Analysis of models of the resonance quantum tunneling of composite systems through potential barriers

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Close-coupling and Kantorovich (Adiabatic) methods

The Schrödinger equation reads as

$$\left(\frac{1}{g_{3s}(x_s)}\hat{H}_2(x_f;x_s)+\hat{H}_1(x_s)+\hat{V}_{fs}(x_f,x_s)-2E\right)\Psi(x_f,x_s)=0,$$

$$\hat{H}_2=-\frac{1}{g_{1f}(x_f)}\frac{\partial}{\partial x_f}g_{2f}(x_f)\frac{\partial}{\partial x_f}+\hat{V}_f(x_f;x_s),\quad \hat{H}_1=-\frac{1}{g_{1s}(x_s)}\frac{\partial}{\partial x_s}g_{2s}(x_s)\frac{\partial}{\partial x_s}+\hat{V}_s(x_s).$$

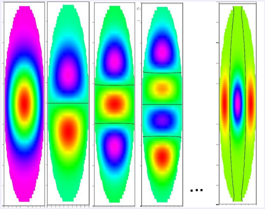
$\hat{H}_2(x_f;x_s)$ is the Hamiltonian of the fast subsystem,
$\hat{H}_1(x_s)$ is the Hamiltonian of the slow subsystem,
$V_{fs}(x_f,x_s)$ is interaction potential.

The Kantorovich expansion of the desired solution of BVP:

$$\Psi(x_f,x_s)=\sum_{j=1}^{j_{\max}}\Phi_j(x_f;x_s)\chi_j(x_s).$$

Example:
prolate spheroid,
ρ is fast variable,
z is slow variable

First wave functions:



BVP for fast subsystem

The equation for the basis functions of the fast variable x_f and the potential curves, $E_i(x_s)$ continuously depend on the slow variable x_s as a parameter

$$\left\{\hat{H}_2(x_f;x_s)-E_i(x_s)\right\}\Phi_i(x_f;x_s)=0,$$

The boundary conditions

$$\lim_{x_f\to x_f^t(x_s)}\left(N_f(x_s)g_{2f}(x_s)\frac{d\Phi_j(x_f;x_s)}{dx_f}+D_f(x_s)\Phi_j(x_f;x_s)\right)=0.$$

The normalization condition

$$\langle\Phi_i|\Phi_j\rangle=\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)}\Phi_i(x_f;x_s)\Phi_j(x_f;x_s)g_{1f}(x_f)dx_f=\delta_{ij}.$$

BVP for slow subsystem

The effective potential matrices of dimension $j_{\max} \times j_{\max}$:

$$U_{ij}(x_s) = \frac{1}{g_{3s}(x_s)} \hat{E}_i(x_s)\delta_{ij} + \frac{g_{2s}(x_s)}{g_{1s}(x_s)} W_{ij}(x_s) + V_{ij}(x_s),$$

$$V_{ij}(x_s) = \int\limits_{x_f^{\min}}^{x_f^{\max}} \Phi_i(x_f; x_s) V_{fs}(x_f, x_s) \Phi_j(x_f; x_s) g_{1f}(x_f) dx_f,$$

$$W_{ij}(x_s) = \int\limits_{x_f^{\min}}^{x_f^{\max}} \frac{\partial \Phi_i(x_f; x_s)}{\partial x_s} \frac{\partial \Phi_j(x_f; x_s)}{\partial x_s} g_{1f}(x_f) dx_f,$$

$$Q_{ij}(x_s) = -\int\limits_{x_f^{\min}}^{x_f^{\max}} \Phi_i(x_f; x_s) \frac{\partial \Phi_j(x_f; x_s)}{\partial x_s} g_{1f}(x_f) dx_f.$$

BVP for slow subsystem

The SDE for the slow subsystem (the adiabatic approximation is a diagonal approximation for the set of ODEs)

$$\mathbf{H}\chi^{(i)}(x_s) = 2E_i\,\mathbf{I}\chi^{(i)}(x_s),$$
$$\mathbf{H} = -\frac{1}{g_{1s}(x_s)}\mathbf{I}\frac{d}{dx_s}g_{2s}(x_s)\frac{d}{dx_s} + \hat{V}_s(x_s)\mathbf{I} + \mathbf{U}(x_s)$$
$$+\frac{g_{2s}(x_s)}{g_{1s}(x_s)}\mathbf{Q}(x_s)\frac{d}{dx_s} + \frac{1}{g_{1s}(x_s)}\frac{dg_{2s}(x_s)\mathbf{Q}(z)}{dx_s},$$

with the boundary conditions

$$\lim_{x_s\to x_s^t}\left(N_s g_{2s}(x_s)\frac{d\boldsymbol{\chi}(x_s)}{dx_s} + D_s\boldsymbol{\chi}(x_s)\right) = 0.$$

The statement of the problem

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

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

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
$\tilde{\mathbf{x}}=(\tilde{x}_1,...,\tilde{x}_A)\in\mathbf{R}^{A\times d}$ 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; $\sum_{i=1}^{A}(y_i \cdot y_i) = \sum_{i=1}^{A}(x_i \cdot x_i) = R^2 \mapsto$ $\sum_{i,j=1}^{A}(x_{ij})^2 = 2A\sum_{i=1}^{A}(y_i)^2 - 2(\sum_{i=1}^{A} x_i)^2 = 2A\sum_{i=1}^{A-1}(y_i)^2$.

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

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

Symmetrized coordinates

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

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

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:

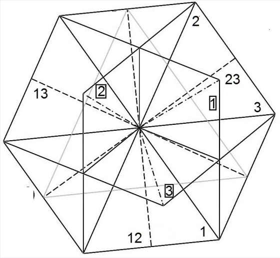
$$M = \begin{pmatrix} b_1^0 & b_1^- \\ b_2^+ & b_2^0 \end{pmatrix} = \begin{pmatrix} (\sqrt{6}-\sqrt{2})/4 & (\sqrt{6}+\sqrt{2})/4 \\ (\sqrt{6}+\sqrt{2})/4 & -(\sqrt{6}-\sqrt{2})/4 \end{pmatrix} = \begin{pmatrix} \sin\phi_1 & \cos\phi_1 \\ \cos\phi_1 & -\sin\phi_1 \end{pmatrix} =$$

$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \cos\phi_1 & -\sin\phi_1 \\ \sin\phi_1 & \cos\phi_1 \end{pmatrix} = \begin{pmatrix} \cos\phi_1 & \sin\phi_1 \\ -\sin\phi_1 & \cos\phi_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = M_1(\phi_1)M_0. \quad (1)$$

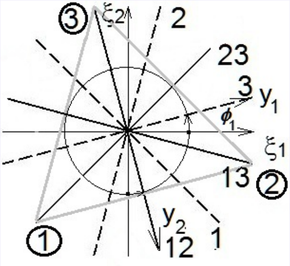
i.e. by permutation of coordinates $(\xi_1, \xi_2) \to (\xi_2, \xi_1)$ and counterclockwise rotation by the angle $\phi_1 = \pi/12$.

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. 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:

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

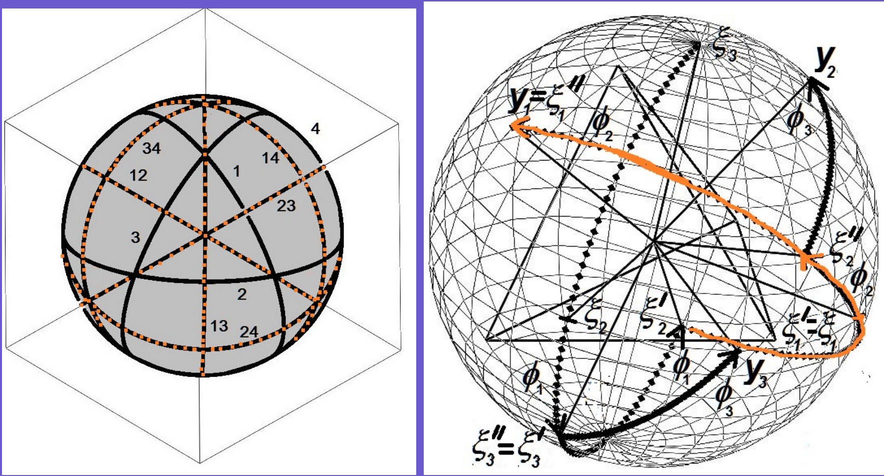
$A = 4$

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

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

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. Note, that the second angle ϕ_2 is supplementary to the angle between an edge and a face of a regular tetrahedron, associated with the system of symmetrized coordinates $\{\xi_1, \xi_2, \xi_3\} \in \mathbf{R}^3$.
This transformation illustrates isomorphism between symmetry operations of the tetrahedron group T_d in $\mathbf{R}^3$ and the permutation group S_4, on four objects ($A = 4$), like [P. Kramer and M. Moshinsky, Nucl. Phys. 82, 241 (1966).].

$A = 4$



Intersections in R^4 of the coordinate spaces R^3 (labelled 1, 2, 3, 4) and the spaces R^3 of pair collisions (labelled 12, etc.) with the sphere S^2 in the center-of-mass space R^3.

$A = 3$

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 $\bar{\Phi}_{[i_1,i_2,...,i_{A-1}]}(\xi_1, ..., \xi_{A-1})$:

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

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

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 $[i_1,i_2,...,i_{A-1}]$, $N_\upsilon\leq A-1$ 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

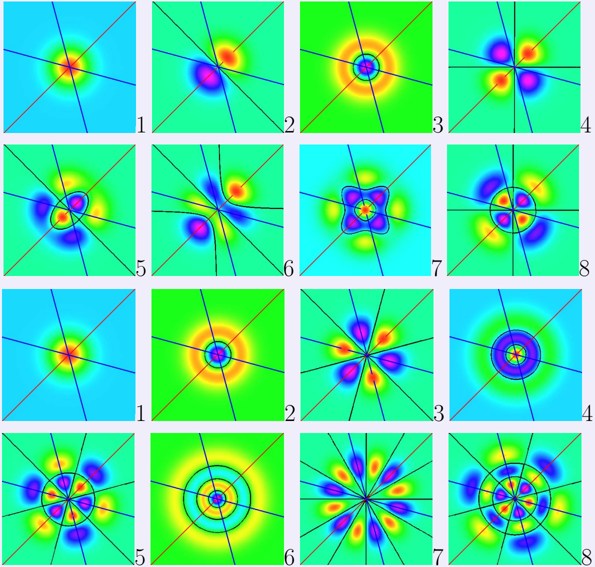
$$x_{ij} \equiv x_i - x_j = \xi_{i-1} - \xi_{j-1} \equiv \xi_{i-1,j-1}, \quad i, j = 2, ..., A, \quad x_1 = \frac{1}{\sqrt{A}} \sum_{i'=0}^{A-1} \xi_{i'}.$$

Symmetrization with respect to permutation of A particles

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

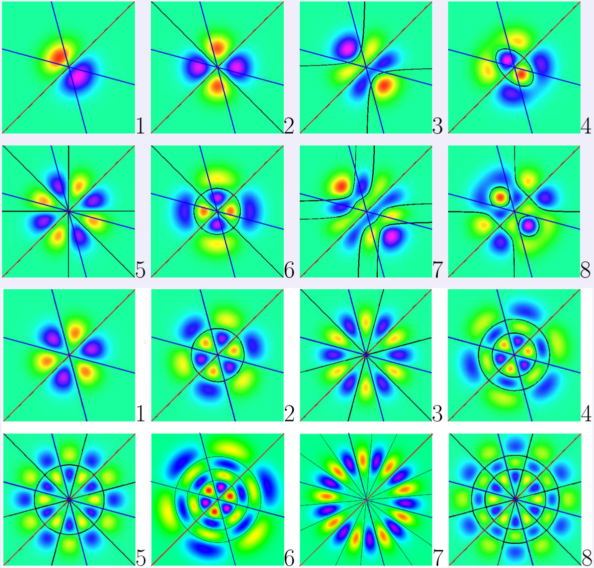
$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \dots \\ \xi_{A-1} \end{pmatrix} = \begin{pmatrix} 1 & a_1 & a_0 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_1 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_0 & a_1 & \cdots & a_0 & a_0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & a_0 & a_0 & a_0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

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.



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

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

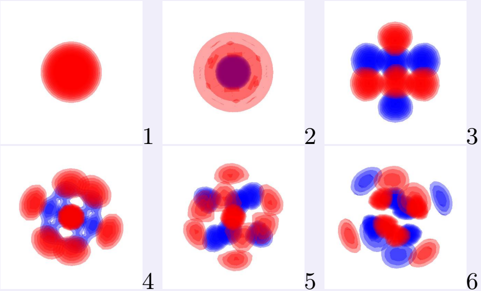


$\Phi^F_{[i_1,i_2]}(\xi_1,\xi_2) = C_{km}(\rho^2)^{3m/2}\exp(-\rho^2/2)\sin(3m(\varphi+\pi/12))L_k^{3m}(\rho^2)$,
$(\xi_1=\rho\cos\varphi,\ \xi_2=\rho\sin\varphi,\ k=0,1,\ldots,\ m=1,2,\ldots)$

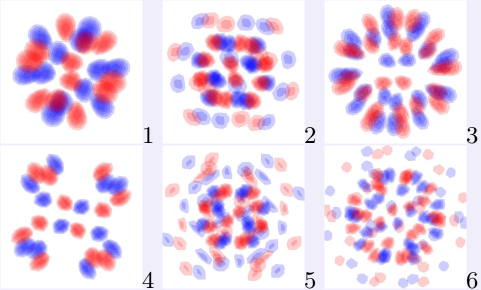
The same but for antisymmetric eigenfunctions.

Eigenfunctions $A=3$, $d=1$ are classified by irrs of symmetry group D_{3m}.

The eigenvalues $\varepsilon^{S(A)}_{k,m}=2(2k+3m+1)$ are degenerate with multiplicity $K+1$, if $\varepsilon^{S(A)}_{k,m}-\varepsilon^{S(A)}_{\text{ground}}=12K+K'$, where $K'=0,4,6,8,10,14$, $\varepsilon^{S}_{\text{ground}}=2$, $\varepsilon^{A}_{\text{ground}}=8$, that is less in ~ 6 times of degenerate multiplicity $p_4(j)$ of eigenvalues without symmetry.



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).

$A = 4$

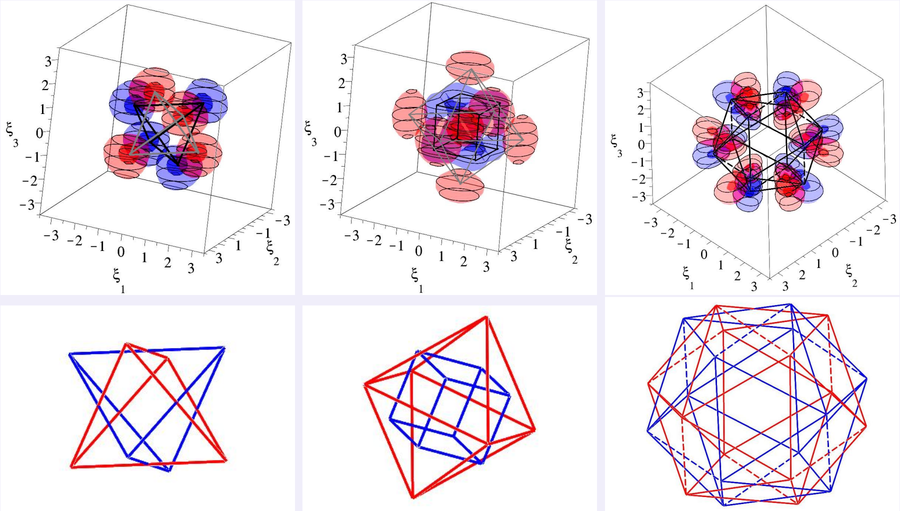
The eigenfunctions $\Phi_j(\xi_1,\ldots,\xi_{A-1})^{S(A)} \equiv \Phi^{S(A)}_{[i_1,i_2,i_3]}(\xi_1,\xi_2,\xi_3)$ of S and A states of a 3D harmonic oscillator are expressed via the eigenfunctions of 1D harmonic oscillator:

$$\Phi^{S(A)}_j(\xi_1,\xi_2,\xi_3) = N^{-1/2}_{[i_1,i_2,i_3]}(\bar{\Phi}_{[i_1,i_2,i_3]} + \bar{\Phi}_{[i_2,i_3,i_1]} + \bar{\Phi}_{[i_3,i_1,i_2]} \pm \bar{\Phi}_{[i_2,i_1,i_3]} \pm \bar{\Phi}_{[i_1,i_3,i_2]} \pm \bar{\Phi}_{[i_3,i_2,i_1]}).$$

Here $i_1 = 0,1,2,\ldots$, $i_2 = i_1, i_1+2,\ldots$, $i_3 = i_2, i_2+2,\ldots$ for S states and $i_1 = 0,1,2,\ldots$, $i_2 = i_1+2, i_1+4,\ldots$, $i_3 = i_2+2, i_2+4,\ldots$ for A states, $N_{[i_1,i_2,i_3]}$ being the number of multiset permutations of i_1, i_2, i_3: $N_{[i_1,i_2,i_3]} = \{6, i_1 < i_2 < i_3; 1, i_1 = i_2 = i_3; 3, \text{otherwise}\}$.

The eigenfunctions of S states with even (odd) i_1 and A states with odd (even) i_1 possess symmetry octahedral (tetrahedral)-type.

The eigenvalues $\varepsilon^{S(A)}_{i_1,i_2,i_3} = 2(i_1+i_2+i_3+3/2)$ are degenerate with multiplicity $3K^2 + (3+K')K + K' + \delta_{0K'}$, if $\varepsilon^{S(A)}_{i_1,i_2,i_3} - \varepsilon^{S(A)}_{\rm ground} = 4(6K+K') + K''$, where $K' = 0,1,2,3,4,5$, $K'' = 0,6$, $\varepsilon^{S}_{\rm ground} = 3$, $\varepsilon^{A}_{\rm ground} = 15$, that is less in ~ 24 times of multiplicity $p_4(j)$ of eigenvalues without symmetry.



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

Close-coupling equations in the SCR

Galerkin expansion in the symmetrized coordinates

$$\Psi_{i_o}(\xi_0)(\xi_0, ..., \xi_{A-1}) = \sum_{j=1}^{j_{\max}} \Phi_j(\xi_1, ..., \xi_{A-1})\chi_{ji_o}(\xi_0),$$

Here $\chi_i(\xi_0)$ are unknown functions

$$\chi_{ji_o}(\xi_0) = \int d\xi_1 ... d\xi_{A-1}\Phi_j(\xi_1, ..., \xi_{A-1})\Psi_{i_o}(\xi_0, ..., \xi_{A-1}),$$

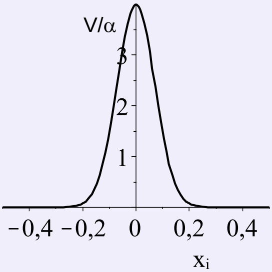
and $\Phi_j(\xi_1, ..., \xi_{A-1})$ are the orthonormalized basis eigenfunctions of the $(A-1)$-dimensional oscillator.

The set of the close-coupling Galerkin equations in symmetrized coordinates

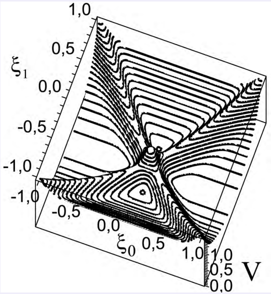
$$\left[-\frac{d^2}{d\xi_0^2} + E_i - E\right]\chi_{ii_o}(\xi_0) + \sum_{j=1}^{j\max}(V_{ij}(\xi_0))\chi_{ji_o}(\xi_0) = 0,$$

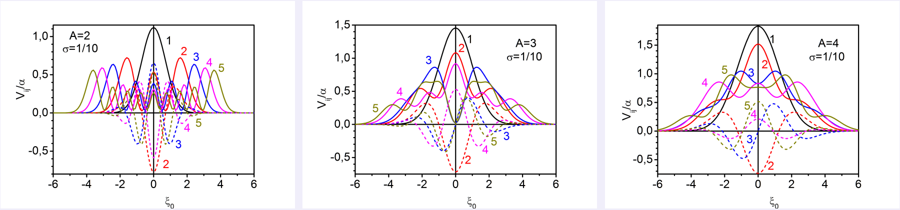
$$V_{ij}(\xi_0) = \int d\xi_1 ... d\xi_{A-1}\Phi_i(\xi_1, ..., \xi_{A-1})\left(\sum_{k=1}^{A} V(x_k(\xi_0, ..., \xi_{A-1}))\right)\Phi_j(\xi_1, ..., \xi_{A-1}),$$

The repulsive barrier is chosen to be a Gaussian potential $V(x_i) = \frac{\alpha}{\sqrt{2\pi}\sigma}\exp(-\frac{x_i^2}{\sigma^2})$.

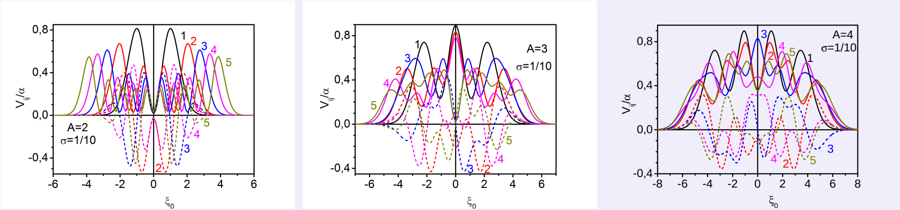


Gaussian-type potential at $\sigma = 0.1$ (in oscillator units) and corresponding 2D barrier potential at $\alpha = 1/10$, $\sigma = 0.1$.





Diagonal V_{jj} (solid lines) and nondiagonal V_{j1}, (dashed lines) effective potentials for $A = 2$, $A = 3$ and $A = 4$ symmetric particles at $\sigma = 1/10$.

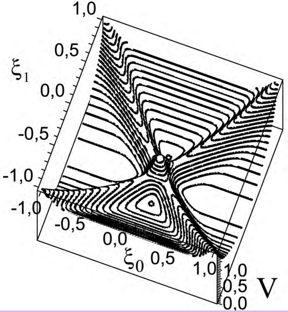


Diagonal V_{jj} (solid lines) and nondiagonal V_{j1}, (dashed lines) effective potentials for $A = 2$, $A = 3$ and $A = 4$ antisymmetric particles at $\sigma = 1/10$.

Asymptotic boundary conditions

$$\left.\frac{d\boldsymbol{F}(\xi_0)}{d\xi_0}\right|_{\xi_0=\xi_{\min}} = \mathcal{R}(\xi_{\min})\boldsymbol{F}(\xi_{\min}), \quad \left.\frac{d\boldsymbol{F}(\xi_0)}{d\xi_0}\right|_{\xi_0=\xi_{\max}} = \mathcal{R}(\xi_{\max})\boldsymbol{F}(\xi_{\max}),$$

$\mathcal{R}(\xi)$ is an unknown $j_{\max} \times j_{\max}$ matrix function,
$\boldsymbol{F}(\xi_0) = \{\boldsymbol{\chi}_{i_o}(\xi_0)\}_{i_o=1}^{N_o} = \{\{\chi_{ji_o}(\xi_0)\}_{j=1}^{j_{\max}}\}_{i_o=1}^{N_o}$ is the required $j_{\max} \times N_o$ matrix solution,
and N_o is the number of open channels, $N_o = \max\limits_{2E \geq E_j} j \leq j_{\max}$.



In asymptotic region:

$$\Psi(\xi_0, ..., \xi_{A-1}; E) = \sum_j \Phi_j(\xi_1, ..., \xi_{A-1}) \frac{\exp\left(+\imath\left(p_j \xi_0\right)\right)}{\sqrt{p_j}}.$$

Open channels: $p_j^2 = E - E_j > 0$ (oscillating solutions).

Closed channels: $p_j^2 = E - E_j < 0$ (exponentially small solutions).

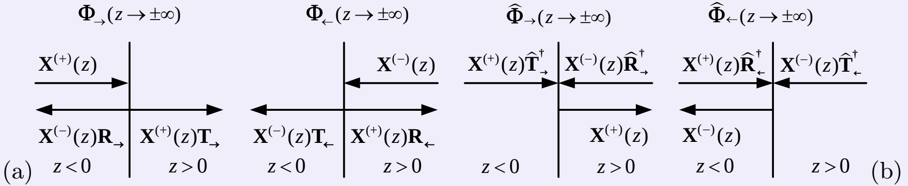
The asymptotic boundary conditions

Matrix-solution $\mathbf{\Phi}_v(z) = \mathbf{\Phi}(z)$ describing the incidence of the particle and its scattering, which has the asymptotic form "incident wave + outgoing waves", is

$$\mathbf{\Phi}_v(z \to \pm\infty) = \left\{ \begin{array}{lll} \left\{ \begin{array}{ll} \mathbf{X}^{(+)}(z)\mathbf{T}_v, & z > 0, \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_v, & z < 0, \end{array} \right. & v = \rightarrow, \\ \left\{ \begin{array}{ll} \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\mathbf{R}_v, & z > 0, \\ \mathbf{X}^{(-)}(z)\mathbf{T}_v, & z < 0, \end{array} \right. & v = \leftarrow, \end{array} \right.$$

where $\mathbf{R}_v$ and $\mathbf{T}_v$ are the reflection and transmission $N_o \times N_o$ matrices, $v = \rightarrow$ and $v = \leftarrow$ denote the initial direction of the particle motion along the z axis.

Schematic diagrams of the continuum spectrum waves having the asymptotic form: (a) "incident wave + outgoing waves", (b) "incident waves + ingoing wave":



The asymptotic boundary conditions

The ABC for the solution $\Psi(y,\mathbf{x}) = \{\Phi_{i_o}(y,\mathbf{x})\}_{i_o=1}^{N_o}$ $(y=\xi_0,\ \mathbf{x}=\{\xi_1,...,\xi_{A-1}\})$

$$\Psi_{i_o}^{\leftarrow}(y\to+\infty,\mathbf{x}) \to \Phi_{i_o}(\mathbf{x})\frac{\exp\left(-\imath\left(p_{i_o}y\right)\right)}{\sqrt{p_{i_o}}} + \sum_{j=1}^{N_o}\Phi_j(\mathbf{x})\frac{\exp\left(+\imath\left(p_j y\right)\right)}{\sqrt{p_j}}R_{ji_o}^{\leftarrow}(E),$$

$$\Psi_{i_o}^{\leftarrow}(y\to-\infty,\mathbf{x}) \to \sum_{j=1}^{N_o}\Phi_j(\mathbf{x})\frac{\exp\left(-\imath\left(p_j y\right)\right)}{\sqrt{p_j}}T_{ji_o}^{\leftarrow}(E),$$

$$\Psi_{i_o}^{\leftarrow}(y,|\mathbf{x}|\to\infty)\to 0;$$

$$\Psi_{i_o}^{\rightarrow}(y\to-\infty,\mathbf{x}) \to \Phi_{i_o}(\mathbf{x})\frac{\exp\left(\imath\left(p_{i_o}y\right)\right)}{\sqrt{p_{i_o}}} + \sum_{j=1}^{N_o}\Phi_j(\mathbf{x})\frac{\exp\left(-\imath\left(p_j y\right)\right)}{\sqrt{p_j}}R_{ji_o}^{\rightarrow}(E),$$

$$\Psi_{i_o}^{\rightarrow}(y\to+\infty,\mathbf{x}) \to \sum_{j=1}^{N_o}\Phi_j(\mathbf{x})\frac{\exp\left(\imath\left(p_j y\right)\right)}{\sqrt{p_j}}T_{ji_o}^{\rightarrow}(E),$$

$$\Psi_{i_o}^{\rightarrow}(y,|\mathbf{x}|\to\infty)\to 0.$$

$v=\leftarrow,\rightarrow$ denotes the initial direction of the particle motion along the y axis, N_o is the number of open channels at the fixed energy $p_{i_o}^2 = E - E_{i_o} > 0$; $R_{ji_o}^{v}$ and $T_{ji_o}^{v}$ are unknown reflection and transmission amplitudes.

S-matrix

ABC in the matrix form

$\mathbf{\Psi} = \mathbf{\Phi}^T \boldsymbol{F}$, describing the "incident wave + outgoing waves" at $y_+ \to +\infty$ and $y_- \to -\infty$ as

$$\begin{pmatrix} \boldsymbol{F}_\to(y_+) & \boldsymbol{F}_\leftarrow(y_+) \\ \boldsymbol{F}_\to(y_-) & \boldsymbol{F}_\leftarrow(y_-) \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{X}^{(-)}(y_+) \\ \mathbf{X}^{(+)}(y_-) & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{X}^{(+)}(y_+) \\ \mathbf{X}^{(-)}(y_-) & \mathbf{0} \end{pmatrix} \mathbf{S},$$

the unitary and symmetric scattering matrix $\mathbf{S}$

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_\to & \mathbf{T}_\leftarrow \\ \mathbf{T}_\to & \mathbf{R}_\leftarrow \end{pmatrix}, \quad \mathbf{S}^\dagger \mathbf{S} = \mathbf{S}\mathbf{S}^\dagger = \mathbf{I}$$

is composed of the above reflection and transmission matrices having the following properties :

$$\mathbf{T}^\dagger_\to \mathbf{T}_\to + \mathbf{R}^\dagger_\to \mathbf{R}_\to = \mathbf{I}_{oo} = \mathbf{T}^\dagger_\leftarrow \mathbf{T}_\leftarrow + \mathbf{R}^\dagger_\leftarrow \mathbf{R}_\leftarrow,$$
$$\mathbf{T}^\dagger_\to \mathbf{R}_\leftarrow + \mathbf{R}^\dagger_\to \mathbf{T}_\leftarrow = \mathbf{0} = \mathbf{R}^\dagger_\leftarrow \mathbf{T}_\to + \mathbf{T}^\dagger_\leftarrow \mathbf{R}_\to,$$
$$\mathbf{T}^T_\to = \mathbf{T}_\leftarrow, \quad \mathbf{R}^T_\to = \mathbf{R}_\to, \quad \mathbf{R}^T_\leftarrow = \mathbf{R}_\leftarrow.$$

In addition, it should be noted that functions $\mathbf{X}^{(\pm)}(z)$ satisfy relations

$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\mp)}(z),\mathbf{X}^{(\pm)}(z)) = \pm 2\imath \mathbf{I}_{oo},\ \ \mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\pm)}(z),\mathbf{X}^{(\pm)}(z)) = \mathbf{0},$$

where $\mathbf{Wr}(\bullet;\mathbf{a}(z),\mathbf{b}(z))$ is a generalized Wronskian with a long derivative defined as

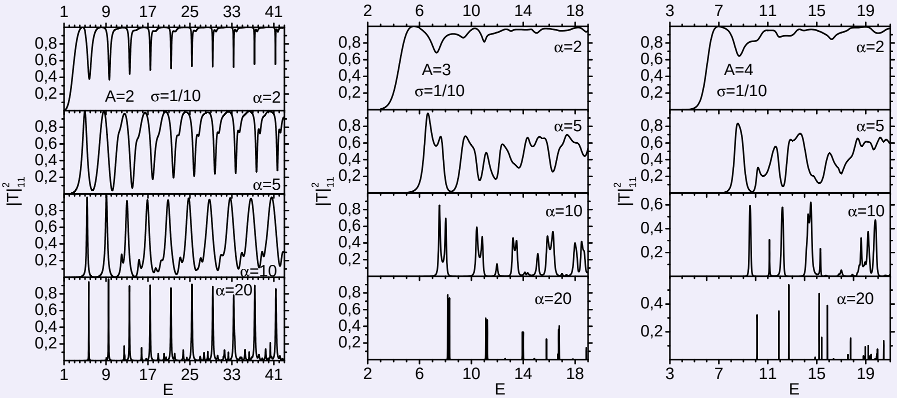
$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{a}(z),\mathbf{b}(z)) = \mathbf{a}^T(z)\left(\frac{d\mathbf{b}(z)}{dz} - \mathbf{Q}(z)\mathbf{b}(z)\right) - \left(\frac{d\mathbf{a}(z)}{dz} - \mathbf{Q}(z)\mathbf{a}(z)\right)^T \mathbf{b}(z).$$

This Wronskian is used to estimate a desirable accuracy of the above expansion.

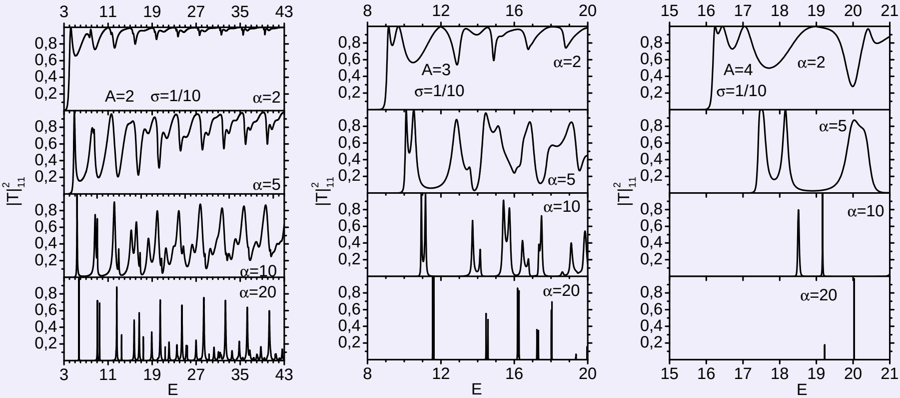
FEM grid details

type	A	$j_{\max}$	$\xi_0^{\max}$	$N_{\rm elem}$	max N_o
S	2	13	9.3	664	10
A	2	13	9.3	664	10
S	3	21	10.5	800	10
A	3	16	10.5	800	7
S	4	39	12.8	976	15
A	4	15	12.8	976	3

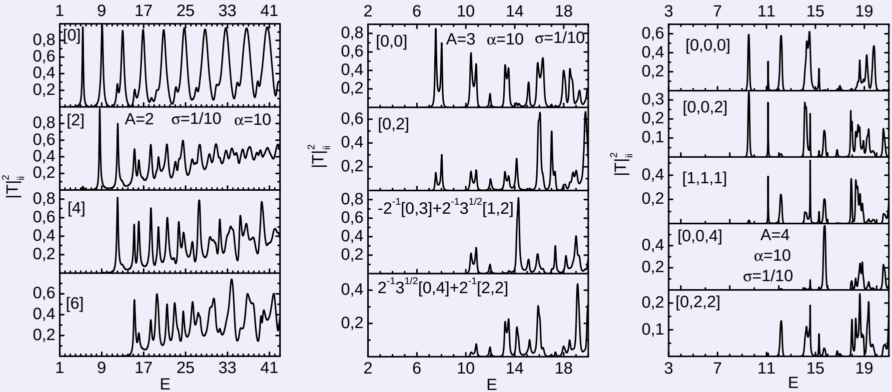
A is number of particles,
$j_{\max}$ is number of Eqs.
$\xi_0^{\max}$ is last point of the finite-element grid $\Omega_\xi\{-\xi_0^{\max},\xi_0^{\max}\}$,
$N_{\rm elem}$ is number of fourth-order Lagrange elements,
max N_o is maximum number of open channels.



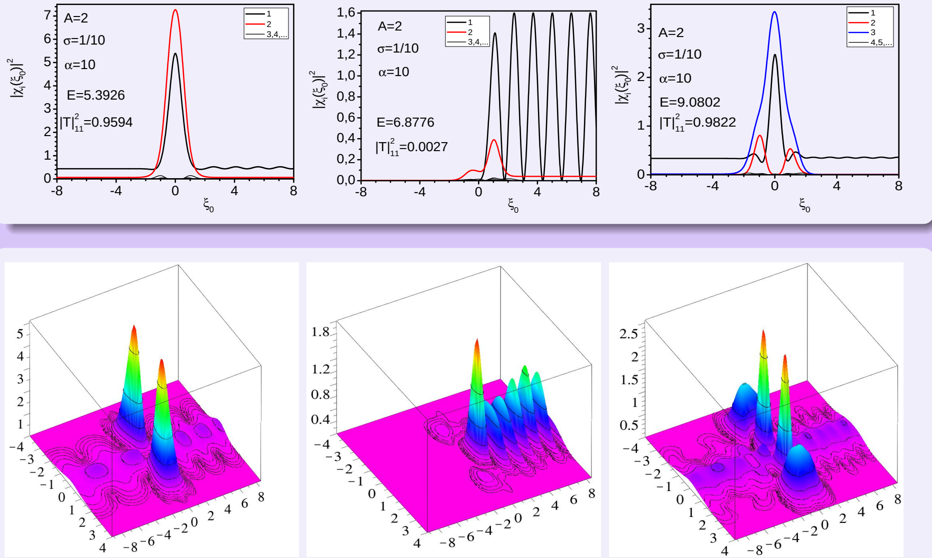
The total transmission probabilities $|T|^2_{11}$ vs energy E (in oscillator units) from the ground state of the system of $A = 2, 3, 4$ of symmetric particles, coupled by the oscillator potential, through the repulsive Gaussian potential barriers $V(x_i) = \frac{\alpha}{\sqrt{2\pi}\sigma} \exp(-\frac{x_i^2}{\sigma^2})$ at $\sigma = 0.1$ and $\alpha = 2, 5, 10, 20$.



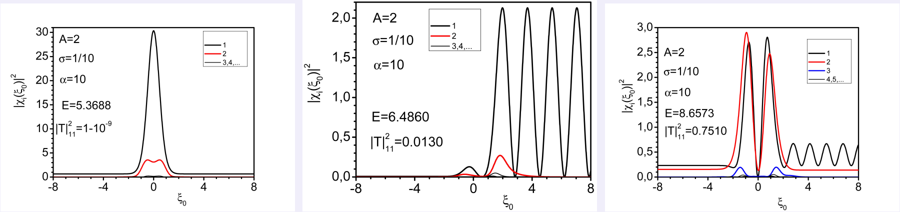
The total transmission probabilities $|T|^2_{11}$ vs energy E (in oscillator units) from the ground state of the system of $A = 2, 3, 4$ of antisymmetric particles, coupled by the oscillator potential, through the repulsive Gaussian potential barriers $V(x_i) = \frac{\alpha}{\sqrt{2\pi}\sigma} \exp(-\frac{x_i^2}{\sigma^2})$ at $\sigma = 0.1$ and $\alpha = 2, 5, 10, 20$.

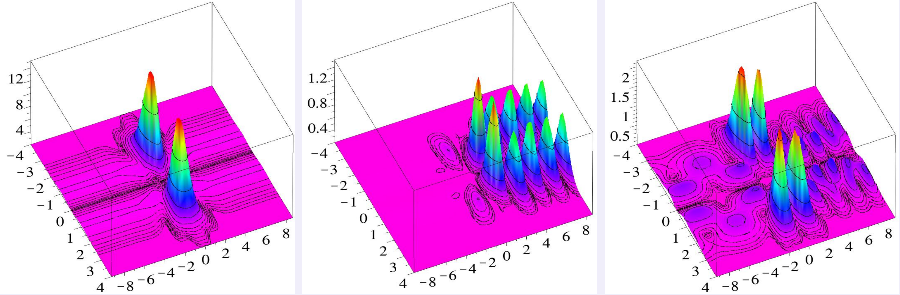


The total penetration probabilities $|T|^2_{ii}$ vs energy E (in oscillator units) from the ground and excited states of the system of $A = 2, 3, 4$ of symmetric particles, coupled by the oscillator potential, through the repulsive Gaussian-type potential barriers $V(x_i) = \frac{\alpha}{\sqrt{2\pi}\sigma} \exp(-\frac{x_i^2}{\sigma^2})$ at $\sigma = 0.1$ and $\alpha = 10$.

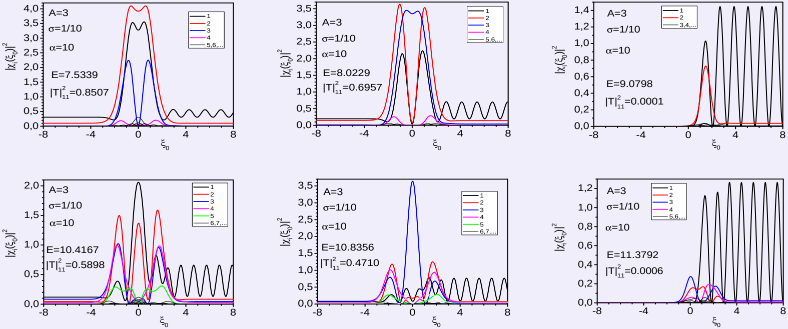


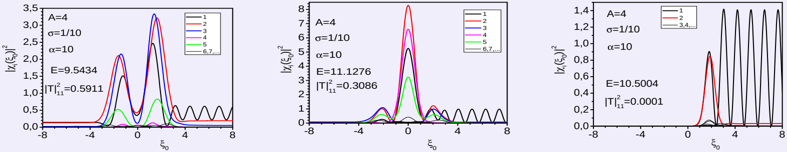
The probability densities $|\chi_i(\xi_0)|^2$ of the coefficient functions and the profiles of probability densities $|\Psi(\xi_0, \xi_1)|^2$ for $A = 2$ symmetric particles.





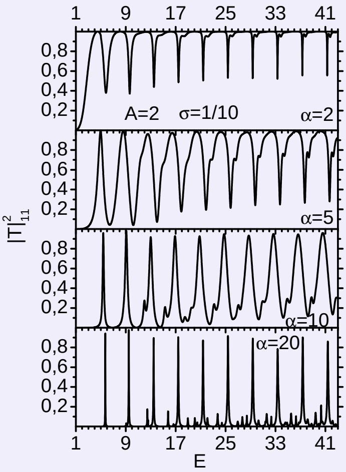
The probability densities $|\chi_i(\xi_0)|^2$ of the coefficient functions and the profiles of probability densities $|\Psi(\xi_0, \xi_1)|^2$ for $A = 2$ antisymmetric particles.

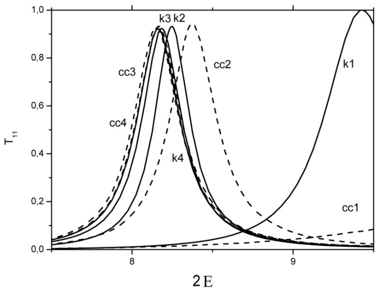




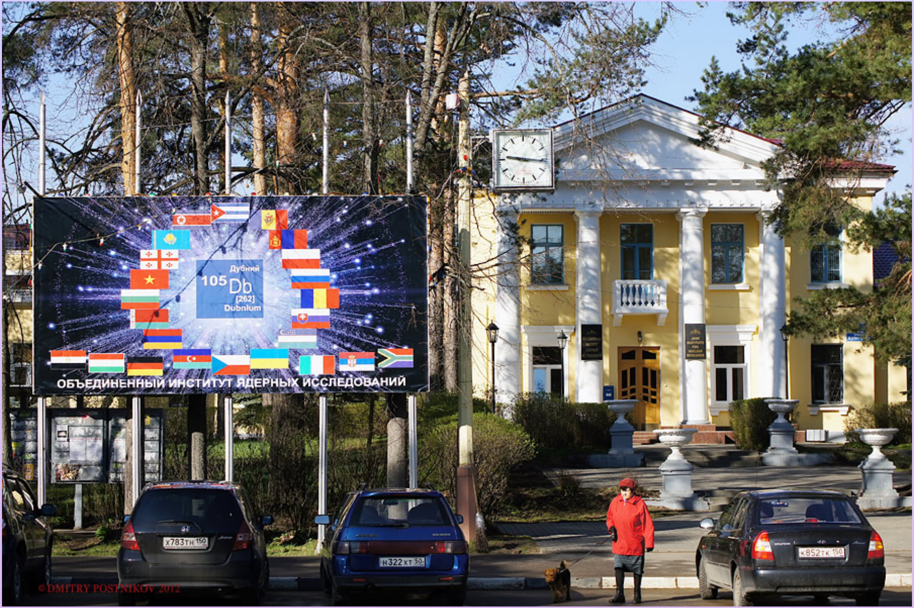
The probability densities $|\chi_i(\xi_0)|^2$ of the coefficient functions for $A = 3$ and $A = 4$ symmetric particles.

The comparison of convergence rate of Galerkin and Kantorovich close-coupling expansions





The comparison of convergence rate of Galerkin (cc*) and Kantorovich (k*) close-coupling expansions in calculations of transmission coefficient $|T|^2_{11}$ for symmetric $A = 2$ at $\alpha = 10$, $\sigma = 0.1$. Results agree with calculations by means of the Numerov method in 2D plane [F.M. Pen'kov, JETP 91, 698 (2000)]



Thank you for your attention!