KANTOROVICH AND CLOSE-COUPLING METHODS IN QUANTUM TUNNELING PROBLEM FOR A COUPLED PAIR OF IONS THROUGH LONG-RANGE POTENTIAL BARRIERS.

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Outline

The problem statement

Let us consider a quantum system of two particles with masses m_1, m_2 and radius-vectors $\tilde{\mathbf{x}}_1$, $\tilde{\mathbf{x}}_2$ describing by the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m_1}\nabla^2_{\tilde{\mathbf{x}}_1} - \frac{\hbar^2}{2m_2}\nabla^2_{\tilde{\mathbf{x}}_2} + \tilde{V}(\tilde{\mathbf{x}}_1 - \tilde{\mathbf{x}}_2) + \tilde{U}_0(\tilde{\mathbf{x}}_1) + \tilde{U}_0(\tilde{\mathbf{x}}_2)$$

We suppose that a pair of particles is coupled by a potential

$$\tilde{V}(\tilde{\mathbf{x}}_1 - \tilde{\mathbf{x}}_2) = \frac{\mu\omega^2}{2}(\tilde{\mathbf{x}}_1 - \tilde{\mathbf{x}}_2)^2,$$

where $\mu = m_1 m_2/(m_1 + m_2)$ is a reduced mass and ω is a frequency of a three-dimensional harmonic oscillator, transmit through a potential barrier $\tilde{U}_0(\tilde{\mathbf{x}}_1) + \tilde{U}_0(\tilde{\mathbf{x}}_2)$ like in heavy ion collisions.

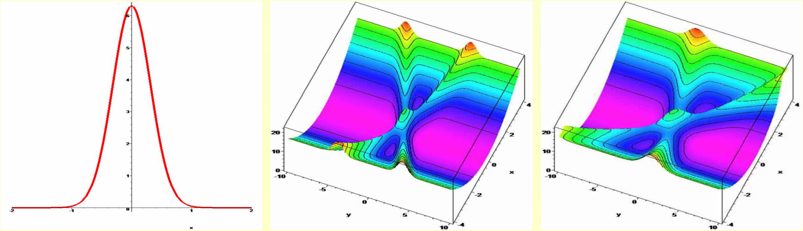
The problem statement

Hamiltonian written in the coordinates of the center of mass of the pair $\tilde{\mathbf{Y}}$ and the internal variable corresponding to the relative motion $\tilde{\mathbf{X}}$,

$$\tilde{\mathbf{Y}} = \frac{m_1\tilde{\mathbf{x}}_1 + m_2\tilde{\mathbf{x}}_2}{M}, \quad \tilde{\mathbf{X}} = \tilde{\mathbf{x}}_1 - \tilde{\mathbf{x}}_2,$$

where $M = m_1 + m_2$ is the total mass, has the form

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla^2_{\tilde{\mathbf{Y}}} - \frac{\hbar^2}{2\mu}\nabla^2_{\tilde{\mathbf{X}}} + \tilde{V}(\tilde{\mathbf{X}}) + \tilde{U}_0(\tilde{\mathbf{x}}_1) + \tilde{U}_0(\tilde{\mathbf{x}}_2)$$



Gaussian-type barrier $\tilde{U}_0(\tilde{x}_i) = \frac{A}{\sqrt{2\pi\sigma}}\exp\left(-\frac{\tilde{x}_i^2}{2\sigma}\right)$, at $a = 5$, $\sigma = 0.1$ and corresponding 2D potentials with $m_1 = 1$, $m_2 = 1$ and $m_1 = 1$, $m_2 = 9$

The problem statement

Using the transformation to dimensionless variables

$$\mathbf{y}=\sqrt{\frac{M\omega}{\hbar}}\,\tilde{\mathbf{Y}}=\sqrt{\frac{M}{\mu}}\frac{\tilde{\mathbf{Y}}}{x_{osc}},\quad \mathbf{x}=\sqrt{\frac{\mu\omega}{\hbar}}\,\tilde{\mathbf{X}}=\frac{\tilde{\mathbf{X}}}{x_{osc}},$$

where $x_{osc}=\sqrt{\frac{\hbar}{\mu\omega}}$ is unit of length, we rewrite the Schrödinger equation with Hamiltonian (1) as the following dimensionless equation:

$$\left(-\nabla^2_{\mathbf{x}}-\nabla^2_{\mathbf{y}}+V(\mathbf{x})+U(\mathbf{x},\mathbf{y})-E\right)\Psi(\mathbf{y},\mathbf{x})=0.$$

Here the energy $E=\tilde{E}/E_{osc}$ and the potential functions

$$V(\mathbf{x})=\mathbf{x}^2,\quad U(\mathbf{x},\mathbf{y})=U_0\left(\tilde{\mathbf{x}}_1\right)+U_0\left(\tilde{\mathbf{x}}_2\right)$$

are given in units of energy $E_{osc}=\hbar\omega/2$ and dimensional variables $\tilde{\mathbf{x}}_i$ are expressed via dimensionless ones $\mathbf{x}_i$

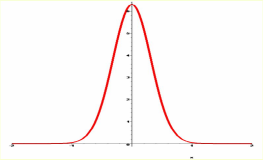
$$\tilde{\mathbf{x}}_1=x_{osc}\mathbf{x}_1=x_{osc}\left(\frac{\sqrt{m_1}\sqrt{m_2}}{M}\,\mathbf{y}+\frac{m_2}{M}\,\mathbf{x}\right),$$

$$\tilde{\mathbf{x}}_2=x_{osc}\mathbf{x}_2=x_{osc}\left(\frac{\sqrt{m_1}\sqrt{m_2}}{M}\,\mathbf{y}-\frac{m_1}{M}\,\mathbf{x}\right).$$

Barriers

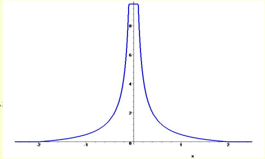
Gaussian-type

$$\tilde{U}_0\left(\tilde{x}_i\right) = \frac{A}{\sqrt{2\pi\sigma}} \exp\left(-\frac{\tilde{x}_i^2}{2\sigma}\right)$$



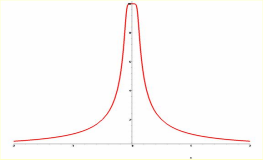
where $\sigma = 0.1$, $m_1 = 1$, $m_2 = 9$, $a = 5$.
Truncated Coulomb potential

$$\tilde{U}_0\left(\tilde{x}_i\right) = \begin{cases} \frac{\hat{Z}_i}{\tilde{x}_{min}} - \frac{\hat{Z}_i}{\tilde{x}_{\max}}, & |\tilde{x}| \leq \tilde{x}_{min}; \\ \frac{\hat{Z}_i}{|\tilde{x}|} - \frac{\hat{Z}_i}{\tilde{x}_{\max}}, & \tilde{x}_{min} < |x| \leq \tilde{x}_{ma} \\ 0 & |\tilde{x}| > \tilde{x}_{max} \end{cases}$$



Coulomb-like potential

$$\tilde{U}_0\left(\tilde{x}_i\right) = \hat{Z}_i(\tilde{x}_i^s + \tilde{x}_{\min}^s)^{-1/s}$$



Close-coupling and Kantorovich (Adiabatic) methods

The Schrödinger equation reads as

$$\left(\frac{1}{g_{3s}(x_s)}\hat{H}_2(x_f;x_s)+\hat{H}_1(x_s)+\hat{V}_{fs}(x_f,x_s)-2E\right)\Psi(x_f,x_s)=0,$$

$$\hat{H}_2=-\frac{1}{g_{1f}(x_f)}\frac{\partial}{\partial x_f}g_{2f}(x_f)\frac{\partial}{\partial x_f}+\hat{V}_f(x_f;x_s),$$

$$\hat{H}_1=-\frac{1}{g_{1s}(x_s)}\frac{\partial}{\partial x_s}g_{2s}(x_s)\frac{\partial}{\partial x_s}+\hat{V}_s(x_s).$$

$\hat{H}_2(x_f;x_s)$ is the Hamiltonian of the fast subsystem,

$\hat{H}_1(x_s)$ is the Hamiltonian of the slow subsystem,

$V_{fs}(x_f,x_s)$ is interaction potential.
The Kantorovich expansion of the desired solution of BVP:

$$\Psi(x_f,x_s)=\sum_{j=1}^{j_{\max}}\Phi_j(x_f;x_s)\chi_j(x_s).$$

BVP for fast subsystem

The equation for the basis functions of the fast variable x_f and the potential curves, $E_i(x_s)$ continuously depend on the slow variable x_s as a parameter

$$\left\{\hat{H}_2(x_f; x_s) - E_i(x_s)\right\}\Phi_i(x_f; x_s) = 0,$$

The boundary conditions

$$\lim_{x_f \to x_f^t(x_s)} \left(N_f(x_s) g_{2f}(x_s) \frac{d\Phi_j(x_f; x_s)}{dx_f} + D_f(x_s)\Phi_j(x_f; x_s)\right) = 0.$$

The normalization condition

$$\langle\Phi_i|\Phi_j\rangle = \int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f; x_s)\Phi_j(x_f; x_s) g_{1f}(x_f) dx_f = \delta_{ij}.$$

BVP for slow subsystem

The effective potential matrices of dimension $j_{\max} \times j_{\max}$:

$$U_{ij}(x_s) = \frac{1}{g_{3s}(x_s)} \hat{E}_i(x_s)\delta_{ij} + \frac{g_{2s}(x_s)}{g_{1s}(x_s)} W_{ij}(x_s) + V_{ij}(x_s),$$

$$V_{ij}(x_s) = \int_{x_f^{\min}}^{x_f^{\max}} \Phi_i(x_f; x_s) V_{fs}(x_f, x_s) \Phi_j(x_f; x_s) g_{1f}(x_f) dx_f,$$

$$W_{ij}(x_s) = \int_{x_f^{\min}}^{x_f^{\max}} \frac{\partial \Phi_i(x_f; x_s)}{\partial x_s} \frac{\partial \Phi_j(x_f; x_s)}{\partial x_s} g_{1f}(x_f) dx_f,$$

$$Q_{ij}(x_s) = -\int_{x_f^{\min}}^{x_f^{\max}} \Phi_i(x_f; x_s) \frac{\partial \Phi_j(x_f; x_s)}{\partial x_s} g_{1f}(x_f) dx_f.$$

BVP for slow subsystem

The SDE for the slow subsystem (the adiabatic approximation is a diagonal approximation for the set of ODEs)

$$\mathbf{H}\chi^{(i)}(x_s) = 2E_i\,\mathbf{I}\chi^{(i)}(x_s),$$
$$\mathbf{H} = -\frac{1}{g_{1s}(x_s)}\mathbf{I}\frac{d}{dx_s}g_{2s}(x_s)\frac{d}{dx_s} + \hat{V}_s(x_s)\mathbf{I} + \mathbf{U}(x_s) + \frac{g_{2s}(x_s)}{g_{1s}(x_s)}\mathbf{Q}(x_s)\frac{d}{dx_s} + \frac{1}{g_{1s}(x_s)}\frac{dg_{2s}(x_s)\mathbf{Q}(z)}{dx_s},$$

with the boundary conditions

$$\lim_{x_s\to x_s^t}\left(N_s g_{2s}(x_s)\frac{d\chi(x_s)}{dx_s} + D_s\chi(x_s)\right) = 0.$$

The scattering problem is solved using the boundary conditions at $d=1$, $z=z_{\min}$ and $z=z_{\max}$:

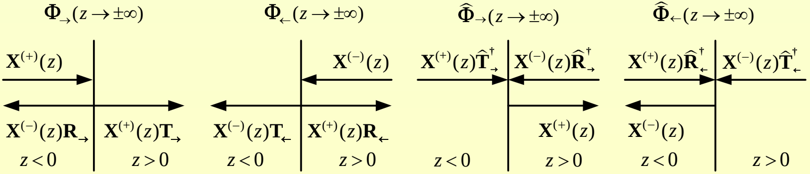
$$\left.\frac{d\Phi(z)}{dz}\right|_{z=z_{\min}}=\mathcal{R}(z_{\min})\Phi(z_{\min}),\ \left.\frac{d\Phi(z)}{dz}\right|_{z=z_{\max}}=\mathcal{R}(z_{\max})\Phi(z_{\max}),$$

where $\mathcal{R}(z)$ is a unknown $N\times N$ matrix-function, $\Phi(z)=\{\chi^{(j)}(z)\}_{j=1}^{N_o}$ is the required $N\times N_o$ matrix-solution and N_o is the number of open channels, $N_o=\max_{2E\geq\epsilon_j} j\leq N$.

Matrix-solution $\mathbf{\Phi}_v(z) = \mathbf{\Phi}(z)$ describing the incidence of the particle and its scattering, which has the asymptotic form “incident wave + outgoing waves”, is

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

where $\mathbf{R}_v$ and $\mathbf{T}_v$ are the reflection and transmission $N_o \times N_o$ matrices, $v = \rightarrow$ and $v = \leftarrow$ denote the initial direction of the particle motion along the z axis.



(a) (b)

Schematic diagrams of the continuum spectrum waves having the asymptotic form: (a) “incident wave + outgoing waves”, (b) “incident waves + ingoing wave”.

Here the leading term of the asymptotic rectangle-matrix functions $\mathbf{X}^{(\pm)}(z)$ has the form

$$X_{ij}^{(\pm)}(z) \to (p_j|z|^{d-1})^{-1/2} \exp\left(\pm\imath\left(p_j z - \frac{Z_j}{p_j}\ln(2p_j|z|)\right)\right)\delta_{ij},$$
$$p_j = \sqrt{2E-\epsilon_j} \quad i=1,\ldots,N, \quad j=1,\ldots,N_o,$$

where $Z_j = Z_j^+$ at $z > 0$ and $Z_j = Z_j^-$ at $z < 0$.

The matrix-solution $\Phi_v(z,E)$ is normalized by

$$\int_{z_0}^{\infty} \Phi^{\dagger}_{v'}(z,E')\Phi_v(z,E)z^{d-1}dz = 2\pi\delta(E'-E)\delta_{v'v}\mathbf{I}_{oo},$$

where $\mathbf{I}_{oo}$ is the unit $N_o \times N_o$ matrix and $z_0 = -\infty$ if $d=1$ or $z_0 > 0$ if $d \geq 2$.

Let us rewrite Eq. (1) in the matrix form at $z_+ \rightarrow +\infty$ and $z_- \rightarrow -\infty$ as

$$\begin{pmatrix} \Phi_{\rightarrow}(z_+) & \Phi_{\leftarrow}(z_+) \\ \Phi_{\rightarrow}(z_-) & \Phi_{\leftarrow}(z_-) \end{pmatrix} = \begin{pmatrix} 0 & \mathbf{X}^{(-)}(z_+) \\ \mathbf{X}^{(+)}(z_-) & 0 \end{pmatrix} + \begin{pmatrix} 0 & \mathbf{X}^{(+)}(z_+) \\ \mathbf{X}^{(-)}(z_-) & 0 \end{pmatrix} \mathbf{S},$$

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

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

is composed of the reflection and transmission matrices.

In addition, it should be noted that functions $\mathbf{X}^{(\pm)}(z)$ satisfy relations

$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\mp)}(z),\mathbf{X}^{(\pm)}(z)) = \pm 2\imath \mathbf{I}_{oo},$$
$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\pm)}(z),\mathbf{X}^{(\pm)}(z)) = \mathbf{0},$$

where $\mathbf{Wr}(\mathbf{Q}(z);\mathbf{a}(z),\mathbf{b}(z))$ is a generalized Wronskian with a long derivative defined as

$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{a}(z),\mathbf{b}(z)) = z^{d-1}\left[\mathbf{a}^T(z)\left(\frac{d\mathbf{b}(z)}{dz} - \mathbf{Q}(z)\mathbf{b}(z)\right)\right.$$
$$\left. - \left(\frac{d\mathbf{a}(z)}{dz} - \mathbf{Q}(z)\mathbf{a}(z)\right)^T \mathbf{b}(z)\right].$$

This Wronskian is used to estimate a desirable accuracy of the above expansion.

From Wronskian conditions, we obtain the following properties of the reflection and transmission matrices:

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

This means that the scattering matrix is symmetric and unitary.

Asymptotic expansions of regular and irregular solutions in longitudinal coordinates

We seek the solution of SDE in the form:

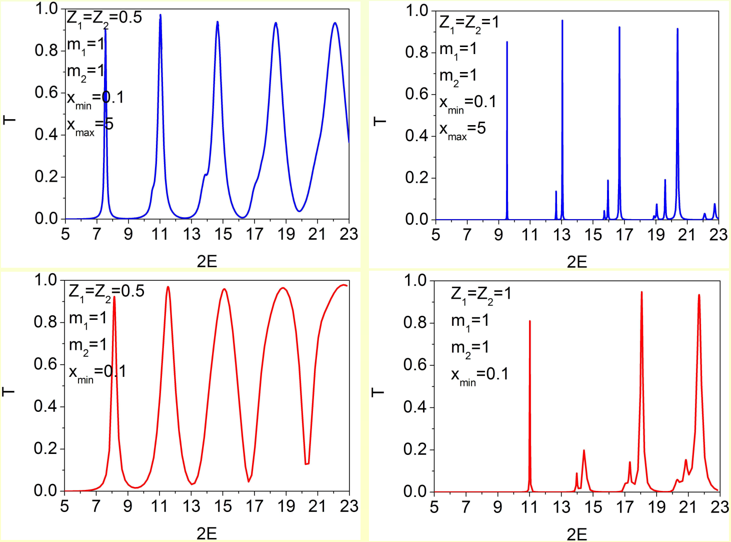
$$\chi_{i'}(x_s) = \phi_{i'}(x_s) R_{i'}(x_s) + \psi_{i'}(x_s) \frac{dR_{i'}(x_s)}{dx_s},$$

where $\phi_{i'}(x_s)$ and $\psi_{i'}(x_s)$ are unknown functions, while $R_{i'}(x_s)$ is known function and $\frac{dR_{i'}(x_s)}{dx_s}$ is derivative of $R_{i'}(x_s)$ with respect to x_s. We choose $R_{i'}(x_s)$ as solutions of auxiliary problem

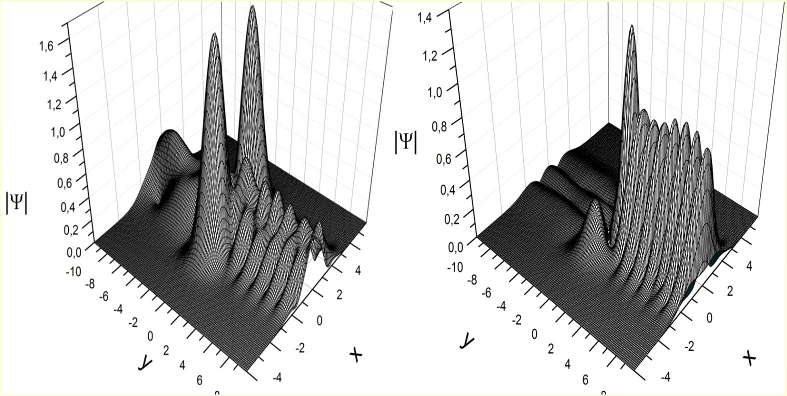
$$\left[-\frac{1}{x_s^{d-1}} \frac{d}{dx_s} x_s^{d-1} \frac{d}{dx_s} + \sum_{l \geq 1} \frac{Z_{i'}^{(l)}}{x_s^l} - k_{i'}^2 \right] R_{i'}(x_s) = 0.$$

Note, if $Z_i^{(l \geq 3)} = 0$ then solutions of last equation are presented via hypergeometric functions, in particular, via exponential, trigonometric, Bessel, Coulomb functions, etc.

Results: 2D model of heavy ion reaction

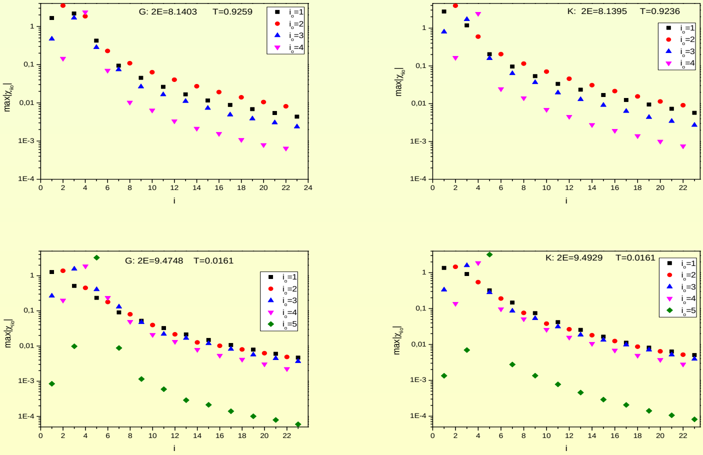


Total probabilities of penetration through Truncated Coulomb and Coulomb-like potential barriers



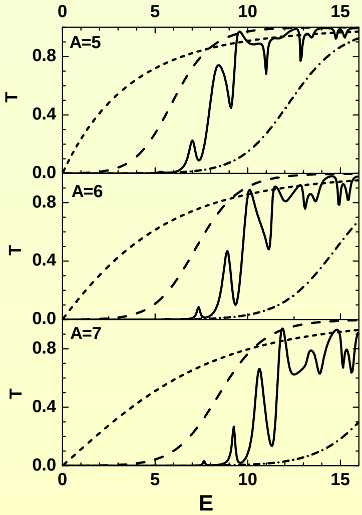
Profiles $|\Psi^{(-)}_{Em\rightarrow}|$ of the total wave functions of the continuous spectrum in the zx plane with $Z_1 = Z_2 = 0.5$, $m_1 = m_2 = 1$ energies $E = 8.1403\,a.u.$ and $E = 9.4748\,a.u.$, demonstrating resonance transmission and total reflection, respectively.

Convergence



The absolute maximum value χ_{j,i_o} vs of number j component of continuum spectrum solution in Close Coupling and Kantorovich expansions.

Results: 2D model of molecular diffusion



Total probabilities T of penetration through the Gaussian barriers at $\sigma = 0.1$, $m_1 = 1$ and $m_2 = 9$. Total probabilities of penetration through the barriers of structured particle (solid line) and for structureless particles with masses $m_1 = 1$ (short dashed line), $m_2 = 9$ (long dashed line) going thought single barrier or $m_3 \equiv M = m_1 + m_2$ (dash-dotted line) going thought twice barrier.

Results: quantum diffusion

Classical diffusion can be considered by following way: transmission probability of particle through the barrier is given by formulae

$$W^{cl}(E) = 1, E \geq E_{cl} \quad W^{cl}(E) = 0, E < E_{cl},$$

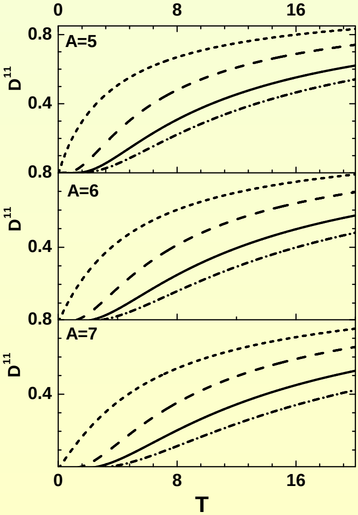
where E_{cl} is height of barrier. Averaging this dependence by Boltzmann law we have the Arenious law

$$D^{cl} = \int_0^\infty W^{cl}(E) e^{-E/T} dE = e^{-E_{cl}/T}.$$

In the case of quantum diffusion it is necessary to substitute in above formula the quantum transmission probability W^{qn}:

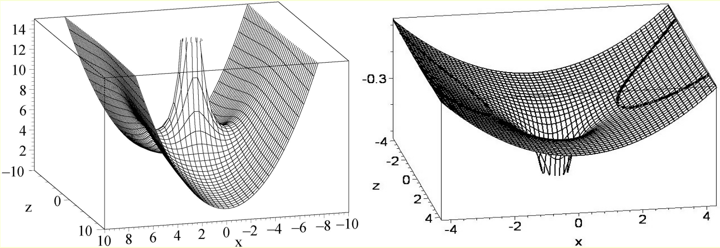
$$D^{qn} = \int_0^\infty W^{qn}(E) e^{-E/T} dE.$$

Results: quantum diffusion



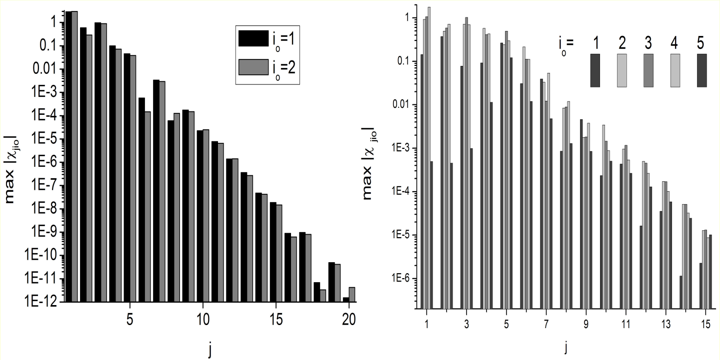
The quantum diffusion corresponding to penetration through the Gaussian barriers at $A = 5$, $\sigma = 0.1$, $m_1 = 1$ and $m_2 = 9$ for structured particle (solid line) and for structureless particles with masses $m_1 = 1$ (short dashed line), $m_2 = 9$ (long dashed line) going thought single barrier or $m_3 \equiv M = m_1 + m_2$ (dash-dotted line) going thought twice barrier.

The channeling model similar or oppositive charged ions



The profile in zx plane of the effective potenial 2U(x,y,z) consisted of sum of 3D Coulomb and 2D oscillator potentials. Left panels similar charges $\boldsymbol{Z = +6}$, $\boldsymbol{\gamma = 1}$ and right panel oppositive charges $\boldsymbol{Z = -1}$, $\boldsymbol{\gamma = 1}$.

Convergence of Kantorovich expansion



The absolute maximum value χ_{j,i_o} vs of number j component of continuum spectrum solution in Kantorovich expansion for channeling model with similar and oppositive charges of ions calculated for BVP of set of $j_{\max} = 16$ ODE on grid Ω.

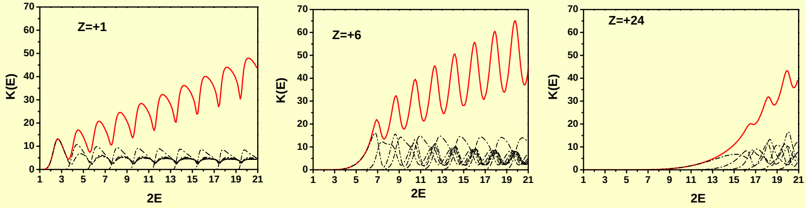
Left panel similar charges ($Z = +6$, $\gamma = 1$, $2E = 0.34$, $j_{\max} = 20$) for two open channels. Right panels oppositive charges ($Z = -1$, $\gamma = 1$, $2E = 10$, $j_{\max} = 15$) for five open channels.

Model of the axis channeling of similar charged ions

The enhancement coefficient – determinates as ratio of square of module of wave functions in the pair impact point $r = 0$ of channeling ions with/without transversal harmonic oscillator field versus the energy E in the c.m.s.[1]:

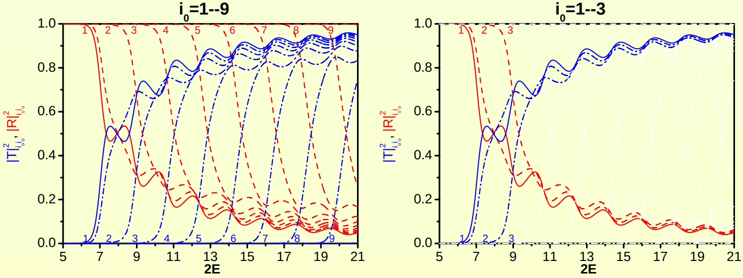
$$K(E) = \frac{|C(2E)|^2}{|C_0(2E)|^2} = \sum_{i=1}^{N_o} \frac{|C_i(2E)|^2}{|C_0(2E)|^2},$$

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

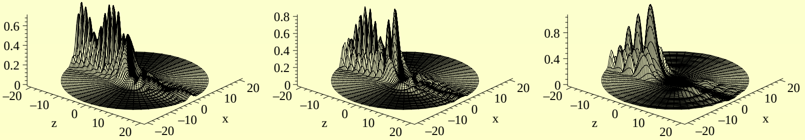


[1] O. Chuluunbaatar, A.A.Gusev, V.L.Derbov, P. M. Krassovitskiy, and S. I. Vinitsky, Channeling Problem for Charged Particles Produced by Confining Environment, Physics of Atomic Nuclei, 2009, Vol. 72, No. 5, pp. 768778.

Results: Transmission and reflection matrices at $Z = +6$

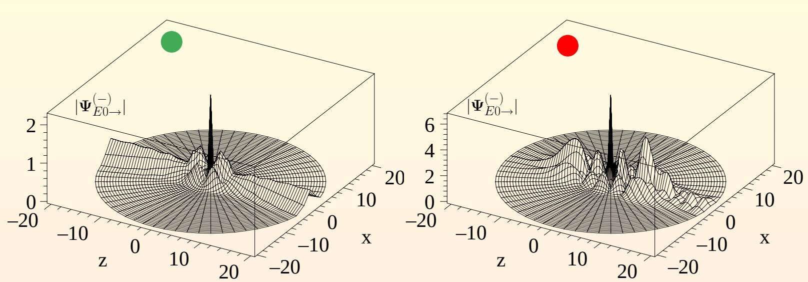


$$|\mathbf{R}|^2 = \begin{pmatrix} \color{red}{0.967329} & 0.004785 & -0.000094 \\ 0.004785 & \color{red}{0.990368} & 0.000074 \\ -0.000094 & 0.000074 & \color{red}{0.999999} \end{pmatrix} \quad \text{at} \quad 2E = 6.552$$



In this way partial transmission and practically total reflection effects for inelastic scattering processes of identical ions in a crystal channel are manifested.

Results: Effects of resonance transmission and total reflection of oppositive charged ions in a transversal oscillator potential

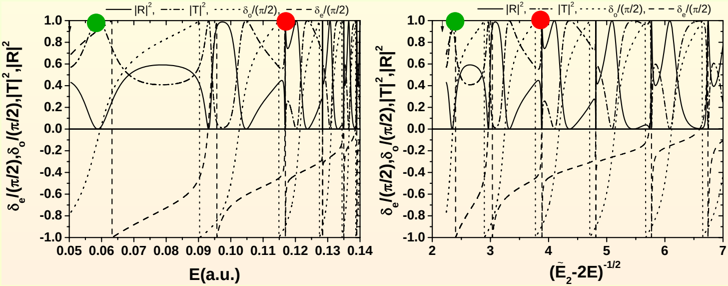


(a) (b)

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

Profiles of the wave function for $Z=1$, $m=0$, $\gamma=0.1$ and $j_{\mathbf{max}}=10$ are shown in Fig. 1 at two fixed values of energy E, corresponding to resonance transmission $|\hat{\mathrm{T}}|^2=\sin^2(\delta_e-\delta_o)=1$ and total reflection $|\hat{\mathrm{R}}|^2=\cos^2(\delta_e-\delta_o)=1$.

Transmission and reflection coefficients



(a) (b)

Transmission $|\hat{\mathbf{T}}|^2$ and reflection $|\hat{\mathbf{R}}|^2$ coefficients, even δ_e and odd δ_o phase shifts versus the energy E (a) and $(\tilde{E}_2 - 2E)^{-1/2}$ (b) for $\gamma = 0.1$ and the final state with $\sigma = -1$, $Z = 1$, $m = 0$. The arrow marks the first Landau threshold $E_1 = \gamma/2$.

Transmission and reflection coefficients are explicitly shown in Fig. 2 together with even δ_e and odd δ_o phase shifts versus the energy E (Fig. 2a) and $(\tilde{E}_2 - 2E)^{-1/2}$ (Fig.2b), where $\tilde{E}_2 = \epsilon^{th}_{m\,2}(\gamma)$ is second threshold shift. The quasi-stationary states imbedded in the continuum correspond to the short-range phase shifts $\delta_{o(e)} = n_{o(e)}\pi + \pi/2$ at $(\tilde{E}_2 - 2E)^{-1/2} = n_{o(e)} + \Delta_{n_{o(e)}}$.

Nonmonotonic behavior of $|\hat{\mathbf{T}}|$ and $|\hat{\mathbf{R}}|$ is seen to manifest the resonance transmission and total reflection effects, related to the existence of these quasistationary states.

Conclusions

• A Schrödinger equation was reduced by Kantorovich or Close-coupling methods to a system of the coupled second-order ODEs on a finite interval with homogeneous third-type BCs for continuous spectrum problem by using derived asymptotic expansion in analytic form with help of symbolic algorithm which realized by CAS MAPLE.

• The effect of quantum transparency consists of nonmonotonical dependence of transmission coefficient at resonance tunneling of coupled pair of particles throughout symmetric/nonsymmetric, short-range/long-range repulsive potential barriers.

• Partial transmission and practically total reflection effects for inelastic scattering processes of identical ions in a crystal channel and the resonance transmission and total reflection effects for scattering processes of oppositive charged ions in uniform magnetic field, related to the existence of these quasistationary states, were manifested.

• Proposed approach, quantum transparency effect and development of software can be used in further **analysis** of **barrier heavy ion reactions**, **molecular diffusion**, etc.

Thank you for your attention !