RESONANCE TUNNELING OF COMPOSITE SYSTEMS THROUGH REPULSIVE BARRIERS

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OUTLINE

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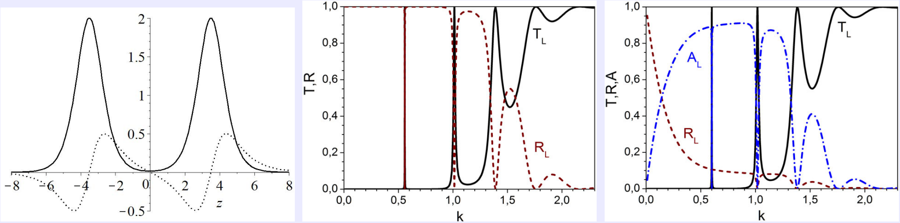
  - Quantum transparency effect
  - Metastable states and their classification
- Resume

Resonance tunneling of a quantum particle through double barriers

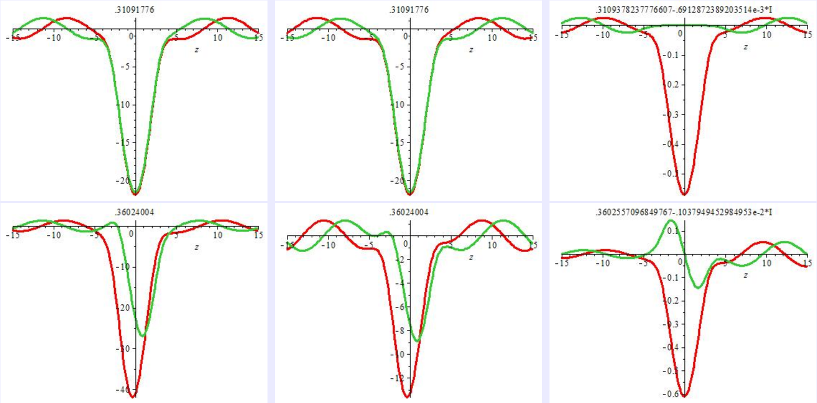


The system of two complex Scarf potentials with $V_1 = 2$, $V_2 = 1$, separated by the distance $d = 7/2$.

$$V(z) = V_{Scarf}(z - d/2) + V_{Scarf}(z + d/2), \qquad V_{Scarf}(z) = \frac{V_1}{\cosh^2 z} + \imath \frac{V_2 \sinh z}{\cosh^2 z}.$$

The solid line shows the real part and the dotted line shows the imaginary part (left-hand panel). The coefficients of transmission $T_L = |T_{\rightarrow}|^2$ (solid line), reflection $R_L = |R_{\rightarrow}|^2$ (dotted line), and absorption A_L (dash-dotted line) versus the wave number $k = \sqrt{2E}$ for the systems of two purely real and complex potentials.

Resonance tunneling of a quantum particle through double barriers



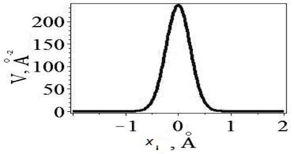
Wave functions of the scattering problem for the first resonance value of energy $2E_1^{\max T}$, corresponding to the full transparency, i.e., the maximal transmission coefficient, for $\Phi_{\rightarrow}$ (left-hand panels) and $\Phi_{\leftarrow}$ (central panels); the functions of resonance metastable states with the energies $2E_1^r$ (right-hand panels).
The upper panels refer to the system of two real Scarf potentials with $V_1 = 2$, $V_2 = 0$, the lower panels refer to the system of two complex Scarf potentials with $V_1 = 2$, $V_2 = 1$. Red and green lines show the real and imaginary parts.

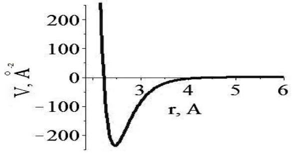
Model of transmission of a diatomic molecule through a barrier

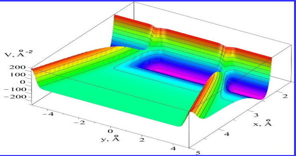
We consider a 2D model of two identical particles with mass m, coupled by pair interaction $\tilde{V}(|x_2 - x_1|)$ and interacting with barrier potentials $\tilde{V}_b(x_1)$ and $\tilde{V}_b(x_2)$. The Schrödinger equation for the wave function $\Psi(x_1, x_2)$ in the s-wave approximation has the form:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2} + \tilde{V}(|x_2 - x_1|) + \tilde{V}_b(x_1) + \tilde{V}_b(x_2) - \tilde{E}\right)\Psi(x_1, x_2) = 0,$$

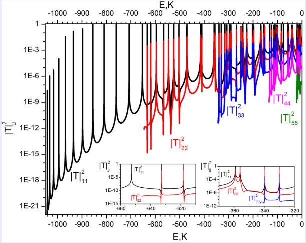
where $\tilde{E}$ is the total energy of the system and $\hbar$ is the Plank constant.



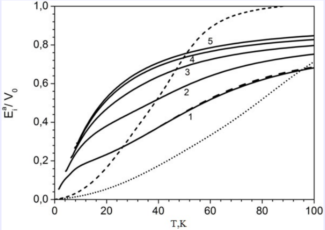




Gaussian-type barrier $V_b(x_i) = \hat{D}\exp\left(-\frac{x_i^2}{2\sigma}\right)$, at $\hat{D} = 236.51\text{Å}^{-2} = (m/\hbar^2)D$, $D = 1280\text{K}$, $\sigma = 5.23 \cdot 10^{-2}\text{Å}^2$, the two-particle interaction potential, $V(r) = \hat{D}\{\exp[-2(r - \hat{x}_{eq})\hat{\rho}] - 2\exp[-(r - \hat{x}_{eq})\hat{\rho}]\}$, $r = |x_2 - x_1|$, $\hat{x}_{eq} = 2.47\text{Å}$, $\hat{\rho} = 2.968\text{Å}^{-1}$ and the corresponding 2D potential in the (x, y) plane.



The total probability of penetration with the transition from the first channels with the energies $E_1 = -1044.8$, $E_2 = -646.1$, $E_3 = -342.7$, $E_4 = -134.7$, $E_5 = -22.1$ (in K) to all five open channels.

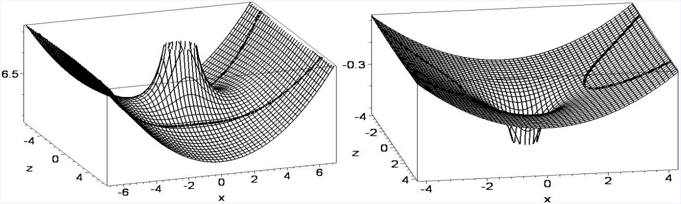


Temperature-dependent activation energy: the partial $E_i^a(T)$ (solid lines) and the total $E^a(T)$ (dashed line) activation energy and its lower (dotted line) and upper (short-dashed line) estimates produced by the corresponding upper and lower estimates of the thermal rate constant $k(T)$.

$$\hat{E}^a(T) = -\frac{1}{\sqrt{\beta}\hat{k}(T)} \frac{d\sqrt{\beta}\hat{k}(T)}{d\beta}, \beta = 1/T.$$

A.A. Gusev, et al. JINR NEWS N1 p. 22 (2014).

Model of channelling for ions with similar or opposite charge

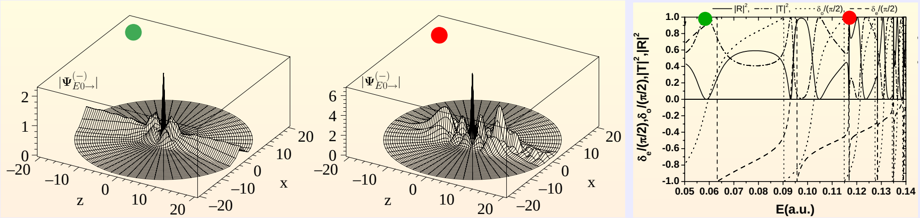


The (z, x)-dependence of the potential $2U(x, y, z)$ equal to a sum of the 3D Coulomb potential and the potential of a 2D oscillator with the frequency $\omega{=}\sqrt{\gamma}$. Left panels - similar charges $q{=}{+}6$, $\gamma{=}1$, right panels - opposite charges $q{=}{-}1$, $\gamma{=}1$. The bold curves are the lines of zero curvature $K(U(x, z)){=}0$ of the potential energy section surface.

The repulsive nonspherical barrier provides the total reflection in the open channels with the numbers $N_o^{sp}{\le}i_o{\le}N_o \equiv N_o(\varepsilon)$, where $N_o^{sp}{\sim}[\max(1, U_o{=}3(q/\sqrt{\gamma})^{2/3}/2)]$ is the number of the open channel $i_o{=}N_o^{sp}$ with the collision energy $\varepsilon = 2E{\approx}2U_o(q/\sqrt{\gamma})$ in the saddle points of the nonspherical barrier with the altitude $2U_0{=}6.24$ for $q/\sqrt{\gamma} = \hat{q}{=}6$, $N_o^{sp} = 3$.

Due to the axial symmetry, the zero-curvature lines $K(U(x, z)) = 0$ correspond to transitions from the regular motion in classical mechanics, $K(U(x, z)) > 0$, to the chaotic one, $K(U(x, z)) < 0$.

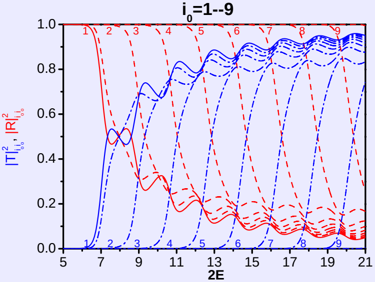
Results: the effects of resonance transmission and total reflection of oppositely charged ions in the transverse oscillator potential

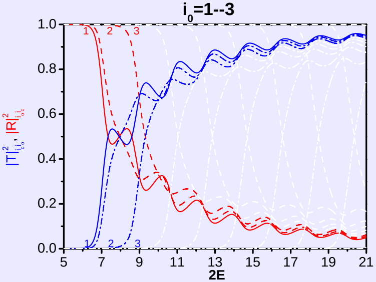


(a) (b)

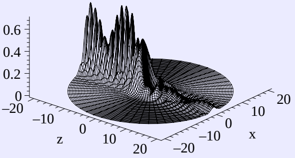
Profiles $|\boldsymbol{\Psi}^{(-)}_{Em\rightarrow}|$ of the total wave functions of the continuous spectrum in the (z, x) plane with $q = -1$, $m = 0$, $\gamma = 0.1$ and the energies $E = 0.05885\,a.u.$ (a) and $E = 0.11692\,a.u.$ (b), demonstrating the resonance transmission and the total reflection, respectively.

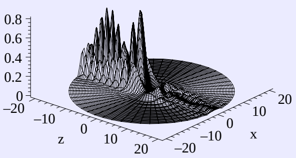
Results: the transmission and reflection matrices at $q = +6$

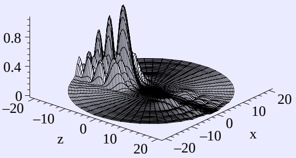




$$|\mathbf{R}|^2 = \begin{pmatrix} 0.967329 & 0.004785 & -0.000094 \\ 0.004785 & 0.990368 & 0.000074 \\ -0.000094 & 0.000074 & 0.999999 \end{pmatrix} \quad \text{at} \quad 2E = 6.552(osc.u.)$$





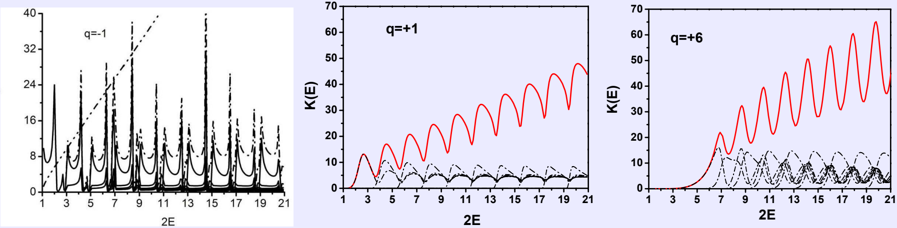


These are manifestations of partial transmission and practically total reflection in the inelastic scattering of identical ions in a crystal channel

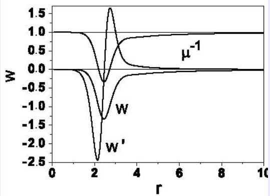
The upper estimate of the enhancement coefficient $K(E)$ is the ratio of squared absolute values of the wave functions in the pair impact point $r = 0$ of the channelled ions with/without the transverse harmonic oscillator field. It is shown versus the energy E (osc. u.) in the c.m.s.[a]:

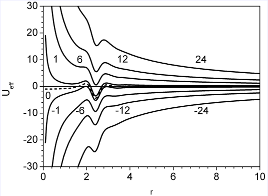
$$K(E) = \frac{|C(2E)|^2}{|C_0(2E)|^2} = \sum_{i=1}^{N_o} \frac{|C_i(2E)|^2}{|C_0(2E)|^2},$$

where $C_i(2E) = \Psi_{1i}(r = 0)$ is the numerical solution at $\gamma \neq 0$; $C_0(2E) = \Psi_{11}(r = 0)$ is the Coulomb function (for $\gamma = 0$).
In the figures $\gamma = 1$ and $1 \leq N_o \leq 10$ is the number of open channels.



[a] O. Chuluunbaatar, A.A.Gusev, V.L.Derbov, P. M. Krassovitskiy, and S. I. Vinitsky, Channeling Problem for Charged Particles Produced by Confining Environment, Physics of Atomic Nuclei, 2009, Vol. 72, No. 5, pp. 768–778.





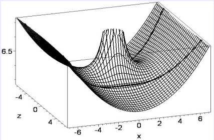
The effective mass correction W_{11}, its derivative W'_{11}, and the inverse effective mass $\mu^{-1}_{i_o i_o}(r) = (1 + W_{i_o i_o}(r))$ (left); the effective potentials $U_{eff} \equiv U^{\rm eff}_{11}(q,r)$ for q=-24,-12,-6,-1,0,1,6,12,24 at $\gamma = 1$ and $m = 0$ for the first even state $i_o = 1$ (right).

The resonance mechanism of ion channelling is explained in effective approximation

$$-\frac{1}{r^2}\frac{d}{dr}\frac{r^2}{\mu_{i_o i_o}(r)}\frac{d}{dr}\chi^{\rm eff}_{i_o i_o}(r) + \frac{\mu'_{i_o i_o}(r)}{\mu^2_{i_o i_o}(r)}\chi^{\rm eff}_{i_o i_o}(r) + [U^{\rm eff}_{i_o i_o}(q,r) - 2\mu E]\chi^{\rm eff}_{i_o i_o}(r,E,q,\gamma) = 0. \quad (1)$$

For the charge values $q = 1$, 6, 12, 24 the effective potential $U^{\rm eff}_{11}$ at the top of the barrier and the potential $2U_0$ of the repulsive nonspherical barrier at the saddle points are roughly equal to the relative energy $\varepsilon = 2E = 2n_o + 1 = 2i_o - 1$ of the open channels with the numbers $i_o = N^{sp}_o = 1, 3, 5, 8$:

$U^{\rm eff}_{11}(q{=}1, r{\approx}2.95){=}1.27{\approx}2U_0{-}1{=}1.89{-}1{=}0.89{\approx}1,$
$U^{\rm eff}_{11}(q{=}6, r{\approx}2.90){=}4.72{\approx}2U_0{-}1{=}6.24{-}1{=}5.24{\approx}5,$
$U^{\rm eff}_{11}(q{=}12, r{\approx}2.85){=}8.90{\approx}2U_0{-}1{=}9.90{-}1{=}8.90{\approx}9,$
$U^{\rm eff}_{11}(q{=}24, r{\approx}2.80){=}17.4{\approx}2U_0{-}1{=}15.7{-}1{=}14.7{\approx}15.$

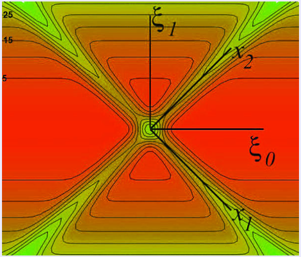


Tunnelling of a system of A identical particles through repulsive barriers

The Schrödinger equation (SE) for penetration of A identical quantum particles coupled by pair potentials $V^{pair}(x_{ij})$ through repulsive barriers $V(x_i)$ (oscillator units)

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

where $U^{pair}(x_{ij})=V^{pair}(x_{ij})-(x_{ij})^2/A$, i.e., if $V^{pair}(x_{ij})=(x_{ij})^2/A$, then $U^{pair}(x_{ij})=0$.



The problem is to find the SE solutions totally symmetric (or antisymmetric) with respect to the permutations of A particles, i.e. the permutations of the coordinates $x_i \leftrightarrow x_j$ at $i,j=1,...,A$, or the symmetry operations of the permutation group S_n.

Barrier potential in the configuration space $A=2$

Symmetrized coordinates for a system of A identical particles

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

where ξ_0 is center-of-mass variable and $\xi_1, ..., \xi_{A-1}$ are relative variables,

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

$a_0 = 1/(1 - \sqrt{A}) < 0$,
$a_1 = a_0 + \sqrt{A} > 0$.
C is an orthogonal and symmetric matrix, $C^2 = I$.

A.A. Gusev, S.I. Vinitsky, O. Chuluunbaatar, et al, Phys. Atom. Nucl. 77, 389 (2014).

For $A = 2$ the SCs are similar to Jacobi coordinates
For $A = 4$ the SCs are similar to the coordinates introduced in [P. Kramer, M. Moshinsky, Nucl. Phys. 82, 241 (1966)]
The SCs are approved in [P. Kramer, T. Kramer, arXiv:1410.4768v2 (2014); Phys. Scr. 90 (2015) 074014 (15pp)]

The SE in the symmetrized coordinates

$$\left[-\frac{\partial^2}{\partial\xi_0^2}+\sum_{i=1}^{A-1}\left[-\frac{\partial^2}{\partial\xi_i^2}+(\xi_i)^2\right]+U(\xi_0,\xi_1,...,\xi_{A-1})-E\right]\Psi(\xi_0,\xi_1,...,\xi_{A-1};E)=0,$$

$$U(\xi_0,\xi_1,...,\xi_{A-1})=\sum_{j=2}^{A}\sum_{i=1}^{j-1}U^{pair}(x_{ij}(\xi_1,...,\xi_{A-1}))+\sum_{i=1}^{A}V(x_i(\xi_0,\xi_1,...,\xi_{A-1})),$$

is invariant under the permutations $\xi_i \leftrightarrow \xi_j$ at $i,j = 1,...,A-1$ (in contrast to the Jacobi coordinates). The invariance of the SE under the permutation $x_i \leftrightarrow x_j$ at $i,j = 1,...,A$ is preserved.

The symmetrized coordinate representation

The expansion of the required solution in the symmetrized coordinates

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

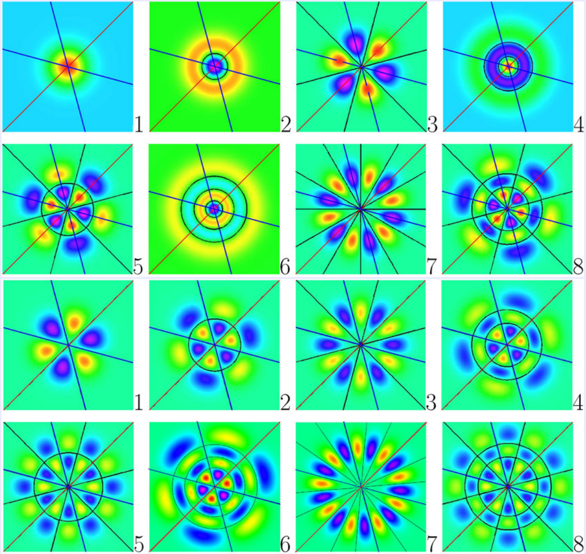
Here $\chi_i(\xi_0)$ are unknown functions of the center-of-mass variable

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

$\Phi_j^{\mathrm{S(A)}}(\xi_1, ..., \xi_{A-1})$ are the orthonormalized basis eigenfunctions of $(A-1)$-dimensional oscillator, symmetric or antisymmetric with respect to the permutations of coordinates $x_i \leftrightarrow x_j$.

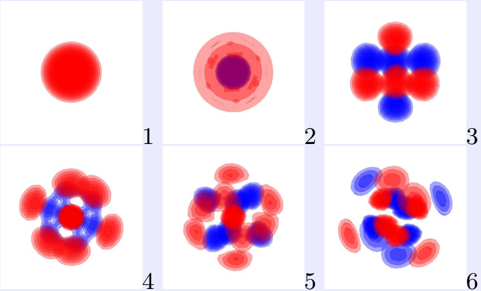
$$\left[\sum_{i=1}^{A-1}\left[-\frac{\partial^2}{\partial \xi_i^2} + (\xi_i)^2\right] - \varepsilon_j^{\mathrm{S(A)}}\right] \Phi_j^{\mathrm{S(A)}}(\xi_1, ..., \xi_{A-1}) = 0, \quad \varepsilon_j^{\mathrm{S(A)}} = 2\sum_{k=1}^{A-1} i_k + A - 1,$$

where the indices i_k, $k = 1, ..., A-1$ take integer values $i_k = 0, 1, 2, 3, ...$. They are sought for in the form of linear combinations of the conventional $(A-1)$-dimensional oscillator eigenfunctions.

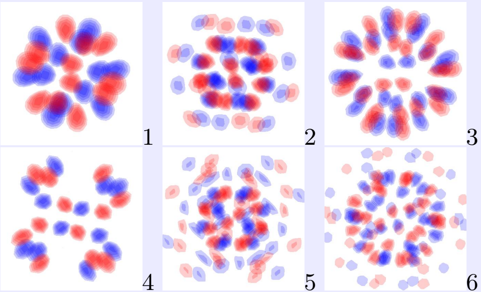


$\Phi^{S(A)}_{[k,m]}(\xi_1,\xi_2) = C_{km}(\rho^2)^{3m/2}\exp(-\rho^2/2)Y^{S(A)}_m(3m(\varphi+\pi/12))L^{3m}_k(\rho^2)$,
$(k = 0,1,\ldots;\ Y^{S}_m(\varphi) = \cos(\varphi),\ m = 0,1,\ldots;\ Y^{A}_m(\varphi) = \sin(\varphi)$,
$m = 1,2,\ldots;\ \varepsilon^{S(A)}_{k,m} = 2(2k+3m+1).)$

Profiles of the first eight oscillator symmetric (upper panels) and antisymmetric (lower panels) eigenfunctions $\Phi_{[i_1,i_2]}(\xi_1,\xi_2)$ at $A=3$ in the coordinate frame (ξ_1,ξ_2).
The black lines show the nodes of eigenfunctions. The red line corresponds to the pair collision $x_2 = x_3$, and the blue lines correspond to pair collisions $x_1 = x_2$ and $x_1 = x_3$ in the projection $(x_1,x_2,x_3) \to (\xi_1,\xi_2)$.



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



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

Close-coupled equations in the symmetrized coordinates

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

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

Scattering problem (real eigenvalues E)

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

where $\mathbf{R}_v$ and $\mathbf{T}_v$ are the reflection and transmission $N_o\times N_o$ matrices, N_o is the number of open channels, v denotes the initial direction of the particle motion, The open channels: $i_o=1,...,N_o$:

$$X_{ii_o}^{(\pm)}(\xi_0)=\frac{\exp\left(\pm\imath\left(p_{i_o}\xi_0\right)\right)}{\sqrt{p_{i_o}}}\delta_{ji_o}$$

The closed channels: $i_c=N_o+1,\ldots,N$: $\chi_{ii_c}(\xi_0)\to 0$

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

The Siegert boundary conditions

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

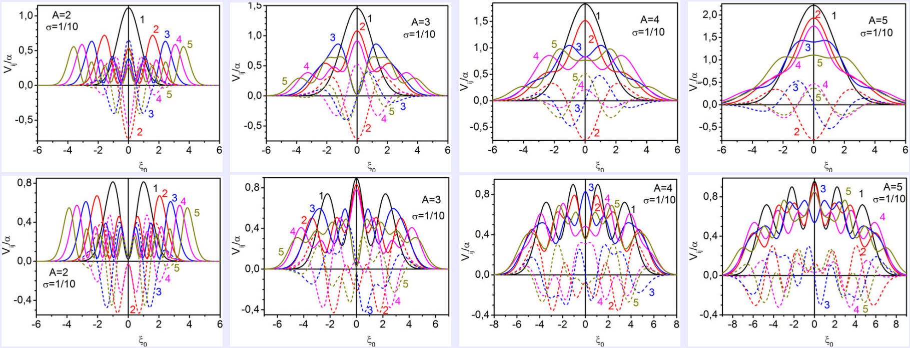
$$t=\min,\max.$$

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

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

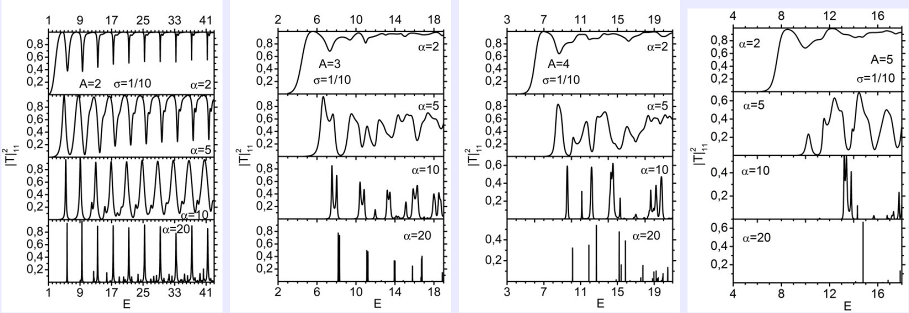
$$p_{i_o}=\sqrt{E-\epsilon_{i_o}^{S(A)}},$$

The repulsive barrier potential is chosen to be Gaussian $V(x_i) = \frac{\alpha}{\sqrt{2\pi}\sigma} \exp(-\frac{x_i^2}{\sigma^2})$. The effective potentials are calculated in the analytical form using Maple.



The diagonal $V_{jj}^{\mathrm{S(A)}}$ (solid lines) and nondiagonal $V_{j1}^{\mathrm{S(A)}}$, (dashed lines) effective potential matrix elements between the symmetric (upper panel) and antisymmetric (lower panel) states of $A = 2, 3, 4, 5$ identical particles for $\sigma = 1/10$.

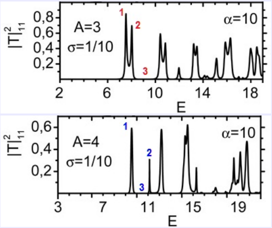
Quantum transparency effect



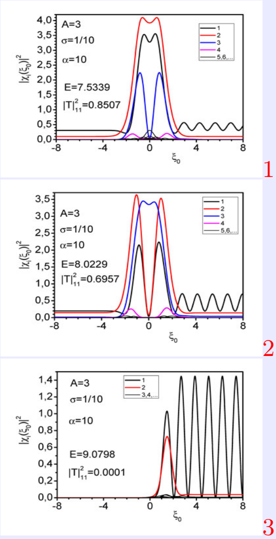
The total probabilities $|T|^2_{11}$ of the transmission through the repulsive Gaussian potential barriers $V(x_i) = \frac{\alpha}{\sqrt{2\pi}\sigma}\exp(-\frac{x_i^2}{\sigma^2})$ with $\sigma = 0.1$ and $\alpha = 2, 5, 10, 20$ for $A = 2, 3, 4, 5$ particles, coupled by the oscillator potential and initially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

Quantum transparency effect

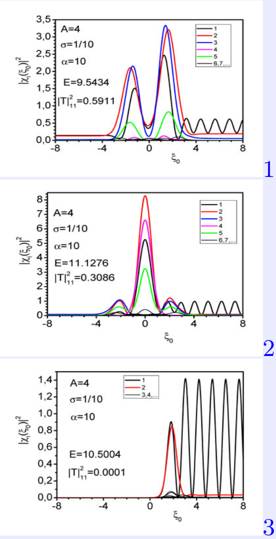
The probability densities $|\chi_i(\xi_0)|^2$ of the coefficient functions of symmetric states for transmission of $A = 3$ and $A = 4$ particles.



$A = 3$



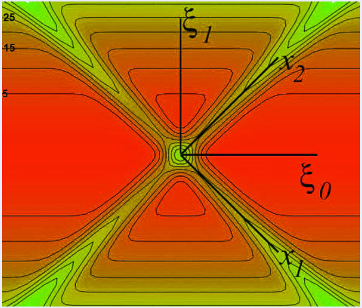
$A = 4$



Classification of the metastable states

The classification problem for metastable states is solved in Cartesian coordinates x_i, $i = 1, ..., A$ (oscillator units)

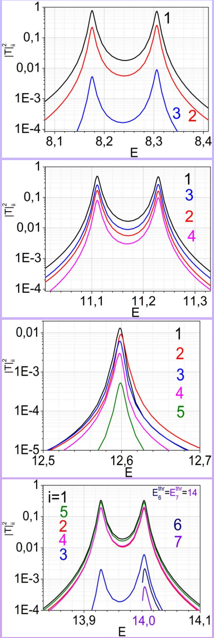
$$\left[-\sum_{i=1}^{A} \frac{\partial^2}{\partial x_i^2} + \sum_{j=2}^{A} \sum_{i=1}^{j-1} \frac{1}{A} (x_{ij})^2 + \sum_{i=1}^{A} V(x_i) - E \right] \Psi(x_1, ..., x_A; E) = 0.$$



The narrow barriers $V(x_i)$ are approximated by impenetrable walls at $x_i = 0$.

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

A.A. Gusev, S.I. Vinitsky, O. Chuluunbaatar, et al, Physica Scripta 89, 054011 (2014); Theor. and Math. Phys. (2015).



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

l	E_l^S	$\lvert T\rvert^2_{11}$	m	$E_m^M = \Re E_m^M + \imath \Im E_m^M$	E_l^{D21}
1	8.175 285	0.775	1	$8.175\ 093-\imath 5.136(-3)$	8.19
	8.305 870	0.737	2	$8.306\ 073-\imath 5.019(-3)$	
2	11.110 524	0.495	3	$11.110\ 270-\imath 5.606(-3)$	11.09
	11.228 868	0.476	4	$11.229\ 133-\imath 5.464(-3)$	
3	12.598 045	0.013	5	$12.598\ 126-\imath 6.417(-3)$	12.51
			6	$12.599\ 124-\imath 6.282(-3)$	
4	13.929 322	0.331	7	$13.929\ 045-\imath 4.508(-3)$	13.86
	14.003 487	0.328	8	$14.003\ 774-\imath 4.636(-3)$	

l	E_l^A	$\lvert T\rvert^2_{11}$	m	$E_m^M = \Re E_m^M + \imath \Im E_m^M$	E_l^{D21}
1	11.551 377	1.000	1	$11.551\ 314-\imath 1.849(-3)$	11.52
	11.610 247	1.000	2	$11.610\ 310-\imath 2.010(-3)$	
2	14.458 786	0.553	3	$14.458\ 718-\imath 2.917(-3)$	14.42
	14.564 450	0.480	4	$14.564\ 528-\imath 2.664(-3)$	
3	16.176 258	0.855	5	$16.176\ 045-\imath 4.070(-3)$	16.11
	16.253 931	0.824	6	$16.254\ 153-\imath 4.152(-3)$	

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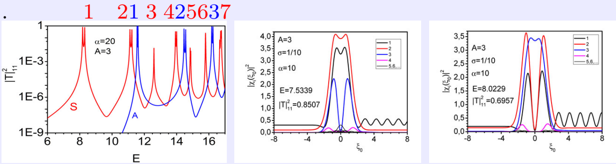


Quantum transmittance induced by metastable states

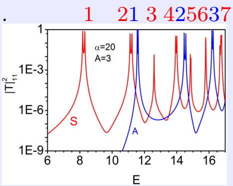
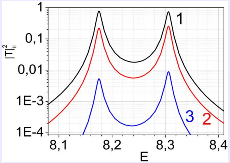
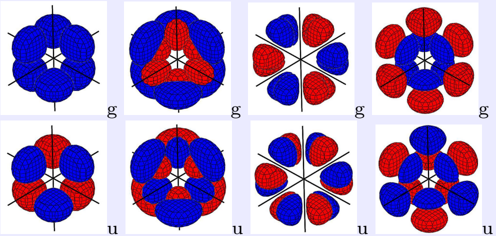


Fig. 1. The transmission coefficient $|T|^2_{11}$ vs the collision energy E (osc. u.) of the symmetric (S) and antisymmetric (A) states for tunnelling of the composite system of three identical particles (A=3) on a line with the pair oscillator interactions through the narrow repulsive Gaussian barrier $V(x_i) = \alpha/(2\pi\sigma^2)^{1/2}\exp(-x_i^2/\sigma^2)$, $\alpha = 20$, $\sigma = 0.1$.

Fig. 2. The transmission coefficients $|T|^2_{ii}$ in the open channels (i=1,2,3) in the vicinity of the first double peak of the pair metastable states with the energies $E_1 = 8.17509 - i0.00514$, $E_2 = 8.30607 - i0.00502$ (osc. u.)





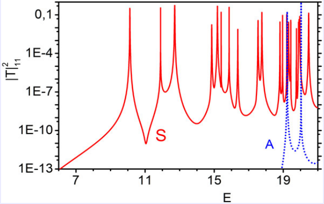
$E_1^S = 8.186$, $E_2^S = 11.09$, $E_1^A = 11.52$, $E_3^S = 12.51$

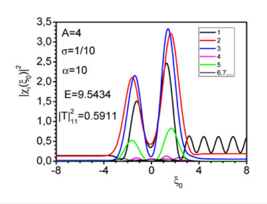
Fig. 3. The first g-u doublets of the symmetric and antisymmetric metastable states with the energies $E^S_{i=1,2,3}$ and $E^A_{i=1}$ (in osc. u.), corresponding to the first four peaks of the transmission coefficient (Fig. 1) for the resonance transmission of a composite system of three identical particles through the repulsive Gaussian barrier.

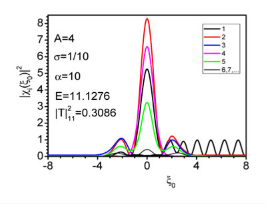
$A = 4,\ \sigma = 1/10,\ \alpha = 20$

l	E_l^{S}	$\lvert T\rvert^2_{11}$	m	$E_m^M = \Re E_m^M + \imath \Im E_m^M$	E_l^{D31}	E_l^{D22}
1	10.120 978	0.321	1	10.119 120$-\imath$4.040($-$3)	10.03	
			2	10.122 850$-\imath$4.041($-$3)		
2	11.896 080	0.349	3	11.896 080$-\imath$ 6.3($-$5)		11.76
3	12.713 101	0.538	4	12.710 127$-\imath$4.504($-$3)	12.59	
			5	12.719 859$-\imath$4.452($-$3)		
4	14.858 432	0.017	6	14.857 342$-\imath$4.330($-$3)	14.71	
			7	14.859 351$-\imath$4.341($-$3)		
5	15.187 817	0.476	8	15.184 665$-\imath$3.866($-$3)	15.04	
			9	15.190 962$-\imath$3.911($-$3)		
6	15.404 657	0.160	10	15.404 657$-\imath$ 1.4($-$5)		15.21
7	15.863 290	0.389	11	15.863 290$-\imath$ 5.3($-$5)		15.64

l	E_l^{A}	$\lvert T\rvert^2_{11}$	m	$E^M = \Re E^M + \imath \Im E^M$	E_l^{D31}	E_l^{D22}
1	19.224 295	0.177	1	19.224 206$-\imath$4.016($-$4)	19.03	
			2	19.224 384$-\imath$4.016($-$4)		
2	20.028 510	0.970	3	20.028 510$-\imath$ 3.3($-$7)		19.77







The solution techniques for the problems presented above

The solution of problems discussed above were obtained using the symbolic-numerical algorithms (SNA), implemented in the problem-oriented complex of programs, available via the Computer Physics Communication Library:

• ODPEVP: A program for computing the eigenvalues, eigenfunctions, and their first derivatives with respect to the parameter of the parametric self-adjoined Sturm-Liouville problem[a]

•POTHMF: A program for computing the potential curves and matrix elements of the coupled adiabatic radial equations for a hydrogen-like atom in a homogeneous magnetic field[b]

• KANTBP & KANTBP 2.0: A program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach[c]

• KANTBP 3.0: The new version of a program for computing the energy levels, reflection and transmission matrices, and the corresponding wave functions in the coupled-channel adiabatic approach [d]

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[a] O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky and A.G. Abrashkevich, CPC 181, 1358-1375 (2009).

[b] O. Chuluunbaatar, A.A. Gusev, V.P. Gerdt, V.A. Rostovtsev, S.I. Vinitsky, A.G. Abrashkevich, M.S. Kaschiev and V.V. Serov, CPC 178, 301-330 (2008).

[c] O. Chuluunbaatar, A.A. Gusev, A.G. Abrashkevich, A. Amaya-Tapia, M.S. Kaschiev, S.Y. Larsen and S.I. Vinitsky, CPC 177, 649-675 (2007);
O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky and A.G. Abrashkevich, CPC 179, 685-693 (2008).

[d] A.A. Gusev, O. Chuluunbaatar, S.I. Vinitsky and A.G. Abrashkevich, CPC 185, pp. 3341–3343 (2014).

Resume

- The analysis of quantum transparency effect in the model of a quantum diffusion of diatomic molecules of beryllium on the copper surface was carried out. The quantum transparency of barriers leads to increasing the thermal rate constants of the quantum tunneling and decreasing the activation energy of the composed molecular system at low temperature below the classical energy barrier.
- The study of the resonance photoionization and laser-stimulated recombination of a hydrogen atom in a uniform magnetic field was performed. The effects of resonance transmission and total reflection of oppositely charged particles in a uniform magnetic field were predicted.
- For the model of axial channeling of similarly charged particles in the effective confining oscillator potential of a crystal the study was carried out. The simulations revealed a non-monotonic dependence of the nuclear reaction rate enhancement coefficient upon the collision energy due to the newly discovered effect of total reflection of channeled ions.
- The analysis of resonance tunneling of a cluster consisting of several identical particles coupled by pair oscillator interactions through repulsive potential barriers was carried out. The quantum transparency effect is a manifestation of metastable states of the cluster arising due to its interaction with barriers.

Thank you for your attention!