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

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The statement of the problem

The Schrödinger equation for the problem of penetration of A identical spinless quantum particles

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{A}\frac{\partial^2}{\partial\tilde{x}_i^2}+\sum_{i,j=1;i<j}^{A}\tilde{V}^{pair}(\tilde{x}_{ij})+\sum_{i=1}^{A}\tilde{V}(\tilde{x}_i)-\tilde{E}\right]\tilde{\Psi}(\tilde{x}_1,\ldots,\tilde{x}_A;\tilde{E})=0.$$

m are masses of particles, $\tilde{E}$ is total energy of system of A particles
$\tilde{P}^2=2m\tilde{E}/\hbar^2$, $\tilde{P}$ is total momentum of system of A particles
$x_i \in \mathbf{R}^d$ are Cartesian coordinates in d-dimensional Euclidian space
$\tilde{\mathbf{x}}=(\tilde{x}_1,\ldots,\tilde{x}_A)\in\mathbf{R}^{A\times d}$ in $A\times d$-dimensional configuration space

$\tilde{V}^{pair}(\tilde{x}_{ij})$ is the pair potential,
$\tilde{x}_{ij}=\tilde{x}_i-\tilde{x}_j$,
for example, $\tilde{V}^{pair}(\tilde{x}_{ij})=\tilde{V}^{hosc}(\tilde{x}_{ij})$;
i.e. $\tilde{V}^{hosc}(\tilde{x}_{ij})=\frac{m\omega^2}{2A}(\tilde{x}_{ij})^2$ is HOP with frequency $\omega/\sqrt{A}$,
$\tilde{V}(\tilde{x}_i)$ potentials of the repulsive potential barriers.

The statement of the problem

Oscillator units

$x_{osc} = \sqrt{\hbar/(m\omega)}$
$p_{osc} = x_{osc}^{-1}$
$E_{osc} = \hbar\omega/2$

$E = \tilde{E}/E_{osc}, \; P^2 = E,$
$P = \tilde{P}/p_{osc} = \tilde{P}x_{osc},$
$x_i = \tilde{x}_i/x_{osc},$
$x_{ij} = \tilde{x}_{ij}/x_{osc} = x_i - x_j.$

$V^{pair}(x_{ij}) = \tilde{V}^{pair}(x_{ij}x_{osc})/E_{osc},$
$V^{hosc}(x_{ij}) = \tilde{V}^{hosc}(x_{ij}x_{osc})/E_{osc} = \frac{1}{A}(x_{ij})^2,$
$V(x_i) = \tilde{V}(x_i x_{osc})/E_{osc}.$
.

SE in Oscillator units

$$\left[-\sum_{i=1}^{A}\frac{\partial^2}{\partial x_i^2} + \sum_{i,j=1;i<j}^{A}\frac{1}{A}(x_{ij})^2 + \sum_{i,j=1;i<j}^{A}U^{pair}(x_{ij}) + \sum_{i=1}^{A}V(x_i) - E\right]\Psi(x_1, ..., x_A; E) = 0.$$

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 $U^{pair}(x_{ij}) = 0$.

The problem under consideration is to find the solutions of SE that are totally symmetric (or antisymmetric) with respect to the permutations of A particles, i.e. the permutations of coordinates $x_i \leftrightarrow x_j$ at $i, j = 1, ..., A$, or symmetry operations of permutation group S_n.

Jacobi coordinates

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{A-1} \\ y_A \end{pmatrix} = J \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{A-1} \\ x_A \end{pmatrix}, \quad \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{A-1} \\ x_A \end{pmatrix} = J^T \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{A-1} \\ y_A \end{pmatrix},$$

Jacobi coordinates [P. Kramer and M. Moshinsky, Nucl. Phys. 82, 241 (1966).]

$$J = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 & 0 & \cdots & 0 \\ 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} & 0 & \cdots & 0 \\ 1/\sqrt{12} & 1/\sqrt{12} & 1/\sqrt{12} & -3/\sqrt{12} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{(A-1)A}} & \frac{1}{\sqrt{(A-1)A}} & \frac{1}{\sqrt{(A-1)A}} & \frac{1}{\sqrt{(A-1)A}} & \cdots & -\frac{A-1}{\sqrt{(A-1)A}} \\ 1/\sqrt{A} & 1/\sqrt{A} & 1/\sqrt{A} & 1/\sqrt{A} & \cdots & 1/\sqrt{A} \end{pmatrix},$$

Properties of Jacobi coordinates

The inverse coordinate transformation is implemented using the transposed matrix

$$J^{-1} = J^T = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{6} & 1/\sqrt{12} & \cdots & 1/\sqrt{(A-1)A} & 1/\sqrt{A} \\ -1/\sqrt{2} & 1/\sqrt{6} & 1/\sqrt{12} & \cdots & 1/\sqrt{(A-1)A} & 1/\sqrt{A} \\ 0 & -2/\sqrt{6} & 1/\sqrt{12} & \cdots & 1/\sqrt{(A-1)A} & 1/\sqrt{A} \\ 0 & 0 & -3/\sqrt{12} & \cdots & 1/\sqrt{(A-1)A} & 1/\sqrt{A} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -(A-1)/\sqrt{(A-1)A} & 1/\sqrt{A} \end{pmatrix},$$

i.e., J is an orthogonal matrix with pairs of complex conjugate eigenvalues, the absolute values of which are equal to one; $\sum_{i=1}^{A}(y_i \cdot y_i) = \sum_{i=1}^{A}(x_i \cdot x_i) = R^2 \mapsto \sum_{i,j=1}^{A}(x_{ij})^2 = 2A\sum_{i=1}^{A}(y_i)^2 - 2(\sum_{i=1}^{A} x_i)^2 = 2A\sum_{i=1}^{A-1}(y_i)^2$.

$$\left[-\frac{\partial^2}{\partial y_A^2} + \sum_{i=1}^{A-1}\left[-\frac{\partial^2}{\partial y_i^2} + (y_i)^2\right] + U(y_1, ..., y_A) - E\right]\Psi(y_1, ..., y_A; E) = 0,$$

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

Symmetrized coordinates

$$\begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \vdots \\ \xi_{A-2} \\ \xi_{A-1} \end{pmatrix} = C \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{A-1} \\ x_A \end{pmatrix}, \quad \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{A-1} \\ x_A \end{pmatrix} = C \begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \vdots \\ \xi_{A-2} \\ \xi_{A-1} \end{pmatrix},$$

$$C = \frac{1}{\sqrt{A}} \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & a_1 & a_0 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_1 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_0 & a_1 & \cdots & a_0 & a_0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & a_0 & a_0 & a_0 & \cdots & a_1 & a_0 \\ 1 & a_0 & a_0 & a_0 & \cdots & a_0 & a_1 \end{pmatrix}, \qquad \begin{aligned} a_0 &= 1/(1-\sqrt{A}) < 0, \\ a_1 &= a_0 + \sqrt{A} > 0. \end{aligned}$$

Properties of symmetrized coordinates

The inverse coordinate transformation is performed using the same matrix $C^{-1} = C$, $C^2 = I$,

$$C^{-1} = C^T = C = \frac{1}{\sqrt{A}} \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & a_1 & a_0 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_1 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_0 & a_1 & \cdots & a_0 & a_0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & a_0 & a_0 & a_0 & \cdots & a_1 & a_0 \\ 1 & a_0 & a_0 & a_0 & \cdots & a_0 & a_1 \end{pmatrix}, \qquad \begin{array}{l} a_0 = 1/(1-\sqrt{A}) < 0, \\ a_1 = a_0 + \sqrt{A} > 0. \end{array}$$

i. e. $C = C^T$ is a symmetric orthogonal matrix with the eigenvalues $\lambda_1 = -1$, $\lambda_{2,\ldots,A} = 1$
$\sum_{i=0}^{A-1}(\xi_i \cdot \xi_i) = \sum_{i=1}^{A}(x_i \cdot x_i) = R^2 \mapsto \sum_{i,j=1}^{A}(x_{ij})^2 = 2A\sum_{i=1}^{A-1}(\xi_i)^2$.

At $A = 2$ similar to Jacobi coordinates (in form of [G.P. Kamuntavičius et al, Nucl. Phys. A 695, 191 (2001)])
At $A = 4$ similar to [D. W. Jepsent and J. O. Hirschfelder, Proc. Natl. Acad. Sci. U.S.A. 45, 249 (1959); P. Kramer and M. Moshinsky, Nucl. Phys. 82, 241 (1966)]

The relative coordinates $x_{ij} \equiv x_i - x_j$ of a pair of particles i and j

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

SE in the symmetrized coordinates

$$\left[-\frac{\partial^2}{\partial \xi_0^2} + \sum_{i=1}^{A-1} \left[-\frac{\partial^2}{\partial \xi_i^2} + (\xi_i)^2 \right] + U(\xi_0, ..., \xi_{A-1}) - E \right] \Psi(\xi_0, ..., \xi_{A-1}; E) = 0,$$

$$U(\xi_0, ..., \xi_{A-1}) = \sum_{i,j=1;i<j}^{A} U^{pair}(x_{ij}(\xi_1, ..., \xi_{A-1})) + \sum_{i=1}^{A} V(x_i(\xi_0, ..., \xi_{A-1})),$$

which is invariant with respect to permutations $\xi_i \leftrightarrow \xi_j$ at $i,j = 1,...,A-1$ as follows from the invariance SE with respect to permutation $x_i \leftrightarrow x_j$ at $i,j = 1,...,A$ is preserved.

However, the direct converse is not true.

The symmetrized coordinates are related with the Jacobi ones as

$$
\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{A-1} \\ y_A \end{pmatrix} = B \begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \vdots \\ \xi_{A-2} \\ \xi_{A-1} \end{pmatrix}, \quad B = JC = \begin{pmatrix} 0 & b_1^0 & b_1^- & b_1^- & b_1^- & \cdots & b_1^- & b_1^- \\ 0 & b_2^+ & b_2^0 & b_2^- & b_2^- & \cdots & b_2^- & b_2^- \\ 0 & b_3^+ & b_3^+ & b_3^0 & b_3^- & \cdots & b_3^- & b_3^- \\ 0 & b_4^+ & b_4^+ & b_4^+ & b_4^0 & \cdots & b_4^- & b_4^- \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & b_{A-1}^+ & b_{A-1}^+ & b_{A-1}^+ & b_{A-1}^0 & \cdots & b_{A-1}^+ & b_{A-1}^0 \\ 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix},
$$

$b_s^+ = 1/((\sqrt{A}-1)\sqrt{s(s+1)})$,
$b_s^- = \sqrt{A}/((\sqrt{A}-1)\sqrt{s(s+1)})$, 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, $y_A = \xi_0$, while the relative coordinates are related via the $(A-1)\times(A-1)$ matrix M having the matrix elements $M_{ij} = B_{i,j+1}$.
The inverse transformation is given by the matrix $B^{-1} = (JC)^{-1} = CJ^T = B^T$, i.e., B is also an orthogonal matrix.

$A = 3$

Note, that at the Jacobi coordinates

$$y_1 = \frac{1}{\sqrt{2}}(x_1 - x_2), \quad y_2 = \frac{1}{\sqrt{6}}(x_1 + x_2 - 2x_3)$$

are related with the symmetrized ones

$$\xi_1 = \frac{1}{\sqrt{3}}(x_1 + \frac{\sqrt{3}-1}{2}x_2 - \frac{\sqrt{3}+1}{2}x_3), \quad \xi_2 = \frac{1}{\sqrt{3}}(x_1 - \frac{\sqrt{3}+1}{2}x_2 + \frac{\sqrt{3}-1}{2}x_3)$$

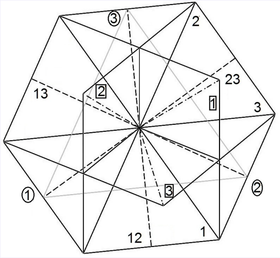
by the orthogonal matrix M:

$$M = \begin{pmatrix} b_1^0 & b_1^- \\ b_2^+ & b_2^0 \end{pmatrix} = \begin{pmatrix} (\sqrt{6}-\sqrt{2})/4 & (\sqrt{6}+\sqrt{2})/4 \\ (\sqrt{6}+\sqrt{2})/4 & -(\sqrt{6}-\sqrt{2})/4 \end{pmatrix} = \begin{pmatrix} \sin\phi_1 & \cos\phi_1 \\ \cos\phi_1 & -\sin\phi_1 \end{pmatrix} =$$
$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos\phi_1 & -\sin\phi_1 \\ \sin\phi_1 & \cos\phi_1 \end{pmatrix} = \begin{pmatrix} \cos\phi_1 & \sin\phi_1 \\ -\sin\phi_1 & \cos\phi_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = M_1(\phi_1)M_0. \quad (1)$$

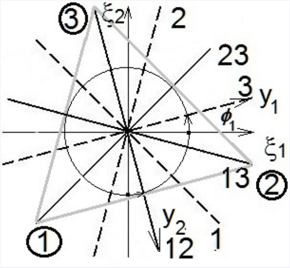
i.e. by permutation of coordinates $(\xi_1, \xi_2) \to (\xi_2, \xi_1)$ and counterclockwise rotation by the angle $\phi_1 = \pi/12$.

This transformation illustrates isomorphism between symmetry operations of the equilateral triangle group D_3 in $\mathbf{R}^2$ and the permutation group S_3, on three objects ($A = 3$), like [V.S. Buslaev et al, Phys. Atom. Nucl. (2013) accepted.].

$A = 3$



The coordinate planes 1, 2, 3, labelled with boxes, the center-of-mass plane in R^3, and the lines of intersection of these planes with the pair-collision planes $x_i = x_j$, corresponding to pair-collision lines $\{x_i = x_j, x_1 + x_2 + x_3 = 0\}$ (labelled 12, 23, 13) in the center-of-mass plane $x_1 + x_2 + x_3 = 0$, belonging to R^2.



The equilateral triangle showing the isomorphism between the group of its symmetry operations D_3 in R^2 and the group of permutations S_3 of three objects 1, 2, 3, labelled with circles. The symmetric (ξ_1, ξ_2) and Jacobi (y_1, y_2) coordinates, related via the transformation (1) in the center-of-mass plane R^2, respectively.

$A = 4$

The Jacobi coordinates

$$y_1 = \frac{1}{\sqrt{2}}(x_1 - x_2), \quad y_2 = 1/\sqrt{6}(x_1 + x_2 - 2x_3), \quad y_3 = 1/\sqrt{12}(x_1 + x_2 + x_3 - 3x_4)$$

are related with the symmetrized ones

$$\xi_1 = 1/2(x_1 + x_2 - x_3 - x_4), \quad \xi_2 = 1/2(x_1 - x_2 + x_3 - x_4), \quad \xi_3 = 1/2(x_1 - x_2 - x_3 + x_4)$$

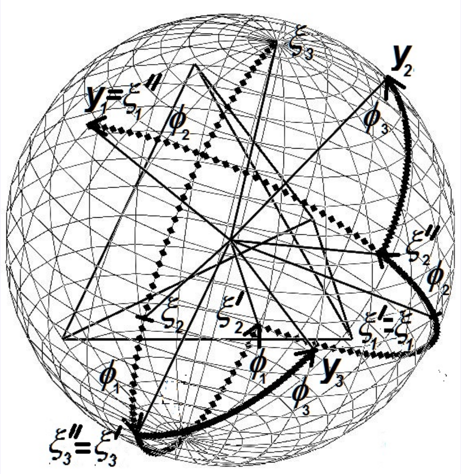
by the orthogonal matrix M:

$$M = \begin{pmatrix} b_1^0 & b_1^- & b_1^- \\ b_2^+ & b_2^0 & b_2^- \\ b_3^+ & b_3^+ & b_3^0 \end{pmatrix} = \begin{pmatrix} 0 & \sqrt{2}/2 & \sqrt{2}/2 \\ \sqrt{6}/3 & -\sqrt{6}/6 & \sqrt{6}/6 \\ \sqrt{3}/3 & \sqrt{3}/3 & -\sqrt{3}/3 \end{pmatrix}.$$

$A = 4$

One of the possible decompositions $M = M_3(\phi_3)M_2(\phi_2)M_1(\phi_1)$ of this matrix is

$$M = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi_3 & \sin\phi_3 \\ 0 & -\sin\phi_3 & \cos\phi_3 \end{pmatrix} \times \begin{pmatrix} \cos\phi_2 & \sin\phi_2 & 0 \\ -\sin\phi_2 & \cos\phi_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \times \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi_1 & \sin\phi_1 \\ 0 & -\sin\phi_1 & \cos\phi_1 \end{pmatrix}.$$



This transformation is a product of three counterclockwise rotations: the first of them by the angle $\phi_1 = 3\pi/4$ about the first old axis, the second one by the angle $\phi_2 = \pi - \arctan(\sqrt{2}) \approx 16\pi/23$ about the third new axis, and the third one by the angle $\phi_3 = \pi/3$ about the first new axis.

Basis tranformation

$A = 3$

Clockwise rotation of the coordinate system (ξ_2, ξ_1) to (y_1, y_2) by the angle $\phi_1 = \pi/12$ induces the transformation of corresponding $A = 2$-oscillator functions

$$< y_1, y_2 | j + m', j - m' >= \sum_{m=-j}^{m=j} d^j_{m'm}(2\phi_1) < \xi_2, \xi_1 | j + m, j - m > .$$

Here $d^j_{m'm}(2\phi_1) = N^j_{m'm} \sin^{|m'-m|} \phi_1 \cos^{|m'+m|} \phi_1 P^{|m'-m|,|m'+m|}_{j-(|m'-m|+|m'+m|)/2}(\cos(2\phi_1))$ are the Wigner functions, $P^{\mu\nu}_s(x)$ are Jacobi polynomials, or

$$\iint_{-\infty}^{\infty} d\xi_2 d\xi_1 < j + m, j - m | \xi_2, \xi_1 >< \xi_2 \cos\phi + \xi_1 \sin\phi, -\xi_2 \sin\phi + \xi_1 \cos\phi | j + m', j - m' > .$$

General case

The transformations of $(A-1)$-dimensional oscillator functions induced by operators of permutation of $A-1$ coordinates and $(A-1)$-dimensional finite rotation, defined as a product of $(A-1)(A-2)/2$ rotations in separate coordinate planes, can be constructed using the diagram method, which reduces the analytic calculations of the $(A-1)$-dimensional oscillator Wigner functions [G. S. Pogosyan, Ya. A. Smorodinsky, and V. M. Ter-Antonyan, J. Phys. A 14, 769 (1981)] to simple geometric operations, similar to the graph method for calculating the Clebsh-Gordan coefficients.

Symmetrized coordinates representation in 1D Euclidian space ($d = 1$)

Eq for $(A-1)$-dimensional oscillator with known eigenfunctions $\Phi_j(\xi_1, ..., \xi_{A-1})$ and eigenenergies E_j

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

where the indices i_k, $k = 1, ..., A-1$ take integer values $i_k = 0, 1, 2, 3, ...$

We define the SCR in the form of linear combinations of the conventional oscillator eigenfunctions $\bar{\Phi}_{[i_1, i_2, ..., i_{A-1}]}(\xi_1, ..., \xi_{A-1})$:

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

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

where $H_{i_k}(\xi_k)$ are Hermite polynomials.

Symmetrization with respect to permutation of $A-1$ particles

The states, symmetric with respect to permutation of $A-1$ particles $i=[i_1,i_2,...,i_{A-1}]$

$$\beta^{(i)}_{[i'_1,i'_2,\ldots,i'_{A-1}]} = \begin{cases} 1/\sqrt{N_\beta}, & [i'_1,i'_2,...,i'_{A-1}] \text{ is a multiset permutation of } [i_1,i_2,...,i_{A-1}], \\ 0, & \text{otherwise.} \end{cases}$$

Here $N_\beta=(A-1)!/\prod_{k=1}^{N_\upsilon}\upsilon_k!$ is the number of multiset permutations of $[i_1,i_2,...,i_{A-1}]$, $N_\upsilon\le A-1$ 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.

The states, antisymmetric with respect to permutation of $A-1$ particles

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

i.e., $\beta^{(i)}_{[i'_1,i'_2,\ldots,i'_{A-1}]}=\varepsilon_{i'_1,i'_2,\ldots,i'_{A-1}}/\sqrt{(A-1)!}$ where $\varepsilon_{i'_1,i'_2,\ldots,i'_{A-1}}$ is a totally antisymmetric tensor.

Symmetrization with respect to permutation of A particles

Case $A = 2$ ($\xi_1 = (x_2 - x_1)/\sqrt{2}$)

Function being even (or odd) with respect to ξ_1 appears to be symmetric (or antisymmetric) with respect to permutation of two particles, i.e. $x_2 \leftrightarrow x_1$.

Case $A \geq 3$

The functions, symmetric (or antisymmetric) with respect to permutations in Cartesian coordinates $x_i \leftrightarrow x_j$, $i, j = 1, ..., A$ become symmetric (or antisymmetric) with respect to permutations of symmetrized coordinates $\xi_i \leftrightarrow \xi_j$, at
$i', j' = 1, ..., A - 1$
$\Phi(..., x_i, ..., x_j, ...) = \pm\Phi(..., x_j, ..., x_i, ...) \to \Phi(..., \xi_{i'}, ..., \xi_{j'}, ...) = \pm\Phi(..., \xi_{j'}, ..., \xi_{i'}, ...)$.

Here and below we use the above property of the symmetrized coordinates

$$x_{ij} \equiv x_i - x_j = \xi_{i-1} - \xi_{j-1} \equiv \xi_{i-1,j-1}, \quad i, j = 2, ..., A, \quad x_1 = \frac{1}{\sqrt{A}} \sum_{i'=0}^{A-1} \xi_{i'}.$$

Symmetrization with respect to permutation of A particles

However, the converse is not true, because we deal with a projection map:

$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \cdots \\ \xi_{A-1} \end{pmatrix} = \begin{pmatrix} 1 & a_1 & a_0 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_1 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_0 & a_1 & \cdots & a_0 & a_0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & a_0 & a_0 & a_0 & \cdots & a_1 & a_0 \\ 1 & a_0 & a_0 & a_0 & \cdots & a_0 & a_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \cdots \\ x_{A-1} \\ x_A \end{pmatrix}$$

Thus, the functions, symmetric (or antisymmetric) with respect to permutations of symmetrized coordinates (i.e. by permutations $x_i \leftrightarrow x_j$ at $i, j = 2, ..., A$), are divided into two types, namely,
the physical symmetric (antisymmetric) solutions, symmetric (or antisymmetric) with respect to permutations $x_1 \leftrightarrow x_{j+1}$ at $j = 1, ..., A-1$
$\Phi(x_1, ..., x_{i+1}, ...) = \pm\Phi(x_{i+1}, ..., x_1, ...)$,
and the nonphysical solutions, $\Phi(x_1, ..., x_{i+1}, ...) \neq \pm\Phi(x_{i+1}, ..., x_1, ...)$, which should be eliminated.
This step is equivalent to only one permutation $x_1 \leftrightarrow x_2$, that simplifies its practical implementation.

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 in the symmetrized and in the Cartesian coordinates;

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;

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 $\Phi_j(\xi_1, ..., \xi_{A-1}) = \Phi_j^{s(a)}(\xi_1, ..., \xi_{A-1})$

$\Phi_j(x_1, ..., x_A) =$subs$((\xi_1, ..., \xi_{A-1}) \rightarrow (x_1, ..., x_A), \Phi_j(\xi_1, ..., \xi_{A-1}))$;

end for

1.4: $p_{i;max} := j$; $p_{i;s(a)} = p_{i;max} - p_{i;min} + 1$;

end for

Local

$i_{min} = 0$ 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;
$p_{s(a)} \equiv p_{i;s(a)}$ are the degeneracy factors of the energy levels $E_i^{s(a)}$ for s(a) functions;
$p_{i;min}$ ($p_{i;max}$)are the lowest (highest) numbers of s(a) functions, belonging to the energy levels $E_i^{s(a)}$;

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.: $\Phi(x_2, x_1, ..., x_A) \mp \Phi(x_1, x_2, ..., x_A) = 0, \rightarrow (\bar{\alpha}_{pj}, j = p_{i;min}, ..., p_{i;max}, p = 1, ..., p_{i;S(A)})$;

2.6.:$P_{i;max} = P_{i;min} - 1 + p_{i;S(A)}$;

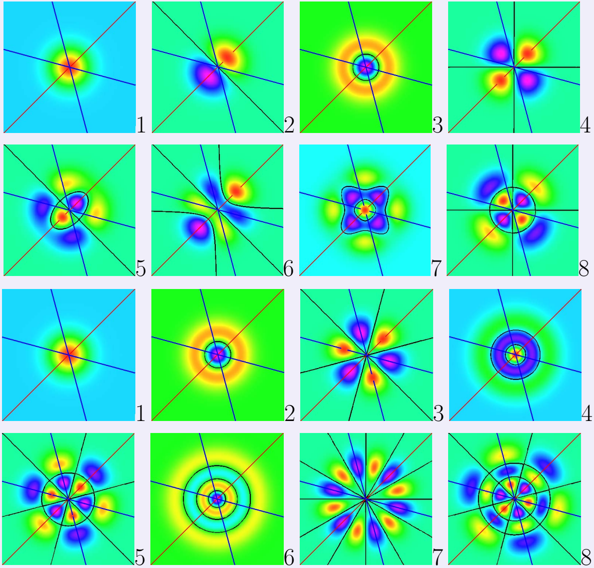
2.7.: Gram–Schmidt procedure for $\Phi(\xi_1, ..., \xi_{A-1})$ $(p = P_{i;min}, ..., P_{i;max}) \rightarrow$

$\Phi_p^{S(A)}(x_1, x_2, ..., x_A) = \sum_{j=p_{i;min}}^{p_{i;max}} \alpha_{pj}^{S(A)} \Phi_j(x_1, x_2, ..., x_A)$; $\Phi_p^{S(A)}(\xi_1, ..., \xi_{A-1}) = \sum_{j=p_{i;min}}^{p_{i;max}} \alpha_{pj}^{S(A)} \Phi_j(\xi_1, ..., \xi_{A-1})$,

end for

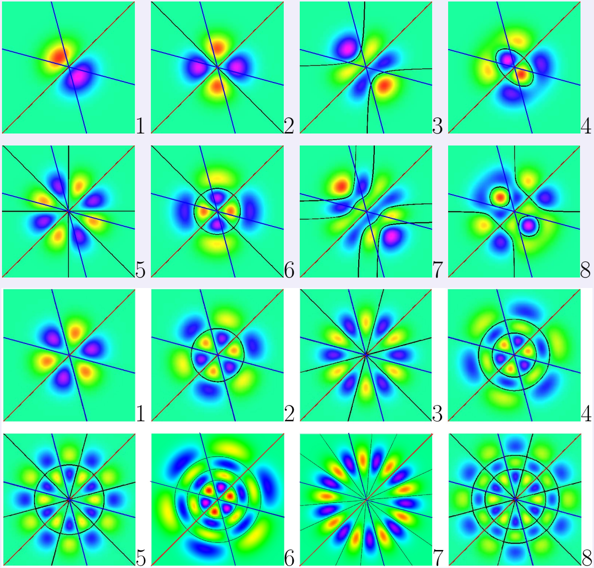
Local

$p_{S(A)} \equiv p_{i;S(A)}$ are the degeneracy factors of the energy levels $E_i^{S(A)}$ for S(A) functions;
$P_{i;min}$ $(P_{i;max})$ are the lowest (highest) numbers of S(A) functions, belonging to the energy levels $E_i^{S(A)}$, respectively;
$\{\bar{\alpha}_j\}$ and $\{\alpha_{pj}^{S(A)}\}$ are the sets of intermediate and desired coefficients;



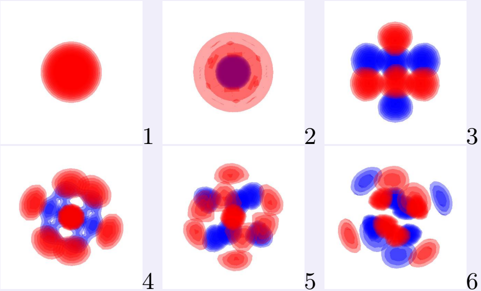
$\Phi^B_{[i_1,i_2]}(\xi_1,\xi_2) = C_{km}(\rho^2)^{3m/2}\exp(-\rho^2/2)\cos(3m(\varphi+\pi/12))L_k^{3m}(\rho^2)$,
$(\xi_1 = \rho\cos\varphi,\ \xi_2 = \rho\sin\varphi,\ k = 0, 1, \ldots,\ m = 0, 1, \ldots.)$

Profiles of the first eight oscillator partial symmetric (upper panels) and symmetric (lower panels) eigenfunctions $\Phi^B_{[i_1,i_2]}(\xi_1,\xi_2)$ at $A = 3$ in coordinate frame (ξ_1,ξ_2). The curves are nodes of the eigenfunctions $\Phi^B_{[i_1,i_2]}(\xi_1,\xi_2)$. Red line correspond to pair collision $x_2 = x_3$, and blue lines correspond to pair collisions $x_1 = x_2$ and $x_1 = x_3$ of projection $(x_1,x_2,x_3) \to (\xi_1,\xi_2)$.

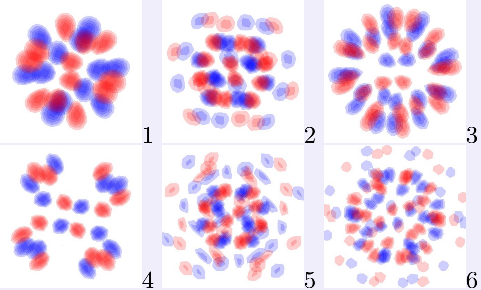


$$\Phi^F_{[i_1,i_2]}(\xi_1,\xi_2) = C_{km}(\rho^2)^{3m/2}\exp(-\rho^2/2)\sin(3m(\varphi+\pi/12))L_k^{3m}(\rho^2),$$
$$(\xi_1=\rho\cos\varphi,\ \xi_2=\rho\sin\varphi,\ k=0,1,\ldots,\ m=1,2,\ldots)$$

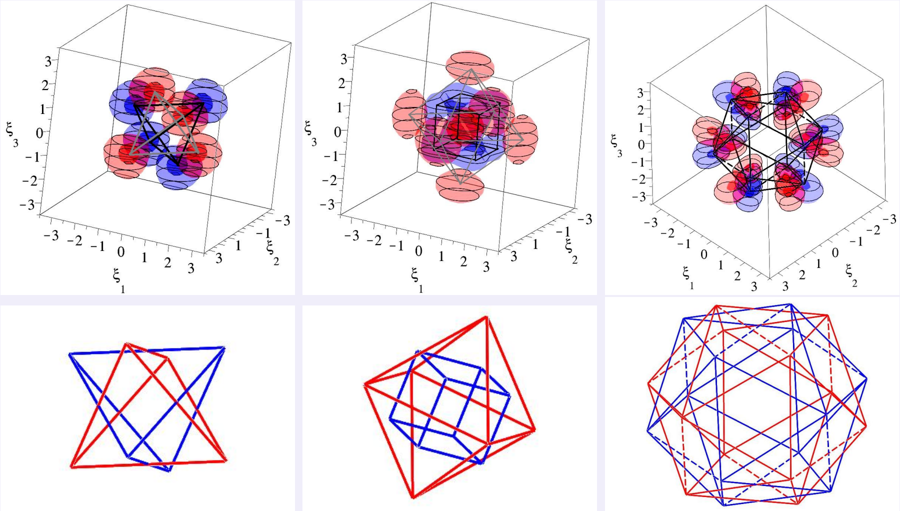
Profiles of the first eight oscillator partial antisymmetric (upper panels) and antisymmetric (lower panels) eigenfunctions $\Phi^F_{[i_1,i_2]}(\xi_1,\xi_2)$ at $A=3$ in coordinate frame (ξ_1,ξ_2). The curves are nodes of the eigenfunctions $\Phi^a_{[i_1,i_2]}(\xi_1,\xi_2)$.
Red line correspond to pair collision $x_2=x_3$, and blue lines correspond to pair collisions $x_1=x_2$ and $x_1=x_3$ of projection $(x_1,x_2,x_3)\to(\xi_1,\xi_2)$.



Profiles of the first six oscillator symmetric eigenfunctions $\Phi^{B}_{[i_1,i_2,i_3]}(\xi_1,\xi_2,\xi_3)$ at $A=4$ in coordinate frame (ξ_1,ξ_2,ξ_3).



Profiles of the first six oscillator antisymmetric eigenfunctions $\Phi^{B}_{[i_1,i_2,i_3]}(\xi_1,\xi_2,\xi_3)$ at $A=4$ in coordinate frame (ξ_1,ξ_2,ξ_3).



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 $A = 4$. Maxima and minima positions of these functions form stella octangula, cube and octahedron, and two polyhedra 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 degeneracy multiplicities p, $p_s = p_a$ 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	$p_{s(a)}$	$p_{S(A)}$	p	$p_{s(a)}$	$p_{S(A)}$	p	$p_{s(a)}$	$p_{S(A)}$	p	$p_{s(a)}$	$p_{S(A)}$	
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

Resume

- 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 algorithm SCR of symmetrizing or antisymmetrizing the $A-1$-dimensional harmonic oscillator basis functions with respect to permutations of A identical particles was described.
- 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 trough barrier potentials of a target is considered in our forthcoming paper.
- 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.

Thank you for your attention!