmetry for the given WF. For k identical particles, there are $k!$ such permutations which form a permutation group Π_k. Calculations of those quantities enable us to find out the symmetry in the general case, i.e. to determine, to which representation of the irreducible group Π_k the wave function Ψ_α belongs. For instance, in the case of two identical particles 1 and 2 – this case is associated with the permutation group Π_2 – there are two one-dimensional representations: symmetric and antisymmetric, for which the quantity $\Lambda_\alpha^{(21)}$ is equal to 1 and -1, respectively. In the case of three identical particles, there are evidently three such Young tableaux: the one-dimensional totally symmetric representation [3], the totally antisymmetric representation $[1^3]$, and the two-dimensional representation [21] of the permutation group Π_3.

3. Calculations of Energy Spectra and Determination of Permutation Symmetry

3.1. Helium atom

As the simplest example, let us consider the calculation of the energy spectrum of a helium atom with zero angular momentum with the use of the variational functions (1) and without previous symmetrization of identical electron coordinates. The Hamiltonian of such a three-particle system looks like (in a.u.)

$$H = \frac{\mathbf{p}_1^2 + \mathbf{p}_2^2}{2} + \frac{\mathbf{p}_3^2}{2M} + \frac{1}{r_{12}} - Z\left(\frac{1}{r_{13}} + \frac{1}{r_{23}}\right) \ , \qquad (4)$$

where $Z = 2$ is the charge of a He nucleus (α-particle), and $M = 7294.299537$ is its mass in terms of electron mass units. Note that the energy spectrum of Hamiltonian (4) is infinite for the given angular momentum, and it has already been studied from various points of view. In addition, the states symmetric (parahelium) and antisymmetric (orthohelium) with respect to the coordinate permutation ($1 \leftrightarrow 2$) alternate (see the discussion in work [8]). In this work, we aim at achieving a reliable accuracy of the energy spectrum calculation and concentrate our main attention on the symmetry properties of WFs with respect to the two-electron permutation ($1 \leftrightarrow 2$) in bases without a symmetry prescribed *a priori*.

The results of calculations of the spectrum and the overlap integral $\Lambda_i^{(21)}$ in the basis containing 300 gaussoids are quoted in Table 1. First, we note that the energy of each level (the second column) calculated with no previously prescribed symmetry has a sufficient accuracy: the corresponding errors for practically all levels in Table 1 comprise several decimal digits in the 5-th to 6-th decimal positions in comparison with the results of precision calculations taken from work [8] (the fourth column). An especially high accuracy was obtained for the ground state which is characterized by the highest symmetry and is separated from the next (antisymmetric) level by a considerable energy interval (gap). Such a situation is typical of the atomic mode. Second, the third column of Table 1 testifies that the corresponding symmetries with respect to the permutation of electrons 1 and 2 were also determined reliably. Should the number of basis functions be increased, the calculation accuracies for energies and corresponding symmetry characteristics would naturally grow. Third, the permutation symmetry of different states was not revealed always monotonously, but with a certain intervening symmetry violation depending on the gradual expanding of nonsymmetrized basis. However, on the average about 50 basis functions (2) were enough for the permutation symmetry to be reliably determined. It is pertinent to emphasize that the distance between a certain antisymmetric level and the previous symmetric one is larger than the distance between the symmetric and previous antisymmetric levels. Note that the degree of the permutation symmetry determination can be also demonstrated by a coincidence of the density distributions for both electrons (see the determination procedure in work [10]). In Fig. 1, an example of the calculation results concerning the electron density distribution for the third excited level (it is the first antisymmetric excited state) is presented; for lower levels, the density distributions and the pair correlation functions calculated with the use of 300 basis functions completely coincide with the exact results taken from work [6]. It follows from Fig. 1 that a helium atom has rather substantial dimensions in the first excited antisymmetric state characterized by the mean-square distance (MSD) of an electron from the center of mass of the helium atom $\langle r^2\rangle_e^{1/2} = 8.289$ (hereafter, in a.u.) and a specific three-mode behavior of the electron density distribution. By the way, the MSD of the α-particle, the mass of which is substantial, with respect to its center of mass is very short, $\langle r^2\rangle_\alpha^{1/2} = 0.0016$; the MSD between electrons is $\langle(\mathbf{r}_1-\mathbf{r}_2)^2\rangle_{ee}^{1/2} = 11.727$; and the MSD between the electron and the α-particle, $\langle(\mathbf{r}_1-\mathbf{r}_3)^2\rangle_{e\alpha}^{1/2} = 8.290$, is close to the electron MSD. Note that the electron density distribution at the third excited level (the first excited antisymmetric level) of a helium atom practically vanishes at $r = r_0 = 5.218$ and has a long halo at farther distances, whereas the correlation function $g_{e\alpha}(r)$ is very close to $\rho_e(r)$ owing to a significant mass of the nucleus. At the same time, as was obtained in work [10], the electron density distributions for the ground and first two excited levels (of both symmetries) do not vanish within a finite distance range because of considerable correlation effects.

In addition, those distributions have two modes: the internal part of the electron distribution repeats itself in all states, but the halo structure of the first excited symmetric state has different characteristic dimensions. For higher excited levels, the electron density distributions are close to the electron–nucleus correlation functions and oscillate with growing r: the density distributions

T a b l e 1. Energy spectrum and overlap integrals $\Lambda_i^{(21)}$ for a helium atom

i	$-E_i$	$\Lambda_i^{(21)}$	$-E_i$ from work [8]
0	2.9033031	0.999952	2.9033044
1	2.1749285	−0.999950	2.17493011
2	2.1456621	0.999929	2.14567849
3	2.0684045	−0.998911	2.06840517
4	2.0609761	0.998858	2.060989
5	2.0362326	−0.994342	2.03623268
6	2.033274	0.994178	2.03330771
7	2.022301	−0.966029	2.022344
8	2.020816	0.964221	2.0208997
9	2.014856	−0.955985	2.01510
10	2.013798	0.953298	2.0142867
11	2.008703	−0.903414	2.01852
12	2.008066	0.907575	2.0103483

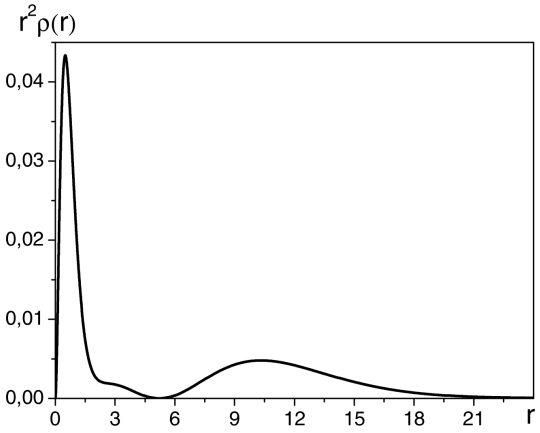

Fig. 1. Electron density distribution in the third excited state of a He atom

for the excited k-th symmetric and excited $(k-1)$-th antisymmetric states have $k-1$ zeros each and rather extended halos. In general, the calculation accuracy obtained for the energy – and, the more so, for the density distributions and other structural functions – in the framework of a scheme with no prescribed symmetry gets worse for higher states, so that the return to the calculation scenario with a prescribed permutation symmetry of two electrons becomes more effective.

3.2. Symmetry properties of states in a system with three gravitating particles

Let us consider the symmetry properties of various states for a system with three self-gravitating particles characterized by the Hamiltonian

$$H = \frac{\mathbf{p}_1^2 + \mathbf{p}_2^2 + \mathbf{p}_3^2}{2} - \left(\frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}}\right) \tag{5}$$

and the zero angular momentum in basis (2) without a prescribed symmetry.

Hamiltonian (5) has infinite energy spectra for a given angular momentum and each permutation symmetry below the corresponding two-particle breakup threshold (see work [6]): $-1/4$ for one-dimensional totally symmetric representation [3] and two-dimensional representation [21] of permutation group Π_3, and $-1/16$ for totally antisymmetric representation $[1^3]$. In this case, the levels with Young tableau [21] are twice degenerate in the exact formulation. How can all that be reproduced in stochastic variational calculations using nonsymmetrized bases?

In the second column of Table 2, the energy spectrum calculated in a nonsymmetrized basis with 750 basis functions (2) is presented. The fourth column contains the results of precision energy calculations obtained in work [6] in the standard scheme with prescribed Young tableaux. First of all, we note the fundamental fact that, in the framework of the approach free of a prescribed permutation symmetry, we have a continuous spectrum above the energy of the lowest two-particle breakup threshold $E_0(2) = -0.25$, where a straightforward variational calculation of bound states with any symmetry has no sense. Then, there exists no possibility to determine even the lowest totally antisymmetric state of three particles in the approach with no prescribed symmetry (see the opposite result obtained for a certain six-particle nuclear problem in work [9]). In the scenario with the prescribed symmetry [6], the known precise energy of the lowest totally antisymmetric state $E_0^a(3) = -0.127445$ lies above the lowest two-particle threshold of -0.25. This fact is also fundamental for other systems with identical particles and a nonsymmetrized scheme of variational calculations, so it does not allow one to rise above the lowest two-particle energy threshold.

Let us dwell on the problems that arise in calculations in the framework of the scheme with no prescribed symmetry for Hamiltonian (5). First, the alternation of singly and approximately twice degenerate (quasidegenerate) excited energy levels is observed: if the basis is expanded and the calculation accuracy is enhanced, the degeneration becomes more and more trustworthy.

Even this fact alone testifies that the twice quasidegenerate levels are related to a series with the Young tableau [21]. Note that, for a system with three self-gravitating particles, the absolutely lowest totally symmetric ground state has a coherent character, being separated by a rather appreciable interval (gap) from the first excited state which is also totally symmetric. Second, for the permutation symmetry of approximately calculated states to be determined reliably, we used additionally several procedures. For instance, we used the amplitudes

$$\left\langle \Psi_\alpha \middle| \sum_{i<j} r_{ij}^2 \middle| \Psi_\beta \right\rangle \tag{6}$$

of monopole transitions between different states α and β. Since the wave function of the ground state is totally symmetric with respect to coordinate permutations, the enhanced transitions (6) between the ground and excited states can be realized only between the states with identical permutation symmetry, being strongly suppressed for states with different permutation symmetries. This technique turned out reliable enough for the first 6 to 10

T a b l e 2. Energy spectrum and dominating probabilities of Young tableaux in nonsymmetrized bases for three gravitating particles

i	$-E_i$	symmetry – $\Gamma_\alpha^{[k]}$	$-E_i$,[6]
0	1.071778933	[3]: 0.99999999	1.07177937297
1	0.5744912	[3]: 0.99999993	0.57449221540
2	0.4528858	[21]: 0.999999909	0.4528869754
3	0.4528850	[21]: 0.99999992	-//-
4	0.393785	[3]: 0.99999951	0.39381649823
5	0.359535	[21]: 0.999999734	0.3595387446
6	0.35952287	[21]: 0.99999763	-//-
7	0.330819	[3]: 0.999979	0.33082419747
8	0.31678	[21]: 0.99999533	0.3167897461
9	0.316771	[21]: 0.99996357	-//-
10	0.3019888	[3]: 0.999831	0.301992565558
11	0.2947328	[21]: 0.999981	0.2947441034
12	0.2947176	[21]: 0.999605	-//-
13	0.2862493	[3]: 0.99773	0.28625287633

levels and confirmed that the first two levels from Table 2 have an identical symmetry, whereas the following two quasidegenerate levels have a different symmetry. Then another symmetric level and two more levels with a different symmetry take place. For higher excited levels, this way gradually loses its reliability, but it remains valid for transitions between neighbor levels. Certainly, transitions (6) between distant states are strongly suppressed and require the very accurate calculations with the use of large bases.

In addition, we systematically considered the determination of a permutation symmetry for the functions obtained which was carried out after variational calculations. For this purpose, the functions $\Psi_\alpha(123)$ obtained for each state were used to construct all irreducible representations: the function that is symmetric with respect to permutations ([3])

$$\Psi^s(123) = \Psi(123) + \Psi(132) + \Psi(213) + \Psi(231) + \\ + \Psi(312) + \Psi(321) \quad (7)$$

the antisymmetric function ([1^3])

$$\Psi^a(123) = \Psi(123) - \Psi(132) - \Psi(213) + \Psi(231) + \\ + \Psi(312) - \Psi(321) \quad (8)$$

and the irreducible representation [21]

$$\Psi'(123) = \frac{\sqrt{3}}{2}\{\Psi(231) + \Psi(213) - \Psi(312) - \Psi(321)\}$$

$$\Psi''(123) = -\frac{1}{2}\{\Psi(213) + \Psi(231) + \Psi(312) + \Psi(321)\} + \\ + \Psi(123) + \Psi(132) \quad (9)$$

(note that the representation [21] has two equivalent realizations). Then the nonsymmetrized functions $\Psi_\alpha(123)$ normalized to 1 can be expanded in series of functions (7)–(9) (also previously normalized to 1) of irreducible representations of the permutation group:

$$\Psi_\alpha = \sum_{[k]} N_\alpha^{[k]} \Psi_\alpha^{[k]} . \quad (10)$$

The squares of the expansion coefficients $N_\alpha^{[k]}$ (the overlap integrals between the wave function Ψ_α with no symmetry prescribed *a priori* and the wave function $\Psi_\alpha^{[k]}$ with reconstructed permutation symmetries), $\Gamma_\alpha^{[k]} = \left(N_\alpha^{[k]}\right)^2$, determine the probabilities for corresponding Young tableaux to be present in the α-state with the normalization condition $\sum_{[k]} \Gamma_\alpha^{[k]} = 1$, where the summation is carried out over all Young tableaux.

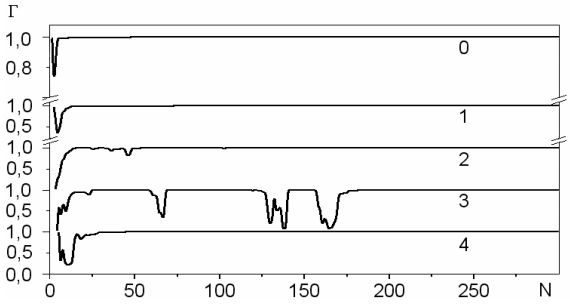

Fig. 2. Dependences of the probabilities of dominating Young tableaux on the number of basis functions for a system with three gravitating particles

The third column in Table 2 displays the dominating probabilities for the corresponding permutation symmetry $\Gamma_\alpha^{[k]}$ calculated in the 750-function basis, which unambiguously evidences the practical purity of the states with respect to permutations. We emphasize that the completely antisymmetric representation is not realized for the examined states, since they are located above the two-particle energy threshold $E_0(2) = -0.25$. Rather interesting are the nonmonotonous dependences of the probabilities of prescribed Young tableaux $\Gamma_\alpha^{[k]}$ on the number of basis functions taken into account. In this case, the absence of the unambiguous correlation between corrections to both the energy and the symmetry (the "symmetry violation" effect) revealed itself. Consider the simplest rather economical scheme of the basis expansion in expression (1), when the basis functions are added one by one, and a large enough stochastic sample (of about 2×10^5) of nonlinear parameters are made only in the added function. In addition, the stochastic minimization over nonlinear parameters was carried out for each state separately. In Fig. 2, the dependence of the dominating probability $\Gamma_\alpha^{[k]}$ of the determined Young tableau [3] on the number of basis functions is depicted for the ground state (curve *0*). As one can see, taking one, two, and three basis functions (2) into account in the framework of the variational method with the stochastic sampling of nonlinear variational parameters gradually improves, to some extent, the energy value, whereas the WF remains totally symmetric and depends only on the squared hyperradius

$$\rho^2 = r_{12}^2 + r_{13}^2 + r_{23}^2. \quad (11)$$

Considering the fourth basis function (2) somewhat improves the energy value obtained, but breaks the symmetry of the ground-state WF (at a level of 0.2%). This effect of the WF symmetry violation at the energy correction is general enough for various interaction potentials and for bases with various dimensions. For larger numbers of basis functions, the nonmonotonous dependence (the symmetry violation) of $\Gamma_0^{[3]}$ on this parameter also takes place (especially, when the number of basis functions is not very large), but about 50 (on the average) basis functions are enough for the totally symmetric character of the ground state WF to be reliably determined. In this case, the quantity $\Gamma_0^{[3]}$ reaches the asymptotic value of 1. For the first excited state, the quantity $\Gamma_1^{[3]}$ also characterizes the dominating totally symmetric character of the WF, and certain oscillations (symmetry violations) reveal themselves again, although there are enough basis functions (of about 50) for the Young tableau [3] to be determined (curve *1* in Fig. 2). Curves *2* and *3* in Fig. 2 show the dependences of the probability of the Young tableau [21] realization on the number of basis functions for the second and third excited states, respectively. Curve *4* corresponds to the probability of the totally symmetric tableau for the fourth excited state. As one can see, the corresponding Young tableaux were authentically found in all those cases (though nonmonotonously and with an insignificant symmetry violation for small numbers of basis functions) with the bases including a little more than 50 functions, when the asymptotics was attained. Similar calculations were also executed for about 10 excited states. In general, higher levels require more basis functions both for obtaining a definite accuracy for the energy value and for determining the valid asymptotics for symmetry coefficients.

Concerning the behavior of the structural functions for three gravitating particles – such as the one-particle distributions of particle density and the pair correlation functions – in the scheme, where bases without symmetrization are used, the situation is rather close to the helium atom problem considered above. Already about 100 basis functions (2) are enough for those structural functions for the ground and first excited levels not to depend on the particle number and to quantitatively coincide with precise results taken from work [6].

One more scenario of the partial symmetrization can be used in this and other problems. In particular, if the wave function is symmetrized with respect to only two arbitrary particles, the number of levels will become approximately half as large, provided that the dimension of the basis used is fixed, and the accuracy of corresponding calculated levels will enhance, as well as the probability of a reconstructed symmetry.

3.3. Analysis of a complete permutation set

Let us consider the overlap integrals $\Lambda_\alpha^{(P)} = \langle \Psi_\alpha | P\Psi_\alpha \rangle$ in more details, but in a smaller basis with regard for the role of all permutations in a system with three identical gravitating particles. The results of calculations obtained with the use of the basis of 220 gaussoids are quoted in Table 3, where the binding energies $\varepsilon_j \equiv -E_j$. The minimization was carried out with respect to the second excited level. Hereafter, the combinations of numbers 123, 132, and so on designate the permutations of particle coordinates $P = \begin{pmatrix} 123 \\ 123 \end{pmatrix}, \begin{pmatrix} 123 \\ 132 \end{pmatrix}$, and so on, respectively. From Table 3, one can see that the ground and first excited states are totally symmetric and realize one-dimensional representations. At the same time, for the second and third excited states, a quasidegeneration is observed, these levels are split, because the calculations were approximate, and a two-dimensional representation that corresponds to a mixed symmetry is realized. Then, we see that the fourth excited state is approximately totally symmetric again.

Let us consider the realization of a two-dimensional representation of the permutation group Π_3 corresponding to the second and third excited states in more details. We construct two-dimensional vectors $f = \begin{pmatrix} \Psi^{(2)} \\ \Psi^{(3)} \end{pmatrix}$ and $f^P = \begin{pmatrix} P\Psi^{(2)} \\ P\Psi^{(3)} \end{pmatrix}$, where $\Psi^{(2)}$ and $\Psi^{(3)}$ are the WFs of the second and third excited states, respectively, and P is a certain permutation of identical particle coordinates. Then, as is known, $f^P = A^P f$, where $A^P = \{a_{ij}^P\}$ are matrices of a two-dimensional irreducible representation of group Π_3. That is, we have a system of equations

$$P\Psi^{(2)} = a_{11}\Psi^{(2)} + a_{12}\Psi^{(3)} ,$$

T a b l e 3. Overlap integrals for the lowest levels and all permutations in a system with three gravitating particles

j	ε_j	Λ_{jj}^P					
		123	132	321	213	231	312
0	1.0717570	1.00	1.00	1.00	1.00	1.00	1.00
1	0.5742926	1.00	1.00	1.00	1.00	1.00	1.00
2	0.4528858	1.00	0.50	−0.50	−1.00	−0.50	−0.50
3	0.4517665	1.00	−0.50	−0.49	1.00	−0.50	−0.50
4	0.3903133	1.00	0.93	0.94	1.00	0.93	0.93

$$P\Psi^{(3)} = a_{21}\Psi^{(2)} + a_{22}\Psi^{(3)} \ . \tag{12}$$

Whence, owing to the orthogonality of WFs, we have

$$a_{ij}^P = \Lambda_{(i+1)(j+1)}^P \ , \quad i,j = \overline{1,2} \ . \tag{13}$$

In Table 4, the calculation results for the quantities Λ and a_{ij}^P and for all permutations are given. The data presented in Table 4 allow us to construct the matrices A^P which look like

$$A^P = \begin{array}{c} 123 \\ \left(\begin{array}{cc} 1.0 & 0 \\ 0 & 1.0 \end{array}\right), \end{array} \quad \begin{array}{c} 132 \\ \left(\begin{array}{cc} 0.50 & -0.86 \\ -0.86 & -0.50 \end{array}\right), \end{array} \quad \begin{array}{c} 321 \\ \left(\begin{array}{cc} 0.50 & 0.87 \\ 0.87 & -0.49 \end{array}\right), \end{array}$$
$$\begin{array}{c} 213 \\ \left(\begin{array}{cc} -1.0 & 0 \\ 0 & 1.0 \end{array}\right), \end{array} \quad \begin{array}{c} 231 \\ \left(\begin{array}{cc} -0.50 & -0.86 \\ 0.86 & -0.50 \end{array}\right), \end{array} \quad \begin{array}{c} 312 \\ \left(\begin{array}{cc} -0.50 & 0.86 \\ -0.86 & -0.50 \end{array}\right). \end{array} \tag{14}$$

Since $\sqrt{3}/2 \approx 0.866025$, one can see that this calculation gives rise to a representation equivalent to the two-dimensional irreducible representation of the permutation group Π_3, where cyclic permutations 231 and 312 are totally reproduced, whereas transpositions 132, 321, and 213 demand that some similar transformation be done:

$$M^{-1}A^PM = \begin{array}{c} 123 \\ \left(\begin{array}{cc} 1.0 & 0 \\ 0 & 1.0 \end{array}\right), \end{array} \quad \begin{array}{c} 132 \\ \left(\begin{array}{cc} -0.50 & 0.86 \\ 0.86 & +0.50 \end{array}\right), \end{array} \quad \begin{array}{c} 321 \\ \left(\begin{array}{cc} -0.49 & -0.87 \\ -0.87 & 0.50 \end{array}\right), \end{array}$$
$$\begin{array}{c} 213 \\ \left(\begin{array}{cc} 1.0 & 0 \\ 0 & -1.0 \end{array}\right), \end{array} \quad \begin{array}{c} 231 \\ \left(\begin{array}{cc} -0.50 & -0.86 \\ 0.86 & -0.50 \end{array}\right), \end{array} \quad \begin{array}{c} 312 \\ \left(\begin{array}{cc} -0.50 & 0.86 \\ -0.86 & -0.50 \end{array}\right), \end{array} \tag{15}$$

where

$$M = \left(\begin{array}{cc} \cos(\pi/2) & -\sin(\pi/2) \\ \sin(\pi/2) & \cos(\pi/2) \end{array}\right) = \left(\begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array}\right) \ ,$$

$$M^{-1} = \left(\begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array}\right) \ . \tag{16}$$

In the calculation with the minimization with respect to the third excited level, the splitting of levels substantially decreases, the representation equivalent to an irreducible one is reproduced as well, but the angle of a similar transformation which reduces either of the representations to the other, can be arbitrary. The results of such calculations in the basis with 204 gaussoids are shown in Table 5. From this table, one can see that the structure of the system states did not change, but the calculation accuracy became substantially better, even for a little smaller basis, since the quasidegenerate states are rather close. The representation which is equivalent to an irreducible one looks like

T a b l e 4. Matrix of the two-dimensional representation a_{ij}^P and overlap integrals for the second and third excited levels for three gravitating particles

		123	132	321	213	231	321
a_{11}^P	Λ_{22}^P	1.00	0.50	0.50	−1.00	−0.50	-0.50
a_{12}^P	Λ_{23}^P	0.00	−0.86	0.87	0.00	0.86	−0.86
a_{22}^P	Λ_{33}^P	1.00	−0.50	−0.49	1.00	-0.50	−0.50
a_{21}^P	Λ_{32}^P	0.00	−0.86	0.87	0.00	−0.86	0.86

T a b l e 5. Calculation results for symmetry properties of the lowest states with regard for the unitary transformations (15) and the minimization with respect to the third excited level

j	ε_j	Λ^P_{jj}					
		123	132	321	213	231	312
0	−1.071751	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
1	−0.5744743	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
2	−0.4528811	1.00000	−0.17706	−0.76381	0.94087	−0.50000	−0.50000
	$\Lambda^P_{23} \to$	1.00000	−0.98420	0.64543	0.33876	−0.86602	0.86602
3	−0.4528810	1.00000	0.17706	0.76381	−0.94087	−0.50000	−0.50000
	$\Lambda^P_{32} \to$	1.00000	−0.98420	0.64543	0.33876	0.86602	−0.86602
4	−0.3935422	1.00000	0.99966	0.99968	0.99979	0.99958	0.99958

$$A^P = \begin{matrix}123\\ \begin{pmatrix} 1.0 & 0 \\ 0 & 1.0 \end{pmatrix},\end{matrix} \quad \begin{matrix}132\\ \begin{pmatrix} -0.17706 & -0.98420 \\ -0.9842 & 0.17706 \end{pmatrix},\end{matrix} \quad \begin{matrix}321\\ \begin{pmatrix} -0.76381 & 0.64543 \\ 0.64543 & 0.76381 \end{pmatrix},\end{matrix}$$
$$\begin{matrix}213\\ \begin{pmatrix} 0.94087 & 0.33876 \\ 0.33986 & -0.94087 \end{pmatrix},\end{matrix} \quad \begin{matrix}231\\ \begin{pmatrix} -0.50000 & -0.86602 \\ 0.86602 & -0.50000 \end{pmatrix},\end{matrix} \quad \begin{matrix}312\\ \begin{pmatrix} -0.50000 & 0.86602 \\ -0.86602 & -0.50000 \end{pmatrix}.\end{matrix} \tag{17}$$

The angle θ of a similarity transformation can be found, e.g., from the relation $\sin 2\theta = 0.33876$. Then, $\theta = 0.1727993296$, and the transformation looks like

$$M = \begin{pmatrix} 0.9851073087 & -0.1719406592 \\ 0.1719406592 & 0.9851073087 \end{pmatrix},$$

$$M^{-1} = \begin{pmatrix} 0.9851073087 & 0.1719406592 \\ -0.1719406592 & 0.9851073087 \end{pmatrix}.$$

Applying this transformation to the matrices A^P, we obtain

$$M^{-1}A^PM = \begin{matrix}123\\ \begin{pmatrix} 1.0 & 0 \\ 0 & 1.0 \end{pmatrix},\end{matrix} \quad \begin{matrix}132\\ \begin{pmatrix} -0.50000 & -0.86603 \\ -0.86603 & 0.50000 \end{pmatrix},\end{matrix} \quad \begin{matrix}321\\ \begin{pmatrix} -0.50000 & 0.86602 \\ 0.86602 & 0.50000 \end{pmatrix},\end{matrix}$$
$$\begin{matrix}213\\ \begin{pmatrix} 1.0000 & 1\cdot 10^{-6} \\ 1\cdot 10^{-6} & -1.0000 \end{pmatrix},\end{matrix} \quad \begin{matrix}231\\ \begin{pmatrix} -0.50000 & -0.86602 \\ 0.86602 & -0.50000 \end{pmatrix},\end{matrix} \quad \begin{matrix}312\\ \begin{pmatrix} -0.50000 & 0.86602 \\ -0.86602 & -0.50000 \end{pmatrix}.\end{matrix} \tag{18}$$

One can see that, in this calculation, the detailed symmetry is determined with rather a high accuracy.

The character of a representation $D(P) = \sum_i A^P_{ii}$ is known to play an important role, because it is not changed at similarity transformations. For two-dimensional irreducible representations of the group Π_3, $D(P)$ has the following values: 2 for the identical permutation (123 in our notation); 0 for transpositions 132, 321, and 213; and −1 for cyclic permutations 231 and 312. The results of our calculations confirm this fact with a high accuracy. Hence, it would be enough to calculate the representation character, rather than to build the matrices of a representation and look for a similarity transformation. The accuracy of such calculations will be the accuracy of the symmetry reconstruction.

The results of corresponding calculations in a gaussoid basis with 542 functions in dimension are presented in Table 6, where $D(P)$ is the exact values of characters of the two-dimensional representation. The minimization was carried out over all levels in turn, increasing

T a b l e 6. Calculated results for the characters of irreducible representations of the permutation group for three gravitating particles

$\hat{D}(P)$		2.0	0.0	0.0	0.0	−1.0	−1.0
j	ε_j	Λ^P_{jj}					
		123	132	321	213	231	312
0	−1.071776	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
1	−0.574488	1.00000	1.00000	1.00000	1.00000	1.00000	1.00000
2	−0.452883	1.00000	−0.994174	0.590427	0.403747	−0.500000	−0.500000
3	−0.452882	1.00000	0.994174	−0.590427	−0.403748	−0.500000	−0.500000
$\lvert D(P)\rvert - \lvert\hat{D}(P)\rvert$		0.32×10^{-13}	0.53×10^{-6}	0.23×10^{-6}	0.50×10^{-7}	-0.68×10^{-6}	-0.68×10^{-6}
4	−0.393803	1.00000	0.999998	0.999998	0.999998	0.999998	0.999998
5	−0.359517	1.00000	0.891803	−0.837704	−0.054097	−0.499998	−0.499998
6	−0.359506	1.00000	−0.891800	0.837707	0.054095	−0.499998	−0.499998
$\lvert D(P)\rvert - \lvert\hat{D}(P)\rvert$		0.25×10^{-13}	0.33×10^{-5}	0.35×10^{-5}	0.26×10^{-5}	-0.39×10^{-5}	-0.39×10^{-5}
7	−0.330728	1.00000	0.999897	0.999904	0.999978	0.999900	0.999900
8	−0.316719	1.00000	0.488361	0.511544	−0.999900	−0.499995	−0.499995
9	−0.316561	1.00000	−0.488158	−0.511320	0.999795	−0.499780	−0.499780
$\lvert D(P)\rvert - \lvert\hat{D}(P)\rvert$		0.75×10^{-13}	0.20×10^{-3}	0.22×10^{-3}	0.11×10^{-3}	-0.22×10^{-3}	-0.22×10^{-3}
10	−0.301797	1.00000	0.999137	0.999024	0.999871	0.999097	0.999097
11	−0.294636	1.00000	0.515815	0.483996	−0.999791	−0.499981	−0.499981
12	−0.294355	1.00000	−0.514688	−0.482861	0.999491	−0.498904	−0.498904
$\lvert D(P)\rvert - \lvert\hat{D}(P)\rvert$		0.31×10^{-13}	0.11×10^{-2}	0.11×10^{-2}	0.30×10^{-3}	-0.11×10^{-2}	-0.11×10^{-2}
13	−0.285861	1.00000	0.997556	0.996175	0.998018	0.996009	0.996009
14	−0.281520	1.00000	0.965797	−0.269215	−0.682057	−0.492610	−0.492610
15	−0.281053	1.00000	−0.954190	0.274642	0.694196	−0.492370	−0.492370
$\lvert D(P)\rvert - \lvert\hat{D}(P)\rvert$		0.51×10^{-11}	0.12×10^{-1}	0.54×10^{-2}	0.12×10^{-1}	-0.15×10^{-1}	-0.15×10^{-1}
16	−0.274792	1.00000	0.930606	0.992712	0.900378	0.913221	0.913221
17	−0.270548	1.00000	0.653855	−0.963852	0.331035	−0.488725	−0.488725
18	−0.268570	1.00000	−0.554538	0.966735	−0.199195	−0.390550	−0.390550
$\lvert D(P)\rvert - \lvert\hat{D}(P)\rvert$		0.18×10^{-10}	0.99×10^{-1}	0.29×10^{-2}	0.13	−0.12	−0.12
19	−0.262261	1.00000	0.272561	0.977084	0.364904	0.314611	0.314611

the number of basis functions and making a stochastic sample of nonlinear coefficients for added functions only. The table demonstrates that, in this calculation, the symmetry is reproduced with a sufficient accuracy up to the 12-th level inclusive. A further enhancement of accuracy could be done by expanding the basis, which would demand, in turn, that computer's word length be increased.

3.4. Examples of other three- and four-particle systems

Similarly to what was done in Section 3 3.2, the three-particle calculations in a scheme without permutation symmetry for the ground and some lowest states were executed for a number of other pair potentials, such as the linear potential $V(r_{ij}) = \gamma r_{ij}$, a superposition of linear and oscillatory potentials, a superposition of the Coulomb and oscillatory potentials, and so on. Let us dwell on a system with three identical particles ($\hbar = M = 1$), with the pair potentials being superpositions of the Coulomb and linear potentials,

$$V(r_{ij}) = \frac{\alpha}{r_{ij}} + \gamma\, r_{ij}\ , \tag{19}$$

which is often used as a model quark–quark confining interaction potential. Consider the case $\alpha = -1$ and $\gamma = 0.1$ where the spectrum (infinite) of three self-gravitating particles (Table 2) shifts upward due to a repulsive potential in formula (19).

The second column in Table 7 shows the calculated energies, as well as the corresponding Young tableaux, for the examined states which were determined by analyzing the monopole transitions (6) and partially using representation (10). It is evident that this problem of three particles has infinite series of energy levels unlimited from above for fixed angular momenta and for each possible permutation symmetry. In the case under consideration, the positions and the permutation symmetries of the lowest levels in the energy spectrum can be determined reliably enough using only the force criterion for the monopole transitions (6). As a general remark, we note that the lower part of the spectrum for potential (19) becomes grouped in such a way that it reminds a spectrum for the case where an oscillatory potential is present: the ground state corresponds to the "zeroth shell", three following levels to the "second main shell", and six following levels to the "fourth main shell". The ground state from the "zeroth shell" is separated from the following first excited state from the "second shell" by a gap, as it also takes place for other attractive potentials, and both the lowest levels are totally symmetric owing to the attractive character of the chosen potential at short distances. The next two quasidegenerate levels are characterized by the Young tableau [21], being located considerably closer to the energy of the previous level (also from the "second shell"). Then, there appears a totally symmetric level separated by a wide gap from the next "fourth shell". The following two pairs of quasidegenerate levels belong to a representation with the mixed symmetry [21]. Afterward, there appears a totally symmetric level which closes the "fourth shell". From subsequent levels, we note the emergence of a totally antisymmetric state (with regard for the degeneracy order, it is the 17-th excited level) which is known [11] to belong to the sixth shell. For its identification, the monopole transitions to neighbor levels were calculated, and its ultimate permutation symmetry was found on the basis of formula (10). On the average, the distances between higher excited levels become shorter and shorter (we recall that we consider a linearly growing potential, for which intervals between levels have to decrease for higher excitations).

The results obtained for the case of a purely linear potential ($\alpha = 0$ in formula (19)), when the attraction potential had been omitted, turned out to be also interesting. The calculated energy levels and their permutation symmetries are listed in the third column of Table 7. By the way, the highest accuracy was achieved for all levels in this example. We also note that the alternation of different symmetries somewhat changes in such a way that the levels with higher symmetry shift upward (taking also into account that the scale is different, since we chose $\gamma = 1$). For example, the lowest antisymmetric level is now at the 16-th place in the general excitation list and belongs to the sixth "shell". For this potential, the level grouping into shells manifests itself pronouncedly enough up to the eighth shell inclusive. We recall that, in the case of three particles with the oscillatory (quadratically dependent on r) potential, the levels are strictly degenerate in each shell, and the first antisymmetric state belongs to the sixth shell [11] (the zeroth shell is nondegenerate, the second one is threefold degenerate, the fourth one is sixfold degenerate, the sixth one is tenfold degenerate, and so on). In addition, should the Coulomb potential be added to a weak oscillatory one, the level arrangement would be similar to that for potential (19), and, in the case with the oscillatory and repulsive Coulomb potentials, the totally antisymmetric level would be the tenth in the level list. Interesting regularities manifest themselves in the case of potential (19) with a repulsive Coulomb term. The results of corresponding calculations with $\alpha = 1$ and $\gamma = 0.$ are listed in the fourth column of Table 7. One can see that, owing to a repulsion at short distances, the levels with higher symmetry are shifted upward much

T a b l e 7. Energy spectra and Young tableaux for three particles with potentials (19) calculated in nonsymmetrized bases

i	$E_i(\alpha = -1,$ $\gamma = 0.1)$	$E_i(\alpha = 0,$ $\gamma = 1)$	$E_i(\alpha = 1,$ $\gamma = 0.1)$
0	−0.5374711 [3]	6.1322623296 [3]	2.35863665 [3]
1	0.4351935 [3]	8.4460183583 [3]	2.6836025 [21]
2	0.6814962 [21]	8.6248514892 [21]	2.6836026 [21]
3	0.6814974 [21]	8.6248514892 [21]	2.7361357 [3]
4	1.088206 [3]	10.468906007 [3]	3.015767 [3]
5	1.225461 [21]	10.572169109 [21]	3.032422 [21]
6	1.225466 [21]	10.572169109 [21]	3.032424 [21]
7	1.466758 [21]	10.799850983 [21]	3.0402091 [21]
8	1.466760 [21]	10.799850983 [21]	3.0402106 [21]
9	1.5075641 [3]	10.970678650 [3]	3.0935262 [3]
10	1.615565 [3]	12.289856674 [3]	3.351440 [1^3]
11	1.6860224 [21]	12.34459748 [21]	3.355503 [3]
12	1.6860522 [21]	12.34459750 [21]	3.360576 [21]
13	1.9215544 [3]	12.577399637 [21]	3.360587 [21]
14	1.9328835 [21]	12.577399664 [21]	3.366835 [21]
15	1.932899 [21]	12.70399441 [3]	3.366839 [21]
16	2.02983147 [3]	12.75225890 [1^3]	3.38232 [21]
17	2.0486622 [1^3]	12.82852283 [3]	3.38232 [21]
18	2.0753597 [3]	12.97594242 [21]	3.39606 [3]
19	2.089238 [21]	12.97594242 [21]	3.43508 [3]

more. Accordingly, the totally antisymmetric states became located relatively lower. For instance, the lowest antisymmetric state became the tenth excited level in the general list (and the lowest in the sixth shell), whereas the next excited totally antisymmetric state became the 20-th one (and the lowest in the eighth shell). The permutation symmetries of all those states were found using the amplitudes of monopole transitions (6) and on the basis of representation (10); however, a basis with about 300 functions was required to be used for higher excited states.

We now consider, in brief, an example of the determination of a permutation symmetry for a system with four particles, in particular, for a hydrogen molecule. Let the Hamiltonian be (in a.u.)

$$H = \frac{\mathbf{p}_1^2 + \mathbf{p}_2^2}{2M} + \frac{\mathbf{p}_3^2 + \mathbf{p}_4^2}{2} + \frac{Z^2}{r_{12}} + \frac{1}{r_{34}} -$$

$$-Z\left(\frac{1}{r_{13}} + \frac{1}{r_{14}} + \frac{1}{r_{23}} + \frac{1}{r_{24}}\right), \qquad (20)$$

where $M = 1836.152701$ is the relative proton mass, and $Z = 1$ is the relative charge. The results of calculations of the spectrum are given in the second column (a nonsymmetrized basis with 1200 components), and the probability of dominating permutation symmetry according to the representation of type (10) is presented in the third column of Table 8. The fourth column gives the energy spectrum (a basis with 1200 components) obtained in the framework of the standard method with prescribed permutations: symmetric with respect to protons and symmetric with respect to electrons (ss). The fifth column exposes the best literature data taken from work [12]. Note that, first, there are no levels with other symmetries different from ss for the zero angular momentum and, second, according to the results of special precise calculations [12] and experimental data obtained for energies below the threshold energy of the breakup into two hydrogen atoms ($4 \to 2+2$, $E_{\text{thres}} = -0.999455679432$), there are actually 15 levels with the ss-symmetry. Our calculation with a gaussoid-like basis containing 1200 functions allows, even in the case of a symmetrized basis, only eight levels to be obtained with an accuracy of 3 to 4 decimal digits. Third, using a nonsymmetrized basis with 1200 gaussoids, we can determine only about 5 energy levels (with an accuracy of 2 to 3 decimal digits); however, their ss-symmetry can be found for sure. This example of a hydrogen molecule demonstrates that the results of calculations for complicated systems with nonsymmetrized bases can be regarded only as qualitative estimations, but the precise calculations demand for special optimizing variational procedures to be elaborated (see work [12]).

T a b l e 8. Comparison of energy levels calculated in nonsymmetrized and symmetrized bases (with 1200 components) with the most accurate literature data taken from work [12]

i	$-E_i$	symmetr. (ss)	$-E_i$(symmetr.)	$-E_i$[12])
0	1.161329	0.99966	1.163501	1.1640250300
1	1.132503	0.99876	1.141878	1.1450653676
2	1.093697	0.99696	1.119645	1.1271779152
3	1.053905	0.99238	1.091461	1.1103404429
4	1.017269	0.97868	1.064515	1.0945391187
5	0.999428	0.4991	1.03230	1.0797693217
6	0.994166	0.5689	1.005119	1.0660370737
7	0.989407	0.5711	0.999522	1.0533604890
8	0.9777	0.1943	0.9983	1.0417726950

To complete a discussion concerning the system with four self-gravitating particles, we note that the calculations with a nonsymmetrized basis allow the order of different levels with reconstructed permutation symmetries to be approximately determined. In particular, the ground state is associated with the totally symmetric Young tableau [4] (see work [6]). The next level which is separated by a substantial interval (gap) is a totally symmetric state too. The subsequent three quasidegenerate levels correspond to the Young tableau [31]. Further, there are located two quasidegenerate levels with the Young tableau [22]. The seventh excited level is also totally symmetric; it belongs already to the fourth "main shell", being separated from the lower levels by a certain gap. The calculations of subsequent levels in the scheme with nonsymmetrized basis reveal considerable errors, and it is expedient to come back to the standard scheme with prescribed permutation symmetries.

4. Conclusions

To summarize, in this work we obtained the following main results.

1. Calculations in the framework of SVM with a nonsymmetrized, with respect to permutations of identical particles, basis allow all low energy states in systems with three or four particles to be determined with a satisfactory accuracy. In addition, the permutation symmetries of those states can be satisfactorily found as well.

2. A nonsymmetrized basis can be used only at energies below the absolutely lowest breakup threshold, in the range of true bound states. The calculations of strongly antisymmetrized states in the approach with-

out a prescribed symmetry cannot be reliable even above the forbidden threshold with a prescribed symmetry, so that the permutation symmetry for identical particles must be prescribed from the very beginning to study such states.

3. In all considered cases with three and four particles, a natural advantage of using the *a priori* symmetrized bases to calculate bound states was observed, when the number of symmetrized basis functions, which were needed to be used to achieve a required accuracy of calculations, was several times less.

4. The variational calculations showed that the expansion of nonsymmetrized variational bases is accompanied not only by an increase of the calculation accuracy for energy levels, but also by the temporary violation of a symmetry of wave functions – especially, if the basis is not very large – although the actual symmetry can be determined more reliably, on the average, for significant bases.

5. For larger numbers of particles and more complicated systems of quantum-mechanical particles, the possibilities to attain a required high accuracy for the energy and other parameters become more and more problematic, both for nonsymmetrized, it is especially true for them, and *a priori* properly symmetrized bases.

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РОЗРАХУНКИ ЗВ'ЯЗАНИХ СТАНІВ
У СТОХАСТИЧНОМУ ВАРІАЦІЙНОМУ
МЕТОДІ З НЕСИМЕТРИЗОВАНИМИ БАЗИСАМИ

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Р е з ю м е

Досліджено можливості встановлення симетрійних властивостей енергетичних станів в системах трьох та чотирьох частинок з нульовим кутовим моментом у стохастичних варіаційних розрахунках без попередньої симетризації станів за координатами тотожних частинок. Виявлено, що у стохастичних варіаційних розрахунках енергетичні спектри включають рівні всіх можливих для даної системи симетрій, якщо це дозволено суперпозицією базисів, що використовуються. Запропоновано локальні та інтегральні схеми встановлення перестановочній симетрії за результатами розрахунків зв'язаних станів. Показано, що для енергетичних станів квантових систем декількох частинок нижче найнижчого порога розвалу на підсистеми перестановочні симетрії (схеми Юнга) можуть бути встановлені з високою точністю. Стани ж вище найнижчого порогу розвалу, якщо він навіть заборонений, можна розглядати лише на відповідно симетризованих базисах.