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Quantum Transparency of Barriers and Reflection from Wells for Clusters of Identical Particles[1]

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Abstract—A method for solving the problem of quantum transmission through potential barriers or potential wells for a compound system consisting of several identical particles coupled via pair oscillator-type potentials in the oscillator representation of the symmetrized coordinates is considered. The efficiency of the proposed approach, algorithms and programs is demonstrated by the examples of calculation of complex energy values and analysis of metastable states of compound systems of two, three, and four identical particles on a straight line, which lead to the effect of quantum transparency of the potential barriers or quantum reflection from the wells.

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INTRODUCTION

The mechanisms of quantum transparency of barriers in the tunneling of a bound pair of particles or a cluster due to metastable states of the composite system “bound pair or cluster + barrier” have been a subject of our earlier studies. With the decreasing number of the molecular degrees of freedom, e.g., in a rigid molecule model, the problem offers a great potential for analytical studies [1]. The analysis of quantum transparency mechanism for a system consisting of n identical particles is of interest for both nuclear and molecular physics, as well as for physics of semiconductor composite nanostructures [2]. The results of the work were applied to the quantum tunneling of clusters consisting of several identical particles placed on a straight line and coupled by pair oscillator-type interactions, through narrow and high Gaussian repulsive barriers, commensurate with the mean size of the incoming cluster. Examples of calculations for various values of the Gaussian repulsive barrier parameters were considered, as well as for a long-range repulsive barrier, including the channeling problem for a pair of ions [3]. The resonance quantum transparency of barriers (or reflection from wells) for a such cluster, caused by the presence of the metastable states, embedded in the continuous energy spectrum and localized near the points where the potential energy of the composite system is minimal were analyzed [4, 5]. This class of problems was shown to require the development of new analytical and numerical methods and computer programs, as well as the upgrade of the existing ones [6].

In this paper we present a brief review of the method for solving the problem of quantum transmission through potential barriers or wells for a cluster of several identical particles coupled via pair oscillator potentials in the oscillator representation of the new symmetrized coordinates. In this representation the wave function of the composite system is sought in the form of expansion over the basis of harmonic oscillator functions symmetric with respect to the permutations of the particles with unknown functions of center mass variable. The efficiency of the proposed approach is demonstrated by the analysis of the shape and Feshbach resonances corresponding to metastable states with complex energies of composite systems of two, three, and four identical particles on a straight line, which give rise to quantum transparency of the repulsive barriers and the resonance reflection from the wells.

1. PROBLEM STATEMENT

We consider the penetration of a cluster of n identical quantum particles with mass m, coupled by oscillator interaction, through a short-range potential barrier or well $V(x_i)$ in the s-wave approximation, corresponding to one-dimensional Euclidian space, $\vec{x} = (x_1,\dots,x_n)^{\mathrm{T}} \in \mathbf{R}^n$. We assume that the spin part of the wave function is known, so that only the spatial part of the wave function $\Psi(\vec{x})$ is to be considered, which may be symmetric or antisymmetric with respect to a permutation of n identical particles. The Schrodinger equation describing the penetration of a

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cluster of n identical spinless quantum particles with energy E in oscillator units has the form

$$\left(-\frac{\partial^2}{\partial\vec{x}^2}+\sum_{i,j=1;i<j}^{n}\frac{(x_i-x_j)^2}{n}+\sum_{i=1}^{n}V(x_i)-E\right)\Psi(\vec{x})=0. \quad (1)$$

Our goal is to find the solutions $\Psi(\vec{x})$ of Eq. (1), which are totally symmetric (or antisymmetric) with respect to the permutations of n particles that belong to the permutation group S_n. The permutation of particles is nothing but a permutation of the Cartesian coordinates $x_i \leftrightarrow x_j$, $i,j=1,\ldots,n$. The reduction is provided by using the appropriately chosen new symmetrized coordinates $\hat{\xi}=(\xi_0,\xi_1,\ldots,\xi_{n-1})^{\mathrm{T}}\in\mathbf{R}^n$, where $\xi_0\in\mathbf{R}^1$ is coordinate of center of masses and $\vec{\xi}=(\xi_1,\ldots,\xi_{n-1})^{\mathrm{T}}\in\mathbf{R}^{n-1}$ are relative coordinates, rather than the conventional Jacobi coordinates [2, 4, 7]. The symmetrized coordinates are determined by the orthogonal transformation $\hat{\xi}=\mathbf{A}\vec{x}$,

$$\mathbf{A}=\frac{1}{\sqrt{n}}\begin{pmatrix}1 & 1 & 1 & \cdots & 1\\ 1 & a_1 & a_0 & \cdots & a_0\\ 1 & a_0 & a_1 & \cdots & a_0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 1 & a_0 & a_0 & \cdots & a_1\end{pmatrix}, \quad (2)$$

where $a_0=1/(1-\sqrt{n})$ and $a_1=a_0+\sqrt{n}$, and $\mathbf{A}=\mathbf{A}^{-1}$. In the symmetrized coordinates Eq. (1) takes the form

$$\left(-\frac{\partial^2}{\partial\xi_0^2}+\sum_{i=1}^{n-1}\left(-\frac{\partial^2}{\partial\xi_i^2}+\xi_i^2\right)+\sum_{i=1}^{n}V(x_i(\xi_0,\vec{\xi}))-E\right)\Psi(\xi_0,\vec{\xi})=0. \quad (3)$$

This equation *is invariant* under the permutations $\xi_i\leftrightarrow\xi_j$ for $i,j=1,\ldots,n-1$, i.e., the *invariance* of Eq. (1) under the permutations $x_i\leftrightarrow x_j$, $i,j=1,\ldots,n$ is conserved, which significantly simplifies the construction of states, symmetric (or antisymmetric) with respect to the operations of permutation of n particles [2, 4, 8], as compared to the Jacobi coordinates in the center-of-mass reference frame [9]. However, the *invariance* of Eq. (3) under the permutations $\xi_i\leftrightarrow\xi_j$ *does not yield the invariance* of Eq. (1) with respect to the permutations $x_i\leftrightarrow x_j$, which is the essence of the problem of constructing translation-invariant models of light nuclei [9].

2. OSCILLATOR REPRESENTATION FOR SEVERAL IDENTICAL PARTICLES

Let us define the set of cluster functions $\langle\vec{\xi}\,|\,j\rangle^{\mathrm{S(A)}}\equiv\Phi_j^{\mathrm{S(A)}}(\vec{\xi})\in\mathbf{L}_2(\mathbf{R}^{n-1})$, symmetric (S) (antisymmetric (A)) under the permutations of n identical particles and the corresponding values of energy $\varepsilon_j^{\mathrm{S(A)}}$ of the spectrum $\varepsilon_1^{\mathrm{S(A)}}\le\varepsilon_2^{\mathrm{S(A)}}\le\ldots\le\varepsilon_j^{\mathrm{S(A)}}\le\ldots$ as the solutions of the eigenvalue problem for the equation

$$\left(-\frac{\partial^2}{\partial\vec{\xi}^2}+\vec{\xi}^2-\varepsilon_j^{\mathrm{S(A)}}\right)\Phi_j^{\mathrm{S(A)}}(\vec{\xi})=0. \quad (4)$$

The desired solutions $\Phi_j^{\mathrm{S(A)}}(\vec{\xi})$ are sought for in the form of linear combinations of the known functions of the $(n-1)$-dimensional harmonic oscillator $\Phi^{\mathrm{osc}}_{[j_1,\ldots,j_{n-1}]}(\vec{\xi})=\prod_{k=1}^{n-1}\Phi_{j_k}(\xi_k)\in\mathbf{L}_2(\mathbf{R}^{n-1})$ in a layer of the corresponding eigenvalues $\varepsilon_j^{\mathrm{S(A)}}=\varepsilon^{\mathrm{S(A)}}_{[j_1,\ldots,j_{n-1}]}=2\left(\left(\sum_{k=1}^{n-1}j_k\right)+(n-1)/2\right)$, $j_k=0,1,\ldots$, at $n=3,4,\ldots$, using the two-step algorithm [2]:

(1) The eigenfunctions symmetric (or antisymmetric) under the permutations $\xi_i\leftrightarrow\xi_j$ $i,j=1,\ldots,n-1$ are generated using the standard method [10]. These functions are also symmetric (or antisymmetric) under the permutations $x_i\leftrightarrow x_j$, $i,j=2,\ldots,n$, but possess no symmetry with respect to the permutations $x_1\leftrightarrow x_j$, $j=2,\ldots,n$.

(2) Using the eigenfunctions obtained at the previous step, the set of linearly-independent functions, symmetric (or antisymmetric) under the permutation $x_2\leftrightarrow x_1$ is constructed, from which we get the desired orthonormalized basis using the Gram–Schmidt procedure.

In the case when $n=2,3,4$, the eigenfunctions $\Phi_j^{\mathrm{S(A)}}(\vec{\xi})$ were calculated in analytic form [4].

In the case when $n=3$, the eigenvalues of energy $\varepsilon_j^{\mathrm{S(A)}}$ are $P^{\mathrm{S(A)}}=K+1$-fold degenerate, where the value of K is determined by the condition of equal energies $\varepsilon_{k,m}^{\mathrm{S(A)}}-\varepsilon_{\mathrm{ground}}^{\mathrm{S(A)}}=12K+K'$ for one of the values $K'=0, 4, 6, 8, 10, 14$; $\varepsilon^{\mathrm{S}}_{\mathrm{ground}}=2$, $\varepsilon^{\mathrm{A}}_{\mathrm{ground}}=8$.

For the case $n=4$, the energy eigenvalues $\varepsilon_j^{\mathrm{S(A)}}$ possess the multiplicity of degeneracy $P^{\mathrm{S(A)}}=3K^2+(3+K')K+K'+\delta_{0K'}$, where the values of K and K' are determined by the condition of equal energies $\varepsilon_{j_1j_2j_3}^{\mathrm{S(A)}}-\varepsilon_{\mathrm{ground}}^{\mathrm{S(A)}}=4(6K+K')+K''$, for one of the values of $K'=0, 1, 2, 3, 4, 5$ and $K''=0,6$; $\varepsilon^{\mathrm{S}}_{\mathrm{ground}}=3$, $\varepsilon^{\mathrm{A}}_{\mathrm{ground}}=15$.

The solution of the problem (3) in the symmetrized coordinates (2) is sought in the form of expansion over the basis of harmonic oscillator functions (4)

$$\Psi_{i_o}^{\mathrm{S(A)}}(\xi_0,\vec{\xi})=\sum_{j=1}^{j_{\max}}\Phi_j^{\mathrm{S(A)}}(\vec{\xi})\chi_{ji_o}(\xi_0). \quad (5)$$

Substituting the expansion (5) into Eq. (3), we get the boundary value problem for a finite set of $j_{\max}$ coupled ordinary differential equations for $\mathbf{F}_v(\xi_0) = (\chi_{1i_o}(\xi_0),\ldots,\chi_{j_{\max}i_o}(\xi_0))^{\mathrm{T}}$

$$\left(-\mathbf{I}\frac{d^2}{d\xi_0^2} + \mathbf{E}^{\mathrm{th}} + \mathbf{V}(\xi_0) - E\mathbf{I}\right)\mathbf{F}_v(\xi_0) = 0, \qquad (6)$$

where $\mathbf{I}$ is unit matrix of dimension $j_{\max}\times j_{\max}$, $\mathbf{E}^{\mathrm{th}}$ and $\mathbf{V}(\xi_0)$ are matrices of dimension $j_{\max}\times j_{\max}$ given by their matrix elements $E_{ij}^{\mathrm{th}} = \varepsilon_j^{\mathrm{S(A)}}\delta_{ij}$ and $V_{ij}(\xi_0)$ calculated in analytic form

$$V_{ij}(\xi_0) = \int d\xi_1\ldots d\xi_{n-1}\Phi_i^{\mathrm{S(A)}}(\vec{\xi})\sum_{i=1}^{n} V(x_i(\xi_0,\vec{\xi}))\Phi_j^{\mathrm{S(A)}}(\vec{\xi}).$$

The rectangular matrix solutions $\mathbf{F}_v(\xi_0)$ describe the transmission and reflection of a particle incident on the barrier or well and have the asymptotic form "incident plane wave + outgoing waves" at $\xi_0 \to \pm\infty$:

$$\begin{aligned}\mathbf{F}_{\rightarrow}(\xi_0) &= \begin{cases}\mathbf{X}^{(+)}(\xi_0)\mathbf{T}_{\rightarrow}, & \xi_0 > 0,\\ \mathbf{X}^{(+)}(\xi_0) + \mathbf{X}^{(-)}(\xi_0)\mathbf{R}_{\rightarrow}, & \xi_0 < 0,\end{cases}\\ \mathbf{F}_{\leftarrow}(\xi_0) &= \begin{cases}\mathbf{X}^{(-)}(\xi_0) + \mathbf{X}^{(+)}(\xi_0)\mathbf{R}_{\leftarrow}, & \xi_0 > 0,\\ \mathbf{X}^{(-)}(\xi_0)\mathbf{T}_{\leftarrow}, & \xi_0 < 0,\end{cases}\end{aligned} \qquad (7)$$

where $\mathbf{R}_v$ and $\mathbf{T}_v$ are the $N_{\mathrm{o}}\times N_{\mathrm{o}}$ transmission and reflection amplitude matrices, N_{o} is the number of open channels for a fixed energy $E > \varepsilon_{i_{\mathrm{o}}}^{\mathrm{S(A)}}$ ($i_{\mathrm{o}} = 1,\ldots,N_{\mathrm{o}}$, $N_{\mathrm{o}} < j_{\max}$), and the subscript v takes the values $\rightarrow$ or $\leftarrow$ and denotes the initial direction of the particle incidence on the barrier or well from the respective left or right side, and $\mathbf{X}^{(\pm)}(\xi_0)$ are rectangular matrix functions with matrix elements

$$X_{ji_{\mathrm{o}}}^{(\pm)}(\xi_0) = p_{i_{\mathrm{o}}}^{-1/2}\exp(\pm ip_{i_{\mathrm{o}}}\xi_0)\delta_{ji_0},\quad p_{i_{\mathrm{o}}} = \sqrt{E - \varepsilon_{i_{\mathrm{o}}}^{\mathrm{S(A)}}},$$
$$j = 1,\ldots,j_{\max} \text{ and } i_{\mathrm{o}} = 1,\ldots,N_{\mathrm{o}}.$$

As a result, we arrive at a multichannel scattering problem for the set of $j_{\max}$ coupled ordinary differential equations for the functions depending on the center-of-mass variable ξ_0 (see, for details [2, 4]).

3. ANALYSIS OF SHAPE AND FESHBACH RESONANCES

The analysis of shape and Feshbach resonances is given for transmission of two, three or four identical particles $n = 2,3,4$ coupled by the harmonic oscillator potential $V(x_t - x_{t'}) = (x_t - x_{t'})^2/n$, $t',t = 1,\ldots,n$ via the Gaussian barrier ($\alpha > 0$) or well ($\alpha < 0$):

$$V(x_t) = \alpha/(\sqrt{2\pi}\sigma)\exp(-x_t^2/\sigma^2). \qquad (8)$$

The case of sub-barrier penetration was considered in [2, 4, 7]. Here we consider the case of over-barrier and over-well transmission (i.e. for $E > 2\alpha$). This is the probability $|\mathbf{T}|_{i_{\mathrm{o}}i_{\mathrm{o}}}^2 = (\mathbf{T}^{\dagger}\mathbf{T})_{i_{\mathrm{o}}i_{\mathrm{o}}} = \sum_{j=1}^{N_{\mathrm{o}}}(T_{ji_{\mathrm{o}}})^* T_{ji_{\mathrm{o}}}$, where the asterisk denotes a complex conjugation, of a transition from the eigenstate i_{o} to any of N_{o} eigenstates in open channels $E > E_j^{\mathrm{th}} = \varepsilon_j^{\mathrm{S(A)}}$ of the boundary-value problem for Eqs. (6), (7) in the Galerkin form and the complex eigenvalues $E_m^{\mathrm{M}} = \mathrm{Re}\,E_m^{\mathrm{M}} + i\,\mathrm{Im}\,E_m^{\mathrm{M}}$ of metastable states are calculated using the program KANTBP [6].

Figure 1 shows that the dependence of the probability $|\mathbf{T}|_{11}^2$ upon the energy E is non-monotonic, and the observed shape resonance peaks are manifestations of the quantum transparency effect below the barrier height (for $E < 2\alpha$). For the symmetric states we have the following threshold energies in oscillator units: $E_j^{\mathrm{th}}(n = 2,\mathrm{S}) = \{4j - 3, j = 1,2,\ldots\}$, $E_j^{\mathrm{th}}(n = 3,\mathrm{S}) = \{2, j = 1; 2j + 2, j = 2,3,\ldots\}$ and $E_j^{\mathrm{th}}(n = 4,\mathrm{S}) = \{3, j = 1; 2j + 3, j = 2,3,\ldots\}$. As can be seen from the figures, up to a certain value of the collision energy E there is almost complete reflection with the exception of small energy regions where resonant transmission (the shape resonance) is observed, and to each maximum of the transmission coefficient there corresponds a metastable state. Above this region there is almost total transmission except for small regions over the energy E where resonance reflection is observed (Feshbach resonance). For systems of three and four particles at small barrier height the peaks corresponding to resonances are smoothed out.

Figure 2 presents the total transmission probability $|\mathbf{T}|_{11}^2$ versus the energy E for the clusters of $n = 2,3,4$ particles coupled by oscillator potential, propagating above the Gaussian well with $\sigma = 1/10$ and $\alpha = -2$. One can see that the resonance structure becomes enriched when the number of transmitted particles increases. In contrast to the case of a barrier, in the vicinity of the well resonance, we see both the resonance reflection and the transmission. Thus, for $n = 2$ we see double-resonance structures, similar to the double-well case. For $n = 3$ and $n = 4$ the double structure can appear when the depth of wells $|\alpha|$ increases. In Table 1 the values of complex energies $E_m^{\mathrm{M}} = \mathrm{Re}\,E_m^{\mathrm{M}} + i\,\mathrm{Im}\,E_m^{\mathrm{M}}$ of the corresponding metastable states for the transmission of $n = 2,3,4$ particles above the Gaussian well at $\alpha = -2$, $\sigma = 1/10$ are summarized that correspondes to some peaks presented in Fig. 2.

Figures 3 and 4 present the probability density profiles $|\Psi(\xi_0,\xi_1)|^2$ for the symmetric states of two particles transmitted above a Gaussian barrier and well at $\alpha = \pm 2$, $\sigma = 1/10$ demonstrating resonance reflection

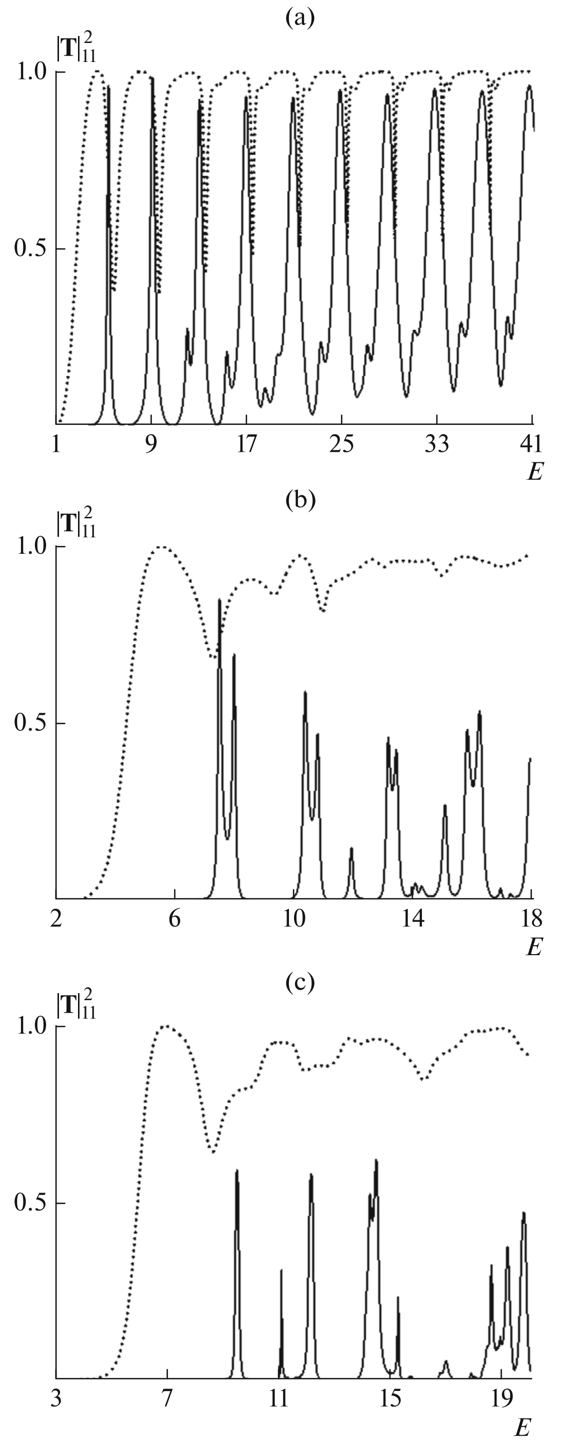

Fig. 1. The total probability $|\mathbf{T}|^2_{11}$ of the transmission through (or above) a Gaussian potential barrier (8) with $\alpha = 2$, $\sigma = 1/10$ (dotted curves) and $\alpha = 10$, $\sigma = 1/10$ (solid curves). versus the energy E (in oscillator units) for the ground state of a cluster of $n = 2, 3, 4$ particles (a, b, c), coupled by the oscillator potential.

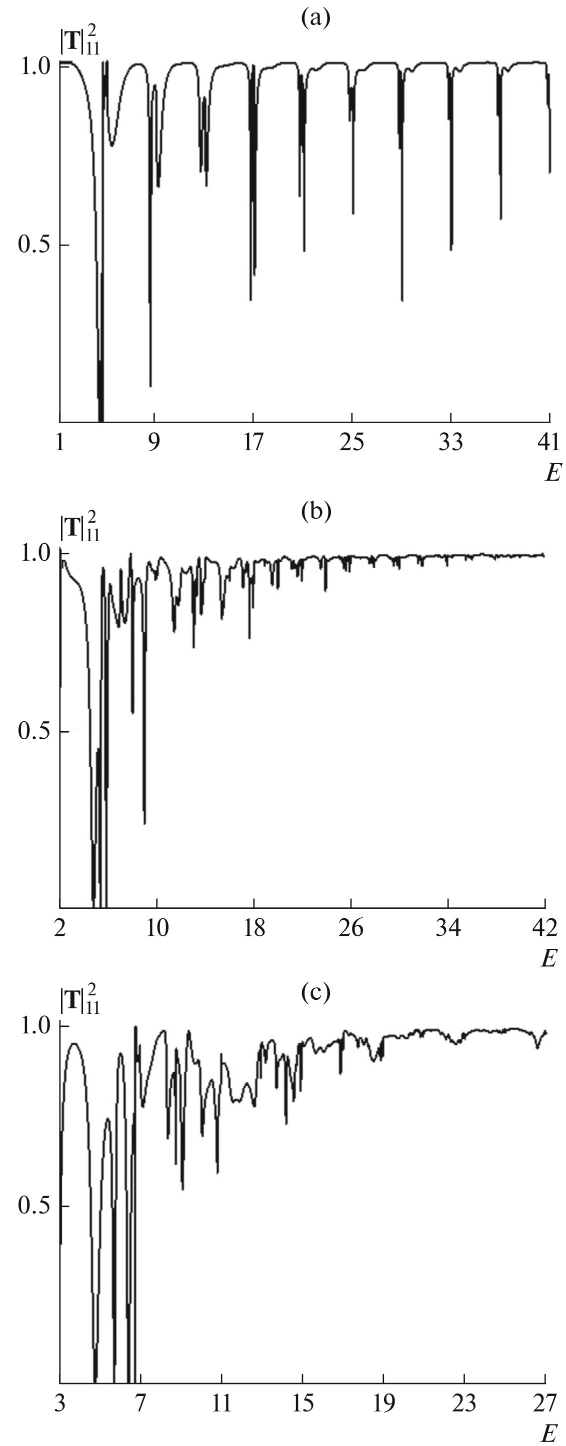

Fig. 2. The total transmission probability $|\mathbf{T}|^2_{11}$ versus the energy E (in oscillator units). The cluster of $n = 2, 3, 4$ particles (a, b, c), coupled by the oscillator potential, propagates above the Gaussian well (8) with $\alpha = -2$ and $\sigma = 1/10$. The cluster is initially in the ground state.

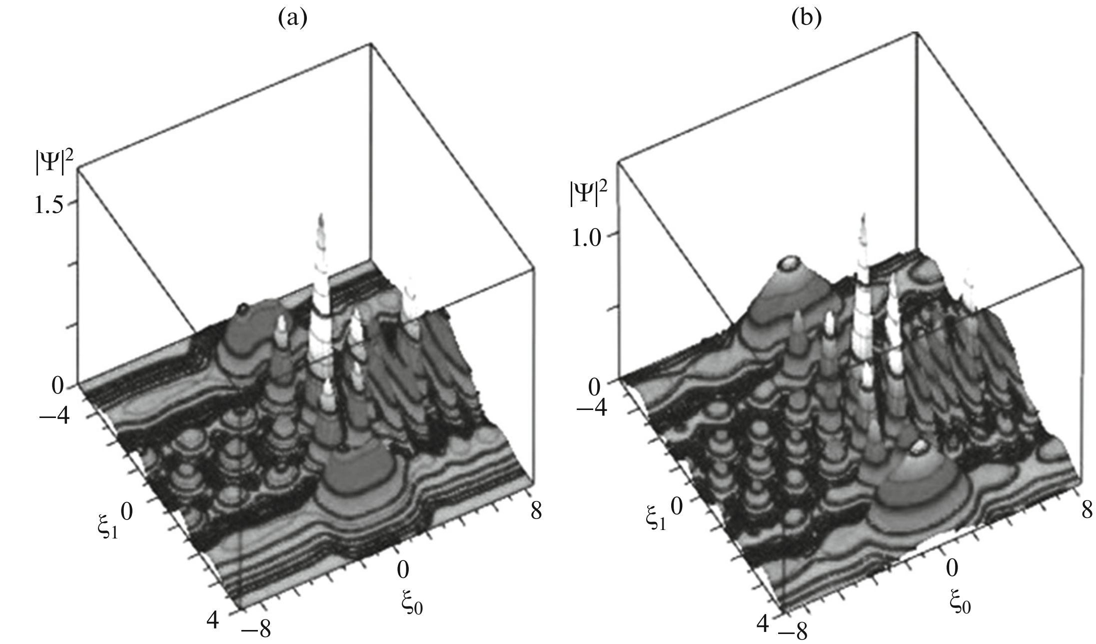

Fig. 3. Profiles of probability densities $|\Psi(\xi_0,\xi_1)|^2$ for symmetric states of the cluster of two particles, transmitted above the Gaussian barrier $\alpha = 2$, $\sigma = 1/10$. The cluster is initially in the ground state. Peak reflection (a) $E = 9.6479$, $|\mathbf{T}|^2_{11} = 0.3779$ and (b) $E = 13.5548$, $|\mathbf{T}|^2_{11} = 0.4765$, reveals itself at the Feshbach resonance energies: $E_1^{\mathrm{M}} = 9.614 - i0.217$ and $E_2^{\mathrm{M}} = 13.505 - i0.144$, respectively (in oscillator units).

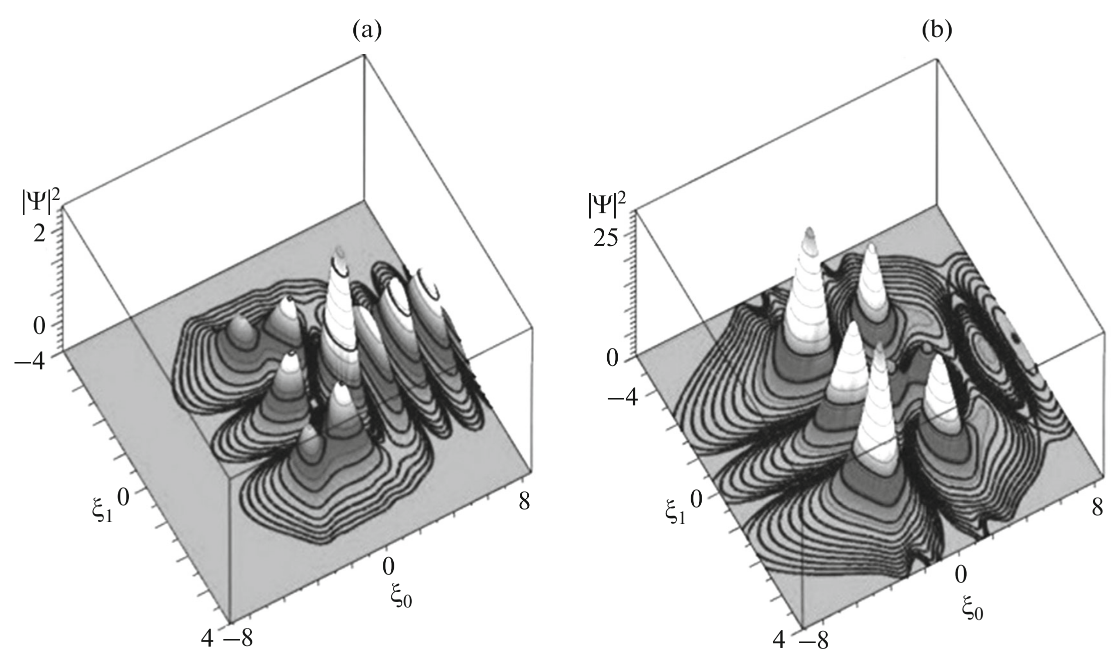

Fig. 4. Profiles of probability densities $|\Psi(\xi_0,\xi_1)|^2$ for symmetric states of the cluster of two particles, transmitted above the Gaussian well $\alpha = -2$, $\sigma = 1/10$. The cluster is initially in the ground state. Peak reflection (a) $E = 4.3954$, $|\mathbf{T}|^2_{11} = 10^{-12}$ and (b) E=4.4726, $|\mathbf{T}|^2_{11} = 10^{-11}$, reveals itself at the Feshbach resonance energies: $E_1^{\mathrm{M}} = 4.4348 - i0.2572$ and $E_2^{\mathrm{M}} = 4.6764 - i0.0058$, respectively (in oscillator units).

Table 1. The threshold energies $E_i^{\rm th}$ and complex energies $E_m^{\rm M} = {\rm Re}\,E_m^{\rm M} + i\,{\rm Im}\,E_m^{\rm M}$ of metastable states in the case of transmission of a cluster comprised by $n = 2$, 3 and 4 particles above the Gaussian well $\alpha = -2$, $\sigma = 1/10$ (in oscillator units)

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

at resonance energies. The series of resonances in the transmission $|\mathbf{T}|_{11}^2$ with the initial ground state $i_o = 1$ are induced by Feshbach metastable states for the closed channels.

CONCLUSIONS

We have formulated a model of cluster of n identical particles bound by the oscillator-type potential under the influence of the external field of a target in the new symmetrized coordinates. As a result the initial problem appears to be reduced to a multichannel scattering problem for the set of coupled-channel equations using harmonic oscillator basis, symmetric with respect to the permutations of the particles. We have proved that the effects of resonance transmission and reflection are due to the existence of metastable states with complex energy, embedded in the continuum, corresponding to shape and Feshbach resonances.

The proposed approach can be adapted and applied to the analysis of quantum transparency or total reflection effects, to the study of the quantum diffusion of molecules and micro-clusters through surfaces, the fragmentation mechanism in neutron-rich light nuclei production.

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