Symbolic-Numerical Algorithm for Generating Cluster Eigenfunctions: Identical Particles with Pair Oscillator Interactions

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Abstract. The quantum model of a cluster, consisting of A identical particles, coupled by the internal pair interactions and affected by the external field of a target, is considered. A symbolic-numerical algorithm for generating $A-1$-dimensional oscillator eigenfunctions, symmetric or antisymmetric with respect to permutations of A identical particles in the new symmetrized coordinates, is formulated and implemented using the MAPLE computer algebra system. Examples of generating the symmetrized coordinate representation for $A-1$ dimensional oscillator functions in one-dimensional Euclidean space are analyzed. The approach is aimed at solving the problem of tunnelling the clusters, consisting of several identical particles, through repulsive potential barriers of a target.

1 Introduction

Quantum harmonic oscillator wave functions have a lot of applications in modern physics, particularly, as a basis for constructing the wave functions of a quantum system, consisting of A identical particles, totally symmetric or antisymmetric with respect to permutations of coordinates of the particles [1]. Various special methods, algorithms, and programs (see, e.g., [1–9]) were used to construct the desired solutions in the form of linear combinations of the eigenfunctions of an $A-1$-dimensional harmonic oscillator that are totally symmetric (or antisymmetric) with respect to the coordinate permutations. However, the implementation of this procedure in closed analytical form is still an open problem [10].

A promising approach to the construction of oscillator basis functions for four identical particles was proposed in [2–4]. It was demonstrated that a clear algorithm for generating symmetric (S) and antisymmetric (A) states can be obtained using the symmetrized coordinates instead of the conventional Jacobi

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coordinates. However, until now this approach was not generalized for a quantum system comprising an arbitrary number A of identical particles.

We intend to develop this approach in order to describe the tunnelling of clusters, consisting of several coupled identical particles, through repulsive potential barriers of a target. Previously this problem was solved only for a pair of coupled particles [11, 12]. The developed approach will be also applicable to the microscopic study of tetrahedral- and octahedral-symmetric nuclei [13] that can be considered in the basis of seven-dimensional harmonic oscillator eigenfunctions [14]. *The aim of this paper is to present a convenient formulation of the problem stated above and the calculation methods, algorithms, and programs for solving it.*

In this paper, we consider the quantum model of a cluster, consisting of A identical particles with the internal pair interactions, under the influence of the external field of a target. We assume that the spin part of the wave function is known, so that only the spatial part of the wave function is to be considered, which can be either symmetric or antisymmetric with respect to a permutation of A identical particles [15–17]. The initial problem is reduced to the problem for a composite system whose internal degrees of freedom describe an $(A-1)\times d$-dimensional oscillator, and the external degrees of freedom describe the center-of-mass motion of A particles in the d-dimensional Euclidean space. For simplicity, we restrict our consideration to the so-called s-wave approximation [11] corresponding to one-dimensional Euclidean space ($d=1$). It is shown that the reduction is provided by using appropriately chosen symmetrized coordinates rather than the conventional Jacoby coordinates.

The main goal of introducing the symmetrized coordinates is to provide the invariance of the Hamiltonian with respect to permutations of A identical particles. This allows construction not only of basis functions, symmetric or antisymmetric under permutations of $A-1$ relative coordinates, but also of basis functions, symmetric (S) or antisymmetric (A) under permutations of A Cartesian coordinates of the initial particles. We refer the expansion of the solution in the basis of such type as the Symmetrized Coordinate Representation (SCR).

The paper is organized as follows. In Section 2, we present the statement of the problem in the conventional Jacobi and the symmetrized coordinates. In Section 3, we introduce the SCR of the solution of the considered problem and describe the appropriate algorithm implemented using the MAPLE computer algebra system. In Section 4, we analyze some examples of generating the symmetrized coordinate representation for $A-1$-dimensional oscillator functions in one-dimensional Euclidean space. In Conclusion, we summarize the results and discuss briefly the prospects of application of the developed approach.

2 Problem Statement

Consider the system of A identical quantum particles with the mass m and the set of Cartesian coordinates $x_i \in \mathbf{R}^d$ in the d-dimensional Euclidean space, considered as the vector $\tilde{\mathbf{x}} = (\tilde{x}_1, ..., \tilde{x}_A) \in \mathbf{R}^{A\times d}$ in the $A\times d$-dimensional

configuration space. The particles are coupled by the pair potential $\tilde{V}^{pair}(\tilde{x}_{ij})$ depending on the relative positions, $\tilde{x}_{ij} = \tilde{x}_i - \tilde{x}_j$, similar to that of a harmonic oscillator $\tilde{V}^{hosc}(\tilde{x}_{ij}) = \frac{m\omega^2}{2}(\tilde{x}_{ij})^2$ with the frequency ω. The whole system is subject to the influence of the potentials $\tilde{V}(\tilde{x}_i)$ describing the external field of a target. The system is described by the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{A}\frac{\partial^2}{\partial\tilde{x}_i^2}+\sum_{i,j=1;i<j}^{A}\tilde{V}^{pair}(\tilde{x}_{ij})+\sum_{i=1}^{A}\tilde{V}(\tilde{x}_i)-\tilde{E}\right]\tilde{\Psi}(\tilde{\mathbf{x}})=0,$$

where $\tilde{E}$ is the total energy of the system of A particles and $\tilde{P}^2 = 2m\tilde{E}/\hbar^2$, $\tilde{P}$ is the total momentum of the system, and $\hbar$ is Planck constant. Using the oscillator units $x_{osc} = \sqrt{\hbar/(m\omega\sqrt{A})}$, $p_{osc} = \sqrt{(m\omega\sqrt{A})/\hbar} = x_{osc}^{-1}$, and $E_{osc} = \hbar\omega\sqrt{A}/2$ to introduce the dimensionless coordinates $x_i = \tilde{x}_i/x_{osc}$, $x_{ij} = \tilde{x}_{ij}/x_{osc} = x_i - x_j$, $E = \tilde{E}/E_{osc} = P^2$, $P = \tilde{P}/p_{osc} = \tilde{P}x_{osc}$, $V^{pair}(x_{ij}) = \tilde{V}^{pair}(x_{ij}x_{osc})/E_{osc}$, $V^{hosc}(x_{ij}) = \tilde{V}^{hosc}(x_{ij}x_{osc})/E_{osc} = \frac{1}{A}(x_{ij})^2$ and $V(x_i) = \tilde{V}(x_i x_{osc})/E_{osc}$, one can rewrite the above equation in the form

$$\left[-\sum_{i=1}^{A}\frac{\partial^2}{\partial x_i^2}+\sum_{i,j=1;i<j}^{A}\frac{1}{A}(x_{ij})^2+\sum_{i,j=1;i<j}^{A}U^{pair}(x_{ij})+\sum_{i=1}^{A}V(x_i)-E\right]\Psi(\mathbf{x})=0, \quad (1)$$

where $U^{pair}(x_{ij}) = V^{pair}(x_{ij}) - V^{hosc}(x_{ij})$, i.e., if $V^{pair}(x_{ij}) = V^{hosc}(x_{ij})$, then $U^{pair}(x_{ij}) = 0$.

Our goal is to find the solutions $\Psi(x_1, ..., x_A)$ of Eq. (1), totally symmetric (or antisymmetric) with respect to the permutations of A particles that belong to the permutation group S_n [16]. The permutation of particles is nothing but a permutation of the Cartesian coordinates $x_i \leftrightarrow x_j$, $i, j = 1, ..., A$. First we introduce the Jacobi coordinates, $y = Jx$, following one of the possible definitions:

$$y_0 = \frac{1}{\sqrt{A}}\left(\sum_{t=1}^{A}x_t\right), \quad y_s = \frac{1}{\sqrt{s(s+1)}}\left(\sum_{t=1}^{s}x_t - sx_{s+1}\right), \quad s = 1,..,A-1. \quad (2)$$

In the matrix form Eqs. (2) read as

$$\begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{A-1} \end{pmatrix} = J\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{A-1} \\ x_A \end{pmatrix}, \quad J = \begin{pmatrix} 1/\sqrt{A} & 1/\sqrt{A} & 1/\sqrt{A} & 1/\sqrt{A} & \cdots & 1/\sqrt{A} \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 & 0 & \cdots & 0 \\ 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} & 0 & \cdots & 0 \\ 1/\sqrt{12} & 1/\sqrt{12} & 1/\sqrt{12} & -3/\sqrt{12} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{A^2-A}} & \frac{1}{\sqrt{A^2-A}} & \frac{1}{\sqrt{A^2-A}} & \frac{1}{\sqrt{A^2-A}} & \cdots & -\frac{A-1}{\sqrt{A^2-A}} \end{pmatrix},$$

The inverse coordinate transformation $x = J^{-1}y$ is implemented using the transposed matrix $J^{-1} = J^T$, i.e., J is an orthogonal matrix with pairs of complex

conjugate eigenvalues, the absolute values of which are equal to one. The Jacobi coordinates have the property $\sum_{i=0}^{A-1}(y_i \cdot y_i) = \sum_{i=1}^{A}(x_i \cdot x_i) = r^2$. Therefore,

$$\sum_{i,j=1}^{A}(x_{ij})^2 = 2A\sum_{i=0}^{A-1}(y_i)^2 - 2(\sum_{i=1}^{A}x_i)^2 = 2A\sum_{i=1}^{A-1}(y_i)^2,$$

so that Eq. (1) takes the form

$$\left[-\frac{\partial^2}{\partial y_0^2} + \sum_{i=1}^{A-1}\left(-\frac{\partial^2}{\partial y_i^2} + (y_i)^2\right) + U(y_0, ..., y_{A-1}) - E\right]\Psi(y_0, ..., y_{A-1}) = 0,$$

$$U(y_0, ..., y_{A-1}) = \sum_{i,j=1;i<j}^{A} U^{pair}(x_{ij}(y_1, ..., y_{A-1})) + \sum_{i=1}^{A} V(x_i(y_0, ..., y_{A-1})),$$

which, as follows from Eq. (2), is *not invariant* with respect to permutations $y_i \leftrightarrow y_j$ at $i, j = 1, ..., A-1$.

Symmetrized Coordinates

The transformation from the Cartesian coordinates to one of the possible choices of the symmetrized ones ξ_i has the form, $\xi = Cx$ and $x = C\xi$:

$$\xi_0 = \frac{1}{\sqrt{A}}\left(\sum_{t=1}^{A}x_t\right),\ \xi_s = \frac{1}{\sqrt{A}}\left(x_1 + \sum_{t=2}^{A}a_0x_t + \sqrt{A}x_{s+1}\right),\ \ s = 1, ..., A-1,$$

$$x_1 = \frac{1}{\sqrt{A}}\left(\sum_{t=0}^{A-1}\xi_t\right),\ \ x_s = \frac{1}{\sqrt{A}}\left(\xi_0 + \sum_{t=1}^{A-1}a_0\xi_t + \sqrt{A}\xi_{s-1}\right),\ \ s = 2, ..., A,$$

or, in the matrix form,

$$\begin{pmatrix}\xi_0\\ \xi_1\\ \xi_2\\ \vdots\\ \xi_{A-2}\\ \xi_{A-1}\end{pmatrix} = C\begin{pmatrix}x_1\\ x_2\\ x_3\\ \vdots\\ x_{A-1}\\ x_A\end{pmatrix},\ \ C = \frac{1}{\sqrt{A}}\begin{pmatrix}1 & 1 & 1 & 1 & \cdots & 1 & 1\\ 1 & a_1 & a_0 & a_0 & \cdots & a_0 & a_0\\ 1 & a_0 & a_1 & a_0 & \cdots & a_0 & a_0\\ 1 & a_0 & a_0 & a_1 & \cdots & a_0 & a_0\\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ 1 & a_0 & a_0 & a_0 & \cdots & a_1 & a_0\\ 1 & a_0 & a_0 & a_0 & \cdots & a_0 & a_1\end{pmatrix}, \qquad (3)$$

where $a_0 = 1/(1-\sqrt{A}) < 0$, $a_1 = a_0 + \sqrt{A}$. The inverse coordinate transformation is performed using the same matrix $C^{-1} = C$, $C^2 = I$, i. e., $C = C^T$ is a symmetric orthogonal matrix with the eigenvalues $\lambda_1 = -1$, $\lambda_2 = 1$, ..., $\lambda_A = 1$ and $\det C = -1$. For $A = 2$, the symmetrized variables (3) are within normalization factors similar to the symmetrized Jacobi coordinates (2) considered in [9], while at $A = 4$ they correspond to another choice of symmetrized coordinates $(\ddot{x}_4, \ddot{x}_1, \ddot{x}_2, \ddot{x}_3)^T = C(x_4, x_1, x_2, x_3)^T$ considered in [2–4] and mentioned earlier

in [5, 18]. We could not find a general definition of symmetrized coordinates for A-identical particles like (3) in the available literature, so we believe that in the present paper it is introduced for the first time. With the relations $a_1 - a_0 = \sqrt{A}$, $a_0 - 1 = a_0\sqrt{A}$ taken into into account, the relative coordinates $x_{ij} \equiv x_i - x_j$ of a pair of particles i and j are expressed in terms of the internal $A-1$ symmetrized coordinates only:

$$x_{ij} \equiv x_i - x_j = \xi_{i-1} - \xi_{j-1} \equiv \xi_{i-1,j-1},$$
$$x_{i1} \equiv x_i - x_1 = \xi_{i-1} + a_0 \sum_{i'=1}^{A-1} \xi_{i'}, \quad i,j = 2,...,A. \tag{4}$$

So, if only the absolute values of x_{ij} are to be considered, then there are $(A-1)(A-2)/2$ old relative coordinates transformed into new relative ones and $A-1$ old relative coordinates expressed in terms of $A-1$ internal symmetrized coordinates. These important relations essentially simplify the procedures of symmetrization (or antisymmetrization) of the oscillator basis functions and the calculations of the corresponding pair-interaction integrals $V^{pair}(x_{ij})$. The symmetrized coordinates are related to the Jacobi ones as $y = B\xi$, $B = JC$:

$$\begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_{A-2} \\ y_{A-1} \end{pmatrix} = B \begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \vdots \\ \xi_{A-2} \\ \xi_{A-1} \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & b_1^0 & b_1^- & b_1^- & b_1^- & \cdots & b_1^- & b_1^- \\ 0 & b_2^+ & b_2^0 & b_2^- & b_2^- & \cdots & b_2^- & b_2^- \\ 0 & b_3^+ & b_3^+ & b_3^0 & b_3^- & \cdots & b_3^- & b_3^- \\ 0 & b_4^+ & b_4^+ & b_4^+ & b_4^0 & \cdots & b_4^- & b_4^- \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & b_{A-1}^+ & b_{A-1}^+ & b_{A-1}^+ & b_{A-1}^+ & \cdots & b_{A-1}^+ & b_{A-1}^0 \end{pmatrix}, \tag{5}$$

where $b_s^+ = 1/((\sqrt{A}-1)\sqrt{s(s+1)})$, $b_s^- = \sqrt{A}/((\sqrt{A}-1)\sqrt{s(s+1)})$, and $b_s^0 = (1+s-s\sqrt{A})/((\sqrt{A}-1)\sqrt{s(s+1)})$. One can see that for the center of mass the symmetrized and Jacobi coordinates are equal, $y_0 = \xi_0$, while the relative coordinates are related via the $(A-1)\times(A-1)$ matrix M with the elements $M_{ij} = B_{i+1,j+1}$ and $\det M = (-1)^{A\times d}$, i.e., the matrix, obtained by cancelling the first row and the first column. The inverse transformation $\xi = B^{-1}y$ is given by the matrix $B^{-1} = (JC)^{-1} = CJ^T = B^T$, i.e., B is also an orthogonal matrix.

In the symmetrized coordinates Eq. (1) takes the form

$$\left[-\frac{\partial^2}{\partial\xi_0^2} + \sum_{i=1}^{A-1}\left(-\frac{\partial^2}{\partial\xi_i^2} + (\xi_i)^2\right) + U(\xi_0,...,\xi_{A-1}) - E\right]\Psi(\xi_0,...,\xi_{A-1}) = 0, \tag{6}$$
$$U(\xi_0,...,\xi_{A-1}) = \sum_{i,j=1;i<j}^{A} U^{pair}(x_{ij}(\xi_1,...,\xi_{A-1})) + \sum_{i=1}^{A} V(x_i(\xi_0,...,\xi_{A-1})),$$

which is *invariant* under permutations $\xi_i \leftrightarrow \xi_j$ at $i,j = 1,...,A-1$, as follows from Eq. (3), i.e., the *invariance* of Eq. (1) under permutations $x_i \leftrightarrow x_j$ at $i,j = 1,...,A$ survives.

Table 1. The first few eigenvalues E_j^S and the oscillator S-eigenfunctions (13) at $E_j^S - E_1^S \leq 10$, $E_1^S = A - 1$. We use the notations $|[i_1, i_2, ..., i_{A-1}]\rangle \equiv \Phi^s_{[i_1,i_2,...,i_{A-1}]}(\xi_1, ..., \xi_{A-1})$ from Eqs. (8) and (10), i.e., $[i_1, i_2, ..., i_{A-1}]$ assumes the summation over permutations of $[i_1, i_2, ..., i_{A-1}]$ in the layer $2\sum_{k=1}^{A-1} i_k + A - 1 = E_i^{s(a)}$.

A=2		A=3		A=4		$E_j^S - E_1^S$
j	$\Phi_j^S(\xi_1)$	j	$\Phi_j^S(\xi_1, \xi_2)$	j	$\Phi_j^S(\xi_1, \xi_2, \xi_3)$	
1	$\|[0]\rangle$	1	$\|[0, 0]\rangle$	1	$\|[0, 0, 0]\rangle$	0
2	$\|[2]\rangle$	2	$\|[0, 2]\rangle$	2	$\|[0, 0, 2]\rangle$	4
		3	$\frac{1}{2}\|[0, 3]\rangle - \frac{\sqrt{3}}{2}\|[1, 2]\rangle$	3	$\|[1, 1, 1]\rangle$	6
3	$\|[4]\rangle$	4	$\frac{\sqrt{3}}{2}\|[0, 4]\rangle + \frac{1}{2}\|[2, 2]\rangle$	4	$\|[0, 0, 4]\rangle$	8
				5	$\|[0, 2, 2]\rangle$	8
		5	$\frac{\sqrt{5}}{4}\|[0, 5]\rangle - \frac{3}{4}\|[1, 4]\rangle - \frac{\sqrt{2}}{4}\|[2, 3]\rangle$	6	$\|[1, 1, 3]\rangle$	10

Table 2. The first few eigenvalues E_j^A and the oscillator A-eigenfunctions (13) at $E_j^A - E_1^A \leq 10$, $E_1^A = A^2 - 1$. We use the notations $|[i_1, i_2, ..., i_{A-1}]\rangle \equiv \Phi^a_{[i_1,i_2,...,i_{A-1}]}(\xi_1, ..., \xi_{A-1})$ from Eq. (11), i.e., $[i_1, i_2, ..., i_{A-1}]$ assumes the summation over the multiset permutations of $[i_1, i_2, ..., i_{A-1}]$ in the layer $2\sum_{k=1}^{A-1} i_k + A - 1 = E_i^{s(a)}$.

$A = 2$, $E_1^A = 3$		$A = 3$, $E_1^A = 8$		$A = 4$, $E_1^A = 15$		$E_j^A - E_1^A$
j	$\Phi_j^A(\xi_1)$	j	$\Phi_j^A(\xi_1, \xi_2)$	j	$\Phi_j^A(\xi_1, \xi_2, \xi_3)$	
1	$\|[1]\rangle$	1	$\frac{1}{2}\|[0, 3]\rangle + \frac{\sqrt{3}}{2}\|[1, 2]\rangle$	1	$\|[0, 2, 4]\rangle$	0
2	$\|[3]\rangle$	2	$\frac{\sqrt{5}}{4}\|[0, 5]\rangle + \frac{3}{4}\|[1, 4]\rangle - \frac{\sqrt{2}}{4}\|[2, 3]\rangle$	2	$\|[0, 2, 6]\rangle$	4
		3	$\frac{1}{4}\|[0, 6]\rangle - \frac{\sqrt{15}}{4}\|[2, 4]\rangle$	3	$\|[1, 3, 5]\rangle$	6
3	$\|[5]\rangle$	4	$\frac{\sqrt{21}}{8}\|[0, 7]\rangle + \frac{3\sqrt{3}}{8}\|[1, 6]\rangle$	4	$\|[0, 4, 6]\rangle$	8
			$- \frac{1}{8}\|[2, 5]\rangle + \frac{\sqrt{5}}{8}\|[3, 4]\rangle$	5	$\|[0, 2, 8]\rangle$	8
		5	$\frac{\sqrt{2}}{4}\|[0, 8]\rangle - \frac{\sqrt{14}}{4}\|[2, 6]\rangle$	6	$\|[1, 3, 7]\rangle$	10

3 The SCR Algorithm: Symmetrized Coordinate Representation

For simplicity, consider the solutions of Eq. (6) in the internal symmetrized coordinates $\{\xi_1, ..., \xi_{A-1}\} \in \mathbf{R}^{A-1}$, $x_i \in \mathbf{R}^1$, in the case of 1D Euclidean space ($d = 1$). The relevant equation describes an $(A - 1)$-dimensional oscillator with the eigenfunctions $\Phi_j(\xi_1, ..., \xi_{A-1})$ and the energy eigenvalues E_j:

$$\left[\sum_{i=1}^{A-1}\left(-\frac{\partial^2}{\partial\xi_i^2} + (\xi_i)^2\right) - E_j\right]\Phi_j(\xi_1, ..., \xi_{A-1}) = 0, \quad E_j = 2\sum_{k=1}^{A-1} i_k + A - 1, \quad (7)$$

where the numbers i_k, $k = 1, ..., A-1$ are integer, $i_k = 0, 1, 2, 3, ...$ The eigenfunctions $\Phi_j(\xi_1, ..., \xi_{A-1})$ can be expressed in terms of the conventional eigenfunctions of individual 1D oscillators as

$$\Phi_j(\xi_1, ..., \xi_{A-1}) = \sum\nolimits_{2\sum_{k=1}^{A-1} i_k + A - 1 = E_j} \beta_{j[i_1, i_2, ..., i_{A-1}]} \bar{\Phi}_{[i_1, i_2, ..., i_{A-1}]}(\xi_1, ..., \xi_{A-1}), \quad (8)$$

$$\bar{\Phi}_{[i_1, i_2, ..., i_{A-1}]}(\xi_1, ..., \xi_{A-1}) = \prod_{k=1}^{A-1} \bar{\Phi}_{i_k}(\xi_k), \quad \bar{\Phi}_{i_k}(\xi_k) = \frac{\exp(-\xi_k^2/2) H_{i_k}(\xi_k)}{\sqrt[4]{\pi}\sqrt{2^{i_k}}\sqrt{i_k!}},$$

where $H_{i_k}(\xi_k)$ are Hermite polynomials [19]. Generally the energy level $E_f = 2f + A - 1$, $f = \sum_{k=1}^{A-1} i_k$, of an $(A-1)$-dimensional oscillator is known [20] to possess the degeneracy multiplicity $p = (A + f - 2)!/f!/(A-2)!$ with respect to the conventional oscillator eigenfunctions $\bar{\Phi}_{[i_1, i_2, ..., i_{A-1}]}(\xi_1, ..., \xi_{A-1})$. This degeneracy allows further symmetrization by choosing the appropriate coefficients $\beta^{(j)}_{[i_1, i_2, ..., i_{A-1}]}$. Degeneracy multiplicity p of all states with the given energy E_j defined by formula

$$p = \sum\nolimits_{2\sum_{k=1}^{A-1} i_k + A - 1 = E_j} N_\beta, \quad N_\beta = (A-1)!/\prod_{k=1}^{N_\upsilon} \upsilon_k!, \quad (9)$$

where N_β is the number of multiset permutations (m.p.) of $[i_1, i_2, ..., i_{A-1}]$, and $N_\upsilon \le A - 1$ is the number of different values i_k in the multiset $[i_1, i_2, ..., i_{A-1}]$, and υ_k is the number of repetitions of the given value i_k.

Step 1. Symmetrization with respect to permutation of A–1 particles For the states $\Phi^s_j(\xi_1, ..., \xi_{A-1}) \equiv \Phi^s_{[i_1, i_2, ..., i_{A-1}]}(\xi_1, ..., \xi_{A-1})$, symmetric with respect to permutation of $A-1$ particles $i = [i_1, i_2, ..., i_{A-1}]$, the coefficients $\beta_{i[i'_1, i'_2, ..., i'_{A-1}]}$ in Eq. (8) are

$$\beta_{i[i'_1, i'_2, ..., i'_{A-1}]} = \begin{cases} \frac{1}{\sqrt{N_\beta}}, \text{ if } [i'_1, i'_2, ..., i'_{A-1}] \text{ is a m. p. of } [i_1, i_2, ..., i_{A-1}], \\ 0, \quad \text{otherwise.} \end{cases} \quad (10)$$

The states $\Phi^a_j(\xi_1, ..., \xi_{A-1}) \equiv \Phi^a_{[i_1, i_2, ..., i_{A-1}]}(\xi_1, ..., \xi_{A-1})$, antisymmetric with respect to permutation of $A-1$ particles are constructed in a conventional way

$$\Phi^a_j(\xi_1, ..., \xi_{A-1}) = \frac{1}{\sqrt{(A-1)!}} \begin{vmatrix} \bar{\Phi}_{i_1}(\xi_1) & \bar{\Phi}_{i_2}(\xi_1) & \cdots & \bar{\Phi}_{i_{A-1}}(\xi_1) \\ \bar{\Phi}_{i_1}(\xi_2) & \bar{\Phi}_{i_2}(\xi_2) & \cdots & \bar{\Phi}_{i_{A-1}}(\xi_2) \\ \vdots & \vdots & \ddots & \vdots \\ \bar{\Phi}_{i_1}(\xi_{A-1}) & \bar{\Phi}_{i_2}(\xi_{A-1}) & \cdots & \bar{\Phi}_{i_{A-1}}(\xi_{A-1}) \end{vmatrix}, \quad (11)$$

i.e., the coefficients $\beta^{(i)}_{[i'_1, i'_2, ..., i'_{A-1}]}$ in (8) are expressed as

$$\beta^{(i)}_{[i'_1, i'_2, ..., i'_{A-1}]} = \varepsilon_{i'_1, i'_2, ..., i'_{A-1}}/\sqrt{(A-1)!},$$

where $\varepsilon_{i'_1, i'_2, ..., i'_{A-1}}$ is a totally antisymmetric tensor. This tensor is defined as follows: $\varepsilon_{i'_1, i'_2, ..., i'_{A-1}} = +1(-1)$, if $i'_1, i'_2, ..., i'_{A-1}$ is an even (odd) permutation of

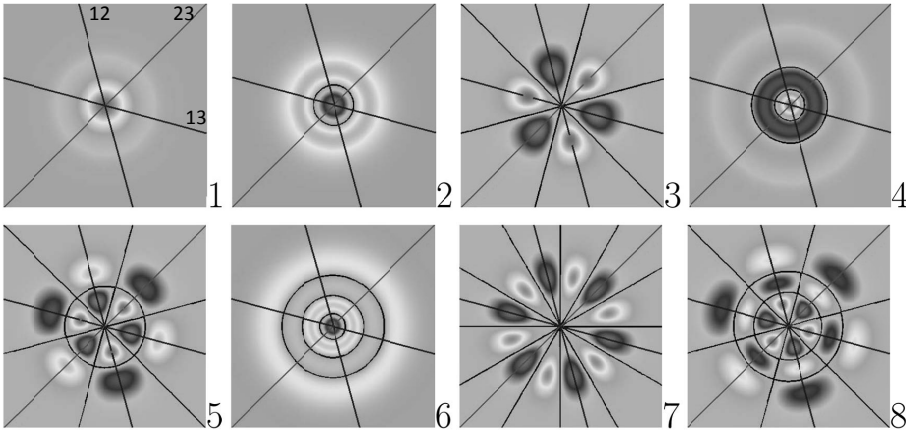

Fig. 1. Profiles of the first eight oscillator S-eigenfunctions $\Phi^S_{[i_1,i_2]}(\xi_1,\xi_2)$, at $A = 3$ in the coordinate frame (ξ_1,ξ_2). The lines correspond to pair collision $x_2 = x_3$, $x_1 = x_2$ and $x_1 = x_3$ of the projection $(x_1,x_2,x_3) \to (\xi_1,\xi_2)$, marked only in the left upper panel with '23', '12', and '13', respectively. The additional lines are nodes of the eigenfunctions $\Phi^S_{[i_1,i_2]}(\xi_1,\xi_2)$.

the numbers $i_1 < i_2 < ... < i_{A-1}$, and $\varepsilon_{i'_1,i'_2,...,i'_{A-1}} = 0$ otherwise, i.e., when some two numbers in the set $i'_1, i'_2, ..., i'_{A-1}$ are equal. Therefore, for antisymmetric states the numbers i_k in Eq. (7) take the integer values $i_k = k-1, k, k+1, ...,$ $k = 1, ..., A-1$.

Here and below s and a are used for the functions, symmetric (antisymmetric) under permutations of $A-1$ relative coordinates, constructed at the first step of the procedure. On the contrary, S and A are used for the functions, symmetric (asymmetric) under permutations of A initial Cartesian coordinates. This is actually the symmetry with respect to permutation of identical particles themselves; in this sense, S and A states may be attributed to boson- and fermion-like particles. However, we prefer to use the S (A) notation as more rigorous.

Step 2. Symmetrization with respect to permutation of A particles

For $A = 2$, the symmetrized coordinate ξ_1 corresponds to the difference $x_2 - x_1$ of Cartesian coordinates, so that a function even (odd) with respect to ξ_1 appears to be symmetric (antisymmetric) with respect to the permutation of two particles $x_2 \leftrightarrow x_1$. Hence, even (odd) eigenfunctions with corresponding eigenvalues $E^s_j = 2(2n)+1$ ($E^a_j = 2(2n+1)+1$) describe S (A) solutions.

For $A \geq 3$, the functions, symmetric (antisymmetric) with respect to permutations of Cartesian coordinates $x_{i+1} \leftrightarrow x_{j+1}$, $i, j = 0, ..., A-1$:

$$\Phi^{S(A)}(..., x_{i+1}, ..., x_{j+1}, ...) \equiv \Phi^{S(A)}(\xi_1(x_1, ..., x_A), ..., \xi_{A-1}(x_1, ..., x_A))$$

$$= \pm\Phi^{S(A)}(..., x_{j+1}, ..., x_{i+1}, ...)$$

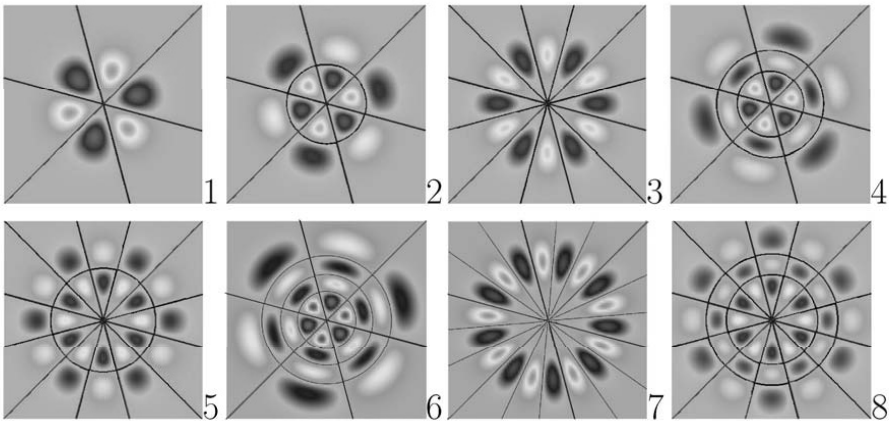

Fig. 2. The same as in Fig. 1, but for the first eight oscillator A-eigenfunctions $\Phi^A_{[i_1,i_2]}(\xi_1,\xi_2)$, at $A=3$

become symmetric (antisymmetric) with respect to permutations of symmetrized coordinates $\xi_i \leftrightarrow \xi_j$, $i,j = 1,...,A-1$:

$$\Phi^{S(A)}(...,\xi_i,...,\xi_j,...) = \pm\Phi^{S(A)}(...,\xi_j,...,\xi_i,...),$$

as follows from Eq. (4). However, the converse statement is not valid,

$$\Phi^{s(a)}(...,\xi_i,...,\xi_j,...) = \pm\Phi^{s(a)}(...,\xi_j,...,\xi_i,...)$$

$$\not\Rightarrow \Phi^{s(a)}(x_1,...,x_{i+1},...) = \pm\Phi^{s(a)}(x_{i+1},...,x_1,...),$$

because we deal with a projection map

$$(\xi_1,...,\xi_{A-1})^T = \hat{C}(x_1,...,x_A)^T, \tag{12}$$

which is implemented by the $(A-1)\times(A)$ matrix $\hat{C}$ with the matrix elements $\hat{C}_{ij} = C_{i+1,j}$, obtained from (3) by cancelling the first row. Hence, the functions, symmetric (antisymmetric) with respect to permutations of symmetrized coordinates, are divided into two types, namely, the S (A) solutions, symmetric (antisymmetric) with respect to permutations $x_1 \leftrightarrow x_{j+1}$ at $j = 1,...,A-1$:

$$\Phi^{S(A)}(x_1,...,x_{j+1},...) = \pm\Phi^{S(A)}(x_{j+1},...,x_1,...)$$

and the other s (a) solutions, $\Phi^{s(a)}(x_1,...,x_{i+1},...) \neq \pm\Phi^{s(a)}(x_{i+1},...,x_1,...)$, which should be eliminated. These requirements are equivalent to only one permutation $x_1 \leftrightarrow x_2$, as follows from (4), which simplifies their practical implementation. With these requirements taken into account in the Gram–Schmidt process, implemented in the *symbolic algorithm SCR*, we obtained the required characteristics of S and A eigenfunctions,

$$\Phi^{S(A)}_i(\xi_1,...,\xi_{A-1}) = \sum_{2\sum_{k=1}^{A-1} i_k + A - 1 = E^{s(a)}_i} \alpha^{S(A)}_{i[i_1,i_2,...,i_{A-1}]} \Phi^{s(a)}_{[i_1,i_2,...,i_{A-1}]}(\xi_1,...,\xi_{A-1}). \tag{13}$$

The algorithm *SCR*:

Input:
A is the number of identical particles;
i_{max} is defined by the maximal value of the energy $E_{i_{max}}$;
$(\xi_1, ..., \xi_{A-1})$ and $(x_1, ..., x_A)$ are the symmetrized and the Cartesian coordinates;

Output:
$\Phi_i^{S(A)}(\xi_1, ..., \xi_{A-1})$ and $\Phi_i^{S(A)}(x_1, ..., x_A)$ are the total symmetric (antisymmetric) functions (13) in the above coordinates connected by (12);

Local:
$E_i^{s(a)} \equiv E_i^{S(A)} = 2\sum_{k=1}^{A-1} i_k + A - 1$ is the $(i+1)^{th}$ eigenenergy;
$i_{min} = 0$ for the symmetric and $i_{min} = (A-1)^2$ for the antisymmetric case;
$\Phi_j \equiv \Phi^{s(a)}_{[i_1,i_2,...,i_{A-1}]}(\xi_1, ..., \xi_{A-1})$ and $\Phi_j \equiv \Phi^{s(a)}_{[i_1,i_2,...,i_{A-1}]}(x_1, ..., x_A)$ are the functions, symmetric (antisymmetric) with respect to $A-1$ Cartesian coordinates;
$p_{s(a)} \equiv p_{i;s(a)}$ and $p_{S(A)} \equiv p_{i;S(A)}$ are the degeneracy factors of the energy levels $E_i^{s(a)}$ and $E_i^{S(A)}$ for s(a) and S(A) functions, respectively;
$p_{i;min}$ ($p_{i;max}$) and $P_{i;min}$ ($P_{i;max}$) are the lowest (highest) numbers of s(a) and S(A) functions, belonging to the energy levels $E_i^{s(a)}$ and $E_i^{S(A)}$, respectively;
$\{\bar{\alpha}_j\}$ and $\{\alpha_{pj}^{S(A)}\}$ are the sets of intermediate and desired coefficients;

1.1 $j := 0$;
for i from i_{min} to i_{max} **do**;
1.2: $p_{i;min} := j + 1$;
1.3: **for each** sorted $i_1, i_2, ..., i_{A-1}$, $2\sum_{k=1}^{A-1} i_k + A - 1 = E_i^{s(a)}$ **do**
$j := j + 1$;
construction $\Phi_j(\xi_1, ..., \xi_{A-1}) = \Phi_j^s(\xi_1, ..., \xi_{A-1})$ from (8), (10)
or $\Phi_j(\xi_1, ..., \xi_{A-1}) = \Phi_j^a(\xi_1, ..., \xi_{A-1})$ from (11)
$\Phi_j(x_1, ..., x_A) =$subs$((\xi_1, ..., \xi_{A-1}) \to (x_1, ..., x_A), \Phi_j(\xi_1, ..., \xi_{A-1}))$;
end for
1.4: $p_{i;max} := j$; $\quad p_{i;s(a)} = p_{i;max} - p_{i;min} + 1$;
end for

2.1.:$P_{min} = 1$;
for i from i_{min} to i_{max} **do**
2.2.:$P_{i;min} = P_{min}$;
2.3.:$\Phi(\xi_1, ..., \xi_{A-1}) = \sum_{j=p_{i;min}}^{p_{i;max}} \bar{\alpha}_j \Phi_j(\xi_1, ..., \xi_{A-1})$;
$\Phi(x_1, ..., x_A) = \sum_{j=p_{i;min}}^{p_{i;max}} \bar{\alpha}_j \Phi_j(x_1, ..., x_A)$;
2.4.: $\Phi(x_2, x_1, ..., x_A) :=$change$(x_1 \leftrightarrow x_2, \Phi(x_1, x_2, ..., x_A)))$;
2.5.: $\Phi(x_2, x_1, ..., x_A) \mp \Phi(x_1, x_2, ..., x_A) = 0$,
$\to \quad (\bar{\alpha}_{pj}, j = p_{i;min}, ..., p_{i;max}, p = 1, ..., p_{i;S(A)})$;
2.6.:$P_{i;max} = P_{i;min} - 1 + p_{i;S(A)}$;
2.7.: Gram–Schmidt procedure for $\Phi(\xi_1, ..., \xi_{A-1}) \quad \to$
$\Phi_p^{S(A)}(x_1, x_2, ..., x_A) = \sum_{j=p_{i;min}}^{p_{i;max}} \alpha_{pj}^{S(A)} \Phi_j(x_1, x_2, ..., x_A)$;
$\Phi_p^{S(A)}(\xi_1, ..., \xi_{A-1}) = \sum_{j=p_{i;min}}^{p_{i;max}} \alpha_{pj}^{S(A)} \Phi_j(\xi_1, ..., \xi_{A-1})$,
at $p = P_{i;min}, ..., P_{i;max}$;
end for

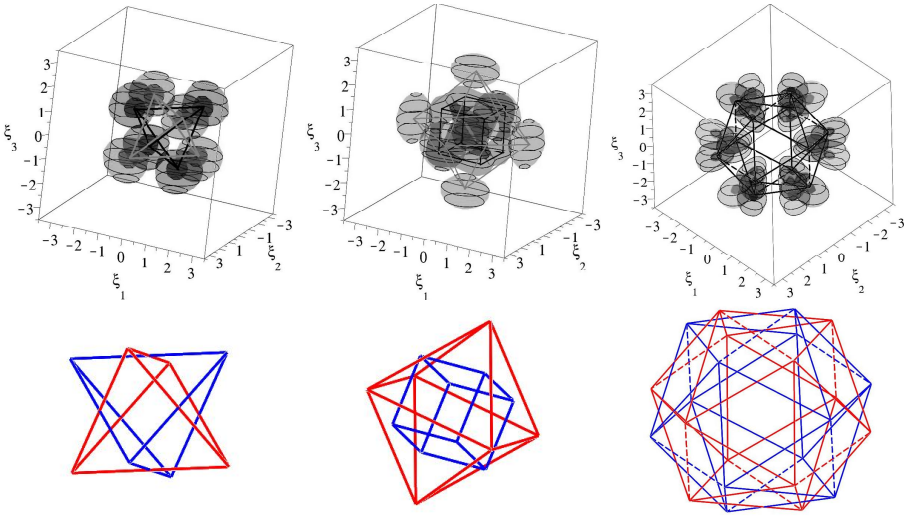

Fig. 3. Upper panel: Profiles of the oscillator S-eigenfunctions $\Phi^S_{[1,1,1]}(\xi_1,\xi_2,\xi_3)$, $\Phi^S_{[0,0,4]}(\xi_1,\xi_2,\xi_3)$ and A-eigenfunction $\Phi^A_{[0,2,4]}(\xi_1,\xi_2,\xi_3)$, at $A=4$ (left, middle, and right panels, respectively). Some maxima and minima positions of these functions are connected by black and gray lines and duplicated in lower panels: two tetrahedrons forming a *stella octangula* for $\Phi^S_{[1,1,1]}(\xi_1,\xi_2,\xi_3)$, a cube and an octahedron for $\Phi^S_{[0,0,4]}(\xi_1,\xi_2,\xi_3)$, and a polyhedron with 20 triangle faces (only 8 of them being equilateral triangles) for $\Phi^A_{[0,2,4]}(\xi_1,\xi_2,\xi_3)$.

4 Examples of the SCR Generation

The SCR algorithm was implemented in MAPLE 14 on Intel Core i5 CPU 660 3.33GHz, 4GB 64 bit, to generate first 11 symmetric (antisymmetric) functions up to $\Delta E_j = 12$ at $A = 6$ with CPU time 10 seconds (600 seconds), that together with a number of functions in dependence of number of particles given in Table 3 demonstrates efficiency and complexity of the algorithm.

The examples of generated total symmetric and antisymmetric $(A-1)$-dimensional oscillator functions are presented in Tables 1 and 2. Note that for $A=4$, the first four states from Table 1 are similar to those of the translation-invariant model without excitation of the center-of-mass variable [3].

As an example, in Figs. 1 and 2 we show isolines of the first eight S and A oscillator eigenfunctions $\Phi^S_{[i_1,i_2]}(\xi_1,\xi_2)$ and $\Phi^A_{[i_1,i_2]}(\xi_1,\xi_2)$ for $A=3$, calculated at the second step of the algorithm. One can see that the S (A) oscillator eigenfunctions are symmetric (antisymmetric) with respect to reflections from three straight lines. The first line (labelled '23') corresponds to the permutation (x_2,x_3) and is rotated by $\pi/4$ counterclockwise with respect to the axis ξ_1. The second and the third lines (labelled '12' and '13') correspond to the permutations (x_1,x_2) and (x_1,x_3) and are rotated by $\pi/3$ clockwise and counterclockwise with respect to the first line. These lines divide the plane into six sectors, while the symmetric (antisymmetric) oscillator eigenfunctions, calculated at the first

Table 3. The degeneracy multiplicities p from (9), $p_s = p_a$ and $p_S = p_A$ of s-, a-, S-, and A-eigenfunctions of the oscillator energy levels $\Delta E_j = E_j^{\bullet} - E_1^{\bullet}$, $\bullet = \emptyset, s, a, S, A$

A=3			A=4			A=5			A=6			ΔE_j
p	p_s, p_a	p_S, p_A	p	p_s, p_a	p_S, p_A	p	p_s, p_a	p_S, p_A	p	p_s, p_a	p_S, p_A	
1	1	1	1	1	1	1	1	1	1	1	1	0
2	1	0	3	1	0	4	1	0	5	1	0	2
3	2	1	6	2	1	10	2	1	15	2	1	4
4	2	1	10	3	1	20	3	1	35	3	1	6
5	3	1	15	4	2	35	5	2	70	5	2	8
6	3	1	21	5	1	56	6	2	126	7	2	10
7	4	2	28	7	3	84	9	3	210	10	4	12

step of the algorithm, which are symmetric (or antisymmetric) with respect to reflections from the first line, generate the division of the plane into two parts. This illustrates the isomorphism between the symmetry group of an equilateral triangle D_3 in $\mathbf{R}^2$ and the 3-body permutation group S_3 (A = 3).

Figure 3 shows examples of profiles of S and A oscillator eigenfunctions for $A = 4$. Note that four maxima (black) and four minima (grey) of the S eigenfunction $\Phi^S_{[1,1,1]}(\xi_1, \xi_2, \xi_3)$ are positioned at the vertices of two tetrahedrons forming a *stella octangula*, with the edges shown by black and grey lines, respectively. Eight maxima and six outer minima for S eigenfunction $\Phi^S_{[0,0,4]}(\xi_1, \xi_2, \xi_3)$ are positioned at the vertices of a cube and an octahedron, the edges of which are shown by black and grey lines, respectively. The positions of twelve maxima of the A oscillator eigenfunction, $\Phi^A_{[0,2,4]}(\xi_1, \xi_2, \xi_3)$ coincide with the vertices of a polyhedron with 20 triangle faces (only 8 of them being equilateral triangles) and 30 edges, 6 of them having the length 2.25 and the other having the length 2.66. The above shapes of eigenfunctions illustrate the isomorphism between the tetrahedron group T_d in $\mathbf{R}^3$ and the 4-particle permutation group S_4 (A = 4), discussed in [2] in the case of $d = 3$.

The degeneracy multiplicity (9), i.e., number p of all states with the given energy E_j of low part of spectra, the numbers p_s (p_a) of the states, symmetric (antisymmetric) under permutations of $A-1$ relative coordinates together with the total numbers p_S (p_A) of the states, symmetric (antisymmetric) under permutations of A initial Cartesian coordinates are summarized in Table 3. Note that the S and A states with $E' = E_1^{S,A} + 2$ do not exist. The numbers p_s (p_a) are essentially smaller than the total number p of all states, which simplifies the procedure of constructing S (A) states with possible excitation of the center-of-mass degree of freedom and allows the use of a compact basis with the reduced degeneracy p_S (p_A) of the S (A) states in our final calculations. For clarity, in the case $A = 3$, $d = 1$, the S(A)-type functions generated by the *SCR* algorithm, in polar coordinates $\xi_1 = \rho\cos\varphi$, $\xi_2 = \rho\sin\varphi$ are expressed as:

$$\Phi^{S(A)}_{k,m}(\rho,\varphi) = C_{km}(\rho^2)^{3m/2}\exp(-\rho^2/2)L_k^{3m}(\rho^2)\begin{matrix}\cos\\ \sin\end{matrix}(3m(\varphi+\pi/12)),$$

where C_{km} is the normalization constant, $L_k^{3m}(\rho^2)$ are the Laguerre polynomials [19], $k = 0, 1, ..., m = 0, 1, ...$ for S states, while $m = 1, 2, ...$ for A states, that are

classified by irr of the D_{3m}-symmetry group. The corresponding energy levels $E^{S(A)}_{k,m} = 2(2k+3m+1) = E^{s(a)}_{[i_1,i_2]} = 2(i_1+i_2+1)$ have the degeneracy multiplicity $K+1$, if the energy $E^{S(A)}_{k,m} - E^{S(A)}_1 = 12K + K'$, where $K' = 0, 4, 6, 8, 10, 14$. For example, in Figs. 1 and 2 we show the wave functions $\Phi^S_{3,0}(\rho, \varphi)$ and $\Phi^S_{0,2}(\rho, \varphi)$ (or $\Phi^A_{3,1}(\rho, \varphi)$ and $\Phi^A_{0,3}(\rho, \varphi)$) labelled with 6 and 7, corresponding to the energy levels $E^{S(A)}_{k,m} - E^{S(A)}_1 = 12$ with the degeneracy $K = 2$, while the functions labelled with $1, 2, 3, 4, 5, 8$ are nondegenerate ($K = 1$). So, the eigenfunctions of the A-identical particle system in one dimension are degenerate in accordance with [21], and this result disagrees with nondegenerate ansatz solutions [10].

5 Conclusion

We considered a model of A identical particles bound by the oscillator-type potential under the influence of the external field of a target in the new symmetrized coordinates. The constructive SCR algorithm of symmetrizing or antisymmetrizing the $A-1$-dimensional harmonic oscillator basis functions with respect to permutations of A identical particles was described. One can see that the transformations of $(A-1)$-dimensional oscillator basis functions from the symmetrized coordinates to the Jacobi coordinates, reducible to permutations of coordinates and $(A-1)$-dimensional finite rotation (5), are implemented by means of the $(A-1)$-dimensional oscillator Wigner functions [23]. Typical examples were analyzed, and a correspondence between the representations of the symmetry groups D_3 and T_d for $A = 3$ and $A = 4$ shapes is displayed. It is shown that one can use the presented SCR algorithm, implemented using the MAPLE computer algebra system, to construct the basis functions in the closed analytical form. However, for practical calculations of matrix elements between the basis states, belonging to the lower part of the spectrum, this is not necessary. The application of the developed approach and algorithm for solving the problem of tunnelling clusters through barrier potentials of a target is considered in our forthcoming paper [22]. The proposed approach can be adapted to the analysis of tetrahedral-symmetric nuclei, quantum diffusion of molecules and micro-clusters through surfaces, and the fragmentation in producing neutron-rich light nuclei.

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