Resonant Tunneling of a Few-Body Cluster Through Repulsive Barriers

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Problem. During a decade the mechanism of quantum penetration of two bound particles through repulsive barriers attracts attention from both theoretical and experiment a viewpoints in relation with such problems as near-surface quantum diffusion of molecules, fragmentation in producing very neutron-rich light nuclei, and heavy ion collisions through multidimensional barriers. The generalization of the two-particle model over a quantum system of A identical particles is of great importance for appropriate description of molecular and heavy-ion collisions as well as a microscopic study of tetrahedral-symmetric nuclei.

Method. We consider the penetration of cluster of A identical quantum particles, coupled by short-range oscillator-like interaction, through a repulsive potential barrier [1, 2, 3]. We assume that the spin part of the wave function is known, so that only the spatial part of the wave function is to be considered, which may be symmetric or antisymmetric with respect to a permutation of A identical particles. The initial problem is reduced to penetration of a composite system with the internal degrees of freedom, describing an (A-1)d-dimensional oscillator, and the external degrees of freedom, describing the center-of-mass motion of A particles in d-dimensional Euclidian space. For simplicity, we restrict our consideration to the so-called s-wave approximation, corresponding to one-dimensional Euclidian space (d=1). It is shown that the reduction is provided by using appropriately chosen symmetrized coordinates, rather than the conventional Jacobi coordinates. The main goal of introducing the symmetrized coordinates is to provide invariance of the Hamiltonian with respect to permutations of A identical particles. This allows construction not only of basis functions, symmetric or antisymmetric under permutations of A-1 relative coordinates, but also of basis functions, symmetric (S) or antisymmetric (A) under permutations of A Cartesian coordinates. We refer the expansion of the solution in this basis as symmetrized coordinate representation (SCR).

Solution. We seek for the solution in the form of Galerkin or Kantorovich expansions [4, 5, 6] with unknown coefficients having the form of matrix functions of the center-of-mass variables in the SCR. As a result the problem is reduced to a boundary-value problem for a system of ordinary second-order differential equations with respect to the center-of-mass variable. Conventional asymptotic boundary conditions are imposed on the desired matrix solution.

A simple and clear way to construct the states keeping the symmetry (antisymmetry) under the permutations of A initial Cartesian coordinates, which we refer as S (A) states, is to use the symmetrized relative coordinates rather than the Jacobi ones. The transformation from the Cartesian coordinates to one of the possible choices of symmetrized ones has the form:

$$\begin{pmatrix} \xi_0 \\ \xi_1 \\ \vdots \\ \xi_{A-1} \end{pmatrix} = \frac{1}{\sqrt{A}} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & a_1 & a_0 & \cdots & a_0 \\ 1 & a_0 & a_1 & \cdots & a_0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & a_0 & a_0 & \cdots & a_1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_A \end{pmatrix},$$

$$a_0 = 1/(1-\sqrt{A}), \qquad a_1 = a_0 + \sqrt{A}.$$

The Schrödinger equation for (A-1)-dimensional oscillator has known solutions. We define the SCR in the form of linear combinations of the conventional oscillator eigenfunctions. The functions, symmetric (or antisymmetric) with respect to permutations of A particles are built in two steps. At first step we construct by standard way the states symmetric (or antisymmetric) with respect to permutations of symmetrized coordinates. These states are symmetric (or antisymmetric) with respect to permutation of $A-1$ particles. And at second step we check symmetry (or antisymmetry) with respect to one permutation $x_2 \leftrightarrow x_1$ only, that simplifies its practical implementation of the method. The examples of first S and A oscillator eigenfunctions for $A = 3$ and $A = 4$ are shown on Figs. 1 and 2.

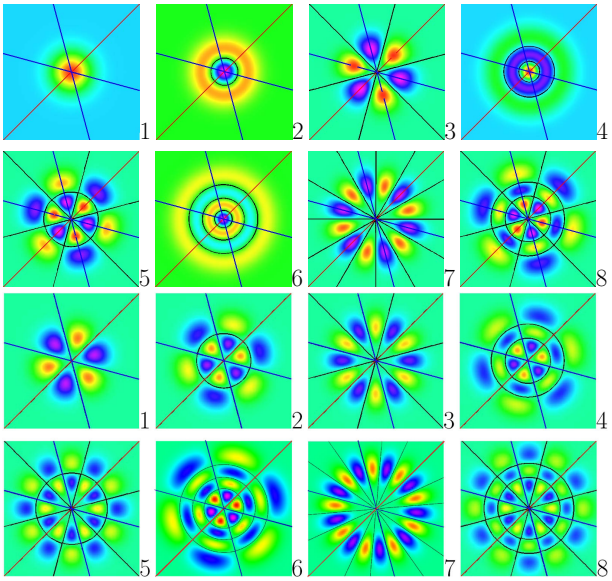

Fig 1. Profiles of the first eight oscillator symmetric (upper panels) and antisymmetric (lower panels) with respect to permutation of A=3 particles eigenfunctions at A = 3 in the plane (ξ_1, ξ_2).

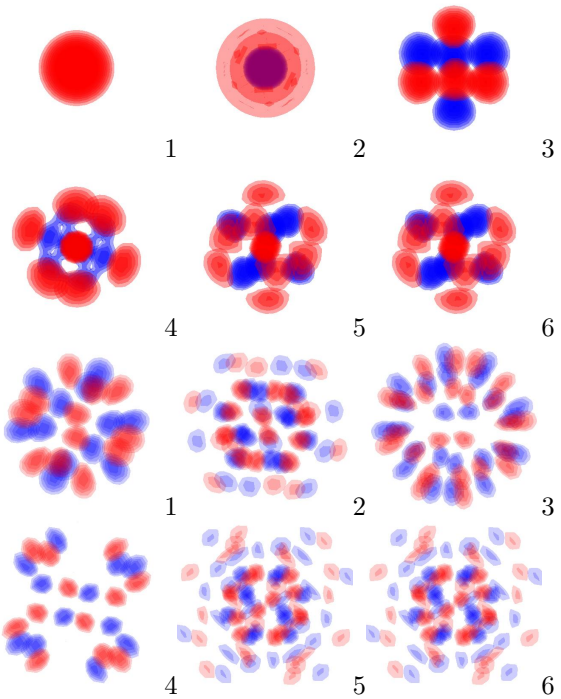

Fig. 2. Profiles of the first six oscillator symmetric (upper) and antisymmetric (lower) with respect to permutation of A=4 particles eigenfunctions at A = 4 in internal 3D space (ξ_1, ξ_2, ξ_3).

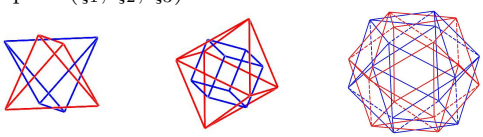

Fig. 3. Maxima and minima positions of functions of third, fourth S and first A states from Fig 2.

Note that four maxima and four minima of the third S eigenfunction coincide with the vertices of two tetrahedrons forming a *stella octangula*. Eight maxima and six outer minima for S eigenfunction (number 4) are positioned at the vertices of a cube and an octahedron, the edges of which are shown by black and grey lines, respectively. The positions of twelve maxima of the first A oscillator eigenfunction coincide with the vertices of a polyhedron with 20 triangle faces (only 8 of them being equilateral triangles) and 30 edges, 6 of them having the length 2.25 and the other having the length 2.66 (see Fig. 3).

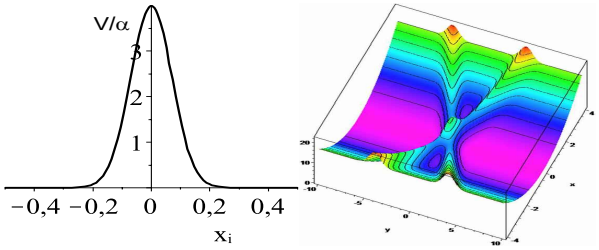

Fig. 4. The Gaussian-type potential $V(x_i) = \frac{\alpha}{\sqrt{2\pi}\sigma}\exp(-\frac{x_i^2}{\sigma^2})$ at $\sigma = 0.1$ (in oscillator units) and the corresponding 2D barrier potential at $\alpha = 1/10$, $\sigma = 0.1$.

We seek for the solution in the form of Galerkin-type expansion in terms of cluster functions in the SCR with unknown coefficients having the form of matrix functions of the center-of-mass variable. As a result the problem is reduced to a boundary-value problem for a system of ordinary second-order differential equations with respect to the center-of-mass variable. Figure 4 illustrates the Gaussian potential and the corresponding barrier potentials in the symmetrized coordinates at $A = 2$. This potential has the oscillator-type shape, and two barriers are crossing at the right angle. In the case $A \geq 3$, the hyperplanes of barriers are crossing at the right angle, too. The corresponding effective potentials are shown in Fig. 5.

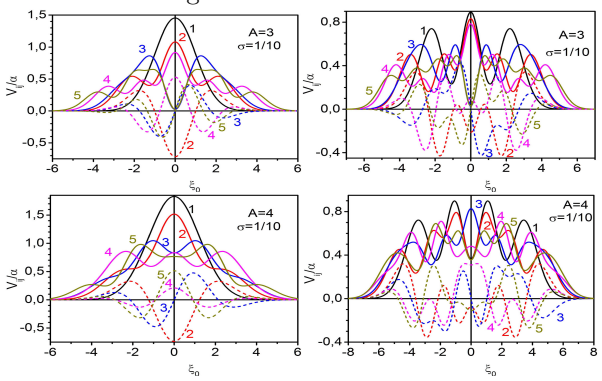

Fig. 5. Diagonal V_{jj} (solid) and nondiagonal V_{j1} (dashed) effective potentials for symmetric (left) and antisymmetric (right) basis states.

The asymptotic boundary conditions involving unknown amplitudes of reflected and transmitted waves are imposed on the desired matrix solution.

The results of calculations are analyzed with particular emphasis on the effect of quantum transparency that manifests itself as nonmonotonic energy dependence of the transmission coefficient due to resonance tunnelling of the bound particles in S (A) states through the repulsive potential barriers (see Fig. 6). This nonmonotonic dependence is explained by existence of sub-barrier quasistationary states, imbedded in the continuum. The probability densities of the coefficient functions for A = 2 symmetric states revealing resonance transmission and total reflection are shown in Fig. 7.

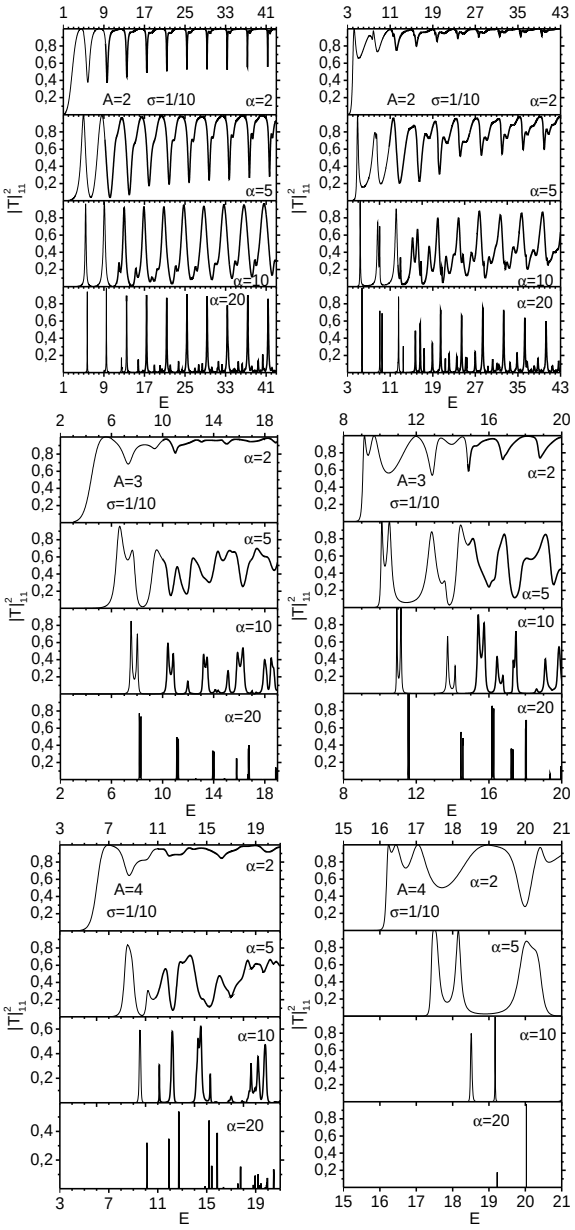

Fig. 6. The total probabilities of transmission through the repulsive Gaussian barriers for the system of A = 2,3,4 particles, coupled by the oscillator potential and being initially in the ground symmetric (left) or antisymmetric (right) state, vs the energy E (in osc.u.).

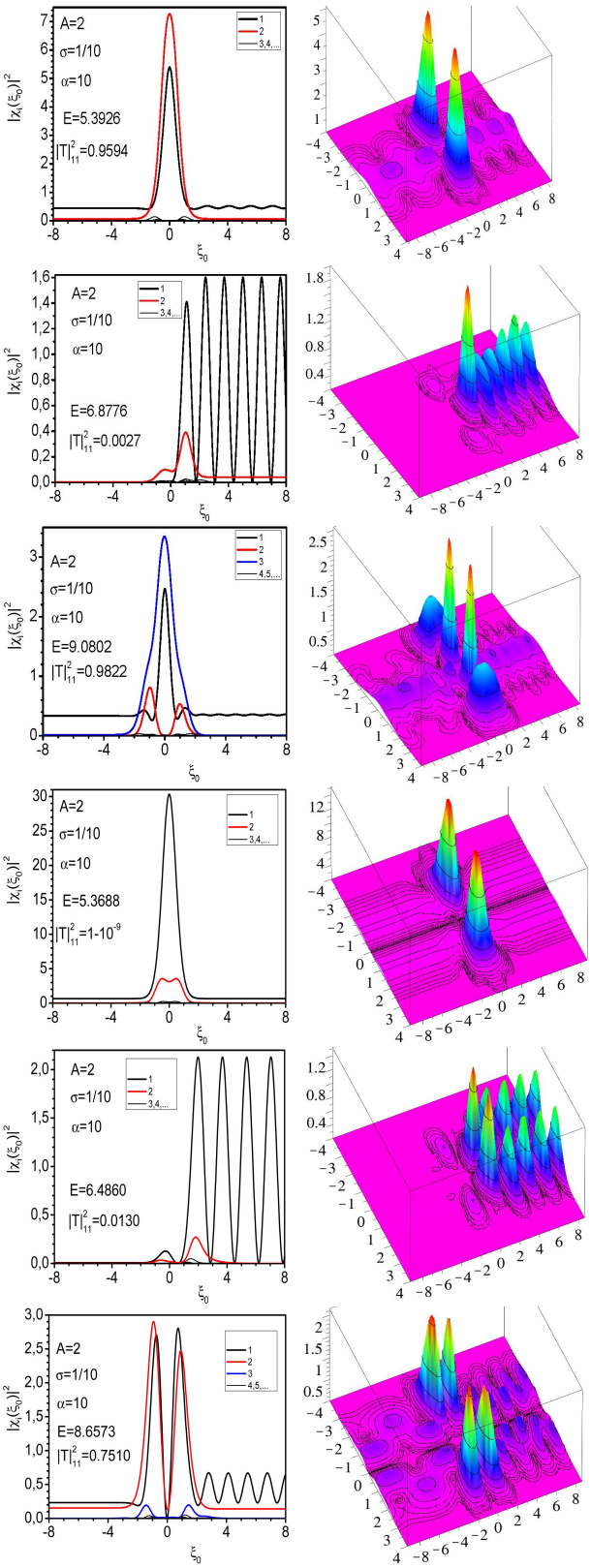

Fig. 7. The sub-barrier enhancement of probability densities of the coefficient functions and profiles of probability densities $|\Psi(\xi_0, \xi_1)|^2$ for the symmetric states of $A = 2$ particles, revealing resonance transmission and total reflection at resonance energies.

Conclusion. We formulated a model of A identical particles bound by the oscillator-type potential under the influence of the external field of a target in the new symmetrized coordinates. The constructive algorithm SCR of symmetrizing or antisymmetrizing the A-1-dimensional harmonic oscillator basis functions with respect to permutations of A identical particles was elaborated. We demonstrated the effect of quantum transparency, i.e., the resonance tunnelling of several bound particles through repulsive potential barriers. We proved that this effect is due to the existence of sub-barrier quasistationary states, imbedded in the continuum.

Prospects. The approach has been applied to the analysis of quantum transparency effect for model of quantum diffusion of molecules [7]. In benchmark calculation we use the Gaussian-type barrier, the Morse potential supported five bound states and a resulting 2D potential is shown in Fig. 8. We present in Fig. 9 effect of quantum transparency, manifesting itself in nonmonotonic resonance-type dependence of the transmission coefficient upon the energy of the diatomic molecule. Finally, in Fig. 9 we show the comparison quantum and classical diffusion coefficient. One can see that the quantum diffusion takes place at low temperature below barrier energy while classical diffusion exists at higher temperature. The approach can be adapted and applied to the analysis of quantum diffusion of micro-clusters through surfaces, and the fragmentation mechanism in producing very neutron-rich light nuclei, as well as trapped-ion quantum simulator. In connection with the intense search for superheavy nuclei, of particular significance is the application of the proposed approach to the mathematically consistent analysis of mechanisms of subbarrier fusion of heavy nuclei and the study of fusion rate enhancement by means of resonance tunneling.

The work was supported by grants 13-602-02 JINR, 11-01-00523 and 13-01-00668 RFBR, 0602/GF MES RK and the Bogoliubov-Infeld program.

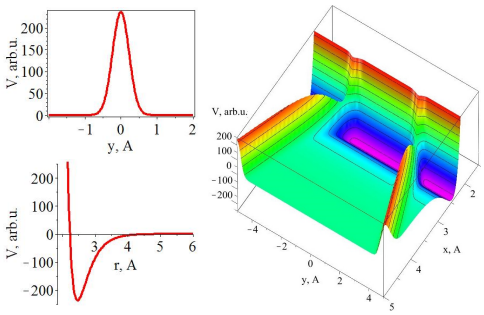

Fig. 8. Gaussian-type barrier $\tilde{U}_0(\tilde{x}_i) = \hat{A}\exp\left(-\frac{\tilde{x}_i^2}{2\sigma}\right)$, at $\hat{A} = 236.510003758401 = 1280K$, $\sigma = 5.23 \cdot 10^{-2}$, t The two-particle interaction potential, $\tilde{V}(\tilde{\mathbf{X}}) = \hat{A}\{\exp[-2(|\tilde{\mathbf{X}}|-\hat{r}_{eq})\hat{\rho}]-2\exp[-(|\tilde{\mathbf{X}}|-\hat{r}_{eq})\hat{\rho}]\}$, $\hat{r}_{eq} = 2.47$, $\hat{\rho} = 2.96812423381643$ and corresponding 2D potential.

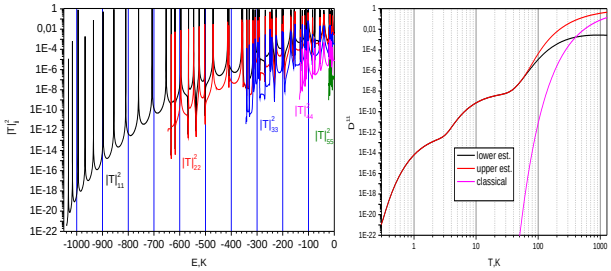

Fig. 9. The total probability of penetration from all 5 channel with energies (in K) to all five open channels, and the diffusion coefficient or thermal rate constant vs. temperature. Comparison with the classical diffusion coefficient.

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