Analysis of models of the resonance quantum tunneling of composite systems through potential barriers

A.A. Gusev

(Laboratory of Information Technologies Joint Institute for Nuclear Research, Dubna, Russia)

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Lection 2

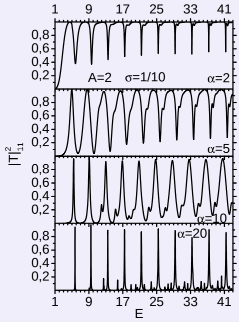
- The classification of quasistationary states
- Resonance tunnelling of diatomic molecule
  - Cartesian coordinates
  - Polar coordinates
    - Three identical particles with pair δ-interaction
- Resume

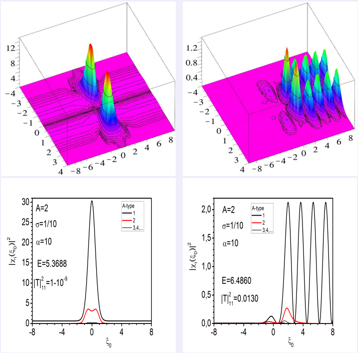
Lection 1

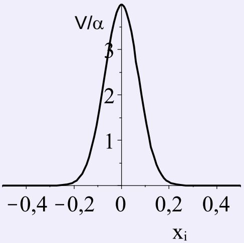
- Close-coupling and Kantorovich (Adiabatic) methods
- The statement of the problem
- Jacobi and Symmetrized coordinates
- Symmetrized coordinates representation
- Close-coupling equations in the SCR
- Asymptotic boundary conditions & multichannel scattering problem
- Resonance transmission of a few coupled particles

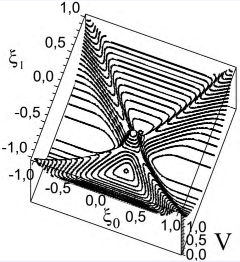
The classification of quasistationary states

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







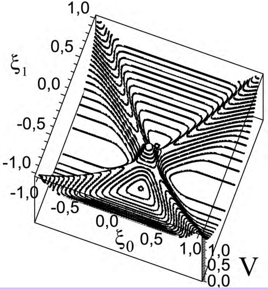


We solve Eq. (*) in the Cartesian coordinates $x_1, \ldots, x_A$ in one of the $2^A - 2$ subdomains, defined as $\sigma_i x_i > 0$, $\sigma_i = \pm 1$ with the Dirichlet conditions (DC):

$$\Psi(x_1,\ldots,x_A)|_{\cup_{i=1}^{A}\{x_i=0\}} = 0 \text{ at } \cup_{i=1}^{A}\{x_i=0\}.$$

The potential barrier $V(x_i)$ is narrow.

The classification of quasistationary states. Algorithm DC ($A = 2$, $d = 1$).



Step. 1. Let us choose coordinates $y_1 = \sigma_1 x_1$, $y_2 = \sigma_2 x_2$, $y_1 > 0$, $y_2 > 0$.
In domains $x_1 < 0$, $x_2 > 0$ and $x_1 > 0$, $x_2 < 0$ we have $\sigma_1 = -1$, $\sigma_2 = 1$ and $\sigma_1 = 1$, $\sigma_2 = -1$, respectively. In both cases Eq. (*) reads as

$$\left[-\frac{\partial^2}{\partial y_1^2} - \frac{\partial^2}{\partial y_2^2} + \frac{y_1^2}{2} + \frac{y_2^2}{2} + y_1 y_2\right] \Psi_s(y_1, y_2) = E_s \Psi_s(y_1, y_2).$$

Step 2. In the terms of new coordinates $y_k = z_k \sqrt[4]{2}$ we have

$$\left[-\frac{\sqrt{2}}{2}\frac{\partial^2}{\partial z_1^2} - \frac{\sqrt{2}}{2}\frac{\partial^2}{\partial z_2^2} + \frac{\sqrt{2}}{2} z_1^2 + \frac{\sqrt{2}}{2} z_2^2 + \sqrt{2} z_1 z_2\right] \Psi_s(z_1, z_2) = E_s \Psi_s(z_1, z_2),$$

$$\int_0^\infty dz_1 \int_0^\infty dz_2 \Psi_s(z_1, z_2) \Psi'_s(z_1, z_2) = \delta_{ss'}.$$

Step 3. We seek solution in of above problem in the form of expansion over orthonormal basis

$$\Psi_s = \sum_{j=1}^{j_{\max}} \Psi_j(z_1, z_2)\Psi_{js}^D \qquad \Psi_i(z_1, z_2) = \bar{\Phi}_{i_1}(z_1)\bar{\Phi}_{i_2}(z_2),$$

where functions

$$\bar{\Phi}_{i_k}(z_k) = \sqrt{2}\frac{\exp(-z_k^2/2)H_{i_k}(z_k)}{\sqrt[4]{\pi}\sqrt{2^{i_k}}\sqrt{i_k!}},$$

are orthonormal solution of 1D harmonic oscillator at odd i_k

$$[-\frac{\partial^2}{\partial z_k^2} + z_k^2]\bar{\Phi}_{i_k}(z_k) = (2i_k + 1)\bar{\Phi}_{i_k}(z_k), \quad \int_0^\infty \bar{\Phi}_{i_k}(z_k)\bar{\Phi}_{i'_k}(z_k) = \delta_{i_k i'_k}.$$

This problem reduces to algebraic eigenvalue problem with unknown E_s and $\Psi_s^D = (\Psi_{1s}^D, ..., \Psi_{Ns}^D)^T$:

$$\mathrm{D}\Psi_s^D = \Psi_s^D E_s, \quad (\Psi_s^D)^T\Psi_{s'}^D = \delta_{ss'},$$

where D is a symmetric completely filled matrix with elements

$$D_{i'i} = \int_0^\infty \int_0^\infty dz_1 dz_2 \bar{\Phi}_{i_1}(z_1)\bar{\Phi}_{i_2}(z_2)\left[D^{(0)} + \sqrt{2}z_1 z_2\right]\bar{\Phi}_{i_1}(z_1)\bar{\Phi}_{i_2}(z_2),$$

$$D^{(0)} = -\frac{\sqrt{2}}{2}\frac{\partial^2}{\partial z_1^2} - \frac{\sqrt{2}}{2}\frac{\partial^2}{\partial z_2^2} + \frac{\sqrt{2}}{2}z_1^2 + \frac{\sqrt{2}}{2}z_2^2.$$

The classification of quasistationary states. Algorithm DC ($A = 2$, $d = 1$).

Step 4. Calculation of integrals:

Using differential equation for 1D oscillator we have

$$D_{i'i} = \int_0^\infty \int_0^\infty dz_1 dz_2 \bar{\Phi}_{i'_1}(z_1)\bar{\Phi}_{i'_2}(z_2)\left[\sqrt{2}(i_1+i_2+1)+\sqrt{2}z_1 z_2\right]\bar{\Phi}_{i_1}(z_1)\bar{\Phi}_{i_2}(z_2).$$

Using orthogonality conditions

$$D_{i'i} = \sqrt{2}(i_1+i_2+1)\delta_{i_1 i'_1}\delta_{i_2 i'_2} + \int_0^\infty \int_0^\infty dz_1 dz_2 \bar{\Phi}_{i'_1}(z_1)\bar{\Phi}_{i'_2}(z_2)\sqrt{2}z_1 z_2 \bar{\Phi}_{i_1}(z_1)\bar{\Phi}_{i_2}(z_2).$$

Integrals are calculated by formula

$$D_{i'i} = \sqrt{2}(i_1+i_2+1)\delta_{i'_1 i_1}\delta_{i'_2 i_2} + \sqrt{2} I(i'_1, i_1) I(i'_2, i_2),$$

$$I(i'_k, i_k) = \int_0^\infty dz_k \bar{\Phi}_{i'_k}(z_k) z_k \bar{\Phi}_{i_k}(z_k) = \frac{2^{(i'_k+i_k-1)/2} {}_2F_1(-i'_k, -i_k; (3-i'_k-i_k)/2; 1/2)}{\Gamma((3-i'_k-i_k)/2)\sqrt{i'_k! i_k!}},$$

where $\Gamma(*)$ is Gamma-function and ${}_2F_1(*, *; *; *)$ is a hypergeometric function.

The classification of quasistationary states. Algorithm DC ($A = 2$, $d = 1$).

Correspondence rule of i and set of indexes $[i_1, i_2]$ is
$i = (i_1 + i_2)(i_1 + i_2 + 2)/8 - (i_2 - 1)/2,\ i_1, i_2 = 1, 3, 5, ...,$.
In numerical calculations are taking into account only such coefficients $D_{i'i}$ for which $i_1 + i_2 \leq i_{\max}$ at conditions $E_i = 2i_1 + 2i_2 + 2 \leq E_{i_{\max}}$, $i_{\max} = 2, 4, ...$ In this case matrix D is dimension of $N \times N$, $N = (i_{\max}(i_{\max} + 2)/8)$.

$$D = \begin{pmatrix} 6.043 & 0.735 & 0.735 & -0.164 & 0.300 & -0.164 & \\ 0.735 & 9.772 & 0.300 & 1.006 & 1.002 & -0.067 & \\ 0.735 & 0.300 & 9.772 & -0.067 & 1.102 & 1.006 & \dots \\ -0.164 & 1.006 & -0.067 & 13.275 & 0.410 & 0.015 & \\ 0.300 & 1.102 & 1.102 & 0.410 & 13.950 & 0.410 & \\ -0.164 & -0.067 & 1.006 & 0.015 & 0.410 & 13.275 & \\ & & \dots & & & & \end{pmatrix}$$

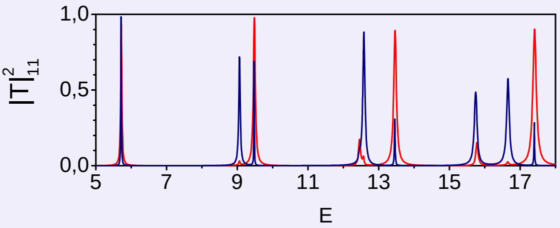
i_1, i_2	1, 1	1, 3	3, 1	1, 5	3, 3	5, 1	
1, 1	6.043	0.735	0.735	−0.164	0.300	−0.164	
1, 3	0.735	9.772	0.300	1.006	1.002	−0.067	
3, 1	0.735	0.300	9.772	−0.067	1.102	1.006	...
1, 5	−0.164	1.006	−0.067	13.275	0.410	0.015	
3, 3	0.300	1.102	1.102	0.410	13.950	0.410	
5, 1	−0.164	−0.067	1.006	0.015	0.410	13.275	
			...				

The classification of quasistationary states.

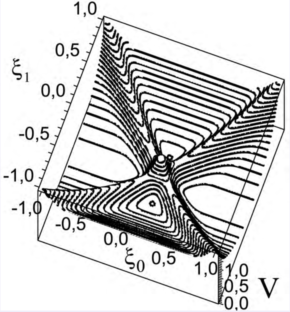
E_{i_1,i_2}	5.756196	9.115926	9.528189	12.52074	12.63792	13.51629
i_1, i_2			$\Psi^D_{s\leftrightarrow i_1,i_2}$			
1, 1	0.965	0.000	0.242	0.047	0.000	0.079
1, 3	−0.176	0.678	0.618	−0.035	0.172	0.270
3, 1	−0.176	−0.678	0.618	−0.035	−0.172	0.270
1, 5	0.045	−0.185	−0.138	−0.599	0.612	0.201
3, 3	0.005	−0.000	−0.351	0.424	0.000	0.680
5, 1	0.045	0.185	−0.138	−0.599	−0.612	0.201
1, 7	−0.015	0.055	0.033	0.193	−0.185	−0.023
3, 5	0.003	−0.030	0.073	0.023	−0.230	−0.360
5, 3	0.003	0.030	0.073	0.023	0.230	−0.360
7, 1	−0.015	−0.055	0.033	0.193	0.185	−0.023

Resonance values of the energy E_S (E_A) for S (A) states for $A = 2$ ($\sigma = 1/10$, $\alpha = 20$) with approximate eigenvalues E_i^D, for the first ten states $i = 1, ..., 10$, calculated using the truncated oscillator basis (D) till $j_{\max} = 136$ at $A = 2$. The asterisk * labels two overlapping peaks of transmission probability.

i	1	2	3	4	5	6	7	8	9	10
E_S	5.72	9.06	9.48	12.46	12.57	13.46	15.74	15.78	16.65	17.41
E_A	5.71	9.06	9.48	12.45	12.57	13.45	15.76*	15.76*	16.66	17.40
E_i^D	5.76	9.12	9.53	12.52	12.64	13.52	15.81	15.84	16.73	17.47



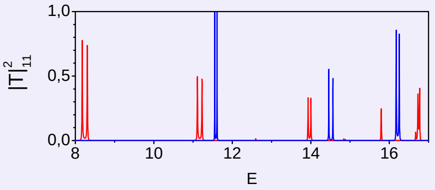
The total transmission probabilities $|T|^2_{11}$ vs energy E (in oscillator units) from the ground state of the system of $A = 2$ of symmetric and antisymmetric particles.



2D barrier potential.

Resonance values of the energy E_S (E_A) for S (A) states for $A = 3$ ($\sigma = 1/10$, $\alpha = 20$) with approximate eigenvalues E_i^D, for the first ten states $i = 1, ..., 10$, calculated using the truncated oscillator basis (D).
The $(i_1 i_2 i_3)$ means the leading components $\bar{\Phi}_{i_1}(x_1)\bar{\Phi}_{i_2}(x_2)\bar{\Phi}_{i_3}(x_3)$ at $p_2 = p_3 = -p_1$ of expansion of quasistationary state solutions Ψ^{D} over harmonic oscillator functions.

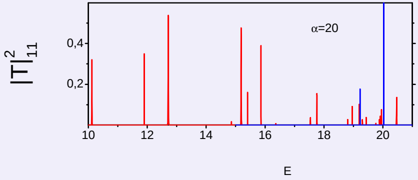
i	1	2	3	4	5	6	7	8	9	10
$A = 3$										
E_S	8.18	11.11		12.60	13.93		14.84	15.79		16.67*
	8.31	11.23			14.00		14.88			16.73(8)*
E_A			11.55			14.46			16.18	
			11.61			14.56			16.25	
E_i^D	8.19	11.09	11.52	12.51	13.86	14.42	14.74	15.67	16.11	16.53
L.c. Ψ^{D} $(i_1 i_2 i_3)$	(111)	(113) +(131)	(113) −(131)	(311)	(133)	(115) −(151)	(133) −(115) −(151)	(313) +(331)	(331) −(313)	(511)



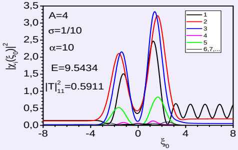
The total transmission probabilities $|T|^2_{11}$ vs energy E (in oscillator units) from the ground state of the system of $A = 3$ of symmetric and antisymmetric particles.

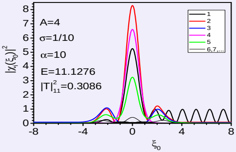
Resonance values of the energy E_S for S states for $A = 4$ ($\sigma = 1/10$, $\alpha = 20$) with approximate eigenvalues E_i^D.

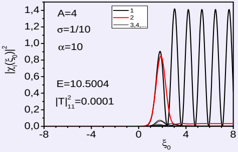
i	1	2	3	4	5	6	7	8	9	10
E_S	10.12	11.89	12.71	14.86	15.19	15.41	15.86	16.37	17.54	17.76
E_i^{D31}	10.03		12.60	14.71	15.04			16.18	17.34	17.56
E_i^{D22}		11.76				15.21	15.64			



The total transmission probabilities $|T|^2_{11}$ vs energy E (in oscillator units) from the ground state of the system of $A = 4$ of symmetric and antisymmetric particles.







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 relevant stationary Schrödinger equation for the wave function $\Psi(x_1, x_2)$ in the s-wave approximation has the form:

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

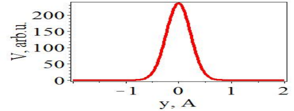
where $\tilde{E}$ is total energy of the system and $\hbar$ is Plank constant. Using the change of variables $x = x_2 - x_1$, $y = x_2 + x_1$, we can rewrite Eq. (1) in the form

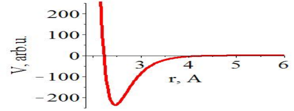
$$\left(-\frac{\hbar^2}{m}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2} + \tilde{V}(x) + \tilde{V}_b(\frac{x+y}{2}) + \tilde{V}_b(\frac{x-y}{2}) - \tilde{E}\right)\Psi(y, x) = 0.$$

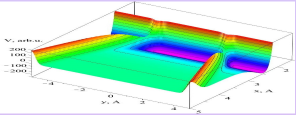
The equation describing the molecular subsystem has the form

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dx^2} + \tilde{V}(x) - \tilde{\varepsilon}\right)\phi(x) = 0.$$

The molecular subsystem considered is assumed to possess the continuous energy spectrum with the eigenvalues $\tilde{\varepsilon} \geq 0$ and eigenfunctions $\phi_{\tilde{\varepsilon}}(x)$ and the discrete energy spectrum with the finite number n of bound states with the eigenfunctions $\phi_j(x)$ and the eigenvalues $\tilde{\varepsilon}_j = -|\tilde{\varepsilon}_j|$, $j = 1, n$.







Gaussian-type barrier $V_b(x_i) = \hat{D}\exp\left(-\frac{x_i^2}{2\sigma}\right)$, at

$\hat{D} = 236.510003758401\text{Å}^{-2} = (m/\hbar^2)\tilde{V}_0 = (m/\hbar^2)D$, $\tilde{V}_0 = D = 1280\text{K}$,
$\sigma = 5.23 \cdot 10^{-2}\text{Å}^2$, the two-particle interaction potential,
$V(r) = \hat{D}\{\exp[-2(r - \hat{r}_{eq})\hat{\rho}] - 2\exp[-(r - \hat{r}_{eq})\hat{\rho}]\}$, $\hat{r}_{eq} = 2.47\text{Å}$,
$\hat{\rho} = 2.96812423381643\text{Å}^{-1}$ and the corresponding 2D potential.
Discrete spectrum energies $E_1 = -1044.879649$, $E_2 = -646.1570935$,
$E_3 = -342.7919791$, $E_4 = -134.7843058$, $E_5 = -22.13407384$ (in K)

The solution of the Eq. is sought for in the form of Galerkin expansion

$$\Psi_{i_o}(y,r) = \sum_{j=1}^{j_{\max}} \phi_j(r)\chi_{ji_o}(y),$$

Here $\chi_{ji_o}(y)$ are unknown functions and the orthonormalized basis functions $\phi_j(r)$ in the interval $0 \le r \le r_{\max}$ are defined as eigenfunctions of the BVP for the equation

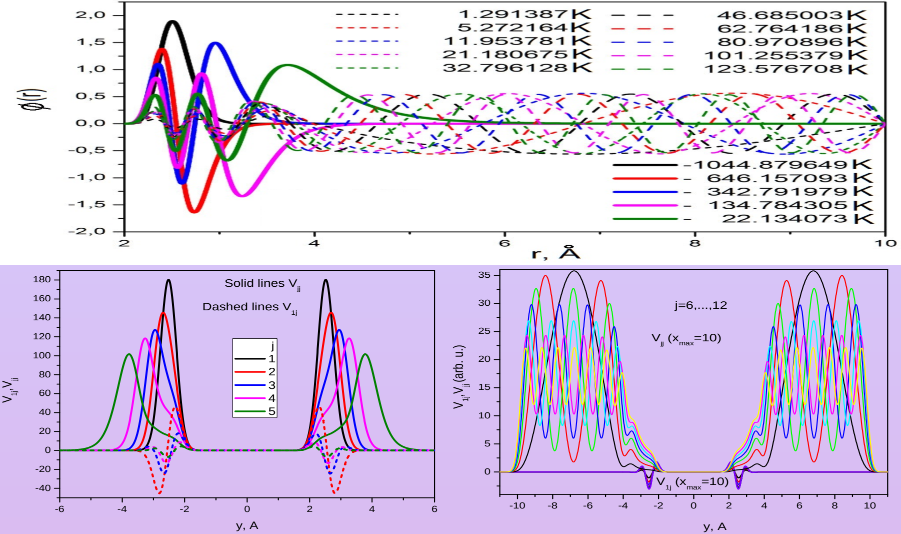
$$\left(-\frac{d^2}{dr^2} + V(r) - \varepsilon_j\right)\phi_j(r) = 0, \quad \phi_j(0) = \phi_j(r_{\max}) = 0, \quad \int_0^{r_{\max}} dr\phi_i(r)\phi_j(r) = \delta_{ij},$$

where $V(r) = (m/\hbar^2)\tilde{V}(x)$, $\varepsilon_j = (m/\hbar^2)\tilde{\varepsilon}_j$.
The set of closed-channel Galerkin equations has the form

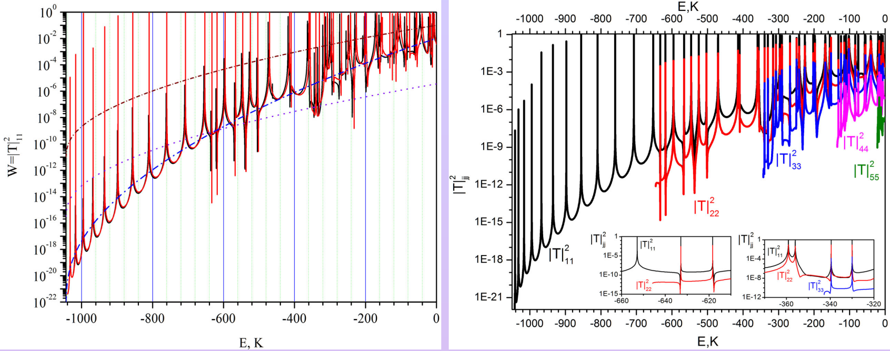
$$\left[-\frac{d^2}{dy^2} + \varepsilon_i - E\right]\chi_{ii_o}(y) + \sum_{j=1}^{j_{\max}} V_{ij}(y)\chi_{ji_o}(y) = 0.$$

The effective potentials $V_{ij}(y)$ are expressed by the integrals

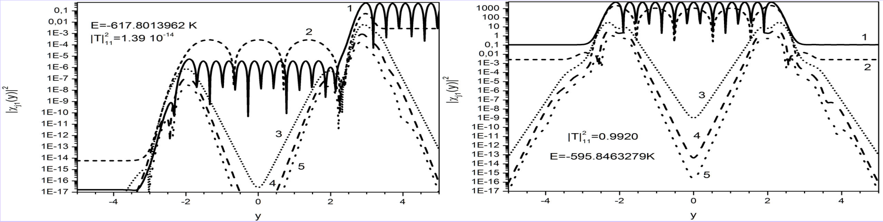
$$V_{ij}(y) = \int_0^{r_{\max}} dr\phi_i(r)(V_b(\frac{r+y}{2}) + V_b(\frac{r-y}{2}))\phi_j(r).$$



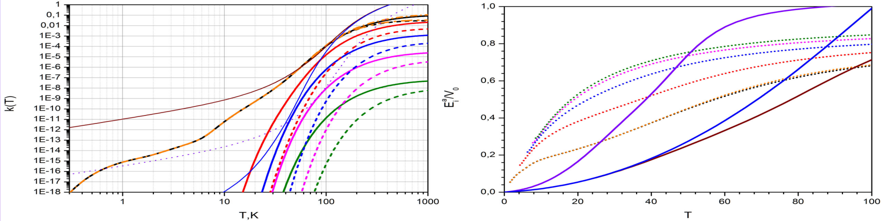
The wave functions $\phi_j(r)$ of the bound states $j = 1, 5$ (solid lines) and pseudostates $j = 6, ..., 15$ (dashed lines) The matrix elements $V_{jj}(y)$ (solid lines) and $V_{j1}(y)$ (dashed lines).



Left panel: Comparison of the total probability of penetration from the first channel to all five open channels simulated by the Galerkin expansion and Numerov calculations ; dotted and dashed curves are probabilities of penetration of one particle through one barrier and one particle through a sequence of two barriers, i.e., upper and lower average, respectively. Right panel: The total probability of penetration from the first channels with the energies $E_1 = -1044.879649$, $E_2 = -646.1570935$, $E_3 = -342.7919791$, $E_4 = -134.7843058$, $E_5 = -22.13407384$ (in K) to all five open channels, simulated by the Galerkin expansion.



The examples of probability $|\chi_{j1}(y)|^2$ of component of vector-functions in the case of total reflection and resonance transmission.



Thermal rate constants vs. temperature: partial $k_i(T)$ (solid curve) and total $\hat{k}(T)$ (dashed lines) and their upper (dotted curves) and lower (short dashed) estimations. andThe temperature-dependent activation energy: partial $E_i^a(T)$ (solid curve) and total $E^a(T)$ (dashed lines) activation energy, and its approximation of lower (dotted curves) and upper (short dashed) estimations that produced by corresponding upper and lower estimations of $k(T)$ of the left panel.

Polar coordinates

Using change of variables $x = \rho \sin\varphi$, $y = \rho\cos\varphi$ we can rewrite the Eq. in polar coordinates (ρ,φ) $\Omega_{\rho,\varphi} = (\rho \in (0,\infty), \varphi \in [0,\pi])$ in dimensionless form

$$\Big(-\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho} - \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + V(\rho\sin\varphi)$$

$$+V_b(\rho\frac{\sin(\varphi-3\pi/4)}{\sqrt{2}}) + V_b(\rho\frac{\sin(\varphi-\pi/4)}{\sqrt{2}}) - E\Big)\Psi(\rho,\varphi) = 0.$$

The solution of the Eq. is sought for in the form of Kantorovich expansion

$$\Psi_{i_o}(\rho,\varphi) = \sum_{j=1}^{j_{\max}} \phi_j(\varphi;\rho)\chi_{ji_o}(\rho),$$

Here $\chi_{ji_o}(\rho)$ are unknown functions and the orthonormalized basis functions $\phi_j(\varphi;\rho)$ in the interval $\varphi \in [0,\pi]$ are defined as eigenfunctions of the BVP for the equation

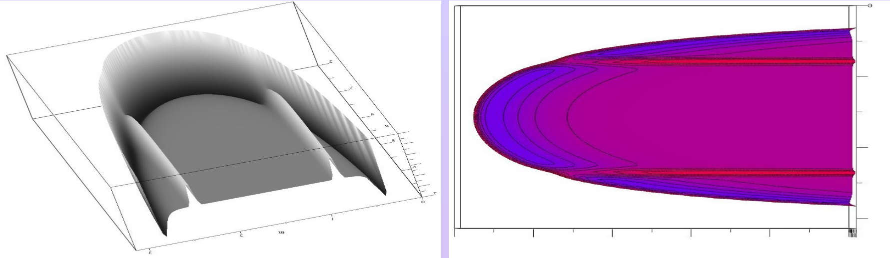
$$\Big(-\frac{\partial^2}{\partial\varphi^2} + \rho^2 V(\rho\sin\varphi) - \varepsilon_j(\rho)\Big)\phi_j(\rho;\varphi) = 0, \qquad \int_0^\pi d\varphi\phi_i(\rho;\varphi)\phi_j(\rho;\varphi) = \delta_{ij}.$$

The set of closed-channel Kantorovich equations has the form

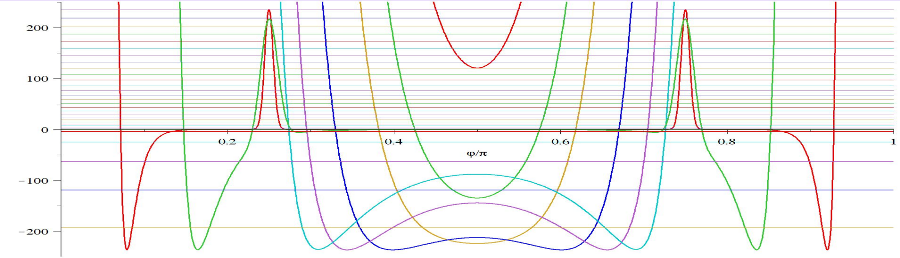
$$\left[-\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho}+\frac{\varepsilon_i(\rho)}{\rho^2}-E\right]\chi_{ii_o}(y)$$
$$+\sum_{j=1}^{j_{\max}}\left[V_{ij}(\rho)\chi_{ji_o}(\rho)+H_{ji}(\rho)\chi_{ji_o}(\rho)+\frac{1}{\rho}\frac{d}{d\rho}\rho Q_{ji}(\rho)\right]\chi_{ji_o}(\rho)=0.$$

where potential curves $\varepsilon_j(\rho)$ and effective potentials $Q_{ij}(\rho)$, $H_{ij}(\rho)$ and $V_{ij}(\rho)$ are determined by integrals

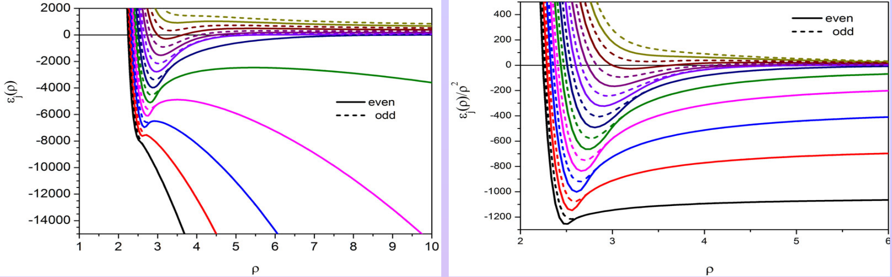
$$Q_{ij}(\rho)=-\int_0^{\pi}d\varphi\phi_i(\rho;\varphi)\frac{d\phi_j(\rho;\varphi)}{d\rho}, H_{ij}(\rho)=\int_0^{\pi}d\varphi\frac{d\phi_i(\rho;\varphi)}{d\rho}\frac{d\phi_j(\rho;\varphi)}{d\rho}$$
$$V_{ij}(\rho)=\int_0^{\pi}d\varphi\phi_i(\rho;\varphi)(V_b(\rho\frac{\sin(\varphi-\pi/4)}{\sqrt{2}})+V_b(\rho\frac{\sin(\varphi-3\pi/4)}{\sqrt{2}}))\phi_j(\rho;\varphi)$$



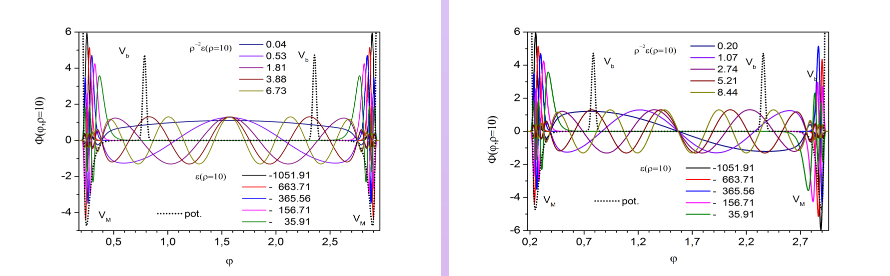
The total potential energy $V^t(\varphi; \rho) = V(\varphi; \rho) + V_b(\varphi; \rho)$.



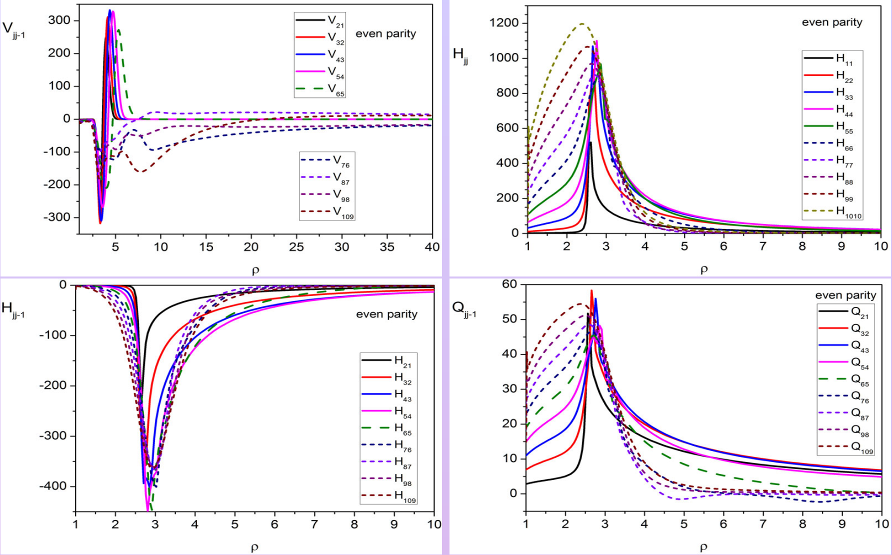
The potential energy $V(\varphi; \rho)$ vs ϕ at $\rho = 2.2, 2.3, 2.4, 2.6, 2.8, 3, 5, 10$



Potential curves $\varepsilon_j(\rho)$ in Å.



Basis functions at $\rho = 10$.



The effective potentials $Q_{ij}(\rho)$, $H_{ij}(\rho)$ and $V_{ij}(\rho)$ vs ρ

Three identical particles with pair δ-interaction

Test desk

We consider three identical particles in the center–of–mass reference frame described by the Jacobi coordinates,

$$\eta = \sqrt{\frac{1}{2}}(x_1 - x_2), \quad \xi = \sqrt{\frac{2}{3}}\left(\frac{x_1 + x_2}{2} - x_3\right), \tag{54}$$

in the plane $\mathbf{R}^2$, where $\{\{x_1, x_2, x_3\} \in \mathbf{R}^3 | x_1 + x_2 + x_3 = 0\}$ are the Cartesian coordinates of the particles on a line. In polar coordinates

$$\eta = \rho\cos\theta,\ \xi = \rho\sin\theta, \ -\frac{\pi}{6} < \theta \le 2\pi - \frac{\pi}{6}, \quad 0 \le \rho < \infty, \tag{55}$$

the Schrödinger equation for the wave function $\Psi(\rho, \theta)$ takes the form

$$-\frac{1}{2}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right)\Psi(\rho,\theta) + \mathrm{U}(\rho,\theta)\Psi(\rho,\theta) = E\Psi(\rho,\theta), \tag{56}$$

where E is the relative energy. To obtain an exact solution which can be used below for a comparison with the numerical results, we involve the sum of delta–functions for describing the pair interactions with identical finite strengths. Thus, $\mathrm{U}(\rho,\theta)$ assumes the form

$$\mathrm{U}(\rho,\theta) = g\sum_{l=-1}^{1}\delta\left(\sqrt{2}\rho\left|\cos\left(\theta - \frac{2\pi}{3}l\right)\right|\right), \tag{57}$$

where $g = \sqrt{2}c\bar{\kappa}$, and $\bar{\kappa} = \pi/6$ is the effective strength of the pair potential[7] [8].

[7] O. Chuluunbaatar, A.A. Gusev, S.Y. Larsen and S.I. Vinitsky, J. Phys. A 35 (2002) L513–L525.

[8] O. Chuluunbaatar, A.A. Gusev, M.S. Kaschiev, V.A. Kaschieva, A. Amaya-Tapia, S.Y. Larsen and S.I. Vinitsky, J. Phys. B 39 (2006) 243–269.

Three identical particles with pair δ-interaction

Test desk

Consider a formal expansion of the solution of Eqs. (56), (57) using the set of one–dimensional orthonormal basis functions $B_j(\theta;\rho) \in W_2^1(-\pi/6, 2\pi - \pi/6)$:

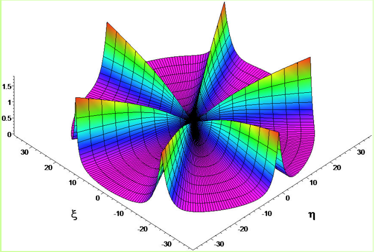
$$\Psi(\rho,\theta) = \sum_{j=1}^{N} B_j(\theta;\rho)\chi_j(\rho), \tag{61}$$

and the functions $B_j(\theta;\rho)$ are determined as solutions of the following one–dimensional parametric eigenvalue problem:

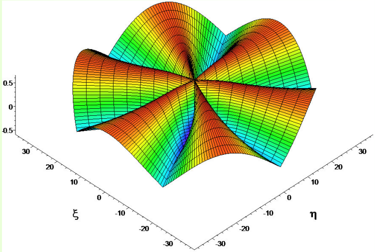
$$\begin{aligned}
&-\frac{1}{\rho^2}\frac{\partial^2 B_j(\theta;\rho)}{\partial\theta^2} = \varepsilon_j(\rho) B_j(\theta;\rho),\\
&\frac{1}{\rho}\frac{\partial B_j(\theta_i;\rho)}{\partial\theta} = (-1)^{i-n} c\bar{\kappa} B_j(\theta_i;\rho), \quad i = n, n+1,\\
&B_j(\theta_{n+1}-0;\rho) = B_j(\theta_{n+1}+0;\rho).
\end{aligned} \tag{62}$$

Three identical particles with pair δ-interaction

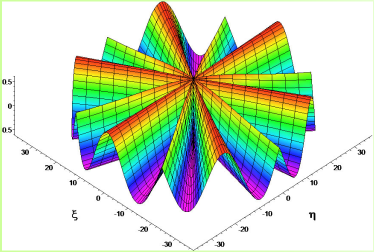
B_1

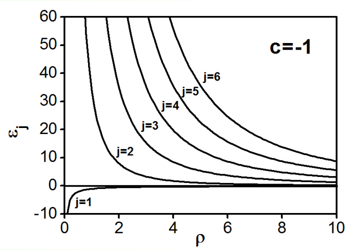


B_2

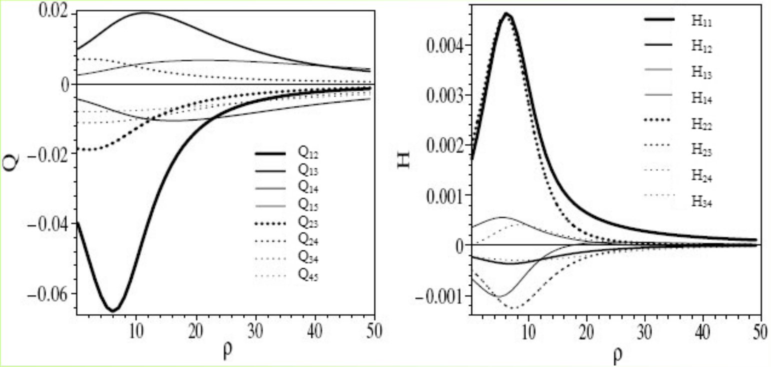


B_3

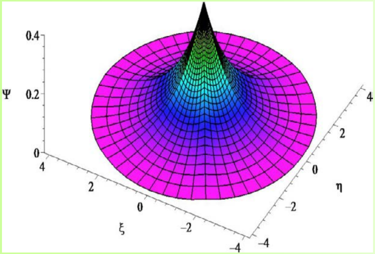




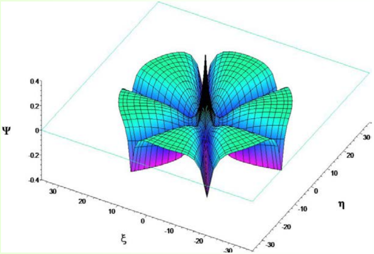
Three identical particles with pair δ-interaction



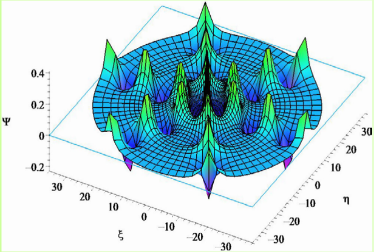
Three identical particles with pair δ-interaction



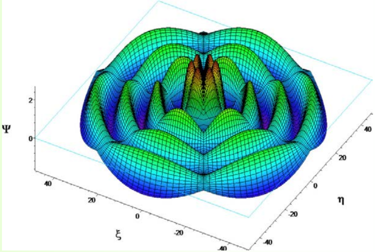
Ground state c=-1



Half bound state c=-1



Scattering c=-1



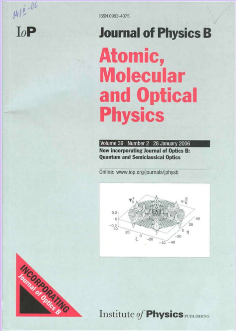
Scattering c=1

Resume

- We formulate a model of quantum tunneling of several bound identical particles interacting via the potential of the oscillator type through the short-range repulsive barrier potentials in the new representation, which we name as symmetrized coordinate representation (SCR).
- The method, algorithm and program for symmetrizing or antisymmetrizing harmonic oscillator basis functions in new symmetrized coordinates is described.
- We considered for clarity a system of several one-dimensional spinless identical particles with discrete spectrum of relative motion of particles in the center-of-mass coordinate system, described by the internal symmetrized variables, and continuous spectrum of the center-of-mass motion (the motion of the system "as a whole"), described by the external variable.
- Multichannel scattering problem for the Schrödinger equation with several short-range repulsive barriers was formulated.
- The elaborated algorithms and program complexes of construction of the effective potentials and solution of the eigenvalue problem in close-coupled method discredited by Finite Element Method [http://wwwinfo.jinr.ru/programs/jinrlib/kantbp/indexe.html], are applied to analyze of the quantum transparency effect in the near-surface quantum diffusion of the diatomic molecules below dissociation threshold.
- We analyzed the effect of quantum transparency consisting in resonance tunneling of the bound particles through the repulsive potential barriers, associated with the existence of barrier quasistationary states, imbedded in the continuum.
- The proposed approach can be adapted and applied to the analysis of quantum transparency effect, to the study of quantum diffusion of molecules, micro-clusters through surfaces, and the fragmentation mechanism in producing very neutron-rich light nuclei, as well as trapped-ion quantum simulator.

A.A. Gusev, e-mail: gooseff@jinr.ru

(Laboratory of Information Technologies, Joint Institute for Nuclear Research, Dubna, Russia)



Thank you for your attention!

- List of Fortran codes:
- http://theor.jinr.ru/~chuka/codes.html
- http://wwwinfo.jinr.ru/programs/jinrlib/kantbp/indexe.html

- O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky and A.G. Abrashkevich, ODPEVP: A program for computing eigenvalues and eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined Sturm-Liouville problem. Comput. Phys. Commun. 181, pp. 1358–1375 (2009). http://cpc.cs.qub.ac.uk/summaries/AEDV_v1_0.html
- O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky and A.G. Abrashkevich, KANTBP 2.0: New version of a program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach, Comput. Phys. Commun. 179, pp. 685–693 (2008). http://cpc.cs.qub.ac.uk/summaries/ADZH_v2_0.html
- O. Chuluunbaatar, A.A. Gusev, V.P. Gerdt, V.A. Rostovtsev, S.I. Vinitsky, A.G. Abrashkevich, M.S. Kaschiev and V.V. Serov, POTHMF: A program for computing potential curves and matrix elements of the coupled adiabatic radial equations for a hydrogen-like atom in a homogeneous magnetic field, Comput. Phys. Commun. 178, pp. 301–330 (2008). http://cpc.cs.qub.ac.uk/summaries/AEAA_v1_0.html
- O. Chuluunbaatar, A.A. Gusev, A.G. Abrashkevich, A. Amaya-Tapia, M.S. Kaschiev, S.Y. Larsen and S.I. Vinitsky, KANTBP: A program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach, Comput. Phys. Commun. 177, pp. 649–675 (2007). http://cpc.cs.qub.ac.uk/summaries/ADZH_v1_0.html