Dependences of the differential cross sections of 2D bosonic and fermionic dipoles scattering on the angles of the dipoles' mutual orientation

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Outline

Introduction: ultracold molecules in 1D and 2D geometries

Dipolar gases are more stable in a quasi-two-dimensional geometry, in contrast with a 3D case, due to the absence of the "head-to-tail"instability[1].
Optical lattices with 2D geometries are prospective candidates for a dipolar gas stabilization, trapping, and dynamics controlling because the dipole-dipole interaction (DDI) is isotropic and repulsive in the case of dipole moments polarized along the frozen direction, whereas tilting of the polarization axis leads to a controllable anisotropy of the interaction[2].
Molecules collisions in one layer of a pancake-shaped trap are modelled by a 2D dynamics of the molecules[3].
The investigations of a dipolar diatomic molecules interaction in a plane are highly relevant due to prospects for one of the possible realisation of a qubit and application to the quantum computing schemes[4].

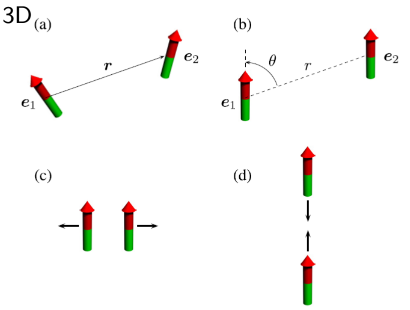
[1] Bohn, J. L. *et al.* English. *Science* **357,** 1002–1010 (2017), Koch, T. *et al.* English. *Nature physics* **4,** 218–222 (2008), Ni, K.-K. *et al.* English. *Nature* **464,** 1324 (2010).

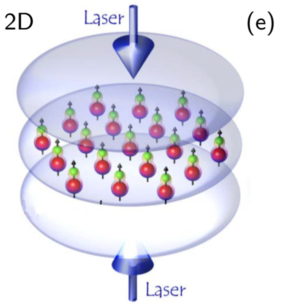
[2] Bohn, J. L. *et al.* English. *Science* **357,** 1002–1010 (2017), De Miranda, M. *et al.* English. *Nature Physics* **7,** 502–507 (2011), Lahaye, T. *et al.* English. *Rep. Prog. Phys.* **72,** 126401 (2009).

[3] De Miranda, M. *et al.* English. *Nature Physics* **7,** 502–507 (2011), Ticknor, C. English. *Physical Review A* **80,** 052702 (2009), Ticknor, C. English. *Physical Review A* **84,** 032702 (2011), Ticknor, C. *et al.* English. *Physical review letters* **106,** 065301 (2011), Volosniev, A. *et al.* English. *Physical review letters* **106,** 250401 (2011), Rosenkranz, M. & Bao, W. English. *Physical Review A* **84,** 050701 (2011), Koval, E. A. *et al.* English. *Physical Review A* **89,** 052710 (2014).

[4] DeMille, D. English. *Physical Review Letters* **88,** 067901 (2002), Ni, K.-K. *et al.* English. *Chemical science* **9,** 6830–6838 (2018).

Introduction: ultracold molecules in 1D and 2D geometries





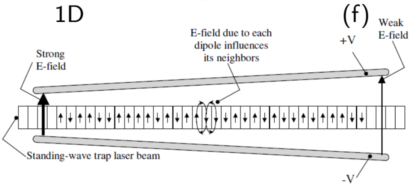


Fig.1 The schematic representation of the polar molecules in 3D (a,b,c,d), 2D (e) and 1D (f) geometries of optical traps.

2D dipole-dipole scattering

The 2D Shrödinger equation for describing quantum dipolar scattering in a plane on anisotropic potential $U(\rho,\phi)$ in polar coordinates (ρ,ϕ) reads:

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right)+U\left(\rho,\phi\right)-E\right]\Psi\left(\rho,\phi\right)=0 \tag{1}$$

with boundary condition in the asymptotic region $\rho\to\infty$:

$$\Psi\left(\rho,\phi\right)\to e^{i\boldsymbol{q}\boldsymbol{\rho}}+f\left(q,\phi,\phi_q\right)\frac{e^{iq\rho}}{\sqrt{-i\rho}}. \tag{2}$$

The relative momentum $\boldsymbol{q}$ is defined by the collision energy E with $q=\sqrt{2\mu E}/\hbar$ and μ denotes the reduced mass of the system. The incoming wave direction $\boldsymbol{q}/q$ is defined by the ϕ_q angle.

A scattering differential cross section is defined by the calculated scattering amplitude $f\left(q,\phi,\phi_q\right)$

$$d\sigma(q,\phi,\phi_q)/d\Omega=|f(q,\phi,\phi_q)|^2, \tag{3}$$

where $d\Omega=d\phi_q d\phi$. A total cross section is obtained by averaging over incoming wave directions (ϕ_q) and integration over scattering angle ϕ:

$$\sigma(q)=\frac{1}{2\pi}\int_0^{2\pi}\int_0^{2\pi}\frac{d\sigma}{d\Omega}d\phi_q d\phi. \tag{4}$$

2D dipolar scattering

A transition to scattering of identical bosons (fermions) is done with the symmetrization $\epsilon = +1$ (antisymmetrization $\epsilon = -1$) of the wave function:

$$\Psi\left(\rho,\phi\right) \to e^{i\mathbf{q}\boldsymbol{\rho}} + \epsilon\, e^{-i\mathbf{q}\boldsymbol{\rho}} + f(\phi)\frac{e^{iq\rho}}{\sqrt{-i\rho}} \tag{5}$$

as well as the differential cross section:

$$d\sigma(\phi)/d\Omega = \left|f(\phi,\phi_q)\right|^2 = \left|f\left(\phi\right) + \epsilon f\left(\left|180^\circ - \phi\right|\right)\right|^2 . \tag{6}$$

The definitions (3) and (6) show, that it leads to an increase for bosons and a decrease for fermions of the differential cross section with respect to the case of distinguishable particles for some scattering angles, e.g., for $\phi + \phi_q = 90^\circ$:

$$\frac{d\sigma_B(\phi+\phi_q)}{d\Omega} = 4\frac{d\sigma(\phi+\phi_q)}{d\Omega} \text{ (for bosons)},$$
$$\frac{d\sigma_F(\phi+\phi_q)}{d\Omega} = 0 \text{ (for fermions)}.$$

2D dipolar scattering

The interaction potential $U(\rho, \phi)$ has the form:

$$U(\rho, \phi) = V_{SR}(\rho) + V_{dd}(\rho, \phi), \tag{7}$$

where for an approximation of the repulsive short-range interaction (SRI) $V_{SR}(\rho)$ we use two different types of potentials: the hard wall potential with the width of ρ_{SR} (so that the wave function is equal to zero at ρ_{SR}) and and the more realistic Lennard-Jones (LJ) potential:

$$V_{SR}^{HW}(\rho) = \begin{cases} \infty, & \rho \leqslant \rho_{SR} \\ 0, & \rho > \rho_{SR} \end{cases} ; \qquad V_{SR}^{LJ}(\rho) = \frac{C_{12}}{\rho^{12}} - \frac{C_6}{\rho^6} \tag{8}$$

A fixed value of the C_6 parameter of the Lennard-Jones potential was taken for polar molecules, e.g., $C_6 = 1.5\ 10^6$ a.u. for the $^{23}Na^{87}Rb$ polar molecule[5]. The dipolar length scale D for polar molecules ($D \approx 182554$ a.u. for $^{23}Na^{87}Rb$) is much larger than the van der Waals length scale $R_6 = (2\mu C_6/\hbar^2)^{1/4}$ ($\mu = 100167$ a.u.; $R_6 \approx 740$ a.u. for $^{23}Na^{87}Rb$) [5] and the Lennard-Jones potential is effectively used as the short-range repulsion potential for the dipole-dipole interaction potential. Increasing the C_{12} at the fixed C_6 leads to an increase of the short-range part of the $U(\rho, \phi)$. So we vary C_{12} to reproduce the change of ρ_{SR}.

[5] Karman, T. *et al.* English. *Physical Review A* **98**, 062502 (2018).

2D dipolar scattering

The long-range interaction potential of the two arbitrarily oriented dipoles $V_{dd}(\rho,\phi)$ in a plane reads:

$$V_{dd}\left(\rho,\phi;\alpha,\beta,\gamma\right)=\frac{d_1 d_2}{\rho^3}[\sin(\alpha)\sin(\gamma)\cos(\beta)+ \\ +\cos(\alpha)\cos(\gamma)-3\sin(\alpha)\sin(\gamma)\cos(\phi)\cos(\phi-\beta)].$$

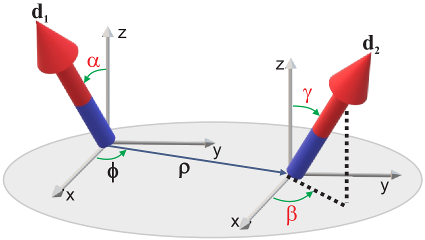


Fig.2 The scheme of mutual orientation of two arbitrarily oriented dipoles $\boldsymbol{d}_1$ and $\boldsymbol{d}_2$, moving in the XY plane.

2D dipolar scattering

In order to compare the results of two types of potential with each other, we need to relate the SRI radius ρ_{SR} with the Lennard-Jones C_6, C_{12} parameters. We define ρ_{SR} for the Lennard-Jones potential as $\rho_{SR} = \min(\rho_0(\phi))$, where $\rho_0(\phi)$ is the positions of the zeros of the potential $U(\rho, \phi)$. From the physical point of view, $\min(\rho_0(\phi))$ — the minimal distance, that molecules could reach at low energies of collision. For the considered polar molecules the term $-C_6/\rho^6$ is small compared to V_{dd}. Thus, ρ_{SR} is found under the condition $C_{12}/\rho^{12} + V_{dd}(\rho, \beta/2) = 0$, from which the next relation follows:

$$\rho_{SR} = \left[\frac{C_{12}(E_D D^3)^{-1}}{\sin(\alpha)\sin(\gamma)\frac{3+\cos(\beta)}{2} - \cos(\alpha)\cos(\gamma)} \right]^{\frac{1}{9}} . \tag{9}$$

Numerical algorithm

To tackle the problem (1)–(2), along with interaction potential (7) we apply the numerical scheme, that we applied to the quantum anisotropic scattering in a plane[6], based on the variation of the discrete-variable representation method, proposed in V.S.Melezhik paper[7] for a solution of the multichannel scattering problem.

The following wave function expansion is applied:

$$\Psi(\rho,\phi) \approx \frac{1}{\sqrt{\rho}} \sum_{m=-M}^{M} \sum_{j=0}^{2M} \xi_m(\phi)\xi_{mj}^{-1}\psi_j(\rho), \tag{10}$$

where $\xi_{mj}^{-1} = \frac{2\pi}{2M+1}\xi_{jm}^{*} = \frac{\sqrt{2\pi}}{2M+1}e^{-im(\phi_j-\pi)}$ — is the inverse matrix to the square matrix $(2M+1)\times(2M+1)$ $\xi_{jm} = \xi_m(\phi_j)$, that is defined on the uniform angular grid $\phi_j = \frac{2\pi j}{2M+1}$(where $j = 0, 1, ..., 2M$). In the angular grid's nodes ϕ_j: $\Psi(\rho,\phi_j) \approx \psi_j(\rho)/\sqrt{\rho}$. $\xi_m(\phi) = \frac{(-1)^m}{\sqrt{2\pi}}e^{im\phi}$ are the eigenfunctions of the operator $h^{(0)}(\phi) = \frac{\partial^2}{\partial\phi^2}$ and serve as a basis of functions for the wave function expansion over the angular variable.

[6] Koval, E. A. *et al.* English. *Physical Review A* **89,** 052710 (2014).

[7] Melezhik, V. S. English. *Journal of Computational Physics* **92,** 67–81 (1991).

Numerical algorithm

In representation (10), the 2D Schrödinger equation transforms in the system of $(2M+1)$ coupled second-order differential equations:

$$\frac{d^2\psi_j(\rho)}{d\rho^2} + \frac{2\mu}{\hbar^2}\left(E - U(\rho,\phi_j) + \frac{\hbar^2}{8\mu\rho^2}\right)\psi_j(\rho) + \\ -\frac{1}{\rho^2}\sum_{j'}\sum_{j''=-M}^{M} j''^2 \xi_{jj''}\xi^{-1}_{j''j'}\psi_{j'}(\rho) = 0. \qquad (11)$$

The seven-point finite difference approximation of six-order accuracy is used for the derivatives discretization. An obtained on each iteration matrix problem is tackled with the matrix modification of the sweep algorithm for the band matrix.

Critical (magic) angle for scattering of arbitrarily oriented dipoles

Domains of the attractive dipolar interaction arise around the points ϕ', that are defined by the expression: $\left.\frac{\partial V_{dd}(\rho,\phi)}{\partial\phi}\right|_{\phi'} = 0$. The *critical tilt angle* $\alpha_c(\beta,\gamma)$ is defined as the angle α, above which values of V_{dd} potential become negative in the points $\phi = \phi'$: $V_{dd}(\rho,\phi) < 0$. Thus, the condition: $V_{dd}(\rho,\phi') = 0$, determines the dependence of the critical tilt angle $\alpha = \alpha_c(\beta,\gamma)$ of the dipole d_1 on the rotation angle β and the tilt angle γ of the dipole d_2:

$$\alpha_c(\beta,\gamma) = \arctan\left(\frac{2\cot(\gamma)}{3+\cos(\beta)}\right). \tag{12}$$

The critical tilt angle $\alpha_c(\beta,\gamma)$ increases as $\beta \to 180^\circ$ (e.g. at $\gamma = 45^\circ$ the angle α_c increases from 26.56° to 45°). It should be noted, that at $\beta = 180^\circ$ the critical tilt angle can be found from a plain ratio $\alpha_c(\beta,\gamma) = 90^\circ - \gamma$, which is indicated in Fig. 3 by the solid red line.
When one considers the aligned dipoles case $\gamma = \alpha$ and $\beta = 0^\circ$, the expression (12) reproduces the known value of the critical (magic) angle $\alpha_c(\beta,\gamma) = \arctan\frac{1}{\sqrt{2}} \approx 35.3^\circ$, as previously mentioned[8].

[8] Ticknor, C. English. *Physical Review A* **84,** 032702 (2011), Giovanazzi, S. *et al.* English. *Physical review letters* **89,** 130401 (2002), Macia, A. *et al.* English. *Physical Review A* **84,** 033625 (2011).

Critical (magic) angle for scattering of arbitrarily oriented dipoles

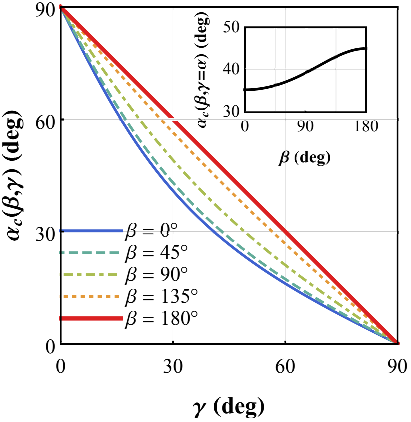


Fig.3 The dependence of the critical tilt angle $\alpha_c(\beta,\gamma)$ of the dipole d_1 on the rotation angle β and on the tilt angle γ of the dipole d_2. The inset presents the critical tilt angle $\alpha_c(\beta,\gamma)$ as a function of the rotation angle β for the case of the dipoles with equal tilt angles ($\gamma = \alpha$).

Angular distributions of differential cross section

• We revealed the strong dependence of the angular distributions of the 2D dipolar scattering differential cross section $d\sigma/d\Omega$ on the value of SRI radius ρ_{SR}.

• The differential cross section angular distributions for bosons exhibit circular shape in the resonant ρ_{SR} points both for $\alpha = 45^\circ$ and $\alpha = 90^\circ$, indicating $s-$wave dominance in the resonance emergence. At dipole tilt angles, which are larger than a critical angle, the $d\sigma/d\Omega$ angular distribution has disturbed resonant-like form at the points of $\sigma(\rho_{SR})$ minimum.

• Whereas at the tilt angle $\alpha = 90^\circ$ angular distributions of $d\sigma/d\Omega$ are strongly anisotropic at the points of a minimum of total cross section dependence $\sigma_B(\rho_{SR})$, indicating that the $s-$wave contribution is suppressed and the scattering is governed by higher partial waves.

• So, in contrast to the central potentials, the 2D low-energy dipolar scattering of bosons is strongly anisotropic and its properties are highly sensitive to the SRI radius as well as dipoles mutual orientation.

Angular distributions of differential cross section: bosons

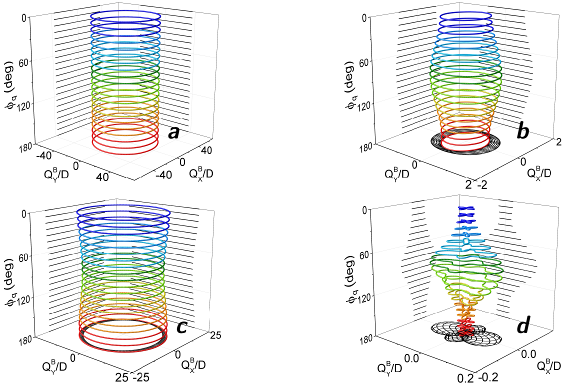


Fig.9 The dependencies of the differential cross sections $d\sigma/d\Omega$ on the scattering angle ϕ at the different values of the incident angle ϕ_q, which is changing along the Z-axis, for the resonant (a, c) and non-resonant (b, d) dipolar scattering of **bosons**. Here $Q_X^B = d\sigma_B/d\Omega\cos(\phi)$, $Q_Y^B = d\sigma_B/d\Omega\sin(\phi)$. The curves are presented for the tilt angles $\alpha = 45^\circ$ (a, b, e, f) and 90° (c, d, g, h) of two aligned $(\beta = 0^\circ; \gamma = \alpha)$ dipoles.

Angular distributions of differential cross section: fermions

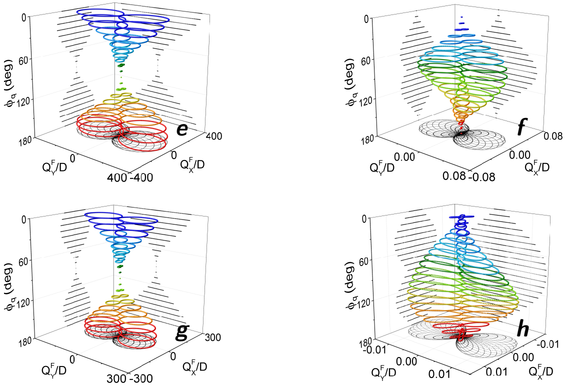


Fig.10 The dependencies of the differential cross sections $d\sigma/d\Omega$ on the scattering angle ϕ at the different values of the incident angle ϕ_q, which is changing along the Z-axis, for resonant (e, g) and non-resonant (f, h) dipolar scattering of **fermions**. Here $Q_X^F = d\sigma_F/d\Omega \cos(\phi)$, $Q_Y^F = d\sigma_F/d\Omega \sin(\phi)$. The curves are presented for the tilt angles $\alpha = 45^\circ$ (a, b, e, f) and 90° (c, d, g, h) of two aligned $(\beta = 0^\circ; \gamma = \alpha)$ dipoles.

SRI-induced resonances in low-energy 2D scattering of bosonic dipoles

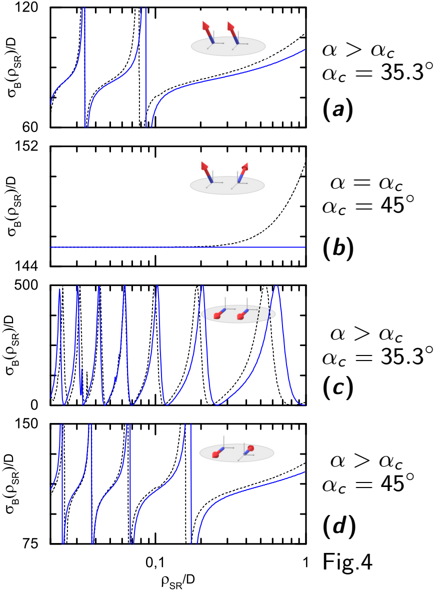


Fig.4

- The distinct narrow resonances in the dependence of the calculated total cross section $\sigma_B(\rho_{SR})$ for bosonic dipoles occur for the scattering of the two *aligned* dipoles ($\beta = 0°$; $\gamma = \alpha$) at tilt angles $\alpha = 45°$.

- The number of resonances in the cross section dependence on the ρ_{SR} is quadrupled with increasing tilt angle α from 45° up to 90°.

- The cross section does not depend on the SRI potential and there are no dipolar scattering resonances at $\alpha \leq \alpha_c(\beta, \gamma)$ and $\rho_{SR}/D \ll 1$. Thus, the rotation of the dipole moment vector d_2 around the Z axis by $\beta \to 180°$ causes the narrowing of the domains, where the dipolar potential is attractive, and the number of the resonances decreases until they disappear at $\beta \to 180°$.

- The resonances emerge also in the case of oppositely oriented dipoles ($\beta = 180°$) lying in the scattering plane at $\alpha \to 90°$.

SRI-induced resonances in low-energy 2D scattering of fermionic dipoles

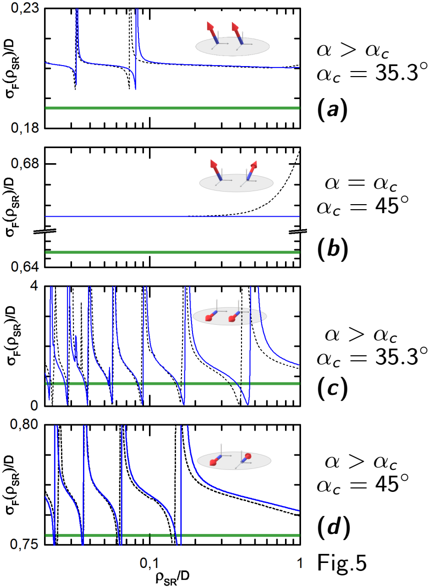


Fig.5

- The fermion scattering is significantly different from the boson scattering at low energies.
- For the case of fermion collisions, the amplitudes of the resonances are two orders of magnitude smaller, than those for bosons, in the case of low energy of the collision.
- The Lennard-Jones potential models short-range repulsion more physically, in the sense of introducing correlations between the different partial waves short-range phases, which shift narrow resonances in high partial waves, as seen in Figs. 4 and 5. But the resonances' structure remains qualitatively the same as when using the hard wall potential, because the resonances are due to the *s*-wave (*p*-wave) dominance in the scattering of bosons (fermions).
- The results for the hard wall potential are marked by a black dashed line, whereas for the Lennard-Jones potential by the blue solid line; Born approx. by a green line.

Energetic dependencies of 2D dipolar scattering cross section

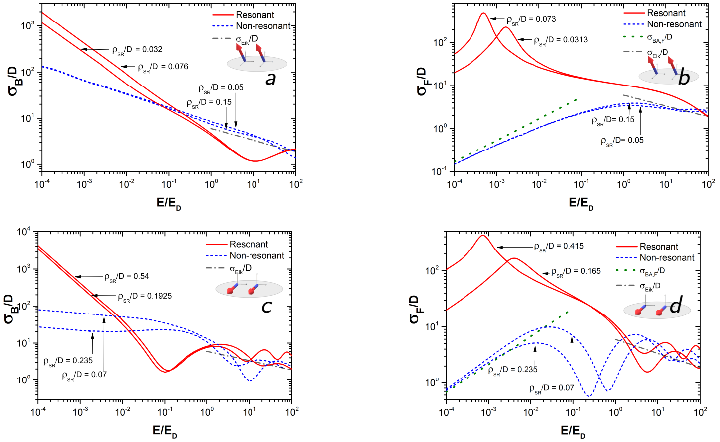


Fig.6 The energy dependencies of the total cross section of the dipolar scattering of identical bosons $\sigma_B(E)$ ($\alpha = 45°$(a), $90°$(c)) and identical fermions $\sigma_F(E)$ ($\alpha = 45°$(b), $90°$(d)) for aligned dipoles configuration $\beta = 0°$ and $\gamma = \alpha$. The tilt angle exceeds the critical angle $\alpha > \alpha_c$ ($\alpha_c = 35.3°$) for such dipole mutual orientations. The curves corresponding to the resonance points are indicated by a red solid line, the non-resonant curves by a blue dashed line; the Born approximation by a green dotted line, the eikonal approximation by a gray dashed line.

Energetic dependencies of 2D dipolar scattering cross section

• The analysis of the dependencies shows that in a low-energy limit, the cross section of resonant cases is at least an order of magnitude greater than the values for non-resonant cases.

• The cross section of identical bosons scattering increases in the $E \to 0$ limit in both cases due to the s-wave, which is caused by the divergence in 2D space[9]. It should be noted, that in the vicinity of resonances the cross section is an order of magnitude greater than those at the absence of resonances.

• All resonant curves of the cross section $\sigma_F(E)$ for the dipolar scattering of fermions demonstrate a peak shape in the low-energy limit, in contrast to the non-resonant curves, that monotonically decrease. These peaks shift to the lower energies with the growing value of its maximums at an increase of ρ_{SR}. The resonances for fermions are narrower than for bosons, due to potential barriers for high partial waves, that suppress the partial cross section in the low-energy limit.

• The boson (fermion) dipoles 2D scattering cross section in the absence of resonances increases (decreases) in the low-energy limit in contrast to the 3D scattering, where the cross section in the absence of resonances has the form of a plateau in the low-energy limit for both bosons and fermions (Refs.[10,11]).

[9] Simon, B. English. *Annals of Physics* **97,** 279–288 (1976).

[10] Roudnev, V. & Cavagnero, M. English. *Journal of Physics B: Atomic, Molecular and Optical Physics* **42,** 044017 (2009).

[11] Bohn, J. *et al.* English. *New Journal of Physics* **11,** 055039 (2009).

Conclusions

• The impact of the short-range interaction on the resonances occurrence in the anisotropic dipolar scattering in a plane was numerically investigated *for different orientations of the dipoles* and for a wide range of collision energies.

• We revealed the strong dependence of the cross section on the radius of short-range interaction, which is modeled by a hard wall potential and by the more realistic Lennard-Jones potential. The results of the numerical calculations of the cross section agree within the low-energy and high-energy limits with the results obtained within the Born and eikonal approximations, respectively.

• It was found, that the $s-$wave ($p-$wave) dominates in the angular distributions of the differential cross section at resonance points in the 2D dipolar scattering of identical bosons (identical fermions), whereas the higher partial waves dominate at non-resonant points and the differential cross sections are highly anisotropic.

• We also defined the critical (magic) tilt angle of one of the dipoles, depending on the direction of the second dipole for arbitrarily oriented dipoles. It was found that resonances arise only when this angle is exceeded.

• In the absence of the resonances the energy dependencies of the boson (fermion) dipolar scattering cross section grows (is reduced) with energy decrease in 2D case, in contrast to the 3D case, where it has the form of a plateau for both bosons and fermions.

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Aspects of arbitrarily oriented dipoles scattering in a plane: Short-range interaction influence

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The impact of the short-range interaction on the resonances' occurrence in the anisotropic dipolar scattering in a plane is numerically investigated for the arbitrarily oriented dipoles and for a wide range of collision energies. We reveal the strong dependence of the cross section of the two-dimensional (2D) dipolar scattering on the radius of short-range interaction, which is modeled by a hard wall potential and by the more realistic Lennard-Jones potential, and on the mutual orientations of the dipoles. We define the critical (magic) tilt angle of one of the dipoles, depending on the direction of the second dipole for arbitrarily oriented dipoles. We find that resonances arise only when this angle is exceeded. In contrast to the three-dimensional (3D) case, the energy dependencies of the boson (fermion) 2D scattering cross section grow (are reduced) with an energy decrease in the absence of the resonances. We show that the mutual orientation of dipoles strongly impacts the form of the energy dependencies, which begin to oscillate with the tilt angle increase, unlike the 3D dipolar scattering. The angular distributions of the differential cross section in the 2D dipolar scattering of both bosons and fermions are highly anisotropic at nonresonant points. The results of the accurate numerical calculations of the cross section agree well with the results obtained within the Born and eikonal approximations.

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Thank you for your attention!