SYSTEM OF IDENTICAL PARTICLES WITH PAIR OSCILLATOR INTERACTIONS IN SYMMETRIC COORDINATES

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OUTLINE

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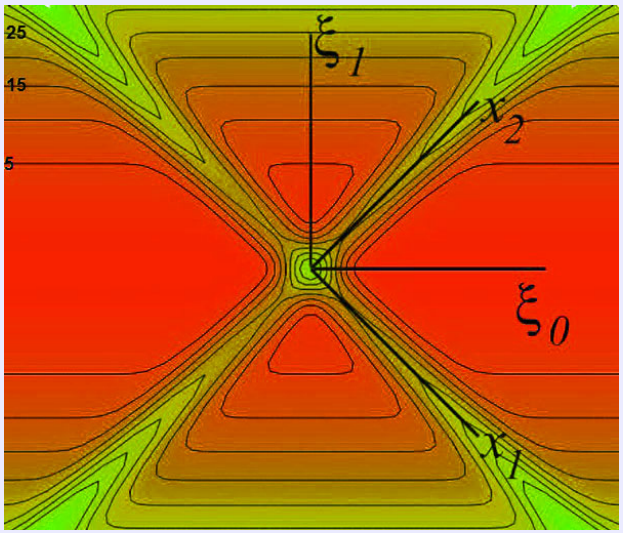
The statement of the problem

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

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



Barrier potential in configuration space $A = 2$

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.

D. W. Jepsent and J. O. Hirschfelder, Proc. Natl. Acad. Sci. U.S.A. 45, 249 (1959)

*SET OF CO-ORDINATE SYSTEMS WHICH DIAGONALIZE THE KINETIC ENERGY OF RELATIVE MOTION**

By Donald W. Jepsen† and Joseph O. Hirschfelder

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Communicated December 15, 1958

A simple scheme is given whereby one can write down any one of a large number of possible sets of co-ordinates, to use in an N-particle problem, which have the property of expressing the relative kinetic energy of the system in diagonal form. This gives a Schrödinger equation without cross-derivatives. These sets of co-ordinates can be visualized in terms of certain "mobile" models. It is easy to construct a "mobile" which leads to a co-ordinate set appropriate to a particular physical problem.

[4] As E. P. Wigner has pointed out to us in private correspondence, if the masses of the four particles are equal, then there is a co-ordinate system which treats each of the four particles in the same manner:

$$(Q_1)_w = \frac{\sqrt{m}}{2}[r_1 + r_2 - r_3 - r_4],$$

$$(Q_2)_w = \frac{\sqrt{m}}{2}[r_1 - r_2 + r_3 - r_4],$$

$$(Q_3)_w = \frac{\sqrt{m}}{2}[r_1 - r_2 - r_3 + r_4],$$

$$(Q_4)_w = \frac{\sqrt{m}}{2}[r_1 + r_2 + r_3 + r_4].$$

Comparing with our co-ordinates of Fig. 4, *b*,

$$\begin{aligned}(Q_1)_w &= Q_3,\\ (Q_2)_w &= -(Q_1 + Q_2)/\sqrt{2},\\ (Q_3)_w &= (Q_2 - Q_1)/\sqrt{2},\\ (Q_4)_w &= Q_4.\end{aligned}$$

There are similar relations between the Wigner co-ordinates and our co-ordinates of Fig. 4, *d*. Wigner states that if the number of particles is a power of 2 and the masses are equal, there is a co-ordinate system of high symmetry in which all particles are treated equally. Unfortunately the form of the potential energy in the collision of diatomic molecules would make these Wigner co-ordinates inconvenient.

P. Kramer and M. Moshinsky,Nucl. Phys. 82, 241 (1966)

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Nuclear Physics **82** (1966) 241—274;

GROUP THEORY OF HARMONIC OSCILLATORS
(III). States with Permutational Symmetry

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Abstract: This article continues the analysis of the problem of n particles in a common harmonic oscillator potential that was initiated in two previous papers under the same general title. The first objective of the paper is to give an analytic procedure for the explicit construction of the states in the $U_{3n} \supset \mathscr{U}_3 \times U_n$, $\mathscr{U}_3 \supset \mathscr{R}_3 \supset \mathscr{R}_2$, $U_n \supset U_{n-1} \supset \ldots \supset U_1$ chain of subgroups, where the $3n$ dimensional unitary group U_{3n} is the symmetry group of the Hamiltonian while $\mathscr{U}_3$ is the symmetry group of the harmonic oscillator, $\mathscr{R}_3$ is the ordinary rotation group, and U_n is the unitary group in n dimensions associated with the particle indices. The second and main objective of this paper is to construct states with definite permutational symmetry. After taking out the centre-of-mass motion the states given in terms of $n-1$ relative Jacobi vectors will be a basis for irreducible representations of the unitary group U_{n-1} and its orthogonal subgroup O_{n-1}. The characterization of the states is completed with the help of the irreducible representations of the symmetric group S_n, which, through its representations $D^{[n-1,\ 1]}(S_n)$, is a subgroup of O_{n-1}. This implies that the states transform irreducibly under the groups in the chain $U_n \supset U_{n-1} \supset O_{n-1} \supset S_n$ rather than under those in the chain $U_n \supset U_{n-1} \supset \ldots \supset U_1$. The states classified in this way contain as particular cases, those of both the shell and the cluster model. Explicit expressions are given for two, three and four particles.

referred to the system $\dot{S} = (\dot{e}_1\dot{e}_2\dot{e}_3)$ of coordinates. We shall use rather the system $\ddot{S} = (\ddot{e}_1\ddot{e}_2\ddot{e}_3)$ which, in turn, corresponds to relative coordinates

$$\begin{aligned} \ddot{\eta}^1 &= \tfrac{1}{2}(\eta^1+\eta^3-\eta^2-\eta^4), \\ \ddot{\eta}^2 &= \tfrac{1}{2}(\eta^1+\eta^4-\eta^2-\eta^3), \\ \ddot{\eta}^3 &= \tfrac{1}{2}(\eta^1+\eta^2-\eta^3-\eta^4). \end{aligned} \tag{6.9}$$

Symmetrized coordinates for system of A identical particles

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

$$C = \frac{1}{\sqrt{A}} \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & a_1 & a_0 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_1 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_0 & a_1 & \cdots & a_0 & a_0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & a_0 & a_0 & a_0 & \cdots & a_1 & a_0 \\ 1 & a_0 & a_0 & a_0 & \cdots & a_0 & a_1 \end{pmatrix},$$

$$a_0 = 1/(1-\sqrt{A}) < 0,$$
$$a_1 = a_0 + \sqrt{A} > 0,$$
$$C^{-1} = C.$$

A.A. Gusev, S.I. Vinitsky, O. Chuluunbaatar, L.L. Hai, V.L. Derbov and P.M. Krassovitskiy, Physics of Atomic Nuclei 77, pp. 389–413 (2014); Lecture Notes in Computer Science 8136, 155–168 (2013).

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Interacting electrons in a magnetic field in a center-of-mass free basis*

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Abstract

We present an extension of the spin-adapted configuration-interaction method (SACI) for the computation of four electrons in a quasi two-dimensional quantum dot. By a group-theoretical decomposition of the basis set and working with relative and center-of-mass (cm) coordinates we obtain an analytical identification of all spurious cm states of the Coulomb-interacting electrons. We find a substantial reduction in the basis set used for numerical computations. At the same time we increase the accuracy compared to the standard SACI due to the absence of distortions caused by an unbalanced cut-off of cm excitations.

Keywords: few-electron quantum dot, variational principle, block-diagonal basis sets

find: all class operators equation (A.2) have diagonal representations, see table A2. This proves:

Prop. All basis states of the irreps of the subgroup D_{2d} in the chosen representations are basis states of irreducible representations of the bigger group $S(4)$.

This remarkable result allows in table A3 , up to certain ambiguities, to almost avoid the use and projection with Young operators for the bigger group $S(4)$. In tables A4, A5 we use it in relation with the full scheme of groups including $SU(3) > O(3, R)$ and subgroups to assign orbital symmetry to the oscillator states.

Of two states separated by |, one and only one can belong to the listed tableau. The states [4], $[1^4]$ are identified as eigenstates under the transposition $T(2, 3)$ with eigenvalue ±1 respectively. If a state is not reproduced under $T(2, 3)$, it necessarily belongs to $f = [22]$ and spin $S = 0$. We conclude that the states equation (A.1) yield all the bases of the orbital Young tableaus.

Appendix B. Symmetrized relative coordinates for $n > 4$ electrons and their permutations

The efficiency of the tetrahedral coordinates raises the question if similar relative coordinates exist for $n > 4$. As a generalization of the tetrahedral coordinates from [13], new symmetrized coordinates for n particles were proposed by Gusev *et al* [8]. The matrix that gives the n new coordinates $(\eta_0, \eta_1, .., \eta_{n-1})$ in terms of the old ones $(x_1, x_2, .., x_n)$ reads

$$C = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & 1 & \dots & 1 & 1 \\ 1 & b & a & a & \dots & a & a \\ 1 & a & b & a & \dots & a & a \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot & \cdot \\ 1 & a & a & a & \dots & b & a \\ 1 & a & a & a & \dots & a & b \end{bmatrix},$$

$$C = C^T,\ C^{-1} = C,\ C^2 = I,$$

$$a = \left[1 - \sqrt{n}\right]^{-1},\ b = a + \sqrt{n}\,. \tag{B.1}$$

The cm coordinate is included as η_0. We shall explore the properties of these coordinates under the action of

SE in the symmetrized coordinates

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

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

Galerkin expansion in the symmetrized coordinates

Galerkin expansion in the symmetrized coordinates

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

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

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

Symbolic-numerical algorithm for generating cluster eigenfunctions: identical particles with pair oscillator interactions in 1D Euclidian space

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.

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

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

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

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

Step 2. 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 $i', j' = 1, ..., A - 1$

$$\Phi(..., x_i, ..., x_j, ...) = \pm\Phi(..., x_j, ..., x_i, ...) \rightarrow \Phi(..., \xi_{i'}, ..., \xi_{j'}, ...) = \pm\Phi(..., \xi_{j'}, ..., \xi_{i'}, ...).$$

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

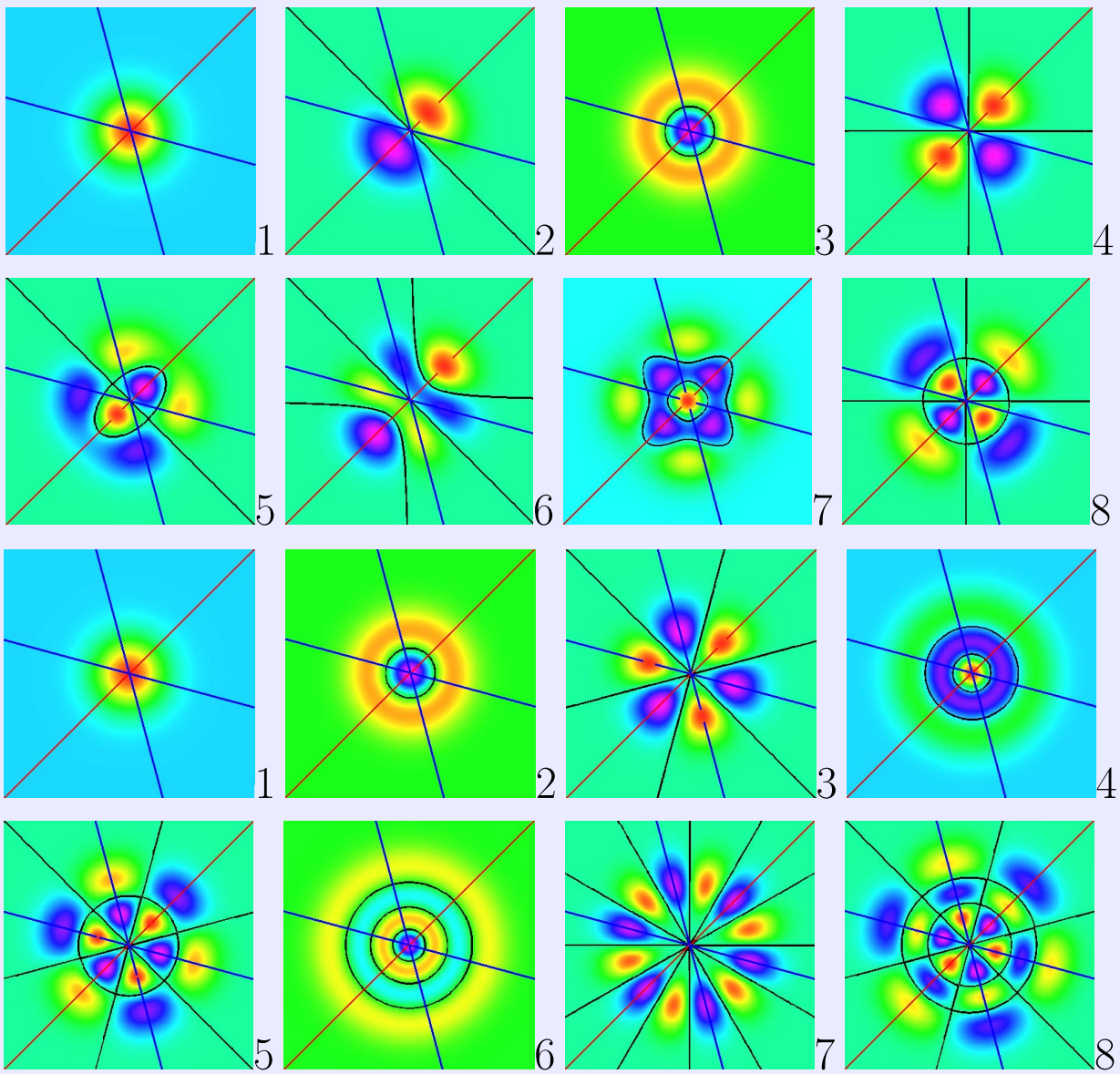
$$x_{ij} \equiv x_i - x_j = \xi_{i-1} - \xi_{j-1} \equiv \xi_{i-1,j-1}, \quad i, j = 2, ..., A, \quad x_1 = \frac{1}{\sqrt{A}} \sum_{i'=0}^{A-1} \xi_{i'}.$$

Step 2. Symmetrization with respect to permutation of A particles

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

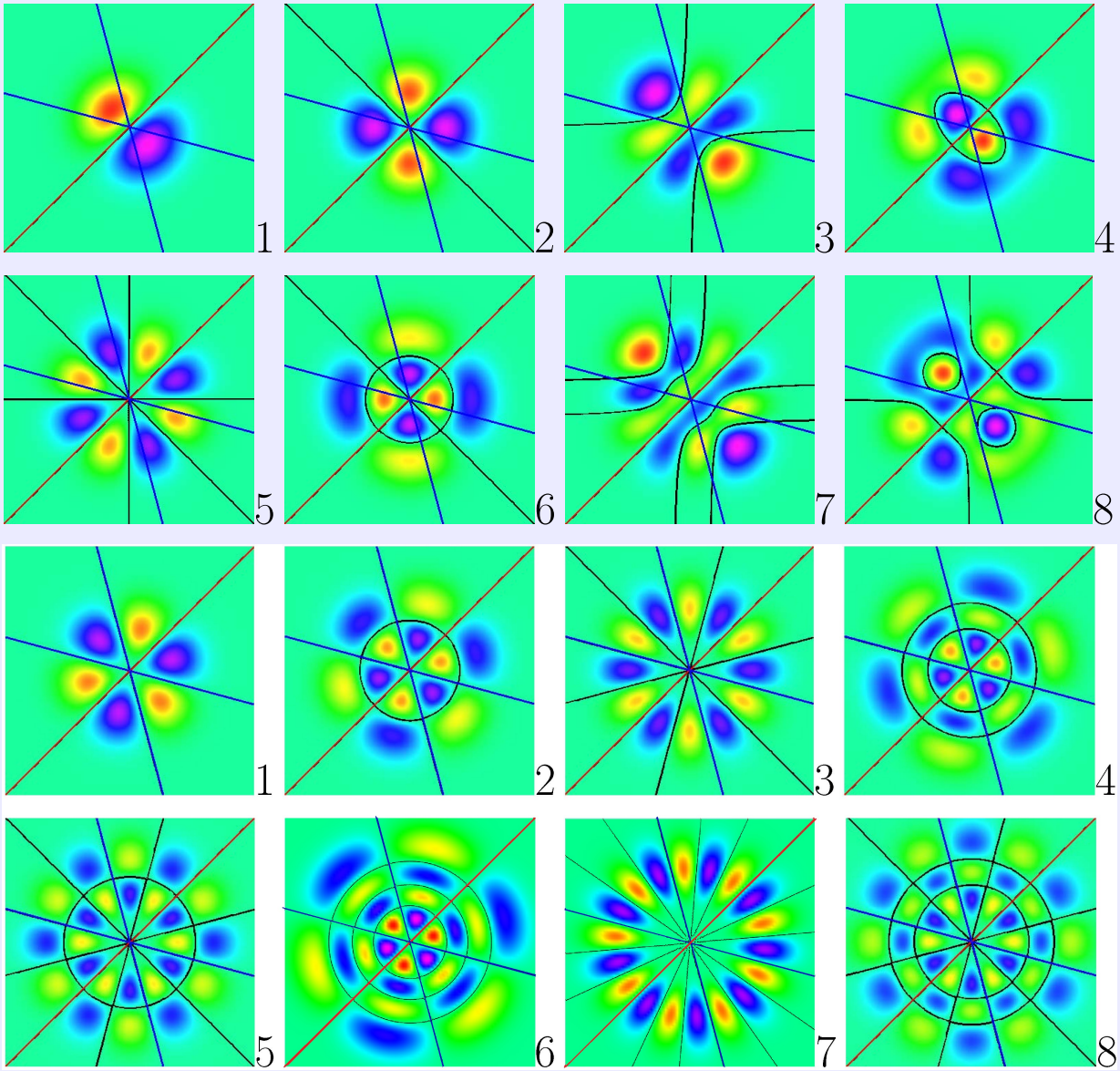
$$\begin{pmatrix} \xi_1 \\ \xi_2 \\ \cdots \\ \xi_{A-1} \end{pmatrix} = \begin{pmatrix} 1 & a_1 & a_0 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_1 & a_0 & \cdots & a_0 & a_0 \\ 1 & a_0 & a_0 & a_1 & \cdots & a_0 & a_0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & a_0 & a_0 & a_0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

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.



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

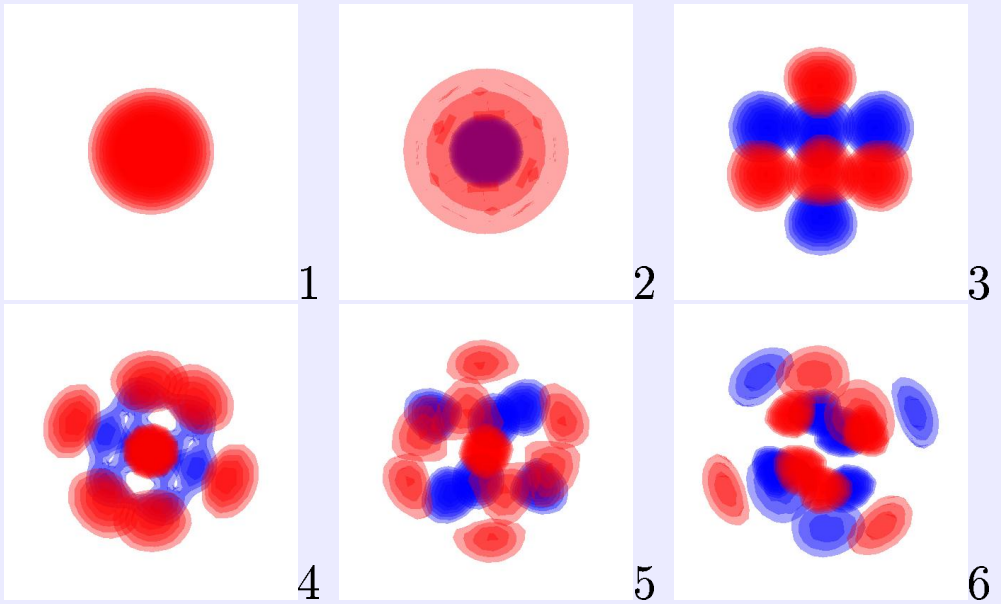
Profiles of the first eight oscillator partial symmetric (upper panels) and symmetric (lower panels) eigenfunctions $\Phi^B_{[i_1,i_2]}(\xi_1,\xi_2)$ at $A = 3$ in coordinate frame (ξ_1,ξ_2). The curves are nodes of the eigenfunctions $\Phi^B_{[i_1,i_2]}(\xi_1,\xi_2)$. Red line correspond to pair collision $x_2 = x_3$, and blue lines correspond to pair collisions $x_1 = x_2$ and $x_1 = x_3$ of projection $(x_1,x_2,x_3) \to (\xi_1,\xi_2)$. From our construction follows: eigenfunctions of the A identical particle system in one dimension are degenerate like in: J.M. Lévy-Leblond, Phys. Lett. A 26, 540 (1968).



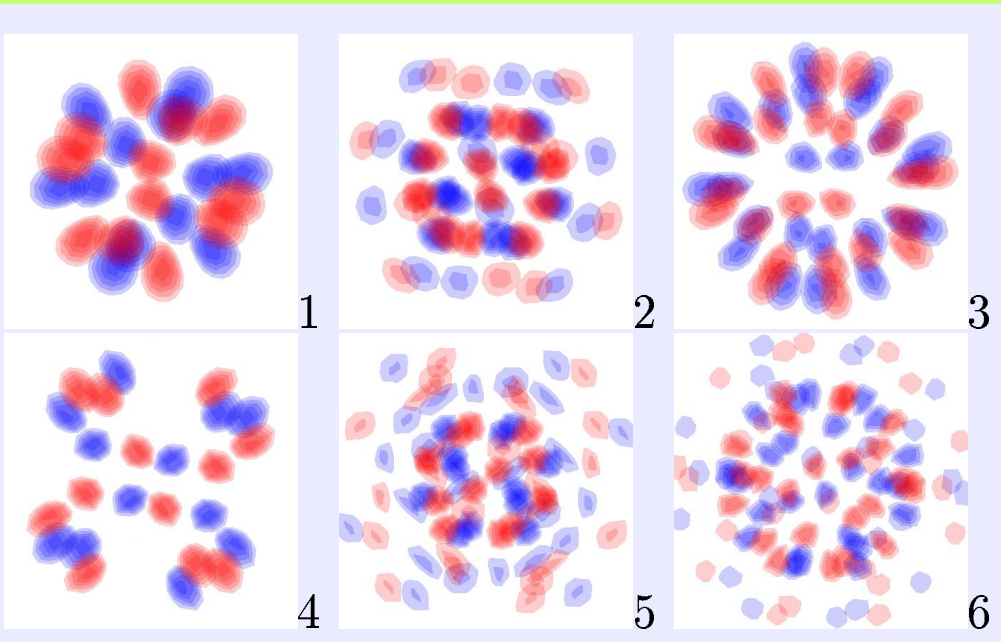
$\Phi^F_{[i_1,i_2]}(\xi_1,\xi_2) = C_{km}(\rho^2)^{3m/2}\exp(-\rho^2/2)\sin(3m(\varphi+\pi/12))L_k^{3m}(\rho^2)$,
$(\xi_1 = \rho\cos\varphi,\ \xi_2 = \rho\sin\varphi,\ k = 0,1,\ldots,\ m = 1,2,\ldots)$

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 $\Phi^a_{[i_1,i_2]}(\xi_1,\xi_2)$.

Our result about degeneracy of the basis disagrees with: Zh.Wang et al., arXiv:1108.1607v4 [math-ph], Commun. Theor. Phys. 58 (2012) 639–644. The latter can be presented as a linear combination of the above S (A)-type functions.

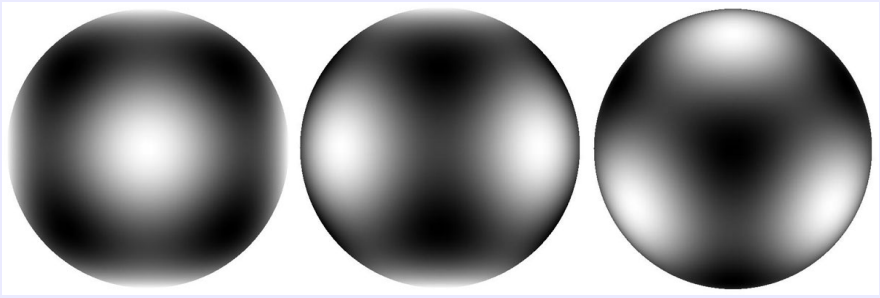


Profiles of the first six oscillator symmetric eigenfunctions $\Phi^{S}_{[i_1,i_2,i_3]}(\xi_1,\xi_2,\xi_3)$ at $A=4$ in coordinate frame (ξ_1,ξ_2,ξ_3).

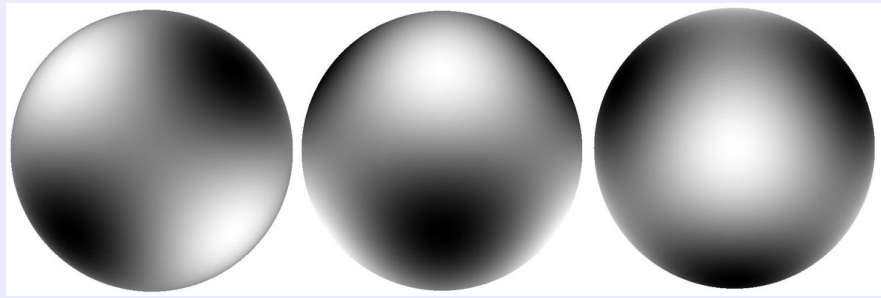


Profiles of the first six oscillator antisymmetric eigenfunctions $\Phi^{A}_{[i_1,i_2,i_3]}(\xi_1,\xi_2,\xi_3)$ at $A=4$ in coordinate frame (ξ_1,ξ_2,ξ_3).

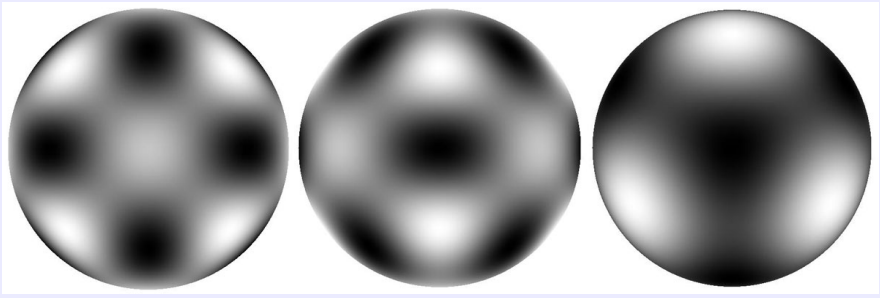
$[c_{40} P_4^0(\eta) + c_{44} P_4^4(\eta) \cos(4\varphi)]$



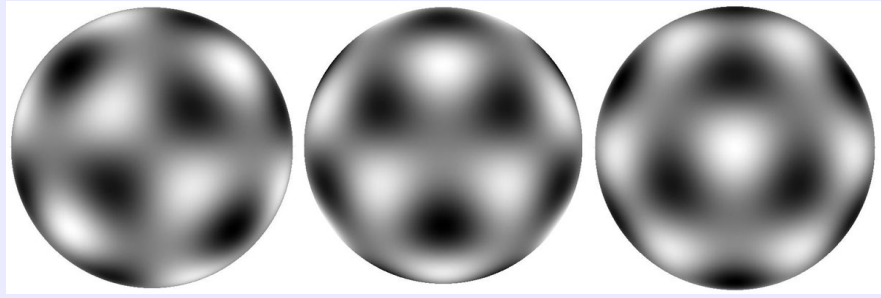
$[c_{32} P_3^2(\eta) \sin(2\varphi)]$



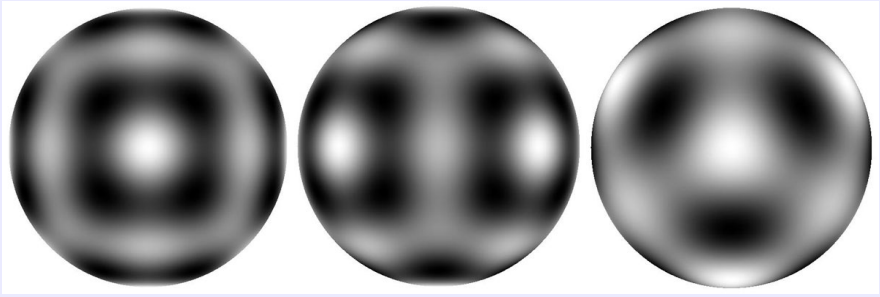
$[c_{60} P_6^0(\eta) + c_{64} P_6^4(\eta) \cos(4\varphi)]$



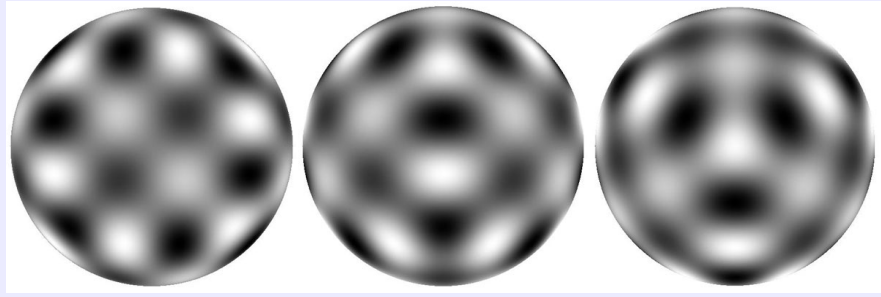
$[c_{72} P_7^2(\eta) \sin(2\varphi) + c_{76} P_7^6(\eta) \sin(6\varphi)]$



$[c_{80} P_8^0(\eta) + c_{84} P_8^4(\eta) \cos(4\varphi) + c_{88} P_8^8(\eta) \cos(8\varphi)]$



$[c_{92} P_9^2(\eta) \sin(2\varphi) + c_{96} P_9^6(\eta) \sin(6\varphi)]$



octahedral symmetry

tetrahedral symmetry

The close-coupling Galerkin equations in symmetrized coordinates

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

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

Scattering problem (with real eigenvalues E)

$$\boldsymbol{\chi}^{v}_{\xi_0\to\pm\infty}=\begin{cases}\begin{cases}\mathbf{X}^{(+)}(\xi_0)\mathbf{T}_v, & \xi_0>0,\\ \mathbf{X}^{(+)}(\xi_0)+\mathbf{X}^{(-)}(\xi_0)\mathbf{R}_v, & \xi_0<0,\end{cases} & v=\rightarrow,\\ \begin{cases}\mathbf{X}^{(-)}(\xi_0)+\mathbf{X}^{(+)}(\xi_0)\mathbf{R}_v, & \xi_0>0,\\ \mathbf{X}^{(-)}(\xi_0)\mathbf{T}_v, & \xi_0<0,\end{cases} & v=\leftarrow,\end{cases}$$

where $\mathbf{R}_v$ and $\mathbf{T}_v$ are the reflection and transmission $N_o\times N_o$ matrices, N_o is number of open channels, v denote the initial direction of the particle motion,
Open channels $i_o=1,\ldots,N_o$:
$X^{(\pm)}_{ii_o}(\xi_0)=\frac{\exp\left(\pm\imath\left(p_{i_o}\xi_0\right)\right)}{\sqrt{p_{i_o}}}\delta_{ji_o}$
Closed channels $i_c=N_o+1,\ldots,N$: $\chi_{ii_c}(\xi_0)\to 0$

Metastable states (with complex eigenvalues $E=\Re E+\imath\Im E$, $\Im E<0$)

Siegert boundary conditions

$$\left.\frac{d\boldsymbol{\chi}(\xi_0)}{d\xi_0}\right|_{\xi_0=\xi_0^t}=\mathcal{R}(\xi_0^t)\boldsymbol{\chi}(\xi_0^t),$$

$t=\min,\max.$

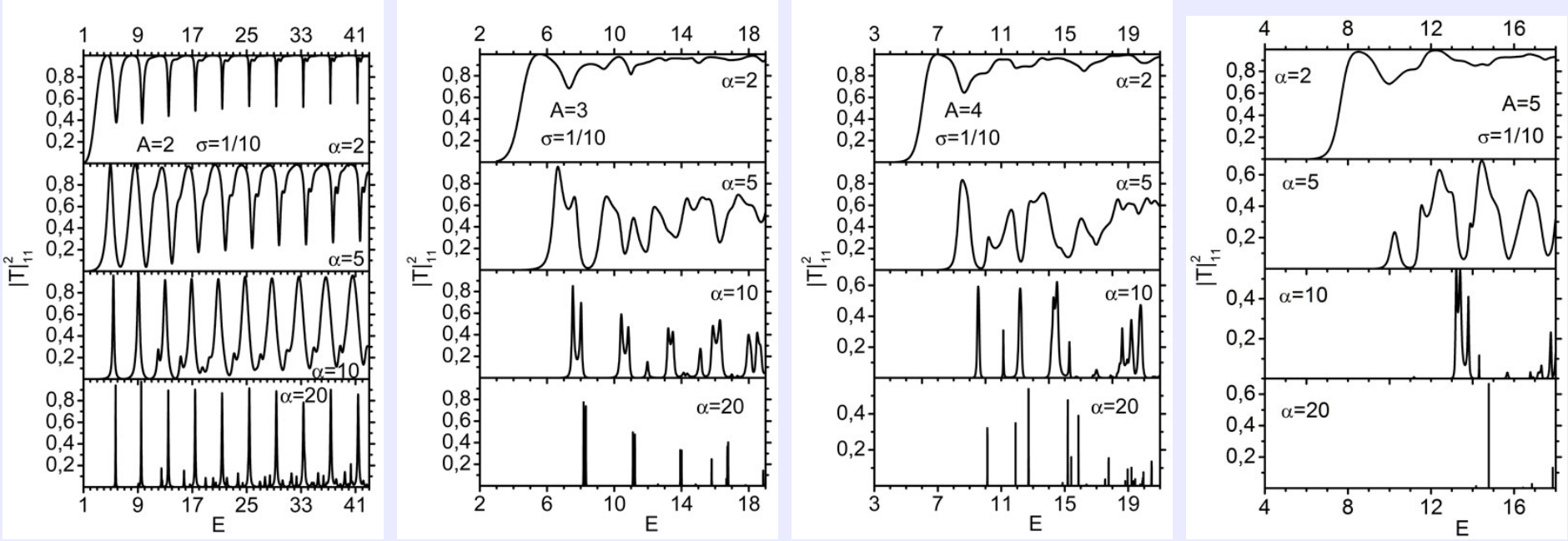
$\mathcal{R}_{i_oi_o}(\xi_0^{\max})=\imath p_{i_o},$

$\mathcal{R}_{i_oi_o}(\xi_0^{\min})=-\mathcal{R}_{i_oi_o}(\xi_0^{\max}),$

$$p_{i_o}=\sqrt{E-E_{i_o}},$$

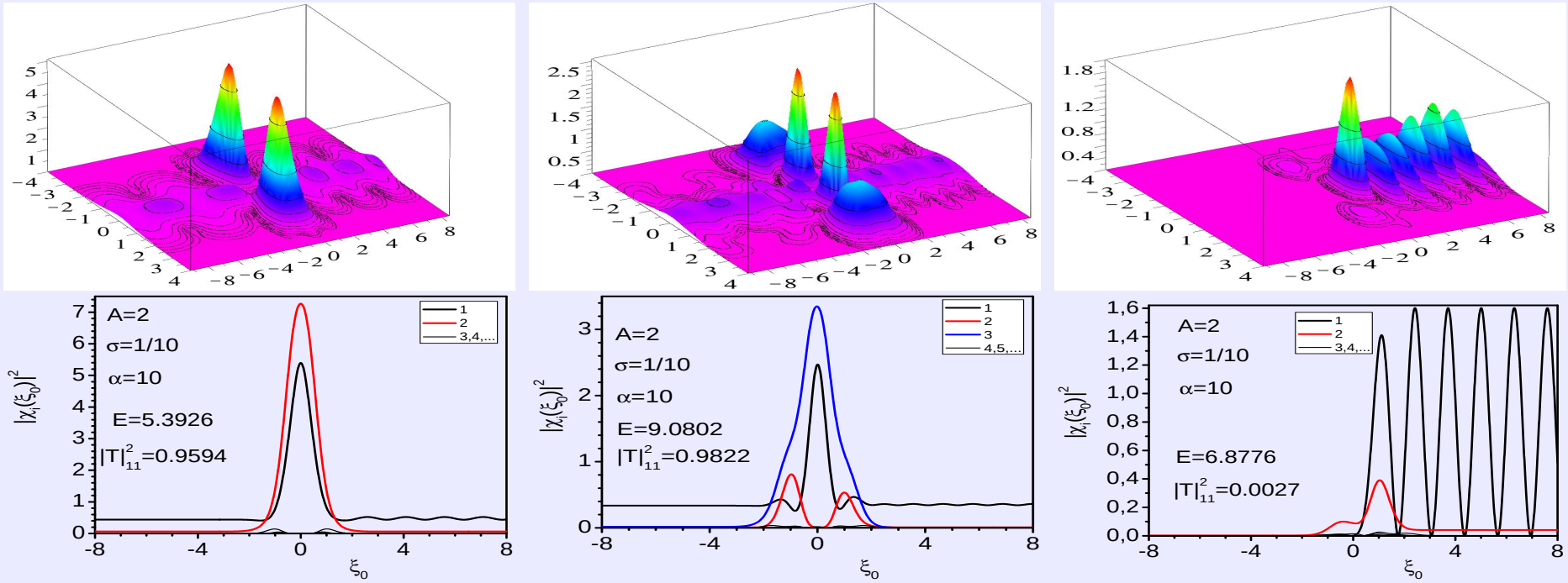
The total transmission probabilities

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



The total transmission probabilities $|T|^2_{11}$ vs energy E (in oscillator units) from the symmetric ground state of the system of $A = 2, 3, 4, 5$ of 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 $\alpha = 2, 5, 10, 20$.

Sub-barrier transmission



The probability densities $|\Psi(\xi_0, \xi_1)|^2$ of functions and their components $|\chi_i(\xi_0)|^2$ of functions of symmetric ground state for $A = 2$ identical particles.

Sub-barrier transmission

$A = 3$, $\sigma = 1/10$, $\alpha = 20$

l	E_l^S	$\lvert T\rvert_{11}^2$	m	E_m^M
1	8.175	0.775	1	$8.175-\imath 5.1(-3)$
	8.306	0.737	2	$8.306-\imath 5.0(-3)$
2	11.111	0.495	3	$11.110-\imath 5.6(-3)$
	11.229	0.476	4	$11.229-\imath 5.5(-3)$
3	12.598	0.013	5	$12.598-\imath 6.4(-3)$
			6	$12.599-\imath 6.3(-3)$

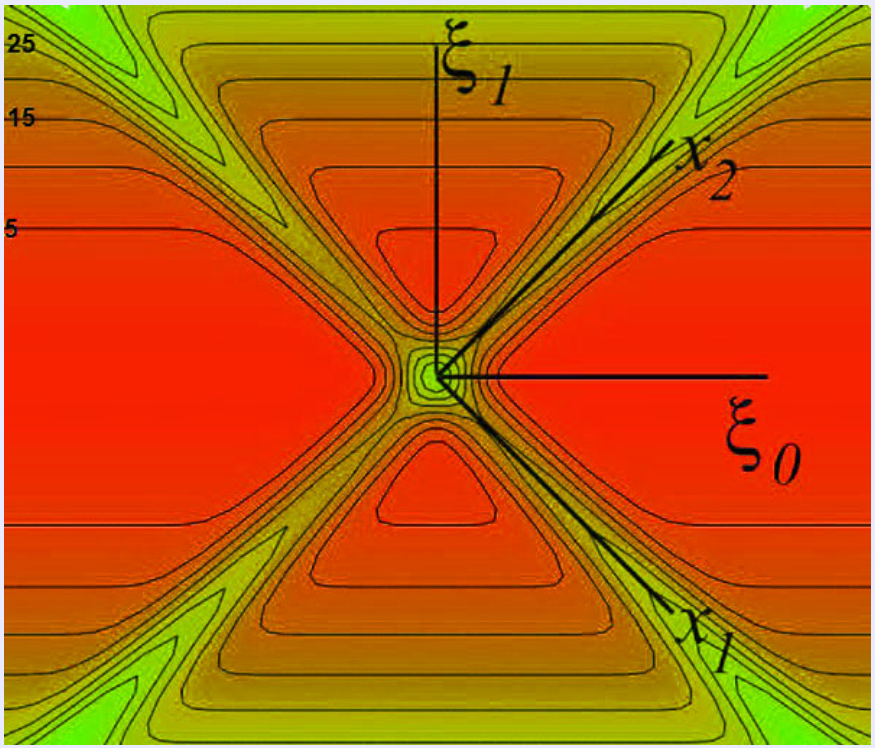
$A = 4$, $\sigma = 1/10$, $\alpha = 20$

l	E_l^S	$\lvert T\rvert_{11}^2$	m	E_m^M
1	10.121	0.321	1	$10.119-\imath 4.0(-3)$
			2	$10.123-\imath 4.0(-3)$
2	11.896	0.349	3	$11.896-\imath 6.3(-5)$
3	12.713	0.538	4	$12.710-\imath 4.5(-3)$
	12.717	0.538	5	$12.720-\imath 4.5(-3)$

$A = 5$, $\sigma = 1/10$, $\alpha = 20$.

l	E_l^S	$\lvert T\rvert_{11}^2$	m	E_m^M
1	11.794	$1.6(-4)$	1	$11.794-\imath 1.3(-3)$
			2	$11.794-\imath 1.3(-3)$
2	14.166	0.014	3	$14.166-\imath 1.1(-3)$
			4	$14.166-\imath 1.1(-3)$
3	14.764	0.666	5	$14.764-\imath 6.6(-6)$
	14.774	0.666	6	$14.774-\imath 5.6(-6)$

Classification of the metastable states



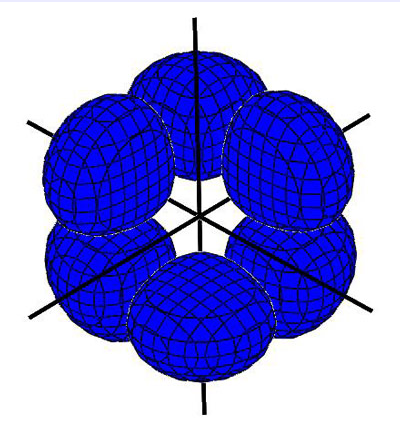
The narrow barriers are approximated by walls $x_i(\xi_0, ..., \xi_{A-1}) = 0$.

The problem is solved in Cartesian coordinates in one of $2^n - 2$ subdomains $\Omega_t = \{x_1, \ldots, x_n | \sigma_i x_i > 0, i = 1, ..., n\}$, where $\sigma_i = \pm 1$ indicates the location of the i-th particle.

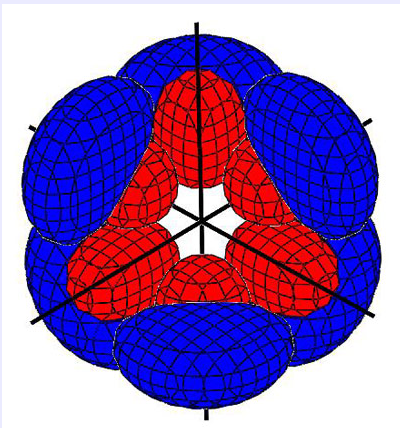
As a truncated oscillator basis we use the odd harmonic oscillator functions centered at the crossing point of walls.

To calculate the eigenfunctions $\Psi_l^D(\mathrm{x})$, S-symmetric (or A-antisymmetric) under the permutations of particles in the entire domain of definition R^n it is necessary and sufficient to ensure that the function in one of the wells $\Psi_l^D(\mathrm{x})$ is symmetric (antisymmetric) with respect to the permutation of the coordinates x_i with similar σ_i.

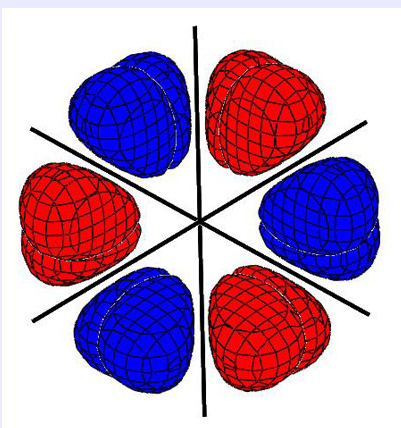
Isosurfaces of first symmetric and antisymmetric doublet states of three identical particles



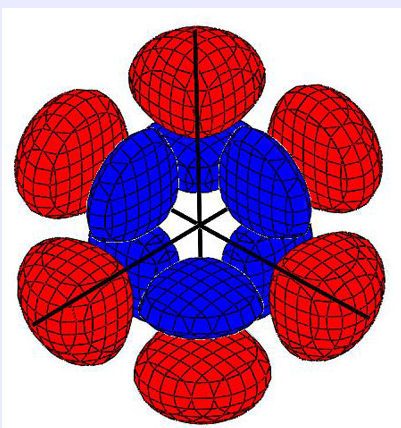
S1g



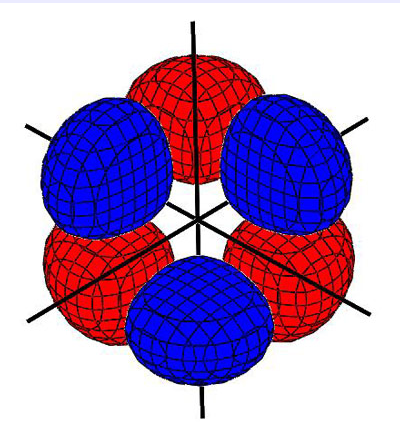
S2g



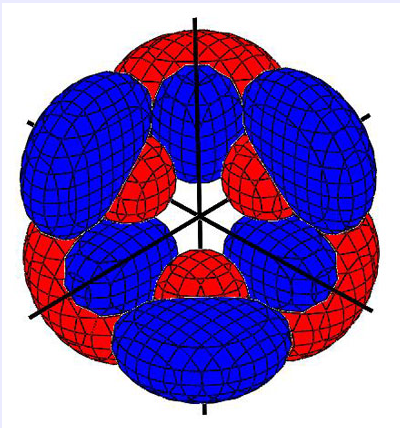
A1g



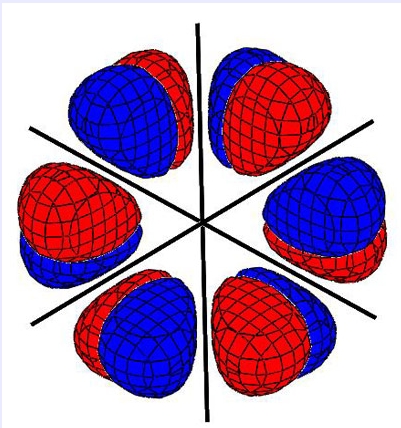
S3g



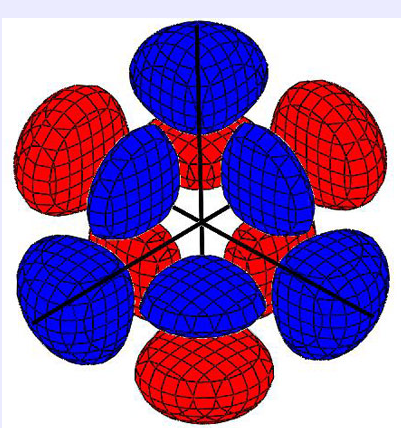
S1u



S2u

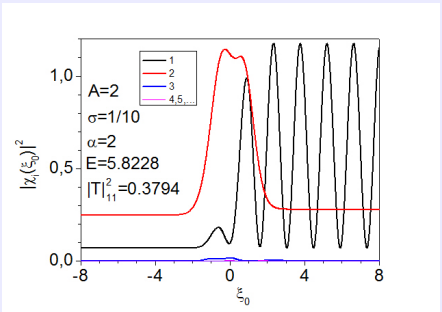


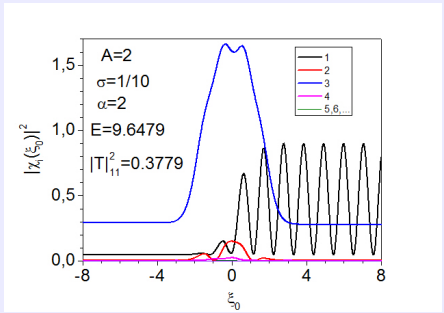
A1u

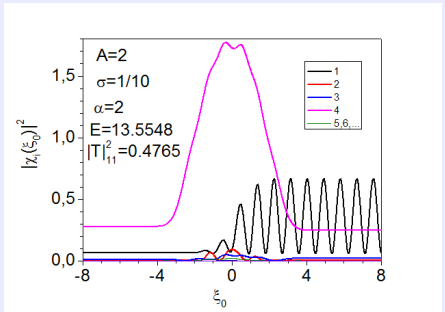


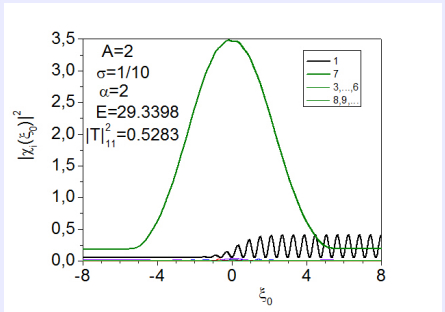
S3u

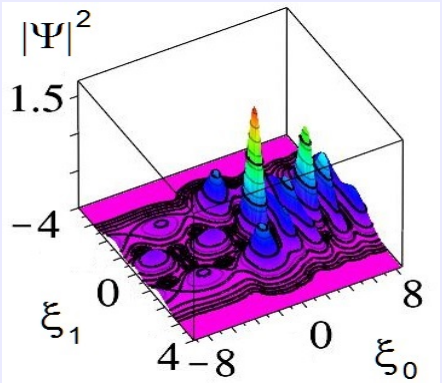
Over-barrier transmission

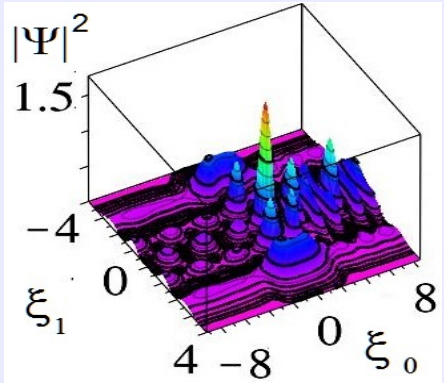


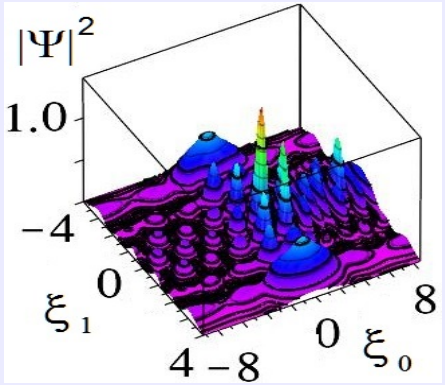


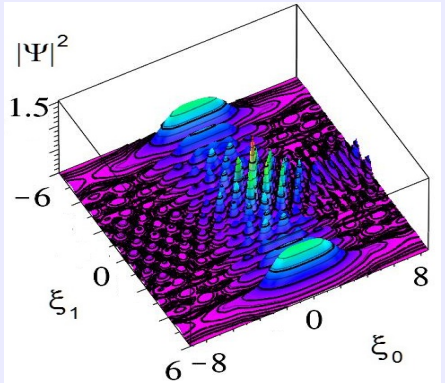


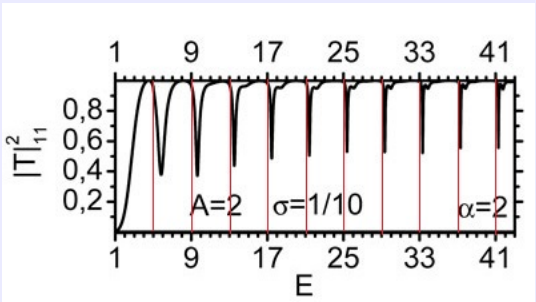








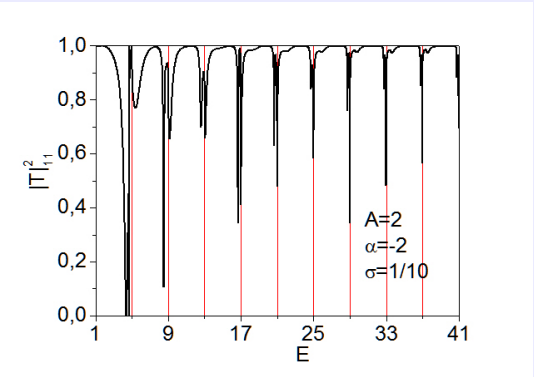


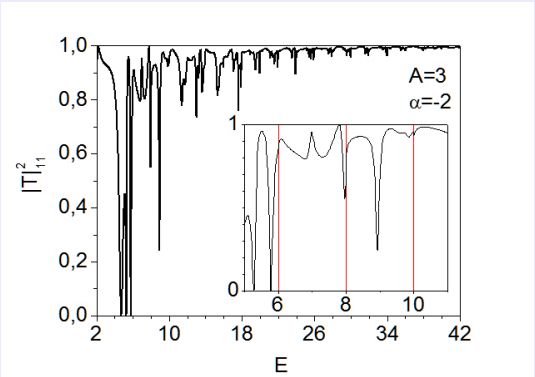


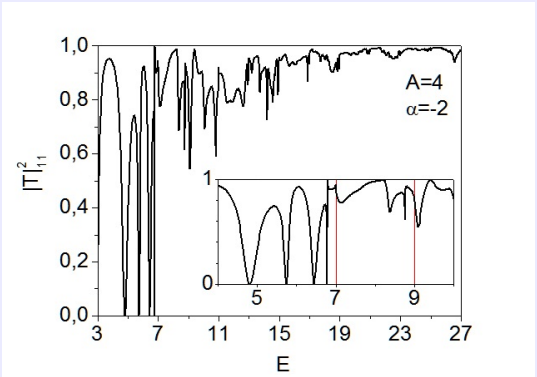
red lines are threshold energies

E_i^S	$\lvert T\rvert^2_{11}$	E_m^M
5.8228	0.3794	
9.6479	0.3779	$9.614-\imath 0.217$
13.5548	0.4765	$13.505-\imath 0.144$
13.9648	$0.8536(\lvert T\rvert^2_{33})$	$14.018-\imath 0.286$
17.4512	0.4874	$17.445-\imath 0.103$

Over-well transmission

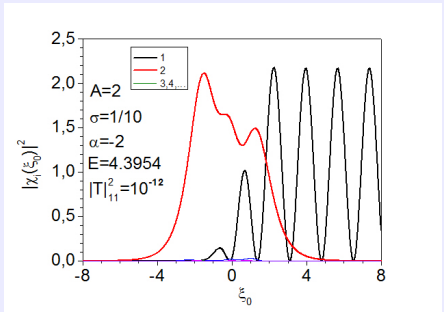


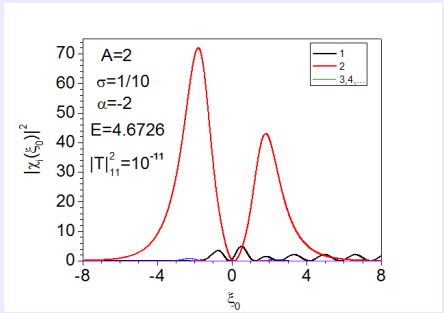


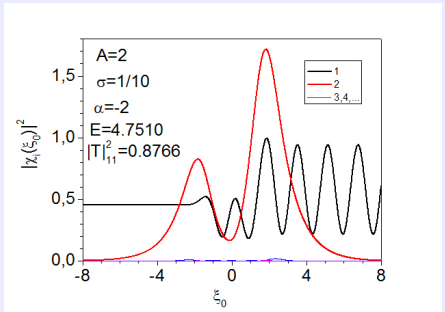


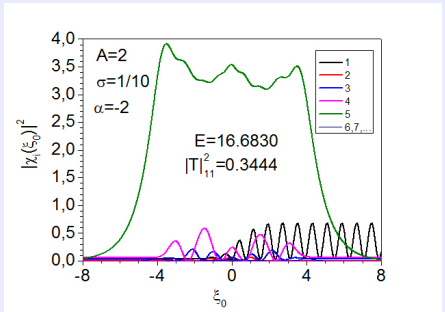
E_i^{th}	$E_m^M(A=2)$	E_i^{th}	$E_m^M(A=3)$	E_i^{th}	$E_m^M(A=4)$
	-0.3588		{-0.2605,1.5082}		{-0.1938, 1.7084 2.7046}
1	$4.4348-\imath 0.2572$	2	$5.3307-\imath 0.0620$	3	$5.7747-\imath 0.0742$
	$4.6764-\imath 0.0058$		$5.7911-\imath 0.0621$		$6.4441-\imath 0.1050$
5	$8.5158-\imath 0.0506$	6	$6.9922-\imath 0.0751$		$6.7934-\imath 0.0033$
	$8.7675-\imath 0.1261$		$7.9457-\imath 0.0565$	7	$8.3668-\imath 0.0651$
9	$12.6009-\imath 0.1215$	8	$8.9601-\imath 0.0588$		$8.7797-\imath 0.0080$
	$12.7330-\imath 0.0142$		$9.4950-\imath 0.2251$	9	$9.4050-\imath 0.1995$
13	$16.6841-\imath 0.0364$		$9.8617-\imath 0.0852$		$9.9926-\imath 0.1225$
	$16.7050-\imath 0.0914$	10	$11.4173-\imath 0.1678$		$10.0755-\imath 0.0676$

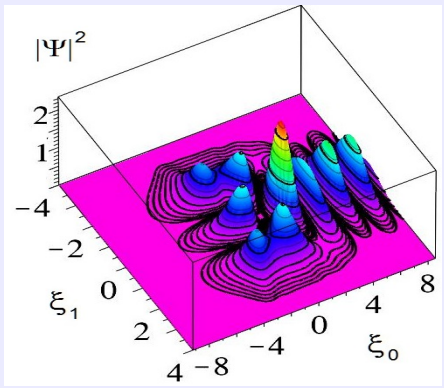
Over-well transmission

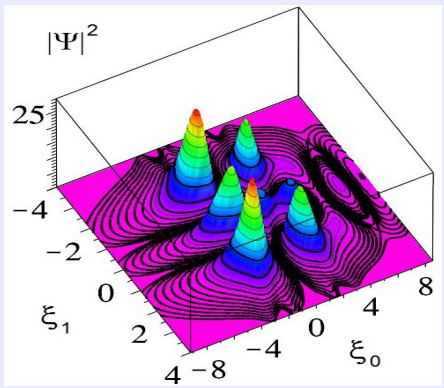


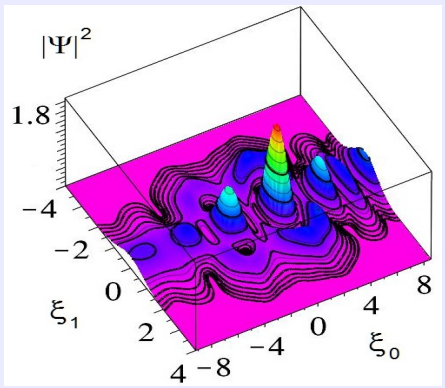


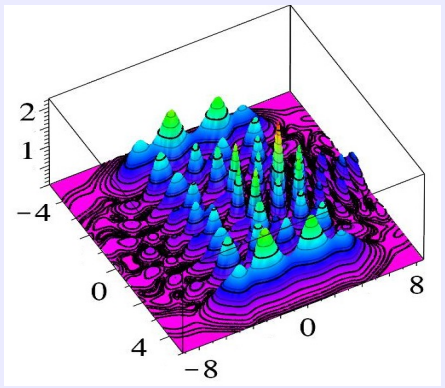












Resume

- Quantum tunnelling of a cluster comprised of several identical particles, coupled via the oscillator-type potential, through short-range repulsive barrier potentials is studied in the s-wave approximation of the symmetrised-coordinate representation.
- A procedure is described that allows construction of states, symmetric or asymmetric with respect to permutations of A identical particles, from the harmonic oscillator basis functions expressed via the newly introduced symmetrized coordinates [Lecture Notes in Computer Science 8136, 155–168 (2013).].
- The description of quantum tunneling (and channeling) of clusters of several identical particles through the barriers and wells in a coupled-channel approximation of symmetrized-coordinate representation of harmonic oscillator basis symmetric or antisymmetric w.r.t. the permutation of particles is presented.
- Efficiency of the proposed approach and computer codes (KANTBP, KANTBP 3.0 & KANTBP 4M) is demonstrated by analysis of metastable states with complex values of energy of composite systems leading to a quantum transparency effect of the barriers and wells in dependence on number of identical particles and type of symmetry of their states.
- The proposed model can be used as a benchmark to test different methods of calculating the metastable states of composite systems of several identical particles and confinement induced resonances in optical traps.

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Thank you for your attention!