INVESTIGATION OF RESONANCES OF 2D TWO-BODY SYSTEMS WITH ANISOTROPIC INTERACTION

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Anisotropic quantum scattering in two dimensions

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Motivation

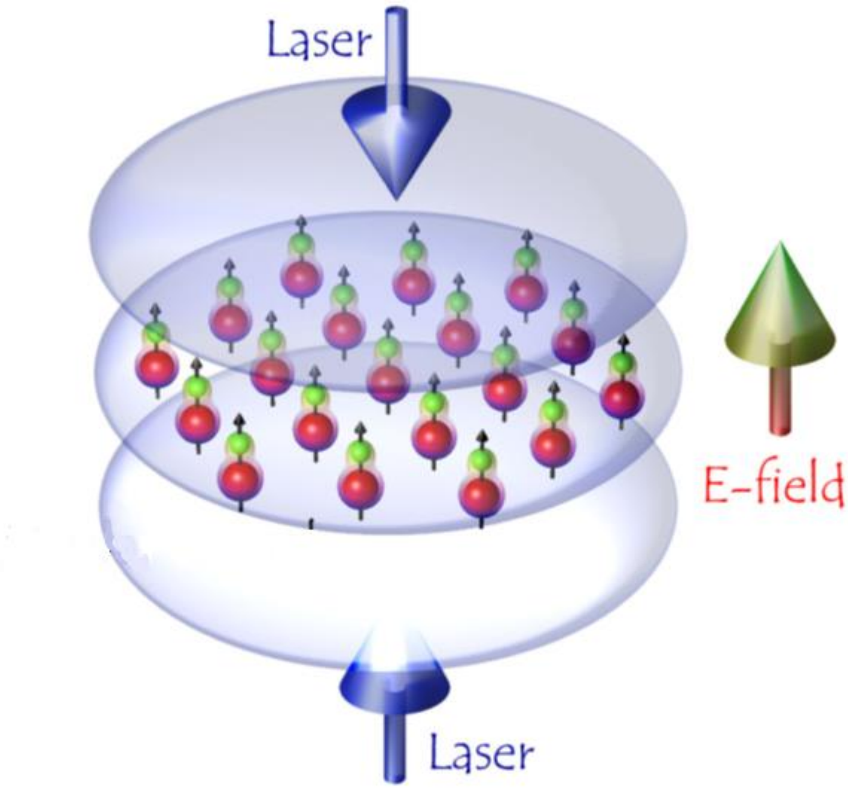
- Ultracold polar molecules collisions problem

  (simulated by dipole-dipole scattering $\sim \frac{1}{\rho^3}$)

- Partial wave expansion becomes inefficient at $q \to 0$:

$$\frac{\tan(\delta_l)}{q} \to const$$

$l = 0, 1, 2 \ldots$



Two-dimensional (2D) stationary scattering problem formulation

- Two-dimensional Schrödinger equation:

$$\begin{cases} H(\rho,\phi)\Psi(\rho,\phi) = E\Psi(\rho,\phi) \\ \Psi(\rho,\phi) \xrightarrow[\rho\to\infty]{} e^{iq\rho\cos(\phi)} + f(q,\phi)\dfrac{e^{iq\rho}}{\sqrt{-i\rho}} \end{cases}$$

- Hamiltonian of the system

$$H(\rho,\phi) = -\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right) + U(\rho,\phi)$$

  - q – the relative momentum, μ - the reduced mass, U – the interaction potential

Time evolution of 2D systems

- Time-dependent two-dimensional Schrödinger equation:

$$\begin{cases} i\dfrac{d\Psi(\rho,\phi|t)}{dt} = H(\rho,\phi)\Psi(\rho,\phi) \\ \Psi(\rho,\phi|t=0) = \Psi_0(\rho,\phi) \end{cases}$$

- Hamiltonian of the system

$$H(\rho,\phi) = -\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)+U(\rho,\phi)$$

Algorithm of numerical solution

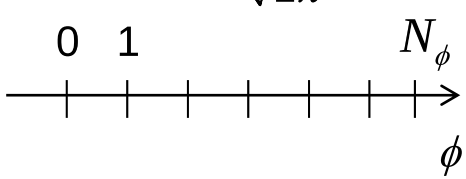
- Transformation of partial differential equations into differential-difference equations:
  - Fourier basis:

$$H_0(\phi)\xi_m(\phi) = -m^2\xi_m(\phi) \equiv \varepsilon_m \xi_m(\phi); \qquad H_0(\phi) = \frac{\partial^2}{\partial \phi^2};$$

  - Special representation of the wave-function:

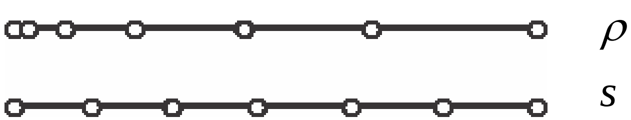
$$\Psi(\rho,\phi) = \frac{1}{\sqrt{\rho}} \sum_{j'=0}^{N_\phi} \sum_{m=-N_\phi/2}^{N_\phi/2} \xi_m(\phi)\xi^{-1}_{mj'}\Psi_{j'}(\rho)$$

$$\xi_{jm} = \xi_m(\phi_j) \to \frac{(-1)^m}{\sqrt{2\pi}} \exp(im\phi_j)$$



$$\Psi(\rho,\phi_j) = \frac{1}{\sqrt{\rho}}\Psi_j(\rho);$$

$$\begin{cases} \rho = \rho_m s^2, \\ \{s_0, s_1, \ldots, s_N\};\ s_0 = 0,\ s_N = 1 \end{cases}$$



Stationary problem

- The system of differential-difference equations has been obtained:

$$\frac{1}{\sqrt{\rho}}\sum_j \sum_m \left[\frac{d^2}{d\rho^2}+\frac{1}{4\rho^2}+\frac{\varepsilon_m}{\rho^2}+\frac{2\mu}{\hbar^2}\left(E-U(\rho,\phi_i)\right)\right]\Psi_j(\rho)\xi_m(\phi_i)\xi_{mj}^{-1}=0$$

after reducing it reads as:

$$\frac{d^2\Psi_i(\rho)}{d\rho^2}+\left[\frac{1}{4\rho^2}+\frac{2\mu}{\hbar^2}\left(E-U(\rho,\phi_i)\right)\right]\Psi_i(\rho)+\frac{1}{\rho^2}\sum_{j=0}^{N_\phi}\left(\sum_{m=-\frac{N_\phi}{2}}^{\frac{N_\phi}{2}}\varepsilon_m\xi_m(\phi_i)\xi_{mj}^{-1}\right)\Psi_j(\rho)=0$$

Hereafter $\hbar = \mu = 1$.

TD Schrödinger equation

- Crank–Nicolson scheme has been employed:

$$\begin{cases} \Psi\left(\rho,\phi \mid t_{n+1}\right)=\left[1+i\dfrac{\delta}{2}H\left(\rho,\phi\right)\right]^{-1}\left[1-i\dfrac{\delta}{2}H\left(\rho,\phi\right)\right]\Psi\left(\rho,\phi \mid t_{n}\right) \\ \Psi\left(\rho,\phi \mid t_{n=0}=0\right)=\Psi_{0}\left(\rho,\phi\right) \end{cases}$$

after reducing time evolution of wave function reads as:

$$\begin{cases} \Psi\left(\rho,\phi \mid t_{n+1}\right)+i\dfrac{\delta}{2}H\left(\rho,\phi\right)\Psi\left(\rho,\phi \mid t_{n+1}\right)=\Psi\left(\rho,\phi \mid t_{n}\right)-i\dfrac{\delta}{2}H\left(\rho,\phi\right)\Psi\left(\rho,\phi \mid t_{n}\right) \\ \Psi\left(\rho,\phi \mid t_{n=0}=0\right)=\Psi_{0}\left(\rho,\phi\right) \end{cases}$$

Hereafter $\hbar=\mu=1$.

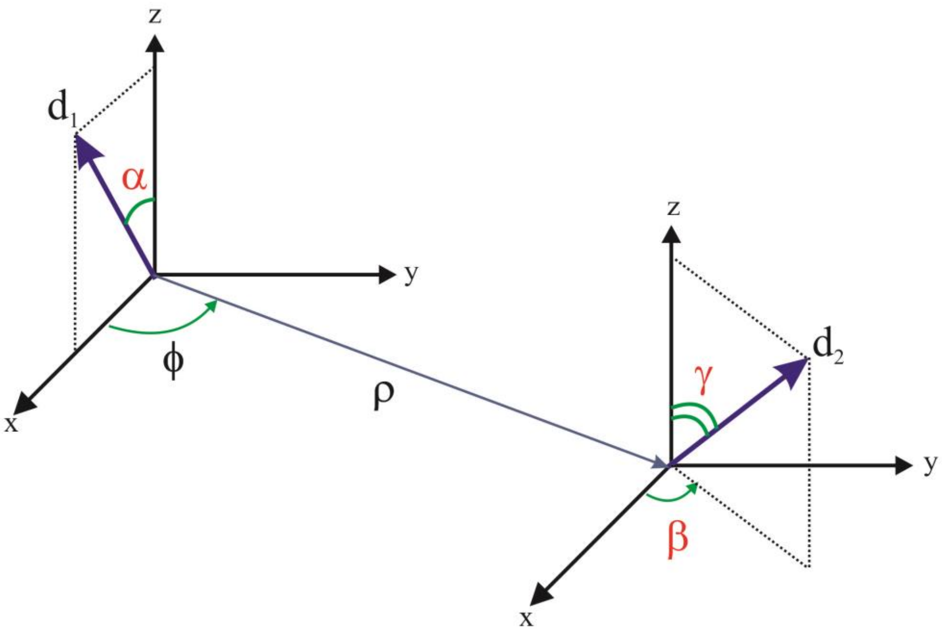
Dipole-dipole scattering

- An example of the physical system with the anisotropic interaction is the dipole-dipole system, that models polar molecules in optical traps.

- For two arbitrary oriented dipoles interaction potential reads:

$$V_{\vec{d}_1\vec{d}_2} = \frac{(\vec{d}_1\vec{d}_2) - 3(\vec{d}_1\vec{e}_r)(\vec{e}_r\vec{d}_2)}{\rho^3},$$

where $\vec{d}_1, \vec{d}_2$ – dipole moments, $(\vec{d}_i\vec{e}_r), i = 1,2$ – their projections onto the collision axis.

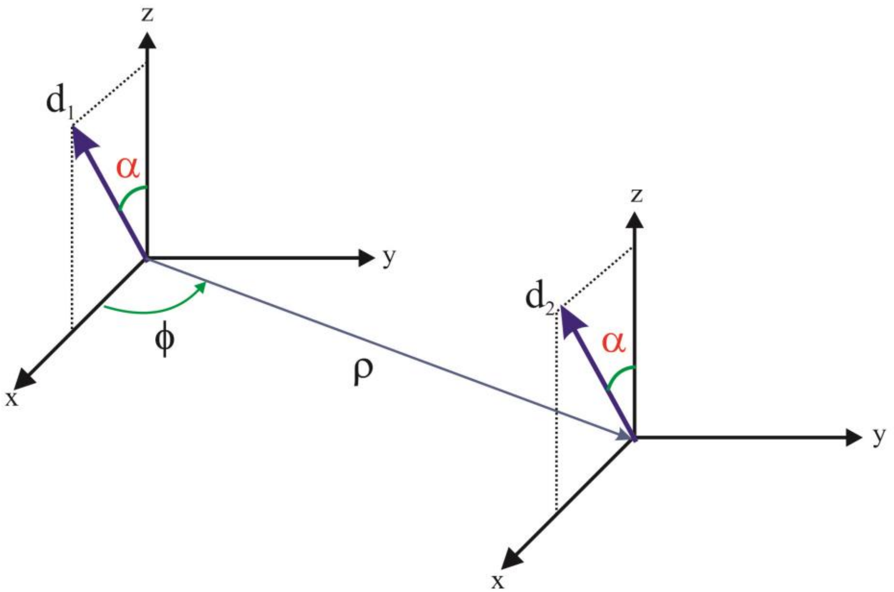


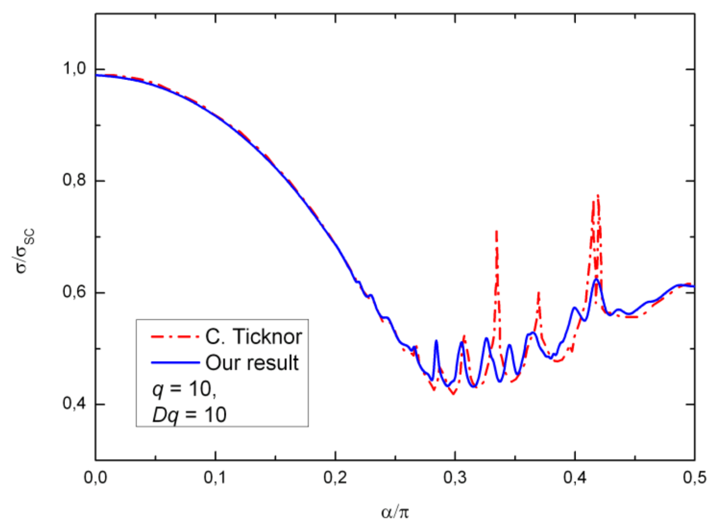
Dipole-dipole scattering

A particular case of parallel dipoles with the polarization axis tilted to the plane of motion $\gamma = \alpha;\ \beta = 0$ with short-range interaction modeled by a hard wall at the origin with the width $\rho_0 / D = 0.1$:

$$V(\rho,\phi,\alpha) = V_{HW}(\rho) + \frac{d_1 d_2}{\rho^3}[1 - 3\sin^2(\alpha)\cos^2(\phi)],$$

was considered in the paper by C. Ticknor [Phys.Rev. A84, 032702 (2011)].





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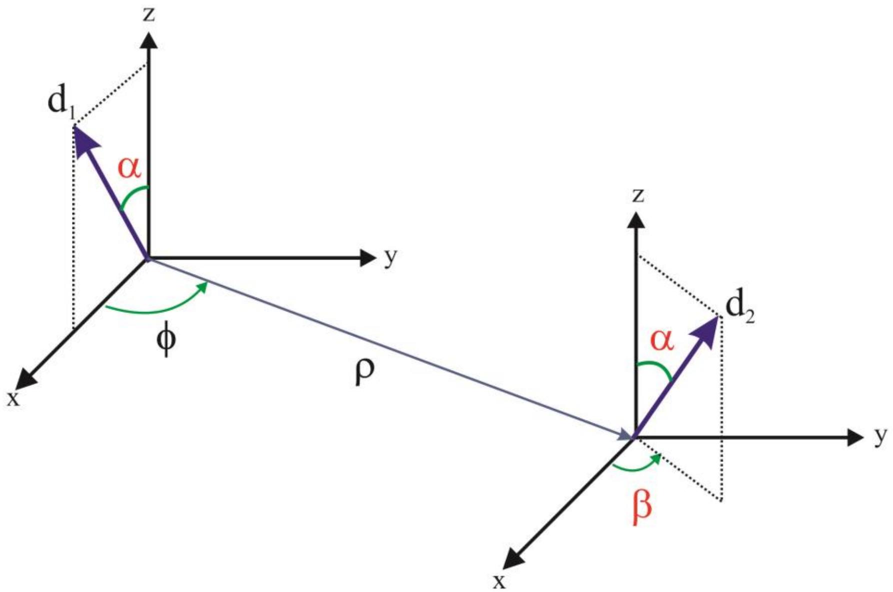

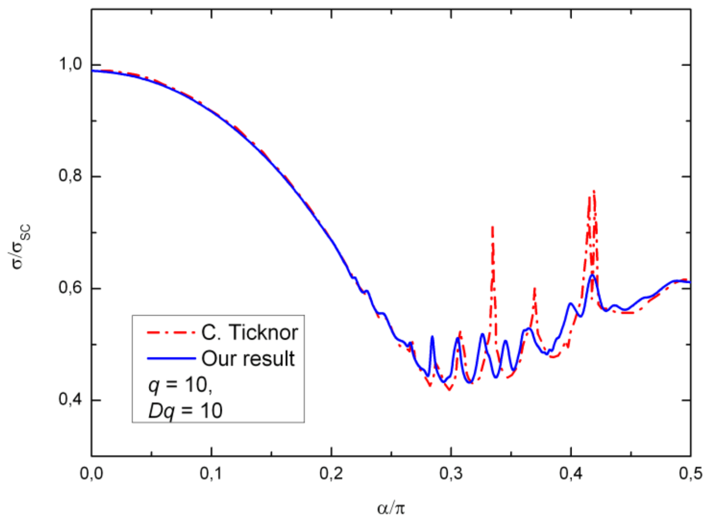

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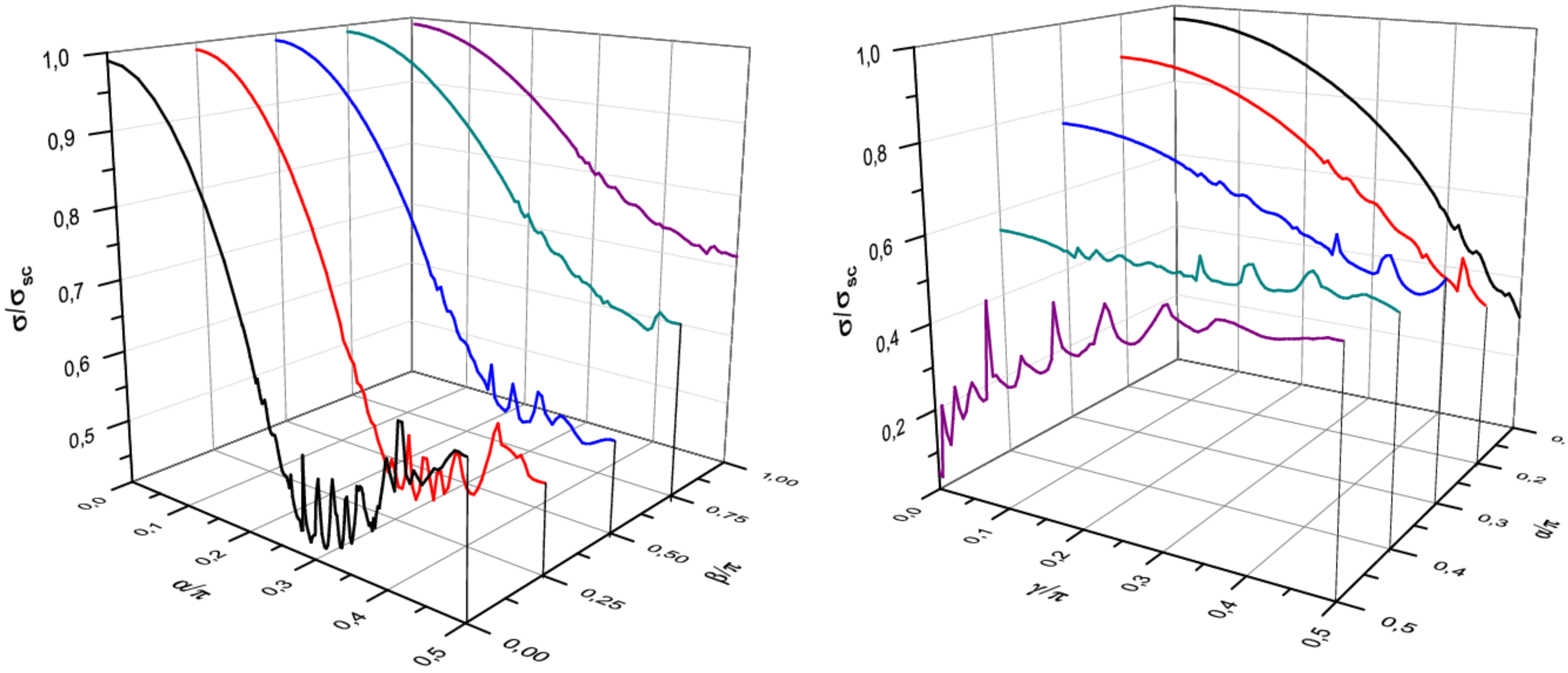
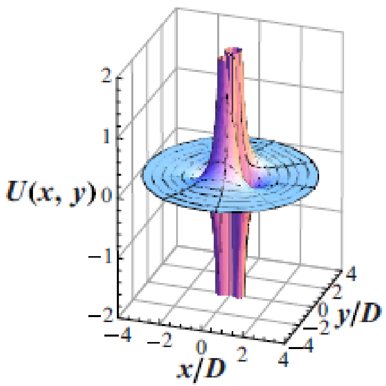
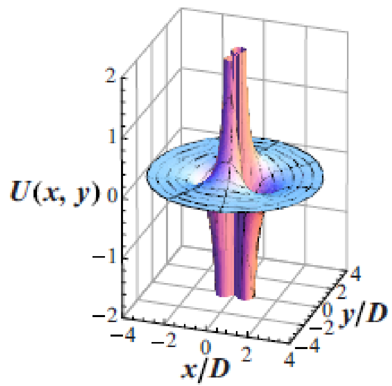


Dipole-dipole scattering

We have analyzed how the found "resonant" structure for the polarized dipoles in the calculated dependence of the scattering cross section on the dipole tilt angle $\gamma = \alpha$ varies with elimination of the polarization.



$\beta = 0,\ \alpha = 0.25\pi$



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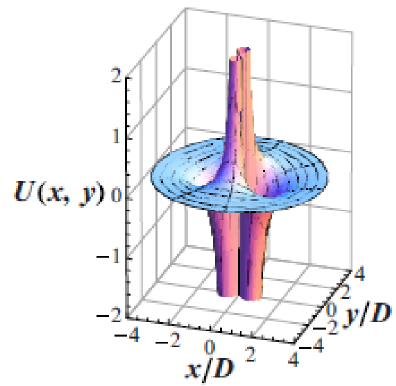
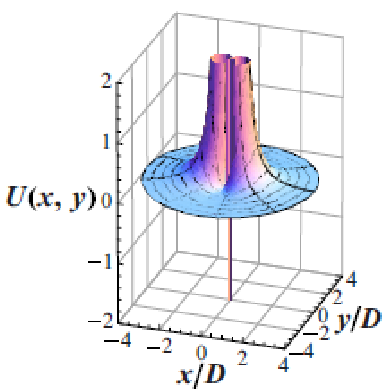
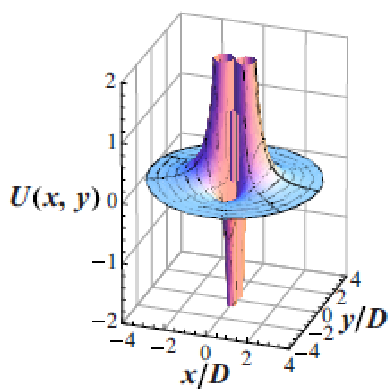


$\beta = 0,\ \alpha = 0.5\pi$



$\beta = \pi,\ \alpha = 0.25\pi$



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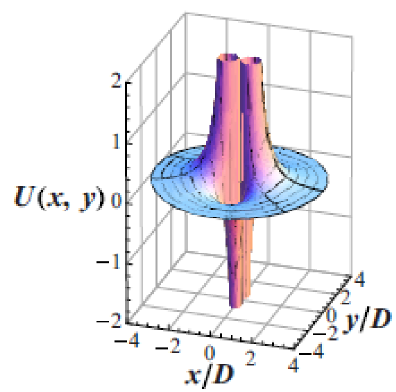


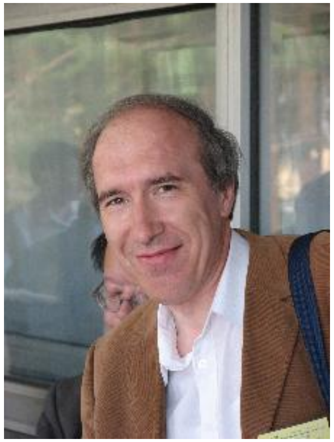
$\beta = \pi,\ \alpha = 0.5\pi$

Conclusions

- Due to advantages the algorithm can be applied for several problems:
  - Numerical simulation of scattering processes in two-particle systems of the ultracold atoms in optical traps
  - Quantum collisions of the diatomic molecules with induced dipole moments.
  - Theoretical investigations of hydrogen atom collisions on the surface of liquid helium.

Thank you
for your attention!

Contacts



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