*Theoretical and Mathematical Physics*, **186**(1): 21–40 (2016)

# METASTABLE STATES OF A COMPOSITE SYSTEM TUNNELING THROUGH REPULSIVE BARRIERS

**A. A. Gusev,[*] S. I. Vinitsky,[*] O. Chuluunbaatar,[*†] V. L. Derbov,[‡] A. Góźdź,[§] and P. M. Krassovitskiy[¶]**

*We consider a method for solving the problem of quantum tunneling through repulsive potential barriers for a composite system consisting of several identical particles coupled via pair oscillator-type potentials in the oscillator symmetrized-coordinate representation. We confirm the efficiency of the proposed approach by calculating complex energy values and analyzing metastable states of composite systems of three, four, and five identical particles on a line, which leads to the effect of quantum transparency of the repulsive barriers.*

**Keywords:** quantum tunneling, system of identical particles, symmetrized-coordinate representation, harmonic oscillator basis, complex energy value, metastable state, quantum transparency

DOI: 10.1134/S0040577916010037

## 1. Introduction

The study of resonance states in reactions with light nuclei is based on the quantum scattering theory for few-particle systems [1], [2]. The more complex problem of studying resonance states arising in the process of scattering light nuclei by heavy target nuclei [3] can be considered in the first approximation as a problem of a composite system tunneling through repulsive barriers. The mechanism of barrier quantum transparency for the tunneling of a coupled pair of particles or ions was interpreted in [4] as a manifestation of metastable states of the composite system "coupled pair of particles + barrier."

We note that the imaginary part of the metastable state energy (or the width of the resonance of the pair transmission probability) is described analytically only in the exceptional case of a rigid molecule model [5]. Therefore, applying both analytic and numerical methods is required for exploring such a

[*]Joint Institute for Nuclear Research, Dubna, Moscow Oblast, Russia, e-mail: gooseff@jinr.ru.

[†]Mongolian National University, Ulaanbaatar, Mongolia.

[‡]Saratov Chernyshevsky State University, Saratov, Russia.

[§]Maria Curie-Skłodowska University, Lublin, Poland.

[¶]Institute of Nuclear Physics, Almaty, Kazakhstan.

This research was supported in part by the Russian Foundation for Basic Research (Grant Nos. 14-01-00420 and 13-01-00668), the Bogoliubov–Infeld program, and the Ministry of Education and Science of the Republic of Kazakhstan (Grant No. 0333/GF4).

Prepared from an English manuscript submitted by the authors; for the Russian version, see *Teoreticheskaya i Matematicheskaya Fizika*, Vol. 186, No. 1, pp. 27–50, January, 2016.

  

class of problems [6], [7]. The analysis of the quantum transparency mechanism in a system of $n$ identical particles is interesting both for nuclear and molecular physics and for the physics of semiconductor composite nanostructures [8].

Here, we formulate a mathematical model for the tunneling of a system of $n$ identical particles coupled by pair oscillator-type interactions in the field of repulsive barrier potentials in the form of a boundary-value problem for an elliptic-type equation and present efficient methods for analyzing its solutions. We assume that the spin part of the wave function is known and therefore consider only the coordinate part of the wave function, which must be symmetric or antisymmetric under a permutation of $n$ identical particles in a $d$-dimensional Euclidean space [9]. We consider the initial problem in the $(n{\times}d)$-dimensional configuration space in the symmetrized coordinates, where the center-of-mass motion for the system of $n$ identical particles is separated as in Jacobi coordinates while the relative coordinates are related to the Jacobi coordinates by an orthogonal transformation [10].

We note that the idea of introducing symmetrized coordinates for a system of four particles was proposed as long as half a century ago [11], but the general case of a system of $n$ identical particles has not been considered in the literature [12]. We recall that the main advantage of introducing symmetrized coordinates compared with traditional Jacobi coordinates or cluster coordinates [13] consists in providing the invariance of the problem under permutations of $n$ identical particles. This property, in comparison with the known cumbersome procedures in Jacobi coordinates (see, e.g., [14]), allows a sufficiently simple construction of not only the basis functions, symmetric or antisymmetric under permutation of $n{-}1$ relative (internal) coordinates, but also the basis functions, symmetric or antisymmetric under permutation of $n$ Cartesian coordinates [15]. The decomposition of the sought solution in such a basis is called the symmetrized-coordinate representation [10].

For clarity of the presentation, we restrict ourself to the case of a one-dimensional Euclidean space ($d = 1$). The solution of the boundary-value problem for the composite system of $n$ identical particles is sought in the form of an expansion over the cluster $(n{-}1)$-dimensional oscillator basis functions [12], symmetric or antisymmetric under permutation of $n$ identical particles in the representation of relative symmetrized coordinates [10], [16], [17]. In this representation, the initial problem reduces to the boundary-value problem for a system of ordinary second-order differential equations for the functions depending on the center-of-mass variable with homogeneous boundary conditions of the third kind. We use the finite-element method implemented in the software package `KANTBP 3.0` [18] to calculate the matrices of transmission and reflection amplitudes and the eigenfunctions of the scattering problem with respect to the center-of-mass variable with fixed real values of the energy in the continuous spectrum.

We demonstrate the efficiency of the approach by analyzing the solutions of the problem of quantum tunneling of clusters, consisting of a few identical particles on a line, through high and narrow Gaussian repulsive barriers, comparable to the mean size of the incident cluster. Example calculations for different parameters of the Gaussian repulsive barrier, as well as of the long-range repulsive barrier, including the channeling problem, were considered in [7], [10], [19]. The quantum transparency effect, i.e., resonance tunneling through repulsive barriers with the transmission coefficient close to unity, was analyzed for a cluster of a few identical particles. The effect is due to the presence of barrier metastable states merged in the continuous spectrum, localized in the vicinity of the potential energy minimums of the composite system.

To calculate metastable states with unknown complex energy eigenvalues, the boundary-value problem for the system of equations mentioned above is formulated on a finite interval with homogeneous boundary conditions of the third kind, depending on the unknown energy eigenvalue, and the appropriate symmetric quadratic functional required for a finite-element discrete formulation of the problem is constructed. In contrast to the scattering problem, the asymptotic solutions for metastable states contain only the

outgoing waves, which are considered on a sufficiently large but finite interval of the spatial variable variation [2], [20], [21]. The complex energy eigenvalues and corresponding eigenfunctions are calculated using the iteration Newton-type method [6] implemented in the program `KANTBP 4.0`. To calculate the energy level positions of the metastable states and to classify them (depending on their number and symmetry type), we use the algorithm of solving the boundary-value problem in the $n$-dimensional domain of a special type based on expanding the solution over the $n$-dimensional oscillator basis in the initial Cartesian coordinates.

The proposed approach is oriented toward analyzing quantum transparency mechanisms for potential barriers in the processes of quantum diffusion of molecules, channeling and tunneling of clusters and ions in crystals, semiconductor composite nanostructures and also toward studying and classifying the metastable states of rare-earth nuclei with tetrahedral and octahedral symmetry [22].

This paper is structured as follows. In Sec. 2, we consider the formulation of the problem and its reduction in the symmetrized coordinates. In Sec. 3, we construct the oscillator representation in the relative symmetrized coordinates. In Sec. 4, we present the equations of the coupled-channel method for functions depending on the center-of-mass coordinate and give the formulation of variational functionals necessary for calculating the transmission and reflection amplitude matrices and the complex eigenvalues and eigenfunctions of metastable states. In Sec. 5, we present the classification of metastable states and the analysis of the quantum transparency effect.

## 2. Symmetrized coordinates

We consider a system of $n$ identical quantum particles with the mass $m$ and the set of Cartesian coordinates $\tilde{x}_i \in \mathbb{R}^d$ in the $d$-dimensional Euclidean space forming the vector $\tilde{\mathbf{x}} = (\tilde{x}_1, \ldots, \tilde{x}_n) \in \mathbb{R}^{n\times d}$ in the $(n\times d)$-dimensional configuration space. We assume that the particles interact via pair potentials $\widetilde{V}^{\rm pair}(\tilde{x}_{ij})$ depending on the relative coordinates $\tilde{x}_{ij} = \tilde{x}_i - \tilde{x}_j$ similar to the harmonic oscillator potential

$$\widetilde{V}^{\rm hosc}(\tilde{x}_{ij}) = \frac{m\omega^2}{2}(\tilde{x}_{ij})^2$$

with the frequency $\omega$. These particles form a composite system (cluster) that tunnels through the repulsive potential barriers $\widetilde{V}(\tilde{x}_i)$. We use the dimensionless coordinates $x_i = \tilde{x}_i/x_{\rm osc}$, $x_{ij} = \tilde{x}_{ij}/x_{\rm osc} = x_i - x_j$, energy $E = \tilde{E}/E_{\rm osc}$, barrier potentials $V(x_i) = \widetilde{V}(x_i x_{\rm osc})/E_{\rm osc}$, and harmonic oscillator potentials

$$V^{\rm hosc}(x_{ij}) = \frac{\widetilde{V}^{\rm hosc}(x_{ij}x_{\rm osc})}{E_{\rm osc}} = \frac{x_{ij}^2}{n},$$

defined in the oscillator units $x_{\rm osc} = \sqrt{\hbar/(m\omega\sqrt{n})}$ and $E_{\rm osc} = \hbar\omega\sqrt{n}/2$. We can then write the Schrödinger equation as

$$\begin{gathered}\left[-\frac{\partial^2}{\partial \mathbf{x}^2} + \sum_{j=2}^{n}\sum_{i=1}^{j-1}\frac{(x_{ij})^2}{n} + U(\mathbf{x}) - E\right]\Psi(\mathbf{x}) = 0,\\ U(\mathbf{x}) = \sum_{j=2}^{n}\sum_{i=1}^{j-1}U^{\rm pair}(x_{ij}) + \sum_{i=1}^{n}V(x_i),\end{gathered} \tag{1}$$

where $U(\mathbf{x})$ is the multidimensional potential barrier, $U^{\rm pair}(x_{ij}) = V^{\rm pair}(x_{ij}) - V^{\rm hosc}(x_{ij})$ is the nonoscillator part of the pair interaction potential such that if $V^{\rm pair}(x_{ij}) = V^{\rm hosc}(x_{ij})$, then $U^{\rm pair}(x_{ij}) = 0$, and $\mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{R}^{n\times d}$.

Below, we use one of the possible definitions of symmetrized coordinates via an orthogonal and symmetric matrix [16]:

$$\begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \vdots \\ \xi_{n-1} \end{pmatrix} = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & a_1 & a_0 & \cdots & a_0 \\ 1 & a_0 & a_1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & a_0 \\ 1 & a_0 & \cdots & a_0 & a_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix}, \tag{2}$$

where $a_0 = 1/(1-\sqrt{n})$, $a_1 = a_0 + \sqrt{n}$, $\xi_0 \in \mathbb{R}^d$ is the center-of-mass coordinate of the system, and $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_{n-1}) \in \mathbb{R}^{(n-1)\times d}$ are the relative coordinates. Taking the relations $a_1 - a_0 = \sqrt{n}$ and $a_0 - 1 = a_0\sqrt{n}$ into account, we can express the relative coordinate $x_{ij} \equiv x_i - x_j$ of a pair of particles $i$ and $j$ using only $n-1$ relative symmetrized coordinates:

$$x_{ij} \equiv x_i - x_j = \xi_{i-1} - \xi_{j-1} \equiv \xi_{i-1,j-1}, \tag{3}$$

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

In the symmetrized coordinates, Eq. (1) becomes

$$\begin{gathered} \left[ -\frac{\partial^2}{\partial \xi_0^2} + \sum_{i=1}^{n-1} \left( -\frac{\partial^2}{\partial \xi_i^2} + \xi_i^2 \right) + U(\xi_0, \boldsymbol{\xi}) - E \right] \Psi(\xi_0, \boldsymbol{\xi}; E) = 0, \\ U(\xi_0, \boldsymbol{\xi}) = \sum_{j=2}^{n} \sum_{i=1}^{j-1} U^{\mathrm{pair}}(x_{ij}(\boldsymbol{\xi})) + \sum_{i=1}^{n} V(x_i(\xi_0, \boldsymbol{\xi})). \end{gathered} \tag{5}$$

This equation is invariant under the permutations $\xi_i \leftrightarrow \xi_j$, $i,j = 1, \ldots, n-1$, i.e., the invariance of Eq. (1) under the permutations $x_i \leftrightarrow x_j$, $i,j = 1, \ldots, n$, is preserved, which significantly simplifies the construction of states symmetric (or antisymmetric) with respect to the operations of permutation of $n$ particles in comparison with the Jacobi coordinates in the center-of-mass reference frame [10], [11], [14], [15]. But the invariance of Eq. (5) under the permutations $\xi_i \leftrightarrow \xi_j$ does not yield the invariance of Eq. (1) under the permutations $x_i \leftrightarrow x_j$, which is the essence of the problem of constructing translation-invariant models of light nuclei [23].

In the case of the one-dimensional Euclidean space considered below ($d = 1$),

$$\xi_0 \in B = [\xi_0^{\min}, \xi_0^{\max}] \subset \mathbb{R}^1, \quad \boldsymbol{\xi} \in \mathbb{R}^{n-1},$$

the solutions $\Psi(\xi_0, \boldsymbol{\xi}; E) \in W_2^2(\Omega)$ of Eq. (5) in the domain $\Omega = B \otimes \mathbb{R}^{n-1}$ satisfy the boundary conditions

$$\begin{aligned} &\lim_{|\boldsymbol{\xi}|\to\infty} \Psi(\xi_0, \boldsymbol{\xi}; E) = 0, && \xi_0 \in [\xi_0^{\min}, \xi_0^{\max}], \\ &\mu_t \frac{\partial \Psi(\xi_0, \boldsymbol{\xi}; E)}{\partial \xi_0} - \lambda_t \, \Psi(\xi_0, \boldsymbol{\xi}; E) = 0, && \xi_0 = \xi_0^t, \quad \boldsymbol{\xi} \in \mathbb{R}^{n-1}, \end{aligned} \tag{6}$$

where the subscript $t = \min, \max$, $\mu_t$ are real-valued constants, and $\lambda_t \equiv \lambda_t(\xi_0^t)$ are real-valued functions depending on $\xi_0^t$ under the condition $\mu_t^2 + \lambda_t^2 \neq 0$.

## 3. Oscillator representation

We restrict ourself to considering only the pair interactions given by harmonic oscillator potentials $V^{\rm pair}(x_{ij}) = V^{\rm hosc}(x_{ij})$ in the case of the one-dimensional Euclidean space ($d = 1$). We define the set of cluster functions

$$\langle \boldsymbol{\xi}|j\rangle^{\rm S(A)} \equiv \Phi_j^{\rm S(A)}(\boldsymbol{\xi}) \in L_2(\mathbb{R}^{n-1}),$$

symmetric (S) or antisymmetric (A) under permutations of $n$ identical particles, and the corresponding energy values $\epsilon_j^{\rm S(A)}$ as solutions of the eigenvalue problem

$$\left(-\frac{\partial^2}{\partial \boldsymbol{\xi}^2} + \boldsymbol{\xi}^2 - \epsilon_j^{\rm S(A)}\right)\Phi_j^{\rm S(A)}(\boldsymbol{\xi}) = 0. \tag{7}$$

We seek solutions $\Phi_j^{\rm S(A)}(\boldsymbol{\xi})$ in the form of linear combinations of known functions of the $(n-1)$-dimensional harmonic oscillator $\Phi^{\rm osc}_{[i_1,\ldots,i_{n-1}]}(\boldsymbol{\xi}) \in L_2(\mathbb{R}^{n-1})$

$$\begin{aligned}
\Phi_j^{\rm S(A)}(\boldsymbol{\xi}) &= \sum_{\{i_1,\ldots,i_{n-1}\}\in\Delta_j} \alpha^{\rm S(A)}_{j[i_1,\ldots,i_{n-1}]}\Phi^{\rm osc}_{[i_1,\ldots,i_{n-1}]}(\boldsymbol{\xi}),\\
\Phi^{\rm osc}_{[i_1,\ldots,i_{n-1}]}(\boldsymbol{\xi}) &= \prod_{k=1}^{n-1}\frac{e^{-\xi_k^2/2}H_{i_k}(\xi_k)}{\sqrt[4]{\pi}\sqrt{2^{i_k}}\sqrt{i_k!}}.
\end{aligned} \tag{8}$$

Here, $H_{i_k}(\xi_k)$ are the Hermite polynomials [24], and the set of subscripts $\Delta_j \equiv \{i_1,\ldots,i_{n-1}\}$ taking natural number values is defined by the condition

$$\Delta_j = \left\{ i_1,\ldots,i_{n-1} \,\middle|\, 2\sum_{k=1}^{n-1} i_k + n - 1 = \epsilon_j^{\rm S(A)} \right\}, \tag{9}$$

which determines their belonging to the set of eigenfunctions $\Phi^{\rm osc}_{[i_1,\ldots,i_{n-1}]}(\boldsymbol{\xi})$ corresponding to the eigenvalue $\epsilon^{\rm osc}_{[i_1,\ldots,i_{n-1}]} \equiv \epsilon^{\rm osc}_f = 2f + n - 1$, $f = \sum_{k=1}^{n-1} i_k$, of the $(n-1)$-dimensional oscillator, which has the degeneracy multiplicity [25]

$$p = \frac{(n+f-2)!}{f!(n-2)!}.$$

This eigenvalue is chosen equal to the sought energy eigenvalue $\epsilon_j^{\rm S(A)} = \epsilon^{\rm osc}_{[i_1,\ldots,i_{n-1}]}$.

The unknown coefficients $\alpha^{\rm S(A)}_{j[i_1,\ldots,i_{n-1}]}$ of expansion (8) for the orthonormalized functions $\Phi_j^{\rm S(A)}(\boldsymbol{\xi})$, the corresponding eigenvalues $\epsilon_j^{\rm S(A)}$, and the multiplicity $p^{\rm S(A)} \ll p$ of their degeneracy were calculated using a two-step algorithm and the program in [16] as follows:

1. The eigenfunctions symmetric or antisymmetric under the permutations $\xi_i \leftrightarrow \xi_j$, $j = 1,\ldots,n-1$ (see relations (3)) were generated using the standard method [9]. These functions are also symmetric or antisymmetric under the permutations $x_i \leftrightarrow x_j$, $i,j = 2,\ldots,n$ but are not symmetric or antisymmetric under the permutations $x_1 \leftrightarrow x_j$, $j = 2,\ldots,n$.

2. Using the eigenfunctions obtained in the preceding step, we construct a set of linearly independent functions, symmetric (or antisymmetric) under the permutation $x_2 \leftrightarrow x_1$ (see relations (4)), from which we construct the sought orthonormalized basis (8) using the Gram–Schmidt procedure.

In the case where $n = 3$ and $d = 1$, the functions $\Phi^{\mathrm{S(A)}}_{k,m}(\rho,\varphi,n) \in L_2(\mathbb{R}^1_+ \times S^1)$ are expressed in the hyperspherical (polar) coordinates $\xi_1 = \rho\cos\varphi$, $\xi_2 = \rho\sin\varphi$ in the analytic form

$$\Phi^{\mathrm{S(A)}}_{k,m}(\rho,\varphi,n)\big|_{n=3} = R_{km}(\rho)Y^{\mathrm{S(A)}}_m\big(3m(\varphi+\pi/12)\big),$$

$$R_{km}(\rho) = \sqrt{\frac{2k!}{(k+3m)!}}(\rho^2)^{3m/2}\,e^{-\rho^2/2}L^{3m}_k(\rho^2),$$

where $k = 0, 1, \ldots$, $L^{3m}_k(\rho^2)$ are the generalized Laguerre polynomials [24], and the functions of the hyperangular variable $\varphi$ for S states

$$Y^{\mathrm{S}}_m(\varphi) = \frac{\cos\varphi}{\sqrt{(1+\delta_{m0})\pi}}, \quad m = 0, 1, \ldots,$$

and for A states

$$Y^{\mathrm{A}}_m(\varphi) = \frac{\sin\varphi}{\sqrt{\pi}}, \quad m = 1, 2, \ldots,$$

are classified with respect to the irreducible representations of the symmetry group $D_{3m}$. The corresponding energy eigenvalues

$$\epsilon^{\mathrm{S(A)}}_{k,m} = 2(2k+3m+1)$$

have the multiplicity $p^{\mathrm{S(A)}} = K+1$, where the value of $K$ is determined by the condition of equal energies $\epsilon^{\mathrm{S(A)}}_{k,m} - \epsilon^{\mathrm{S(A)}}_{\mathrm{ground}} = 12K + K'$ for one of the values $K' = 0, 4, 6, 8, 10, 14$, $\epsilon^{\mathrm{S}}_{\mathrm{ground}} = 2$, $\epsilon^{\mathrm{A}}_{\mathrm{ground}} = 8$.

In the case where $n = 4$ and $d = 1$, the energy eigenvalues

$$\epsilon^{\mathrm{S(A)}}_{i_1,i_2,i_3} = 2\left(i_1 + i_2 + i_3 + \frac{3}{2}\right)$$

have the multiplicity $p^{\mathrm{S(A)}} = 3K^2 + (3+K')K + K' + \delta_{0K'}$, where the values of $K$ and $K'$ are determined by the condition of equal energies $\epsilon^{\mathrm{S(A)}}_{i_1,i_2,i_3} - \epsilon^{\mathrm{S(A)}}_{\mathrm{ground}} = 4(6K+K') + K''$ for one of the values of $K' = 0, 1, 2, 3, 4, 5$ and $K'' = 0, 6$, $\epsilon^{\mathrm{S}}_{\mathrm{ground}} = 3$, $\epsilon^{\mathrm{A}}_{\mathrm{ground}} = 15$. Here, $i_1$, $i_2$, and $i_3$ take the values

$$i_1 = 0, 1, \ldots, \qquad i_2 = i_1, i_1+2, \ldots, \qquad i_3 = i_2, i_2+2, \ldots$$

for S states and

$$i_1 = 0, 1, \ldots, \qquad i_2 = i_1+2, i_1+4, \ldots, \qquad i_3 = i_2+2, i_2+4, \ldots$$

for A states. The S states with even quantum numbers $i_1$, $i_2$, and $i_3$ and the A states with odd quantum numbers have octahedral symmetry, while the A states with even values of the quantum numbers $i_1$, $i_2$, and $i_3$ and S states with odd quantum numbers have tetrahedral symmetry [26].

## 4. Coupled channels equations

We restrict ourself to considering the one-dimensional Euclidean space. The asymptotic solution $\mathbf{\Psi}^{\mathrm{S(A)}}(\xi_0, \boldsymbol{\xi}) = \{\Psi^{\mathrm{S(A)}}_{i_\mathrm{o}}(\xi_0, \boldsymbol{\xi})\}^{N_\mathrm{o}}_{i_\mathrm{o}=1}$ of Eq. (5), describing the incident and the outgoing wave as $\xi^+_0 \to +\infty$ and $\xi^-_0 \to -\infty$, in the oscillator basis $\mathbf{\Phi}^{\mathrm{S(A)}}(\boldsymbol{\xi}) = \{\Phi^{\mathrm{S(A)}}_j(\boldsymbol{\xi})\}^{j_{\max}}_{j=1}$ can be written in the matrix form $\mathbf{\Psi}^{\mathrm{S(A)}} = (\mathbf{\Phi}^{\mathrm{S(A)}})^{\mathrm{T}}\mathbf{F}$, where the superscript T denotes matrix transposition.

The matrix solutions $\mathbf{F}_v(\xi_0) = \mathbf{F}(\xi_0)$ describe the transmission and reflection of a particle incident on the barrier and have the asymptotic form "incident plane wave + outgoing waves"

$$\mathbf{F}_v(\xi_0)\big|_{\xi_0\to\pm\infty} = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(\xi_0)\mathbf{T}_v, & \xi_0 > 0, \\ \mathbf{X}^{(+)}(\xi_0) + \mathbf{X}^{(-)}(\xi_0)\mathbf{R}_v, & \xi_0 < 0, \end{cases} & v = \rightarrow, \\ \begin{cases} \mathbf{X}^{(-)}(\xi_0) + \mathbf{X}^{(+)}(\xi_0)\mathbf{R}_v, & \xi_0 > 0, \\ \mathbf{X}^{(-)}(\xi_0)\mathbf{T}_v, & \xi_0 < 0, \end{cases} & v = \leftarrow, \end{cases} \tag{10}$$

where $\mathbf{R}_v$ and $\mathbf{T}_v$ are the $N_\mathrm{o}\times N_\mathrm{o}$ transmission and reflection amplitude matrices, $N_\mathrm{o}$ is the number of open channels for a fixed energy $E > \epsilon_{i_\mathrm{o}}^{\mathrm{S(A)}}$ ($i_\mathrm{o} = 1, \ldots, N_\mathrm{o}$), and the subscript $v$ takes the values $\rightarrow$ or $\leftarrow$ and denotes the initial direction of the particle incidence on the barrier from the respective left or right side. The leading terms of the asymptotic form of the rectangular matrix function $\mathbf{X}^{(\pm)}(z)$ in the presence of a long-range repulsive Coulomb potential barrier are

$$\begin{aligned} &X_{ji_\mathrm{o}}^{(\pm)}(\xi_0) \to p_{i_\mathrm{o}}^{-1/2} \exp\left\{\pm\imath\left(p_{i_\mathrm{o}}\xi_0 - \frac{Z_{i_\mathrm{o}}}{p_{i_\mathrm{o}}}\log(2p_{i_\mathrm{o}}|\xi_0|)\right)\right\}\delta_{ji_\mathrm{o}}, \\ &p_{i_\mathrm{o}} = \sqrt{2E - \epsilon_{i_\mathrm{o}}^{\mathrm{S(A)}}}, \quad j = 1, \ldots, j_{\max}, \quad i_\mathrm{o} = 1, \ldots, N_\mathrm{o}, \end{aligned} \tag{11}$$

where $Z_{i_\mathrm{o}} = Z_{i_\mathrm{o}}^{+}$ for $\xi_0 > 0$ and $Z_{i_\mathrm{o}} = Z_{i_\mathrm{o}}^{-}$ for $\xi_0 < 0$, i.e., when the effective charges are located to the left or right of the repulsive long-range Coulomb potential barrier. The corresponding calculations for the problem of ion pair ($n = 2$) tunneling through a long-range repulsive Coulomb barrier for $Z_{i_\mathrm{o}}^{\pm} \neq 0$ were presented in [7]. Taking the limited volume of this paper taken into account, we restrict ourself in the calculations presented below to considering only tunneling through short-range potential barriers, $Z_{i_\mathrm{o}}^{\pm} = 0$.

The solution matrix $\mathbf{F}_v(\xi_0, E)$ is normalized by the condition

$$\int_{-\infty}^{\infty} \mathbf{F}_{v'}^{\dagger}(\xi_0, E')\mathbf{F}_v(\xi_0, E)\, d\xi_0 = 2\pi\delta(E' - E)\delta_{v'v}\mathbf{I}_{\mathrm{oo}}, \tag{12}$$

where $\mathbf{I}_{\mathrm{oo}}$ is the $N_\mathrm{o}\times N_\mathrm{o}$ unit matrix.

As $\xi_0^{\pm} \to \pm\infty$, we can write Eq. (10) in the matrix form as

$$\begin{pmatrix} \mathbf{F}_{\rightarrow}(\xi_0^{+}) & \mathbf{F}_{\leftarrow}(\xi_0^{+}) \\ \mathbf{F}_{\rightarrow}(\xi_0^{-}) & \mathbf{F}_{\leftarrow}(\xi_0^{-}) \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{X}^{(-)}(\xi_0^{+}) \\ \mathbf{X}^{(+)}(\xi_0^{-}) & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{X}^{(+)}(\xi_0^{+}) \\ \mathbf{X}^{(-)}(\xi_0^{-}) & \mathbf{0} \end{pmatrix} \mathbf{S}, \tag{13}$$

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

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix}, \qquad \mathbf{S}^{\dagger}\mathbf{S} = \mathbf{S}\mathbf{S}^{\dagger} = \mathbf{I}, \tag{14}$$

consisting of the amplitudes of reflected and transmitted waves $\mathbf{R}_v = \mathbf{R}_v(E)$ and $\mathbf{T}_v = \mathbf{T}_v(E)$, the $N_\mathrm{o}\times N_\mathrm{o}$ matrices, for which the required relations follow from the property of Wronskian preservation on the solutions, ensuring that the matrix $\mathbf{S}$ is unitary and symmetric:

$$\begin{aligned} &\mathbf{T}_{\rightarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{R}_{\rightarrow} = \mathbf{I}_{\mathrm{oo}} = \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{T}_{\leftarrow} + \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{R}_{\leftarrow}, \\ &\mathbf{T}_{\rightarrow}^{\dagger}\mathbf{R}_{\leftarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{T}_{\leftarrow} = \mathbf{0} = \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{R}_{\rightarrow}, \\ &\mathbf{T}_{\rightarrow}^{\mathrm{T}} = \mathbf{T}_{\leftarrow}, \qquad \mathbf{R}_{\rightarrow}^{\mathrm{T}} = \mathbf{R}_{\rightarrow}, \qquad \mathbf{R}_{\leftarrow}^{\mathrm{T}} = \mathbf{R}_{\leftarrow}. \end{aligned} \tag{15}$$

The matrix solutions $\widehat{\mathbf{F}}_v(\xi_0) = \widehat{\mathbf{F}}(\xi_0)$ describing the time-reversed tunneling process have the asymptotic form "ingoing waves + outgoing plane wave"

$$\widehat{\mathbf{F}}_v(\xi_0)\big|_{\xi_0\to\pm\infty} = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(\xi_0) + \mathbf{X}^{(-)}(\xi_0)\widehat{\mathbf{R}}_v^\dagger & \xi_0 > 0, \\ \mathbf{X}^{(+)}(\xi_0)\widehat{\mathbf{T}}_v^\dagger, & \xi_0 < 0, \end{cases} & v = \rightarrow, \\ \begin{cases} \mathbf{X}^{(-)}(\xi_0)\widehat{\mathbf{T}}_v^\dagger, & \xi_0 > 0, \\ \mathbf{X}^{(-)}(\xi_0) + \mathbf{X}^{(+)}(\xi_0)\widehat{\mathbf{R}}_v^\dagger, & \xi_0 < 0, \end{cases} & v = \leftarrow . \end{cases} \tag{16}$$

We note that from the equality of the solutions $\widehat{\mathbf{F}}^*_{\leftrightarrows}(z) = \widehat{\mathbf{F}}_{\leftrightarrows}(z)$ normalized by condition (12), relations between the amplitudes necessarily follow,

$$\widehat{\mathbf{R}}_{\rightarrow} = \mathbf{R}_{\leftarrow}, \qquad \widehat{\mathbf{R}}_{\leftarrow} = \mathbf{R}_{\rightarrow}, \qquad \widehat{\mathbf{T}}_v = \mathbf{T}_v,$$

which were obtained in (15) from the Wronskian preservation condition. Therefore, we consider only the solutions $\mathbf{F}_v(z)$ below.

The solution of problem (5) in symmetrized coordinates (2) is sought in the form of the expansion

$$\Psi^{\mathrm{S(A)}}_{i_\mathrm{o}}(\xi_0, \boldsymbol{\xi}) = \sum_{j=1}^{j_{\max}} \Phi^{\mathrm{S(A)}}_j(\boldsymbol{\xi}) \chi^{\mathrm{S(A)}}_{ji_\mathrm{o}}(\xi_0), \tag{17}$$

where $\chi^{\mathrm{S(A)}}_{ji_\mathrm{o}}(\xi_0)$ are the elements of the sought matrix function of size $j_{\max} \times N_\mathrm{o}$ and $\Phi^{\mathrm{S(A)}}_j(\boldsymbol{\xi})$ are cluster basis functions (8). In oscillator representation (8), the set of coupled ordinary differential equations for functions depending on the center-of-mass variable has the form

$$\sum_{j=1}^{j_{\max}} \left[ \left( -\frac{d^2}{d\xi_0^2} - (E - \epsilon^{\mathrm{S(A)}}_i) \right) \delta_{ij} + V^{\mathrm{S(A)}}_{ij}(\xi_0) \right] \chi^{\mathrm{S(A)}}_{ji_\mathrm{o}}(\xi_0) = 0, \tag{18}$$

where $V^{\mathrm{S(A)}}_{ij}(\xi_0) = V^{\mathrm{S(A)}}_{ji}(\xi_0)$ are the elements of the symmetric matrix $\mathbf{V}^{\mathrm{S(A)}}(\xi_0)$ of effective potentials of size $j_{\max} \times j_{\max}$ expressed as the integrals

$$V^{\mathrm{S(A)}}_{ij}(\xi_0) = \int \Phi^{\mathrm{S(A)}}_i(\boldsymbol{\xi}) \left( \sum_{k=1}^{n} V(x_k(\xi_0, \boldsymbol{\xi})) \right) \Phi^{\mathrm{S(A)}}_j(\boldsymbol{\xi})\, d\boldsymbol{\xi}. \tag{19}$$

For Gaussian potentials $V(x_i) = (\alpha/\sqrt{2\pi}\sigma)\exp(-x_i^2/\sigma^2)$, the integrals can be calculated analytically and are $V_{ij}(\xi_0)/\alpha$, shown in Fig. 1.

Averaging boundary conditions (6) in orthonormalized basis (8)

$$\int \Phi^{\mathrm{S(A)}}_i(\boldsymbol{\xi}) \left( \mu_t^{(i_\mathrm{o})} \frac{\partial \Psi_{i_\mathrm{o}}(\xi_0, \boldsymbol{\xi})}{\partial \xi_0} - \lambda_t^{(i_\mathrm{o})}\, \Psi_{i_\mathrm{o}}(\xi_0, \boldsymbol{\xi}) \right) d\boldsymbol{\xi} = 0, \qquad \xi_0 = \xi_0^t, \tag{20}$$

we obtain the homogeneous boundary conditions of the third kind for solutions (18),

$$\mu_t^{(i_\mathrm{o})} \mathbf{I} \frac{d}{d\xi_0} \boldsymbol{\chi}^{(i_\mathrm{o})}(\xi_0) - \lambda_t^{(i_\mathrm{o})} \boldsymbol{\chi}^{(i_\mathrm{o})}(\xi_0) = 0, \qquad \xi_0 = \xi_0^t, \tag{21}$$

where $t = \min, \max$.

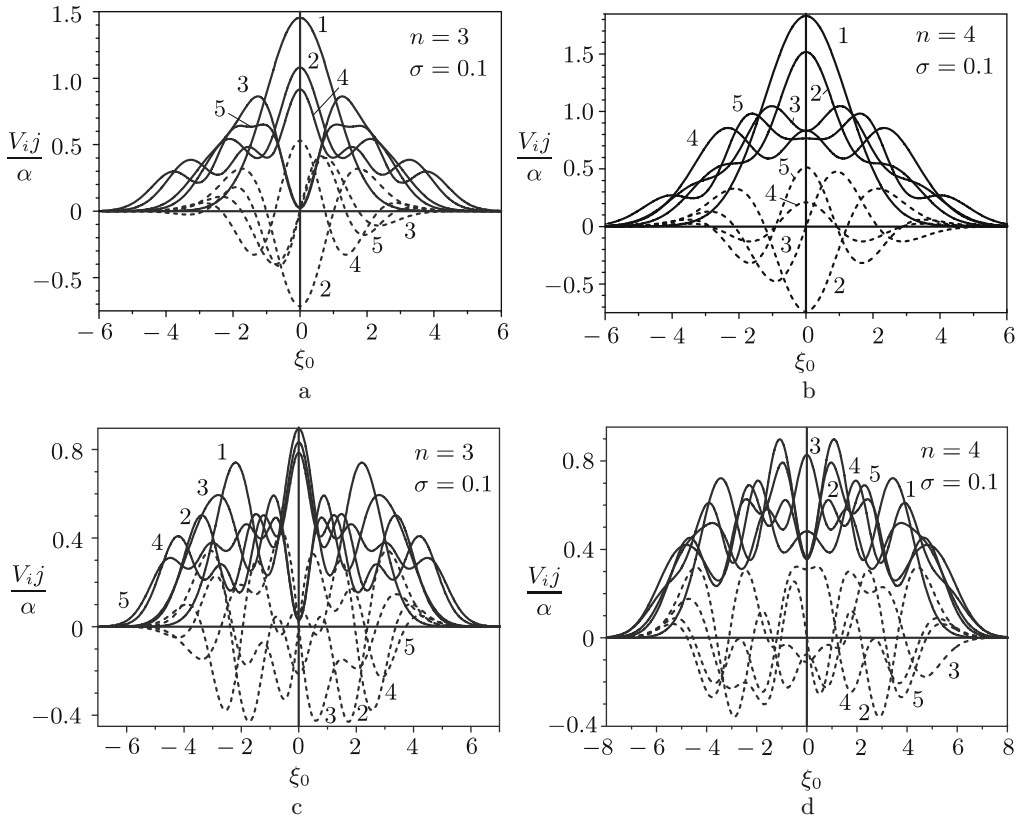


**Fig. 1**. Diagonal elements $V_{jj}$ (solid lines) and nondiagonal elements $V_{j1}$ (dashed lines) of the effective potential matrix for (a,b) S states and (c,d) A states for (a,c) $n = 3$ and (b,d) $n = 4$ particles at $\sigma = 0.1$.

For the scattering problem, according to [27], conditions (21) can be transformed into the boundary conditions for $\xi_0 = \xi_0^t$:

$$\left.\frac{d\mathbf{F}(\xi_0)}{d\xi_0}\right|_{\xi_0=\xi_0^t} = \mathcal{R}(\xi_0^t)\mathbf{F}(\xi_0^t). \tag{22}$$

Here, $\mathcal{R}(\xi)$ is the unknown matrix function of size $j_{\max} \times j_{\max}$, and

$$\mathbf{F}(\xi_0) = \{\boldsymbol{\chi}^{(i_o)}(\xi_0)\}_{i_o=1}^{N_o} = \{\{\chi_{ji_o}(\xi_0)\}_{j=1}^{j_{\max}}\}_{i_o=1}^{N_o}$$

is the desired matrix solution of boundary-value problem (18)–(22) with asymptotic behavior (13), (14) and the size $j_{\max} \times N_o$, $j_{\max} \geq N_o$.

We solve the scattering problem with a fixed energy $E$ for the set of Eqs. (18) with boundary conditions (22) independently in two cases. The wave is incident from the left $v =\rightarrow$, $\xi_0 < 0$ in the first case and from the right $v =\leftarrow$, $\xi_0 > 0$ in the second case. We use the fact that because of Eq. (13) for $\xi_0 = \xi_0^{\max} > 0$, $v =\rightarrow$ or $\xi_0 = \xi_0^{\min} < 0$, $v =\leftarrow$, the matrices $\mathcal{R}(\xi_0)$ are expressed in terms of the known set of linearly independent asymptotic solutions $\widetilde{\mathbf{F}}_v(\xi_0)$ of Eqs. (18):

$$\mathcal{R}(\xi_0) = \frac{d\widetilde{\mathbf{F}}_v(\xi_0)}{d\xi_0}(\widetilde{\mathbf{F}}_v(\xi_0))^{-1}. \tag{23}$$

For open channels $\epsilon_{i_o}^{\mathrm{S(A)}} < E$, the set consists of linearly independent asymptotic solutions $\widetilde{\mathbf{F}}_v(\xi_0) = \{\boldsymbol{\chi}^{(i_o)}(\xi_0)\}_{i_o=1}^{j_{\max}}$ with the components

$$\boldsymbol{\chi}^{(i_o)}(\xi_0) = (\tilde{\chi}_{1i_o}(\xi_0), \ldots, \tilde{\chi}_{j_{\max}i_o}(\xi_0))^{\mathrm{T}}$$

for $\xi_0 > 0$, $v = \rightarrow$ or $\xi_0 < 0$, $v = \leftarrow$:

$$\widetilde{\mathbf{F}}_{\rightarrow}(\xi_0) = \widetilde{\mathbf{X}}^{(+)}(\xi_0), \quad \xi_0 > 0, \qquad \widetilde{\mathbf{F}}_{\leftarrow}(\xi_0) = \widetilde{\mathbf{X}}^{(-)}(\xi_0), \quad \xi_0 < 0,$$
$$\widetilde{X}^{(\pm)}_{ii_\mathrm{o}}(\xi_0) = X^{(\pm)}_{ii_\mathrm{o}}(\xi_0), \quad i = 1, \ldots, j_{\max}, \quad i_\mathrm{o} = 1, \ldots, N_\mathrm{o}, \tag{24}$$

where $X^{(\pm)}_{ii_\mathrm{o}}(\xi_0)$ are given by expression (11). If for a fixed energy value $E$, there are closed channels $\epsilon^{\mathrm{S(A)}}_{i_\mathrm{o}} > E$ with the numbers $i_\mathrm{o} = N_\mathrm{o} + 1, \ldots, j_{\max}$, then set (24) includes additional linearly independent asymptotic functions $\widetilde{X}^{(+)}_{ii_\mathrm{o}}(\xi_0)$ for $\xi_0 > 0$ or $\widetilde{X}^{(-)}_{ii_\mathrm{o}}(\xi_0)$ for $\xi_0 < 0$, which in the presence of a long-range repulsive Coulomb potential barrier have the form

$$\widetilde{X}^{(\pm)}_{ii_\mathrm{o}}(\xi_0) \to q^{-1/2}_{i_\mathrm{o}} \exp\left\{\mp\left(q_{i_\mathrm{o}}\xi_0 + \frac{Z^{\pm}_j}{q_{i_\mathrm{o}}}\log(2q_{i_\mathrm{o}}|z|)\right)\right\}\delta_{ii_\mathrm{o}},$$
$$q_{i_\mathrm{o}} = \sqrt{\epsilon^{\mathrm{S(A)}}_{i_\mathrm{o}} - E}, \quad i = 1, \ldots, j_{\max}, \quad i_\mathrm{o} = N_\mathrm{o} + 1, \ldots, j_{\max}. \tag{25}$$

Boundary-value problem (18)–(22) was solved using the finite-element method with the symmetric quadratic functional [27]–[29]

$$\Xi(\mathbf{F}, E, \xi^{\min}_0, \xi^{\max}_0) = \int_{\xi^{\min}_0}^{\xi^{\max}_0}\left[\frac{d\mathbf{F}^{\mathrm{T}}(\xi_0)}{d\xi_0}\frac{d\mathbf{F}(\xi_0)}{d\xi_0} + \mathbf{F}^{\mathrm{T}}(\xi_0)V(\xi_0)\mathbf{F}(\xi_0) - E\mathbf{F}^{\mathrm{T}}(\xi_0)\mathbf{F}(\xi_0)\right]d\xi_0 -$$
$$- \mathbf{F}^{\mathrm{T}}(\xi^{\max}_0)\mathcal{R}(\xi^{\max}_0)\mathbf{F}(\xi^{\max}_0) + \mathbf{F}^{\mathrm{T}}(\xi^{\min}_0)\mathcal{R}(\xi^{\min}_0)\mathbf{F}(\xi^{\min}_0). \tag{26}$$

The solution sought in the class of functions $W^1_2(B)$ was discretized and boundary-value problem (18)–(22) was reduced to an algebraic problem on the finite-element grid $\Omega_h = (\xi^{\min}_0(N_{\mathrm{el}})\xi^{\max}_0)$ with the step $h = (\xi^{\max}_0 - \xi^{\min}_0)/N_{\mathrm{el}}$, where $N_{\mathrm{el}}$ is the number of Lagrange elements of the order $k$ in the interval $(\xi^{\min}_0, \xi^{\max}_0)$, ensuring the required accuracies of the orders $O(h^{k+1})$ for the approximate eigenfunction solution and $O(h^{2k})$ for the eigenvalue [30].

For the scattering problem with a fixed real energy value $E$, the eigenfunctions $\mathbf{F}(E, \xi_0)$ satisfy boundary conditions (22) of the third kind, and the function $\mathbf{F}^{\mathrm{T}}(E, \xi_0)$ in functional (26) is replaced with the Hermitian conjugate function $\mathbf{F}^{\dagger}(E, \xi_0)$ corresponding to the definition of scalar product (12). The asymptotic solutions of the scattering problem for $|\xi^{\max}_0| \le |\xi_0| < \infty$ contain the incident wave and the unknown matrices $\mathbf{T}(E)$ and $\mathbf{R}(E)$ of transmitted and reflected wave amplitudes (13) and (14), which are calculated together with the approximate numerical solution $\mathbf{F}_h$ on the grid $\Omega_h$ and the matrices of its logarithmic derivatives $\mathcal{R}(\xi^{\min}_0) = \mathcal{R}_{\leftarrow}(\xi^{\min}_0)$ or $\mathcal{R}(\xi^{\max}_0) = \mathcal{R}_{\rightarrow}(\xi^{\max}_0)$ at the boundary points of the interval $(\xi^{\min}_0, \xi^{\max}_0)$. The matrix $\mathcal{R}(\xi^{\max}_0) = \mathcal{R}_{\leftarrow}(\xi^{\max}_0)$ or $\mathcal{R}(\xi^{\min}_0) = \mathcal{R}_{\rightarrow}(\xi^{\min}_0)$ is calculated from Eq. (23) and substituted in functional (26).

The solutions of the boundary-value problem were discretized on the finite-element grid

$$\Omega_h = (-10.5(800)10.5) \quad \text{for } n = 3,$$
$$\Omega_h = (-12.8(976)12.8) \quad \text{for } n = 4,$$
$$\Omega_h = (-14.0(1080)14.0) \quad \text{for } n = 5$$

with the Lagrange elements of the fourth order ($k = 4$). The boundary points of the interval $\xi^t_0$ were chosen corresponding to the required accuracy of the approximate solution

$$\max_{i,j=1,\ldots,j_{\max}}\left|\frac{V_{ij}(\xi^t_0)}{\alpha}\right| < 10^{-8}.$$

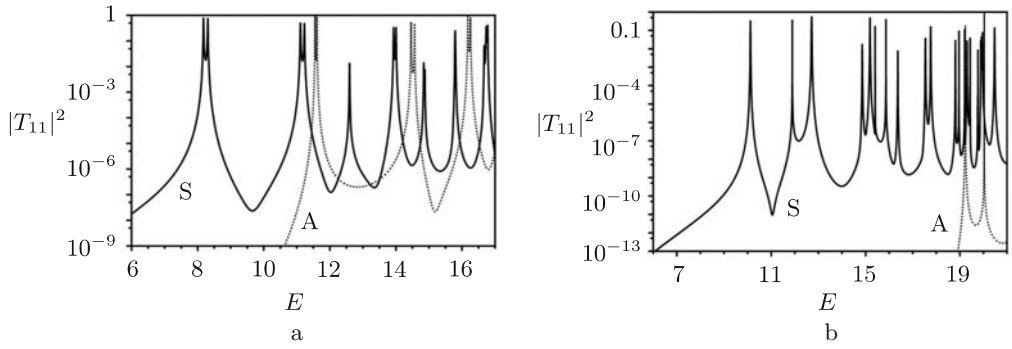


**Fig. 2**. The dependence of the total probability $|T|^2_{11}$ of transmission through a repulsive Gaussian barrier on the energy $E$ (in oscillator units) at $\sigma = 0, 1$ and $\alpha = 20$ for the system of (a) three ($n = 3$) and (b) four ($n = 4$) identical particles initially in the in the ground symmetric (solid lines) and antisymmetric (dashed lines) states.

The number $j_{\max}$ of the cluster basis functions in expansion (17) and, correspondingly, the number of equations in set (18) at $n = 3, 4, 5$ was chosen equal to $j_{\max} = 21, 39, 37$ for S states and at $n = 3, 4$ was chosen equal to $j_{\max} = 16, 15$ for A states. The convergence of the results with respect to the number $j_{\max}$ necessary for achieving the required accuracy was studied previously [17]. The results of the calculations at $n = 3$ and $n = 4$ are shown in Fig. 2. The resonance energy values $E^{\mathrm{S(A)}}$ and the corresponding maximum values of the transmission coefficient $|T|^2_{11}$ are presented in Tables 1 and 2, and the resonance energy values $E^{\mathrm{S}}$ for $n = 5$ are presented in Table 3.

For metastable states, the eigenfunctions satisfy boundary conditions (22) of the third kind, where the matrices $\mathcal{R}(\xi_0^t) = \mathrm{diag}(\mathcal{R}(\xi_0^t))$ depend on the sought complex energy eigenvalue $E \equiv E_m = \mathrm{Re}\, E_m + \imath\, \mathrm{Im}\, E_m$, $\mathrm{Im}\, E_m < 0$, and are given by

$$\mathcal{R}_{i_\circ i_\circ}(\xi_0^{\max}) = \begin{cases} \imath p_m, & \mathrm{Re}\, E_m \geq \epsilon_j^{\mathrm{S(A)}}, \\ \imath q_m, & \mathrm{Re}\, E_m < \epsilon_j^{\mathrm{S(A)}}, \end{cases} \qquad \mathcal{R}_{i_\circ i_\circ}(\xi_0^{\min}) = -\mathcal{R}_{i_\circ i_\circ}(\xi_0^{\max}),$$
$$p_m = \sqrt{E_m - \epsilon_{i_\circ}^{\mathrm{S(A)}}}, \qquad q_m = \imath\sqrt{\epsilon_{i_\circ}^{\mathrm{S(A)}} - E_m}, \tag{27}$$

because the asymptotic solutions of this problem contain only outgoing waves in the open channels. In this case, the eigenfunctions satisfy the orthogonality and normalization conditions

$$(\mathbf{F}_m|\mathbf{F}_{m'}) = (\imath p_m + \imath p_{m'})\left[\int_{\xi_0^{\min}}^{\xi_0^{\max}} \mathbf{F}_m^{\mathrm{T}}(\xi_0)\mathbf{F}_{m'}(\xi_0)\, d\xi_0 - \delta_{mm'}\right] + C_{mm'} = 0,$$
$$C_{mm'} = -\mathbf{F}_m^{\mathrm{T}}(\xi_0^{\max})\mathbf{F}_{m'}(\xi_0^{\max}) + \mathbf{F}_m^{\mathrm{T}}(\xi_0^{\min})\mathbf{F}_{m'}(\xi_0^{\min}). \tag{28}$$

We note that the orthogonality condition results from calculating the difference of variational functionals (26) with the eigenvalues $E_m$ and $E_{m'}$, the eigenfunctions $\mathbf{F}_m(\xi_0)$ and $\mathbf{F}_{m'}(\xi_0)$, and the elements of the matrices $\mathcal{R}(\xi_0^{\max})$ and $\mathcal{R}(\xi_0^{\min})$ given by (27) substituted in them. In this case, the normalization condition agrees with the choice in [2].

For the method of exterior complex scaling, the orthogonality and normalization relations were chosen according to [21]:

$$(\mathbf{F}_m|\mathbf{F}_{m'})_C = \int_C \mathbf{F}_m^{\mathrm{T}}(\xi_0)\mathbf{F}_{m'}(\xi_0)\, d\xi_0 - \delta_{mm'} = 0, \tag{29}$$

**Table 1**

| $l$ | $E_l^{\mathrm{S}}$ | $\lvert T\rvert_{11}^2$ | $m$ | $E_m^{\mathrm{M}}$ | $E_l^{\mathrm{D21}}$ |
|---|---|---|---|---|---|
| 1 | 8.175 | 0.775 | 1 | $8.175 - \imath 5.1(-3)$ | 8.19 |
| | 8.306 | 0.737 | 2 | $8.306 - \imath 5.0(-3)$ | |
| 2 | 11.111 | 0.495 | 3 | $11.110 - \imath 5.6(-3)$ | 11.09 |
| | 11.229 | 0.476 | 4 | $11.229 - \imath 5.5(-3)$ | |
| 3 | 12.598 | 0.013 | 5 | $12.598 - \imath 6.4(-3)$ | 12.51 |
| | | | 6 | $12.599 - \imath 6.3(-3)$ | |
| 4 | 13.929 | 0.331 | 7 | $13.929 - \imath 4.5(-3)$ | 13.86 |
| | 14.003 | 0.328 | 8 | $14.004 - \imath 4.6(-3)$ | |
| 5 | 14.841 | 0.014 | 9 | $14.841 - \imath 3.5(-3)$ | 14.74 |
| | 14.877 | 0.008 | 10 | $14.878 - \imath 3.5(-3)$ | |
| 6 | 15.794 | 0.246 | 11 | $15.788 - \imath 6.0(-3)$ | 15.67 |
| | | | 12 | $15.799 - \imath 6.3(-3)$ | |
| 7 | 16.670 | 0.065 | 13 | $16.666 - \imath 2.9(-3)$ | 16.53 |
| | | | 14 | $16.669 - \imath 4.3(-3)$ | |
| 8 | 16.731 | 0.361 | 15 | $16.730 - \imath 7.0(-3)$ | 16.59 |
| | 16.77 | 0.404 | 16 | $16.775 - \imath 5.2(-3)$ | |
| $l$ | $E_l^{\mathrm{A}}$ | $\lvert T\rvert_{11}^2$ | $m$ | $E_m^{\mathrm{M}}$ | $E_l^{\mathrm{D21}}$ |
| 1 | 11.551 | 1.000 | 11 | $111.551 - \imath 1.8(-3)$ | 11.52 |
| | 11.610 | 1.000 | 12 | $11.610 - \imath 2.0(-3)$ | |
| 2 | 14.459 | 0.553 | 3 | $14.459 - \imath 2.9(-3)$ | 14.42 |
| | 14.564 | 0.480 | 4 | $14.565 - \imath 2.7(-3)$ | |
| 3 | 16.176 | 0.855 | 5 | $16.176 - \imath 4.7(-3)$ | 16.11 |
| | 16.254 | 0.824 | 6 | $16.254 - \imath 4.2(-3)$ | |

The sets of the first resonance energy values $E_l^{\mathrm{S(A)}}$ at which the maximum of the transmission coefficient $\lvert T\rvert_{11}^2$ is achieved, the complex energy eigenvalues $E_m^{\mathrm{M}} = \mathrm{Re}\, E_m^{\mathrm{M}} + \imath\, \mathrm{Im}\, E_m^{\mathrm{M}}$ of the metastable states, and their approximations $E_l^{\mathrm{D21}}$ for S and A states of $n = 3$ particles at $\sigma = 0.1$ and $\alpha = 20$.

where $C$ is the appropriate integration contour in the complex plane of the independent variable $\xi_0$. In variational functional (26), we integrated over $\xi_0$ along the same contour $C$ continued into the complex plane beyond the integration interval $[\xi_0^{\min}, \xi_0^{\max}]$, ensuring the decay of the sought solution with the required

**Table 2**

| $l$ | $E_l^{\mathrm{S}}$ | $\lvert T\rvert_{11}^2$ | $m$ | $E_m^{\mathrm{M}}$ | $E_l^{\mathrm{D31}}$ | $E_l^{\mathrm{D22}}$ |
|---|---|---|---|---|---|---|
| 1 | 10.121 | 0.321 | 1 | $10.119-\imath 4.0(-3)$ | 10.03 | |
| | | | 2 | $10.123-\imath 4.0(-3)$ | | |
| 2 | 11.896 | 0.349 | 3 | $11.896-\imath 6.3(-5)$ | | 11.76 |
| 3 | 12.713 | 0.538 | 4 | $12.710-\imath 4.5(-3)$ | 12.60 | |
| | 12.717 | 0.538 | 5 | $12.720-\imath 4.5(-3)$ | | |
| 4 | 14.858 | 0.017 | 6 | $14.857-\imath 4.3(-3)$ | 14.71 | |
| | | | 7 | $14.859-\imath 4.3(-3)$ | | |
| 5 | 15.188 | 0.476 | 8 | $15.185-\imath 3.9(-3)$ | 15.04 | |
| | | | 9 | $15.191-\imath 3.9(-3)$ | | |
| 6 | 15.405 | 0.160 | 10 | $15.405-\imath 1.4(-5)$ | | 15.21 |
| 7 | 15.863 | 0.389 | 11 | $15.863-\imath 5.3(-5)$ | | 15.64 |
| $l$ | $E_l^{\mathrm{A}}$ | $\lvert T\rvert_{11}^2$ | $m$ | $E_m^{\mathrm{M}}$ | $E_l^{\mathrm{D31}}$ | $E_l^{\mathrm{D22}}$ |
| 1 | 19.224 | 0.177 | 1 | $19.224-\imath 4.0(-4)$ | 19.03 | |
| | | | 2 | $19.224-\imath 4.0(-4)$ | | |
| 2 | 20.029 | 0.970 | 3 | $20.029-\imath 3.3(-7)$ | | 19.24 |

The same as in Table 1 but for $n=4$ particles.

accuracy. The solutions of the boundary-value problem were discretized on the finite-element grid

$$\Omega_h = (-10.5(150) - 3.5(300)3.5(150)10.5) \quad \text{for } n=3,$$

$$\Omega_h = (-12.8(220) - 4.2(440)4.2(220)12.8) \quad \text{for } n=4,$$

$$\Omega_h = (-15.0(250) - 5.0(500)5.0(250)14.0) \quad \text{for } n=5$$

with the Lagrange elements of the fifth order ($k=5$). The algebraic eigenvalue problem was solved using the Newton method with the optimal choice of the iteration step [6], [31], [32] using the additional condition $\Xi_h(\mathbf{F}_m, E_m, \xi_0^{\min}, \xi_0^{\max}) = 0$, obtained as a result of discretizing functional (26) and ensuring the estimates from above for the approximate eigenvalue. Using the alternative condition $(\mathbf{F}_m|\mathbf{F}_{m'}) = 0$ yields lower estimates of the approximate eigenvalue [6]. The real eigenvalues and eigenfunctions orthonormalized by the condition that the expression in square brackets in Eq. (28) is zero were used as the initial approximation. They were found using the program `KANTBP 3.0` as a result of solving the bound-state problem with functional (26) at $\mathcal{R}(\xi_0^t) = 0$ on the grid

$$\Omega_h = (-3.5(300)3.5) \quad \text{for } n=3,$$

**Table 3**

| $l$ | $E_l^{\mathrm{S}}$ | $\lvert T\rvert_{11}^2$ | $m$ | $E_m^{\mathrm{M}}$ | $E_l^{\mathrm{D41}}$ | $E_l^{\mathrm{D32}}$ |
|---|---|---|---|---|---|---|
| 1 | 11.794 | 1.6(-4) | 1 | $11.794 - \imath 1.3(-3)$ | 11.61 | |
| | | | 2 | $11.794 - \imath 1.3(-3)$ | | |
| 2 | 4.166 | 0.014 | 3 | $14.166 - \imath 1.1(-3)$ | 13.94 | |
| | | | 4 | $14.166 - \imath 1.1(-3)$ | | |
| 3 | 14.764 | 0.666 | 5 | $14.764 - \imath 6.6(-6)$ | | 14.42 |
| | 14.774 | 0.666 | 6 | $14.774 - \imath 5.6(-6)$ | | |
| 4 | 16.429 | 0.005 | 7 | $16.429 - \imath 3.3(-3)$ | 16.16 | |
| | | | 8 | $16.429 - \imath 3.3(-3)$ | | |

The same as in Table 1 but for $n = 5$ particles.

$$\Omega_h = (-4.2(440)4.2) \quad \text{for } n = 4,$$

$$\Omega_h = (-5.0(500)5.0) \quad \text{for } n = 5.$$

The results of the calculations with variational functional (26), (28), defined both in the interval $[\xi_0^{\min}, \xi_0^{\max}]$ and on the contour $C$ for complex values of the energy of metastable states $E_m^{\mathrm{M}} \equiv E_m = \operatorname{Re} E_m + \imath \operatorname{Im} E_m$ for $n = 3$, $n = 4$, and $n = 5$ are presented in Tables 1–3.

These metastable states are responsible for the resonance energy values corresponding to the maximum values of the transmission coefficient, i.e., the quantum transparency of the barriers.

The position of peaks shown in Fig. 2 is seen to agree quantitatively with the real part $\operatorname{Re} E$, and the geometric half-width of the $|T|_{11}^2(E)$ peaks agrees in order of magnitude with the imaginary part $\Gamma = -2 \operatorname{Im} E$ of the complex energy eigenvalues $E = \operatorname{Re} E + \imath \operatorname{Im} E$ of the metastable states.

## 5. Classification of the metastable states

Because narrow Gaussian peaks were chosen as the potential barriers $V(x_i)$, $i = 1, \ldots, n$,

$$V(x_i) = \frac{\alpha}{\sqrt{2\pi}\sigma} e^{-x_i^2/\sigma^2},$$

for the approximate calculation of the real part $E_l^{\mathrm{D}} \approx \operatorname{Re} E_m$ of the energy eigenvalues for metastable S and A states, we restrict ourself to the solution of problem (1) with $d = 1$ using the approximation of the potential barriers $V(x_i)$ by infinitely high impenetrable walls.

In this approach, we seek the approximate solution in one of the potential wells, neglecting the tunneling through the barriers separating the wells. Hence, we cannot calculate the splitting inherent in the exact eigenvalues of the metastable S and A states. Nevertheless, we can explain the mechanism of their appearance and classify them, which is an important characteristic of the spectrum. To simplify the notation, we omit the indexes S and A in this section.

To find the square-integrable solutions $\Psi(\mathbf{x})$ localized in the vicinity of one of the $2^n-2$ local minimums of the multidimensional barrier $U(x_1,\ldots,x_n)$ from (1), we restrict ourself to solving the eigenvalue problem for Eq. (1) in the $n$-dimensional domain $\Omega_t$ of a special type, i.e., to finding the set of eigenvalues $E_1^{\mathrm{D}} < E_2^{\mathrm{D}} < \cdots < E_{l_{\max}}^{\mathrm{D}}$ and the corresponding set of orthonormal eigenfunctions

$$\Psi_1^{\mathrm{D}}(x_1,\ldots,x_n),\ \Psi_2^{\mathrm{D}}(x_1,\ldots,x_n),\ \ldots,\ \Psi_{l_{\max}}^{\mathrm{D}}(x_1,\ldots,x_n),$$

$$\int_{\Omega_t} \Psi_l^{\mathrm{D}}(x_1,\ldots,x_n)\Psi_{l'}^{\mathrm{D}}(x_1,\ldots,x_n)\,d\Omega_t = \delta_{ll'}.$$

This problem is solved in the Cartesian coordinates $x_1,\ldots,x_n$ in one of the $2^n-2$ subdomains

$$\Omega_t = \{x_1,\ldots,x_n \mid \sigma_i x_i > 0,\ i=1,\ldots,n\}, \qquad \sigma_i = \pm 1,$$

with the Dirichlet conditions $\Psi^{\mathrm{D}}(x_1,\ldots,x_n)|_{\partial\Omega_t} = 0$ both at the inner boundary $\partial\Omega_t^{\mathrm{in}} = \cup_{i=1}^n\{x_i = 0\}$ and at the outer boundary $\partial\Omega_t^{\mathrm{out}}$ of the chosen subdomain $\Omega_t$. The value $\sigma_i = -1$ or $\sigma_i = 1$ indicates the location of the $i$th particle to the respective right or left of the barrier $V(x_i)$ with respect to the variable $x_i$.

We seek the desired solution $\Psi_l^{\mathrm{D}}(\mathbf{x}) = \Psi_l^{\mathrm{D}}(x_1,\ldots,x_n) \in L_2(\overline{\Omega}_t)$ in the domain $\overline{\Omega}_t = \Omega_t \cup \partial\Omega_t^{\mathrm{in}} \cup \partial\Omega_t^{\mathrm{out}} \subset \mathbb{R}^n$ in the form of an expansion with the matrix of unknown coefficients $\mathbf{\Psi}^{\mathrm{D}} = \{\Psi_{jl}^{\mathrm{D}}\}$ at

$$j \in \Delta = \left\{ i_1,\ldots,i_n \,\middle|\, \sum_{k=1}^n i_k \le i^{\max},\ \frac{i_k+1}{2} \in \mathbb{N} \text{ for } k=1,\ldots,n \right\},$$

$$\Psi_l^{\mathrm{D}}(\mathbf{x}) = \sum_{j\in\Delta} \bar{\Phi}_j^{\mathrm{D}}(\mathbf{x})\Psi_{jl}^{\mathrm{D}}, \tag{30}$$

in the orthonormal basis of the $n$-dimensional oscillator $\bar{\Phi}_j^{\mathrm{D}}(\mathbf{x}) \in L_2(\overline{\Omega}_t)$ in the domain $\overline{\Omega}_t$:

$$\begin{aligned} \bar{\Phi}_j^{\mathrm{D}}(\mathbf{x}) &= \sum_{\{i_1,\ldots,i_n\}\in\bar{\Delta}_j} \bar{\alpha}_{j[i_1,\ldots,i_n]} \bar{\Phi}^{\mathrm{osc}}_{[i_1,i_2,\ldots,i_n]}(\mathbf{x}), \\ \bar{\Phi}^{\mathrm{osc}}_{[i_1,i_2,\ldots,i_n]}(\mathbf{x}) &= \prod_{k=1}^n \bar{\Phi}_{i_k}(x_k), \qquad \bar{\Phi}_{i_k}(x_k) = \sqrt{2}\,\frac{e^{-x_k^2/2}H_{i_k}(x_k)}{\sqrt[4]{\pi}\sqrt{2^{i_k}}\sqrt{i_k!}}. \end{aligned} \tag{31}$$

The limit for the functions $\bar{\Phi}_{i_k}(x_k)$ follows from the Dirichlet conditions $\bar{\Phi}_{i_k}(x_k)|_{x_k=0} = 0$ at the inner boundaries $\partial\Omega_t^{\mathrm{in}}$, namely, their subscripts $i_k$ should be even. The functions $\bar{\Phi}_{i_k}(x_k)$ then satisfy the orthogonality and normalization conditions on the half-axis $\sigma_i x_i \in \mathbb{R}_+^1$. The set of indices $\bar{\Delta}_j \equiv \{i_1,\ldots,i_n\}$ taking odd values is defined by the condition

$$\bar{\Delta}_j = \left\{ i_1,\ldots,i_n \,\middle|\, 2\sum_{k=1}^n i_k + n = \epsilon_j^{\mathrm{D}} \right\}$$

of belonging to the set of the eigenfunctions $\bar{\Phi}^{\mathrm{osc}}_{[i_1,\ldots,i_n]}(\mathbf{x})$ corresponding to the eigenvalue of the $n$-dimensional oscillator chosen equal to the desired energy eigenvalue $\epsilon_j^{\mathrm{D}} = \epsilon^{\mathrm{osc}}_{[i_1,\ldots,i_n]}$.

To calculate the eigenfunctions $\Psi_l^{\mathrm{D}}(\mathbf{x})$ symmetric (or antisymmetric) under permutations of particles in the entire domain $\mathbb{R}^n$, it is necessary and sufficient to ensure that the function $\Psi_l^{\mathrm{D}}(\mathbf{x})$ is symmetric (antisymmetric) with respect to permutation of the coordinates $x_i$ with the same $\sigma_i$ in one of the wells. The basis functions $\bar{\Phi}_j^{\mathrm{D}}(\mathbf{x})$ satisfying this condition and expressed as linear combination (31) with the coefficients $\bar{\alpha}_{j[i_1,\ldots,i_n]}$ were generated using a program implementing the standard method [9].

As a result, we obtain the algebraic eigenvalue problem

$$\mathbf{D}\mathbf{\Psi}^{\mathrm{D}} = \mathbf{\Psi}^{\mathrm{D}}\mathbf{E}^{\mathrm{D}},$$

where the real symmetric matrix $\mathbf{D}$ has the size $N_{\mathrm{D}} \times N_{\mathrm{D}}$, which was solved by the diagonalization method using the subroutines `imtql2` and `tred2` in [33]. In the calculations, $i_k$ took odd values $1, 3, \ldots, 21$, hence $i^{\max} = 20 + n$, and for $n = 3$, $n = 4$ and $n = 5$, the number of rows (columns) $N_{\mathrm{D}}$ of the matrix $\mathbf{D}$ respectively did not exceed 161, 336, and 489.

For the known local solution $\Psi^{\mathrm{D}}(\mathbf{x}) \equiv \Psi_l^{\mathrm{D}(n-k)(k)}(\mathbf{x})$ in one of the subdomains $\overline{\Omega}_t$ with $k$ particles to the left of the barrier and $n-k$ particles to the right of it, for example, for $\sigma_1 = \cdots = \sigma_k = -1$ and $\sigma_{k+1} = \cdots = \sigma_n = 1$, i.e., $\omega_t \equiv \sum_{i=1}^n \sigma_i = n - 2k$, the solution $\Psi(\mathbf{x}) \in W_2^1(\overline{\Omega})$ in the entire domain $\overline{\Omega} = \bigcup_t \overline{\Omega}_t \subset \mathbb{R}^n$ is calculated using a three-step algorithm and program.

**Step 1.** The calculated local solution in one of the subdomains $\overline{\Omega}_t$ is continued into all subdomains $\overline{\Omega}_{t'}$ for which $\omega_{t'} = \omega_t$ ($k$ particles are to the left of the barrier and $n-k$ particles are to the right of it) using the symmetry (antisymmetry) of the sought solution under permutations of the particles ($x_i \leftrightarrow x_j$, $i, j = 1, \ldots, n$):

$$\Psi_l^{\mathrm{D}(n-k)(k)}(\ldots, x_i, \ldots, x_j, \ldots) = \pm\Psi_l^{\mathrm{D}(n-k)(k)}(\ldots, x_j, \ldots, x_i, \ldots)$$

(the sign + denotes S states and − denotes A states).

**Step 2.** If $\omega_{t'} \neq 0$, then the solution found in Step 1 is continued into all subdomains $\overline{\Omega}_{t''}$ for which $\omega_{t''} = -\omega_t$ ($n-k$ particles are to the left of the barrier and $k$ are to the right of it) by coordinate inversion, thus producing even (gerade), $\Psi_l^{\mathrm{D}(n-k)(k)}(-\mathbf{x}) = \Psi_l^{\mathrm{D}(n-k)(k)}(\mathbf{x})$, and odd (ungerade), $\Psi_l^{\mathrm{D}(n-k)(k)}(-\mathbf{x}) = -\Psi_l^{\mathrm{D}(n-k)(k)}(\mathbf{x})$, solutions.

**Step 3.** In the remaining $2^n - n!/(k!(n-k)!) \cdot (2 - \delta_{0\omega_{t'}})$ subdomains, the sought solution is equal to zero.

In the case $n = 3$, there are six identical potential wells. The symmetry with respect to the plane $\xi_0 = 0$ in which the barriers are localized explains the presence of doublets (see Fig. 2) similar to the pairs of even (g) and odd (u) solutions with exponential splitting for symmetric double-well molecular potentials. In contrast to the case where $n = 2$, there is one additional condition, related to the presence of the symmetry condition, namely, to construct the solution symmetric or antisymmetric under permutation of two particles in the subdomain (octant) bounded by the planes of pair collisions 12 and 13, i.e., the first particle is to the left of the barrier, $\sigma_1 = -1$, and the second and the third particle are to the right of it, $\sigma_2 = \sigma_3 = 1$, it is necessary and sufficient to ensure that the eigenfunction of the problem is symmetric or antisymmetric under the permutation $x_2 \leftrightarrow x_3$. In other words, the solutions should satisfy different boundary conditions for $x_2 = x_3$: the Neumann condition for S states and the Dirichlet condition for A states. It hence follows that the energy levels of symmetric and antisymmetric states differ.

For example, the first three symmetric solutions and the first antisymmetric solution of the problem corresponding to the energy eigenvalues in Table 1 in the above octant have the following leading components in expansion (30) in the domain $x_1 < 0$, $x_2 > 0$, $x_3 > 0$:

$$\Psi_{1;\mathrm{S}}^{\mathrm{D}21}(x_1, x_2, x_3) \approx \bar{\Phi}_1(|x_1|)\bar{\Phi}_1(|x_2|)\bar{\Phi}_1(|x_3|),$$

$$\Psi_{2;\mathrm{S}}^{\mathrm{D}21}(x_1, x_2, x_3) \approx \bar{\Phi}_1(|x_1|)\,\frac{\bar{\Phi}_1(|x_2|)\bar{\Phi}_3(|x_3|) + \bar{\Phi}_3(|x_2|)\bar{\Phi}_1(|x_3|)}{\sqrt{2}},$$

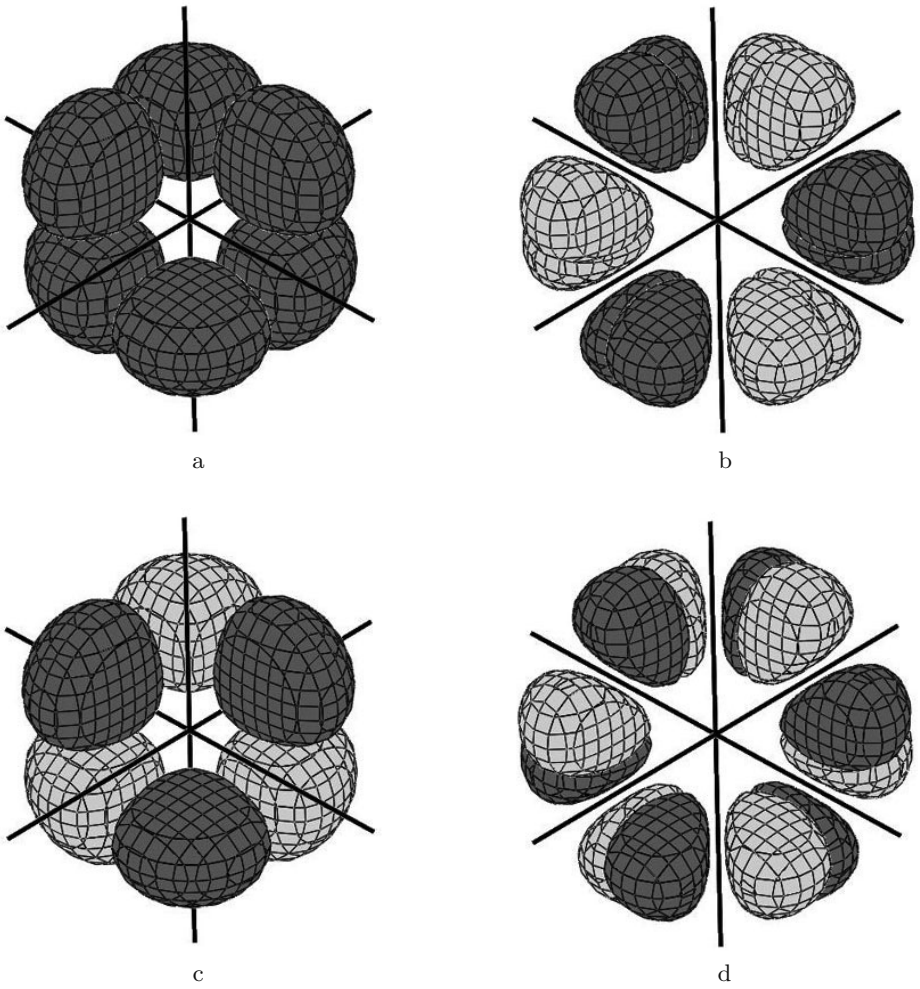


**Fig. 3**. Isosurfaces of the eigenfunctions of the (a,c) S1 states, (b,d) A1 states, (a,b) g states, and (c,d) u states of three identical particles in Cartesian coordinates $x_1$, $x_2$, $x_3$ of the three-dimensional configuration space $\mathbb{R}^3$: positive and negative values of the functions are respectively shown by dark and light shading.

$$\Psi^{\mathrm{D}21}_{3;\mathrm{S}}(x_1,x_2,x_3) \approx \bar{\Phi}_3(|x_1|)\bar{\Phi}_1(|x_2|)\bar{\Phi}_1(|x_3|),$$

$$\Psi^{\mathrm{D}21}_{1;\mathrm{A}}(x_1,x_2,x_3) \approx \bar{\Phi}_1(|x_1|)\,\frac{\bar{\Phi}_1(|x_2|)\bar{\Phi}_3(|x_3|) - \bar{\Phi}_3(|x_2|)\bar{\Phi}_1(|x_3|)}{\sqrt{2}}.$$

Continuing each of these solutions into the other five wells (octants), after multiplying by the normalizing factor $1/\sqrt{6}$, we correspondingly obtain six symmetric solutions (three even and three odd) and two antisymmetric solutions (one even and one odd). Hence, the lower levels of the energy spectrum of S and A states form sequences of g-u doublets.

The isosurfaces of the eigenfunctions of the first symmetric (S1) and antisymmetric (A1) doublet (g-u) states corresponding to the energy values $E_l^{D21}$ presented in Table 1 for three identical particles in Cartesian coordinates of the three-dimensional configuration space are shown in Fig. 3. In the presented projection, the planes of pair collisions are perpendicular to the plane of the figure and pass through three straight lines (projections of the coordinate axes) crossing in the center. It can be seen from the figure that in the case of

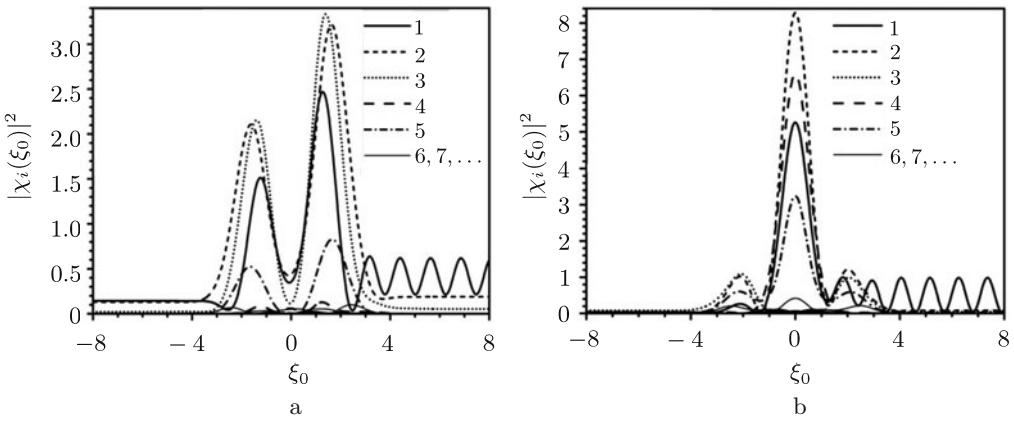


**Fig. 4**. Probability density $|\chi_i(\xi_0)|^2$ for the components (17) of the wave function expansion in the center-of-mass coordinate of the ground S state of a four-particle cluster at the collision energy $E$ corresponding to the (a) first, $E = 9.543$, $|T|^2_{11} = 0.591$, and (b) second, $E = 11.128$, $|T|^2_{11} = 0.309$, maximums of the transmission coefficient: the Gaussian barrier parameters are $\alpha = 10$ and $\sigma = 0.1$.

symmetric (antisymmetric) states of the particles, the eigenfunctions are symmetric (antisymmetric) with respect to these lines. This g-u degeneration of the energy levels $E_l^{\mathrm{D}}$ of the symmetric (antisymmetric) states is removed in the calculation of the corresponding complex energy values of the metastable states presented in Table 1.

For $n = 4$, there are 14 potential wells. Six of them in the center correspond to the case where two particles are on one side of the barrier and the other two particles are on the other side. They are denoted by the symbol D22. The remaining eight wells located at the edges of the central six-well area correspond to the case where one particle is on one side of the barrier and the other three particles are on the other side. These states are labeled with the symbol D31. Because the well D22 is narrower than D31, the energy levels $E_l^{\mathrm{D22}}$ are higher than the corresponding levels $E_l^{\mathrm{D31}}$ (see Table 2). The peaks corresponding to localizing the wave function in the wells D22 are singlet because in the vicinity of the symmetry space $\xi_0 = 0$, there are no barriers except the coordinate origin. Two groups of wells D31, in analogy with the case of three particles $n = 3$, are separated by the barriers, and doublets occur in this case. But they are not seen in Fig. 2, because the separation between the levels in the doublet is of the order of their width, i.e., essentially smaller than in the case of three particles, which is explained because two groups of D31 wells are separated by two barriers while they are separated by only one barrier in the case of three particles.

As can be seen from Table 2, for doublet D31 states at $l = 2$, we can observe two peaks of the transmission coefficient, and a local minimum of $|T|^2_{11}$ is located in the middle between these peaks, its value being smaller by a few thousandths. For doublet states D31 with $l = 1, 4, 5$, for which the width of the energy levels is nearly the same but the levels are closer to each other, one maximum of the transmission coefficient is observed exactly in the middle between the real parts of the complex energy values $E_m^{\mathrm{M}}$. We note that the components $\boldsymbol{\chi}_{j1}^{\mathrm{S}}(\xi_0)$ of the eigenfunction $\Psi_1^{\mathrm{S}}(\xi_0, \boldsymbol{\xi})$ given by (17) corresponding to the first maximum of the transmission coefficient (see Fig. 4) have minimums in the vicinity of zero, i.e., the function $\Psi_1^{\mathrm{S}}(\xi_0, \boldsymbol{\xi})$ is localized in the D31 wells, while the components of the eigenfunction corresponding to the second maximum are localized in the vicinity of zero, i.e., the function is localized in the D22 wells, which is confirmed by the last columns in Table 2. Similarly to the case $n = 3$, for D31 states, this g-u degeneracy of the energy levels $E_l^{\mathrm{D}}$ for the symmetric (antisymmetric) states is removed in the calculation of the appropriate complex energy values of metastable states. We note that the width of the singlet D22 levels is smaller than that of the D31 levels by an order of magnitude, which is related to the fact that the

D22 wells are separated from the free motion domain by two barriers.

Similarly, for $n = 5, 6, \ldots$, there are $2^n - 2$ potential wells. For odd $n$, there are groups $\mathrm{D}(n-k)(k)$, $k = 1, \ldots, (n-1)/2$, each including $2n!/k!(n-k)!$ wells separated by barriers as in the case $n = 3$, and only doublet states exist in this case. For example, if $n = 5$, then there are four groups of wells: five D41 wells and ten D32 wells corresponding to the case where one or two particles are to the left of the barrier and two similar groups corresponding to one or two particles are to the right of the barrier. This is analogous to the case of the four-well symmetric potential, where two central wells differ from the two peripheral wells. For example, if $n = 5$ (see Table 3), then the complex energies of the doubled D41 states are close to each other (the separation between them being $10^{-4}$), and the individual maximums of the transmission coefficient are not resolved, while for doublet D32 states, the separation between the levels is greater than their width and double peaks are hence observed. For even $n$, in addition to the groups $\mathrm{D}(n-k)(k)$, $k = 1, \ldots, (n-2)/2$, there is a group of $n!/((n/2)!)^2$ wells located in the vicinity of the coordinate frame origin, i.e., $n/2$ particles are on one side of the barrier and $n/2$ are on the other side, which yields singlet states. In this case, the separation between the complex energy values in the doublets for a fixed number $n$ of particles in the cluster grows as the number $k$ of particles located on one side of the barrier increases because the number of barriers separating the groups of wells decreases, and the level width decreases because of the increasing number of barriers separating the wells from the domain of "free motion" of the entire cluster of $n$ particles, and the singlet levels have the minimum width. In particular, it can be seen from Tables 1–3 that the energy level widths for the corresponding doublet states D21, D31, and D41 with $n = 3, 4, 5$, which are separated from the domain of free motion by only a single barrier, are nearly similar and amount to $10^{-3}$.

As expected, for $n = 3, 4, 5$ with the considered narrow high barrier, the approximation by impermeable walls yields an estimate with an error smaller than 2% for the calculated resonance energies $E_l^{\mathrm{S(A)}}$ and the real part of the energy $E_m^{\mathrm{M}}$ of metastable states presented in Tables 1–3.

**Acknowledgments.** The authors thank S. N. Ershov, F. M. Pen'kov, I. V. Puzynin, A .K. Motovilov, and the participants of the seminar "Few-body systems" of the Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, for the fruitful discussions.

## REFERENCES

1. S. P. Merkuriev and L. D. Faddeev, *Quantum Scattering Theory for Several Particle Systems* [in Russian], Nauka, Moscow (1985); English transl.: L. D. Faddeev and S. P. Merkuriev (Math. Phys. Appl. Math., Vol. 11), Kluwer, Dordrecht (1993).
2. V. I. Kukulin, V. M. Krasnopolsky, and J. Horáček, *Theory of Resonances*: *Principles and Applications* (Reidel Texts Math. Sci., Vol. 3), Springer, Netherlands (1989).
3. S. N. Ershov, B. V. Danilin, and J. S. Vaagen, *Phys. Rev. C*, **64**, 064609 (2001).
4. F. M. Pen'kov, *JETP*, **91**, 698–705 (2000).
5. P. M. Krassovitskiy and F. M. Pen'kov, *J. Phys. B*, **47**, 225210 (2014); arXiv:1412.3905v1 [quant-ph] (2014).
6. I. V. Puzynin, T. L. Boyadzhiev, S. I. Vinitskii, E. V. Zemlyanaya, T. P. Puzynina, and O. Chuluunbaatar, *Phys. Part. Nucl.*, **38**, 70–116 (2007).
7. A. A. Gusev, S. I. Vinitsky, O. Chuluunbaatar, V. P. Gerdt, and V. A. Rostovtsev, "Symbolic-numerical algorithms to solve the quantum tunneling problem for a coupled pair of ions," in: *Computer Algebra in Scientific Computing* (Lect. Notes. Comp. Sci., Vol. 6885, V. P. Gerdt, W. Koepf, E. W. Mayr, and E. V. Vorozhtsov, eds.), Springer, Berlin (2011), pp. 175–191.
8. J. G. Muga, J. P. Palao, B. Navarro, and I. L. Egusquiza, *Phys. Rep.*, **395**, 357–426 (2004).
9. V. A. Fock, *Z. Phys.*, **61**, 126–148 (1930).
10. A. A. Gusev, S. I. Vinitsky, O. Chuluunbaatar, L. L. Hai, V. L. Derbov, A. Góźdź, and P. M. Krassovitskiy, *Phys. Atom. Nucl.*, **77**, 389-413 (2014).
11. P. Kramer and M. Moshinsky, *Nucl. Phys.*, **82**, 241–274 (1966).

12. M. Moshinsky and Yu. F. Smirnov, *The Harmonic Oscillator in Modern Physics* (Contemp. Concepts Phys., Vol. 9), Harwood, Amsterdam (1996).
13. K. Wildermut and Y. C. Tang, *A Unified Theory of the Nucleus*, Vieweg, Braunschweig (1977).
14. A. Novoselsky and J. Katriel, *Ann. Phys.*, **196**, 135–149 (1989).
15. P. Kramer and T. Kramer, *Phys. Scr.*, **90**, 074014 (2015); arXiv:1410.4768v2 [cond-mat.mes-hall] (2014).
16. A. Gusev, S. Vinitsky, O. Chuluunbaatar, V. A. Rostovtsev, L. L. Hai, V. Derbov, A. Gozdz, and E. Klimov, "Symbolic-numerical algorithm for generating cluster eigenfunctions: Identical particles with pair oscillator interactions," , Berlin, 155–168 (2013).
17. A. A. Gusev, *Vestn. RUDN. Ser. Matematika. Informatika. Fizika*, No. 1, 52–70 (2014).
18. A. A. Gusev, O. Chuluunbaatar, S. I. Vinitsky, and A. G. Abrashkevich, *Comput. Phys. Commun.*, **185**, 3341–3343 (2014).
19. O. Chuluunbaatar, A. A. Gusev, V. L. Derbov, P. M. Krassovitskiy, and S. I. Vinitsky, *Phys. Atom. Nucl.*, **72**, 768–778 (2009).
20. A. J. F. Siegert, *Phys. Rev.*, **56**, 750–752 (1939).
21. C. W. McCurdy and C. K. Stroud, *Comput. Phys. Commun.*, **63**, 323–330 (1991).
22. A. Dobrowolski, A. Góźdź, K. Mazurek, and J. Dudek, *Internat. J. Mod. Phys. E*, **20**, 500–506 (2011).
23. V. G. Neudachin and Yu. F. Smirnov, *Nuclear Clusters in Light Nuclei* [in Russian], Nauka, Moscow (1969).
24. M. Abramowitz and I. A. Stegun, eds., *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (Natl. Bur. Stds. Appl. Math. Ser., Vol. 55), Dover, New York (1972).
25. G. A. Baker Jr., *Phys. Rev.*, **103**, 1119–1120 (1956).
26. A. A. Gusev, S. I. Vinitsky, O. Chuluunbaatar, A. Góźdź, and V. L. Derbov, *Phys. Scr.*, **89**, 054011 (2014).
27. O. Chuluunbaatar, A. A. Gusev, A. G. Abrashkevich, A. Amaya-Tapia, M. S. Kaschiev, S. Y. Larsen, and S. I. Vinitsky, *Comput. Phys. Commun.*, **177**, 649–675 (2007).
28. Yu. N. Demkov, *Variational Principles in Collision Theory* [in Russian], GIFML, Moscow (1958); English transl., NASA, Washington (1965).
29. O. A. Ladyzhenskaya, *The Boundary Value Problems of Mathematical Physics* [in Russian], Nauka, Moscow (1973); English transl. (Appl. Math. Sci., Vol. 49), Springer, New York (1985).
30. G. Strang and G. J. Fix, *An Analysis of the Finite Element Method*, Prentice-Hall, Englewood Cliffs, N. J. (1973).
31. T. Zhanlav, R. Mijiddorj, and O. Chuluunbaatar, *Vestn. gos. un-ta. Ser. Prikladnaya matematika*, **2**, No. 9, 27–37 (2008).
32. T. Zhanlav, O. Chuluunbaatar, and V. Ulziibayar, *Appl. Math. Comput.*, **236**, 239–246 (2014).
33. J. H. Wilkinson and C. Reins, eds., *Handbook for Automatic Computation*: *Linear Algebra* (Grundlehren Math. Wiss., Vol. 186), Springer, New York (1971).