Anisotropic quantum scattering in plane

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We study the quantum scattering in two spatial dimensions (2D). Our computational scheme allows to quantitatively analyze the scattering parameters for the strong anisotropy of the interaction potential. High efficiency of the method is demonstrated for the 2D scattering on the cylindrical potential with the elliptical base and dipole-dipole collisions in the plane. We reproduce the result for the 2D scattering of polarized dipoles in binary collisions obtained recently by Ticknor [Phys. Rev. A 84, 032702 (2011)] and explore the 2D collisions of unpolarized dipoles.

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I. INTRODUCTION

In recent years, the problem of anisotropic quantum scattering in two spatial dimensions (2D) attracts increasing interest. It is stimulated by spectacular proposals for prospects to create exotic and highly correlated quantum systems with dipolar gases [1, 2]. Particularly, there were considered anisotropic superfluidity [3], 2D dipolar fermions [4], and few-body dipolar complexes [5]. The recent experimental production of ultracold polar molecules in confined geometry of optical traps [6, 7] has opened up ways to realize these phenomena. Noteworthy also is rather long history of research of 2D quantum systems with dipolar gases [1, 2]. Particularly, it permits analysis of the 2D quantum scattering on a long-range strongly anisotropic scatterer. Particularly, it permits the description of the 2D collisions of unpolarized dipoles. Our approach is based on the method suggested in [21] for the few-dimensional scattering which was successfully applied to the dipole-dipole scattering induced by an elliptically polarized laser field in the 3D free-space [15].

The key elements of the method are described in Section II. In Section III, we apply the method to the 2D scattering on the cylindrical potential with the elliptical base and the 2D dipole-dipole scattering of unpolarized dipoles. We reproduce the threshold formula [22, 23] for the scattering amplitude on the cylinder potential with the circular base and the results of [16, 17] for the 2D scattering of polarized dipoles. High efficiency of the method has been found in all problems being considered. The last Section contains the concluding remarks. Some important details of the computational scheme and illustration of the convergence are given in Appendices.

II. 2D SCATTERING PROBLEM IN ANGULAR GRID REPRESENTATION

The quantum scattering on the anisotropic potential $U(\rho, \phi)$ in the plane is described by the 2D Schrödinger equation in polar coordinates $(\rho, \phi)$

$$H(\rho, \phi) \Psi (\rho, \phi) = E \Psi (\rho, \phi)$$

with the scattering boundary conditions

$$\Psi (\rho, \phi) \rightarrow e^{iq\rho} + f (q, \phi, \phi_q) \frac{e^{iq\rho}}{\sqrt{-iq\rho}}$$

in the asymptotic region $\rho \rightarrow \infty$ and the Hamiltonian of the system

$$H(\rho, \phi) = -\frac{\hbar^2}{2\mu} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} h^{(0)}(\phi) \right) + U(\rho, \phi).$$
The unknown wave function $\Psi(\rho, \phi)$ and the scattering amplitude $f(q, \phi, \phi_q)$ are searched for the fixed momentum $q$ defined by the colliding energy $E \equiv \sqrt{2\mu E/h}$ and the direction $q/q$ of the incident wave (defined by the angle $\phi_q$) and for the scattering angle $\phi$. Here $\mu$ is the reduced mass of the system. In the polar coordinates, the angular part of the kinetic energy operator in $H(\rho, \phi)$ has a simple form $h^{(0)}(\phi) = \frac{\rho^2}{2\mu}$. The interaction potential $U(\rho, \phi)$ can be anisotropic in the general case, i.e. to be strongly dependent on $\phi$. It is clear that varying the direction of the incident wave $q/q$ can be replaced by the rotation $U(\rho, \phi) \to U(\rho, \phi + \phi_q)$ of the interaction potential by the angle $\phi_q$, for the fixed direction of the incident wave, which we choose to be coincident with the $x$-axis. Thus, in the case of anisotropic potential $U(\rho, \phi)$ the task is to solve the problem in with the interaction potential $U(\rho, \phi + \phi_q)$ for all possible $\phi_q$ and fixed $E$ with the scattering boundary conditions

$$
\Psi(\rho, \phi) = \exp\{iq\rho \cos(\phi)\} + f(q, \phi, \phi_q) \frac{e^{iq\rho}}{\sqrt{\rho}} \tag{3}
$$

If the scattering amplitude $f(q, \phi, \phi_q)$ is found, one can calculate the differential scattering cross section

$$
d\sigma(q, \phi, \phi_q)/dΩ = |f(q, \phi, \phi_q)|^2 \tag{4}
$$

where $d\Omega = d\phi d\phi_q$, as well as the total cross section

$$
\sigma(q) = \frac{1}{2\pi} \int_0^{2\pi} \int_0^{2\pi} d\sigma d\phi
$$

by averaging over all possible orientations $\phi_q$ of the scatterer and integration over the scattering angle $\phi$.

To integrate the problem (1), (2), we use the method suggested in [21] to solving a few-dimensional scattering problem and applied in [15] for the dipole-dipole scattering in the 3D free-space. Following the ideas of these works we choose the eigenfunctions

$$
\xi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im(\phi - \pi)} = \frac{(-1)^m}{\sqrt{2\pi}} e^{im\phi} \tag{6}
$$

of the operator $h^{(0)}(\phi)$ as a Fourier basis for the angular grid representation of the searched wave-function $\Psi(\rho, \phi)$. We introduce the uniform grid $\phi_j = \frac{2\pi j}{2M+1}$ (where $j = 0, 1, ..., 2M$) over the $\phi$ and $\phi_q$-variables and search the wave function as expansion

$$
\Psi(\rho, \phi) = \frac{1}{\sqrt{\rho}} \sum_{j=0}^{2M} \sum_{m=-M}^{M} \xi_m(\phi) \tilde{\xi}_{m,j}^{-1} \psi_j(\rho) = \frac{2\pi}{\sqrt{\rho}} \left( \frac{1}{2M+1} \right) \sum_{j=0}^{2M} \sum_{m=-M}^{M} e^{im(\phi - \phi_j)} \psi_j(\rho) \tag{7}
$$

where $\xi_m^{-1} = \frac{2\pi}{2M+1} \xi_{m,j} = \frac{2\pi}{2M+1} \left( e^{-im\phi_j} \right)$ is the inverse matrix to the $(2M+1) \times (2M+1)$ square matrix $\xi_{m,j}$ defined on the angular grid $\phi_j$.

In the representation (7) the unknown coefficients $\psi_j(\rho)$ are defined by the values of the searched wave function on the angular grid $\psi_j(\rho) = \sqrt{\rho} \Psi(\rho, \phi_j)$, any local interaction is diagonal

$$
U(\rho, \phi) \Psi(\rho, \phi) \big|_{\phi = \phi_j} = \frac{2\pi}{(2M+1)\sqrt{\rho}} U(\rho, \phi_j) \sum_{j'=0}^{2M} \sum_{m=-M}^{M} e^{im(\phi_j - \phi_{j'})} \psi_{j'}(\rho) \tag{8}
$$

and the angular part $h^{(0)}(\phi)$ of the kinetic energy operator has a simple form

$$
h^{(0)}(\phi) \Psi(\rho, \phi) \big|_{\phi = \phi_j} = \frac{2\pi}{(2M+1)\sqrt{\rho}} \sum_{j'=0}^{2M} \sum_{m=-M}^{M} e^{im(\phi_j - \phi_{j'})} \psi_{j'}(\rho) \tag{9}
$$

Note that the presence in the interaction potential of the "nonlocal" angular part (i.e. the integration or differentiation over angular variable) leads to destroying the diagonal structure in (8).

Thus, the 2D Schrödinger equation (11) is reduced in the angular grid representation (7) to the system of $2M + 1$ coupled ordinary differential equations of the second order:

$$
\frac{d^2\psi_j(\rho)}{d\rho^2} + \frac{2\mu}{h^2} \left( E - U(\rho, \phi_j) + \frac{h^2}{8\mu\rho^2} \right) \psi_j(\rho) + \frac{1}{\rho^2} \sum_{j'} h^{(0)}_{jj'} \psi_{j'}(\rho) = 0. \tag{10}
$$

Since the wave function $\Psi(\rho, \phi_j) = \psi_j(\rho)$ must be finite at the origin (where $\psi_j(0) \to const.$), the “left-side” boundary condition for the functions $\psi_j(\rho)$ reads as

$$
\psi_j(\rho \to 0) \to const. \sqrt{\rho} \quad (j = 0, 1, ..., 2M). \tag{11}
$$

In the asymptotic region $\rho \to \infty$ the scattering boundary condition (11) accepts the form

$$
\sqrt{\rho}(2M+1) \sum_{j=0}^{2M} \sum_{m=-M}^{M} e^{im(\phi - \phi_j)} \psi_j(\rho) = \exp\{i\rho \cos(\phi)\} + f(q, \phi, \phi_q) \frac{e^{iq\rho}}{\sqrt{\rho}}. \tag{12}
$$

1. Hereafter we use the definition of the scattering amplitude introduced in [24].

2. To calculate the inverse matrix $\xi_m^{-1}$, we use the completeness relation for the Fourier basis

$$
\sum_{m=-\infty}^{\infty} \xi_m(\phi_j) \xi^*_m(\phi_j) = \delta(\phi_j - \phi_{j'}), \quad \text{which in our grid representation reads}
\sum_{m=-M}^{M} \xi_m(\phi_j) \xi^*_m(\phi_j) = \frac{2M+1}{2\pi} \delta_{jj'}.
$$
By using the Fourier expansion for the plane wave \( \exp\{iq\rho \cos(\phi)\} \) and the scattering amplitude \( f(q, \phi, \phi_0) \) we have

\[
\exp\{iq\rho \cos(\phi)\} = \sum_{m'=-M}^{M} i^{m'} J_{m'}(q\rho) e^{im'\phi} \tag{13}
\]

\[
f(q, \phi, \phi_0) = \frac{1}{\sqrt{2\pi}} \sum_{m'=-M}^{M} f_{m'}(\phi_0) e^{im'\phi} \tag{14}
\]

we eliminate the angular dependence from the asymptotic equation (12) and represent the “right-side” boundary condition for the functions \( \psi_j(\rho \to \infty) \) in the form

\[
\frac{2\pi}{(2M+1)\sqrt{\rho}} \sum_{j=0}^{2M} e^{-i\rho\phi_j}(\rho) = i^{m} J_{m}(q\rho)\sqrt{2\pi} + \frac{f_{m}(\phi_0)}{\sqrt{q}} e^{iq\rho}. \tag{15}
\]

To solve the boundary-value problem [10], [11] and [15], we introduce the grid over the \( \rho \)-variable \( \{\rho_n\} \) \( n = 0, 1, \ldots, N \) and reduce the system of differential equations [10] by using the finite-difference approximation of the sixth order to the system of \((N+1) \times (2M+1)\) algebraic equations

\[
\hat{A}\psi = 0 \tag{16}
\]

with the band-structure of the matrix \( \hat{A} \) with the width \((2M+1) \times 7\) of the band. By using the asymptotic equations [15] in the last two points \( \rho_{N-1} \) and \( \rho_N \) one can eliminate the unknown vector \( f_{m}(\phi_0) \) from equation (15) and rewrite the “right-side” boundary condition in the form

\[
\sum_{j'} \{ A_{jj',NN-1}\psi_{j'}(\rho_{N-1}) + A_{jj',NN}\psi_{j'}(\rho_N) \} = F_{j,N}(q, \rho_{N-1}, \rho_N). \tag{17}
\]

Analogously, one can eliminate unknown constant from expression [11] by considering asymptotic equations [11] at the first points \( \rho_0, \rho_1 \) and \( \rho_1 \). The acquired “left-side” boundary condition reads

\[
\sum_{j'} \{ A_{jj',11}\psi_{j'}(\rho_1) + A_{jj',12}\psi_{j'}(\rho_2) \} = F_{j,1}(q, \rho_1, \rho_2). \tag{18}
\]

Thus, the scattering problem is reduced to the boundary value problem (16) [15]

\[
\hat{A}\psi = F, \tag{19}
\]

which can be efficiently solved with standard computational techniques such as the sweeping method [26] or the LU-decomposition [27]. The detailed structure of the matrix of the coefficients \( A_{jj',nn'} \) is discussed in Appendix A. After the solving of Eq. (19) and finding the wave function \( \psi_j(\rho) \) the scattering amplitude \( f(q, \phi, \phi_0) \) is constructed according to Eqs. (15) and (14).

III. RESULTS AND DISCUSSIONS

A. Scattering on anisotropic scatterer

First, we have analyzed the 2D scattering on the cylindrical potential barrier with the elliptical base

\[
U(\rho, \phi) = \begin{cases} U_0, & \rho \leq a(\phi) \\ 0, & \rho > a(\phi) \end{cases}. \tag{20}
\]

The case of the circular base \( a(\phi) = a_0 \) was considered in [22] [24], where analytic formula for the scattering amplitude

\[
f(q) \to \sqrt{\frac{\pi}{2q}} \ln \left( \frac{1}{2q} \right) + i\frac{\pi}{2} \tag{21}
\]

was obtained in the zero-energy limit \( q \to 0 \). Here \( \gamma = \exp(C) \) and \( C = 0.577 \ldots \) is the Euler constant. We have analyzed the scattering on the potential barrier with circular base \( a(\phi) = a_0 \) for arbitrary momentum \( q \). The results of calculation presented in Figs. 1 and 2 confirm the convergence of the scattering amplitude \( f(q, \phi, \phi_0) \) to the analytical value (21) at \( q \to 0 \). Hereafter all the calculations were performed in the units \( h = \mu = 1 \).

In the limiting case of the infinitely high potential barrier [20] with the circular base \( a(\phi) = a_0 \) the asymptotic formula (21) becomes exact for arbitrary \( q \). This is confirmed by investigation presented in Table 1 which illustrates the convergence of the numerical values \( f(q, \phi, \phi_0) \) with increasing \( (U_0 \to \infty) \) and narrowing \( (a_0 \to 0) \) of the potential barrier to the analytic result (21). In the limit case \( U_0 \to \infty \) and \( a_0 \to 0 \) we obtain \( a_{2D} \to a_0 \) for the scattering length \( a_{2D} \) extracted from the calculated amplitude \( f(q) \) by the formula (21), what is in agreement to the estimate given in [22]. The range of applicability of Eq. (21) was investigated recently in [25].

Then, we have applied our scheme for calculation of the scattering cross section \( d\sigma = \sigma(q, \phi, \phi_0) / d\Omega \) for the isotropic \( a(\phi) = a_0 \) and anisotropic \( a(\phi) = \pi/2 \) scattering. In Fig. 3 the differential cross section, calculated for the circular base \( a(\phi) = a_0 \) of the scatter [20], is given as a function of \( q \) and \( \phi \). The dependence of the cross

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3 Here \( J_{m}(q\rho) \) are the first kind Bessel functions of integer order. Their asymptotic behavior [29]:

\[
J_{m}(z) \xrightarrow{|z| \to \infty} \sqrt{\frac{2}{\pi z}} \cos \left( z - \frac{m\pi}{2} \right) e^{\pm i\pi/4}, \quad (|\arg(z)| < \pi)
\]
can be written in the polar coordinates projections onto the collision axis. The expression (22)

where \( \alpha \), \( \beta \), and \( \gamma \) denote the tilt of dipoles to the scattering plane \( XY \), and the angle \( \phi \) defines the mutual orientation of the dipole polarization planes \( Zd_1 \) and \( Zd_2 \) in Fig. 3.

If we consider the scenario when the polarization of colliding molecules is orthogonal to the plane of motion \( (\alpha = \beta = \gamma = 0) \), interaction is fully isotropic and repulsive

\[
U(\rho) = \frac{d_1 d_2}{\rho^3}, \tag{24}
\]

section on \( \phi \) disappears with decreasing momentum \( q \) and the dependence on \( \phi \) is absent for any \( q \) due to the spherical symmetry of the potential (20) if \( a(\phi) = a_0 \). Further, the analysis was extended to more general case of elliptical base of the potential barrier (20). In Figs. 4 and 5 the calculated differential cross sections on the anisotropic scatter (20) are presented for the cases of weak \((a(\phi = \pi/2)/a(\phi = 0) = 1.1)\) and strong anisotropy \((a(\phi = \pi/2)/a(\phi = 0) = 2)\). Here, we observe more sharp dependence on \( \phi \) and \( q \) in the cross section with increasing anisotropy of the scatterer. The anisotropy in the scattering cross sections appears with increasing \( q \) earlier for the anisotropic potential barrier than for the barrier with circular base.

B. Dipole-dipole scattering in plane

Here we analyze the 2D quantum scattering on the long-range anisotropic scatterer defined by the dipole-dipole interaction. This problem simulates the collisions of polar molecules in pancake optical traps. The interaction potential between two arbitrarily oriented dipoles reads

\[
U(\rho, d_1, d_2) = \frac{1}{\rho^3} \left( (d_1 d_2) - 3 \frac{(d_1 \rho)(d_2 \rho)}{\rho^2} \right), \tag{22}
\]

where \( d_i \), \( i = 1, 2 \) – dipole moments and \( (d_i \rho)/\rho \) – their projections onto the collision axis. The expression (22) can be written in the polar coordinates

\[
U(\rho, \phi; \alpha, \beta, \gamma) = \frac{d_1 d_2}{\rho^3} \left[ \sin(\alpha) \sin(\gamma) \cos(\beta) + \cos(\alpha) \cos(\gamma) - 3 \sin(\alpha) \sin(\gamma) \cos(\phi) \cos(\phi - \beta) \right], \tag{23}
\]

where the angles \( \alpha \) and \( \gamma \) define the tilt of dipoles to the scattering plane \( XY \) and the angle \( \beta \) denotes the mutual orientation of the dipole polarization planes \( Zd_1 \) and \( Zd_2 \) in Fig. 3.

If we consider the scenario when the polarization of colliding molecules is orthogonal to the plane of motion \( (\alpha = \beta = \gamma = 0) \), interaction is fully isotropic and repulsive

\[
U(\rho) = \frac{d_1 d_2}{\rho^3}, \tag{24}
\]

This case was intensively studied in the previous works [16, 18].

For dipoles oriented in the plane \( (\alpha = \gamma = \frac{\pi}{2}) \), anisotropy

| \( U_0 \) | \( f(q, 0, 0) \) | \( q = 0.125 \) | \( f(q, \pi, 0) \) | \( f(q, 0, 0) \) | \( q = 1 \) | \( f(q, \pi, 0) \) |
|------|---------|----------------|---------|---------|----------------|---------|
| 10^4 | -0.42692 + i0.08772 | -0.42693 + i0.08772 | -0.19832 + i0.05304 | -0.19837 + i0.05304 |
| 10^5 | -0.47906 + i0.11141 | -0.47961 + i0.11141 | -0.22999 + i0.07362 | -0.23016 + i0.07362 |
| 10^6 | -0.49055 + i0.11846 | -0.49040 + i0.11846 | -0.23995 + i0.07992 | -0.23920 + i0.07998 |
| 10^7 | -0.49408 + i0.11846 | -0.49409 + i0.11849 | -0.23999 + i0.07992 | -0.23925 + i0.07992 |

Eq. (21)
arises and the interaction potential reads
\[ U(\rho, \phi, \beta) = \frac{d_1 d_2}{\rho^3} \left[ \cos(\beta) - 3 \cos(\phi) \cos(\phi - \beta) \right]. \tag{25} \]

A particular case of parallel dipoles with the polarization axis tilted to the plane of motion (\(\alpha = \gamma;\ \beta = 0\)) with short-range interaction modeled by a hard wall at the origin
\[ V_{HW}(\rho) = \begin{cases} \infty, & \rho \leq \rho_{HW} \\ 0, & \rho > \rho_{HW} \end{cases} \tag{26} \]
with the width \(\rho_{HW}/D = 0.1\)

\[ U(\rho, \phi, \alpha) = V_{HW}(\rho) + \frac{\rho^2}{\rho^3} [1 - 3 \sin^2(\alpha) \cos^2(\phi)] \tag{27} \]
was considered in paper [17]. We have investigated this case with our approach and have obtained good agreement with the results of paper [17]. This is illustrated by Fig. 7, where the calculated total cross section $\sigma(q, \alpha)$ [2] is given in the units of $\sigma_{SC}$. Here $D$ is the dipolar length $D = \mu a^2/\hbar^2 (d = d_1 = d_2)$ and $\sigma_{SC} = \frac{1}{2} \sqrt{\pi D q}$ is the value of the total scattering cross section in the eikonal approximation that is valid in the high-energy regime, $D q \gg 1$ [17]. All calculations in this section were performed for the following parameters: $M = 40$, $N = 1.2 \times 10^5$ and $\rho_N = 60$; the number of grid points on $\phi_q$ was $2Mq + 1 = 101$.

![Graph](image)

**FIG. 7.** (Color online) A comparison of the total cross section (in the units of $\sigma_{SC}$) with the result of C. Ticknor [17] calculated for potential [27] at $D = 1$, $D q = 10$.

Then, we have analyzed how the found “resonant” structure for the polarized dipoles (see Fig. 7) in the calculated dependence of the scattering cross section on the dipole tilt angle $\alpha = \gamma$ varies with destroying the polarization. Depolarization was simulated by rotating the angle $\beta$ between the dipole polarization planes $Zd_1$ and $Zd_2$ (see Fig. 5). We found progressive narrowing of the “resonance” area with a simultaneous decrease of the amplitudes of the “resonance” oscillations with increasing angle $\beta$ from 0 to $\pi$ (see Fig. 5). When approaching the point $\pi$ the “resonant” structure disappears, the cross section becomes smooth relative to $\alpha$ and reaches its maximum value. This effect is due to the fact that when approaching the angle $\beta = \pi$ repulsive feature of the dipole-dipole interaction becomes dominant (see Fig. 5). With decreasing $\beta$ from $\pi$ to 0 the attractive part $U(\rho, \phi) < 0$ appears for some $\rho$ and $\phi$. It leads to appearing the “resonant” part in the scattering cross section. Note, that the presented cross sections were obtained for distinguishable particles. The effect of symmetrization/antisymmetrization $f_{s,a}(\phi) = (f(\phi) \pm f(\phi - \pi))/\sqrt{2}$ (i.e. transition to identical particles) is shown in Fig. 10 for $\alpha = 0.2\pi$ and $\beta$ varying from 0 to $2\pi$, where we observe the strong dependence of the total cross sections on the angle $\beta$ with the maximal enhancement at $\beta = \pi$.

**IV. CONCLUSION**

We have developed a computational scheme for quantitative analysis of the 2D quantum scattering on the long-range anisotropic potentials. High efficiency of the method was demonstrated in the analysis of scattering on the cylindrical potential with the elliptical base and dipole-dipole collisions in the plane. In the last case we found the strong dependence of the scattering cross section on the mutual orientation of dipoles.

The method can be applicable for analyzing the collisional dynamics of the polarized as well as unpolarized polar molecules in the plane. A natural application is the quantitative analysis of the confinement-induced resonances (CIR) in one-dimensional traps. Particularly, this analysis can resolve the puzzle with the position of...
FIG. 9. (Color online) The dependence of the dipole-dipole potential $U(x, y, z, \rho, d_1, d_2)$ (23) in the units of $E_D = \hbar^2/\mu d^4$ ($d = d_1 = d_2$) on the tilt angle $\alpha$ for two extreme mutual orientations $\beta = 0$ and $\pi$ of the dipole polarization planes $Z_{d_1}$ and $Z_{d_2}$.

FIG. 10. (Color online) The total cross section $\sigma$ (solid line), bosonic cross section $\sigma_g$ (dashed line) and fermionic cross section $\sigma_u$ (dash-dot line) calculated for potential (23) as a function of the angle $\beta$ for the fixed $\alpha = 0.2\pi$ at $D = 1, Dq = 10$ (in the units of $\sigma_{SC}$).

FIG. 11. (Color online) The total cross sections $\sigma$ in the units of $\sigma_{SC}$ as a function of the dipole tilt angles $\alpha$ and $\gamma$ calculated for potential (23) at $D = 1, Dq = 10$. The rotational angle $\beta$ is equal to $\pi/2$.

the 2D CIR measured recently [29], which is under intensive discussions.
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Appendix A: Finite-difference approximation for boundary-value problem (10), (11) and (15)

The boundary-value problem [10], [11] and [15], obtained in Section II in the angular grid representation [7], reads in a matrix form as:

\[
\begin{align*}
\frac{d^2}{d\rho^2} \psi_{n}(\rho) + \left[ \frac{i}{2} \hat{I} + \frac{2\mu}{h^2} \right] \psi_{n}(\rho) + \frac{\hat{h}^{(0)}}{2} \psi_{n}(\rho) &= 0, \\
\hat{h}^{(0)} &= -\frac{2\pi}{(2M+1)^2} \sum_{m=-M}^{M} m^2 e^{im\phi_{1}} \psi_{j}(\rho) = im J_m(\rho) \sqrt{2\pi} + J_m(\rho) \psi_{j}(\rho) ,
\end{align*}
\]

(A1)

where \( h^{(0)} \) is given by (18) in the first two points \( n = 1, 2 \), and, analogously, the “left-side” boundary condition in the form (18) in the last three grid points \( n = N - 2, N - 1, N \) and, analogously, the “left-side” boundary condition in the form (18) in the last three grid points \( n = N - 2, N - 1, N \).

The block structure of the system (A4) provides several significant advantages. The block matrix can be stored in a packed form, which allows the use of optimal resource. The system (A4) can be efficiently solved by a fast implicit matrix algorithm based on the idea of the block sweep method [20].

Appendix B: Convergence of computational scheme

In the Table I, we illustrate the convergence of the calculated scattering amplitude \( f(q, \phi, \phi_{q}) \) over the number of angular grid points \( M + 1 \) for the scatterers with weak and essential anisotropy at \( a_0(\pi/2)/a_0(0) = 1.1 \) and 2 in the potential barrier [20]. For the case \( a_0(\pi/2)/a_0(0) = 1.1 \), the accuracy of four significant digits in the scattering amplitude on the angular grids with \( M = 5 \). For stronger anisotropy \( a_0(\pi/2)/a_0(0) = 2 \) the accuracy of two significant digits was reached at \( M = 30 \).

The number of radial grids \( N \) and the border of integration \( \rho_{N} \) were chosen to keep the accuracy of four significant digits in the calculated amplitudes.

(17) in the last three grid points \( n = N - 2, N - 1, N \) and, analogously, the “left-side” boundary condition in the form (18) in the first two points \( n = 1, 2 \), the detailed structure of the matrix \( \hat{A} \) is represented as

\[
\begin{align*}
\sum_{n'=n+1}^{n+3} \hat{A}_{nn'} \psi_{n'} &= F_{n}, \quad n = 1, 2 \\
\sum_{n'=n+3}^{n+6} \hat{A}_{nn'} \psi_{n'} &= 0, \quad n = 3, 4, ..., N - 3 \\
\sum_{n'=n+1}^{n+3} \hat{A}_{nn'} \psi_{n'} &= F_{n}, \quad n = N - 2, N - 1, N .
\end{align*}
\]

(A4)
TABLE II. The dependence of the scattering amplitude $f(q, \phi, \phi_q)$ on the number of angular grid points for the scatterer with elliptical base. Calculations were performed for $q = 1.5$ with the parameters: $U_0 = 10^3$, $N = 10^4$, and $\rho_N = 15$.

| $M$ | $f(q, 0, 0) a_0(\pi/2)/a_0(0) = 1.1$ | $f(q, \pi, 0)$ | $f(q, 0, 0) a_0(\pi/2)/a_0(0) = 2.0$ | $f(q, \pi, 0)$ |
|-----|----------------------------------|----------------|----------------------------------|----------------|
| 1   | 0.94212 - i0.36446               | -0.53027 + 11.24225 | -0.95099 - i0.52976                | 0.36649 + 11.04884 |
| 2   | 0.65276 – i0.30331              | -0.61946 + 11.30336 | -0.31229 + i1.24236                | -1.49373 + 10.79349 |
| 3   | 0.68693 – i0.30254              | -0.65902 + 11.29149 | 0.36649 + i1.04884                 | -0.90133 + 11.68129 |
| 4   | 0.68794 – i0.30507              | -0.65940 + 11.29164 | -0.50155 + i0.05523                | -0.87486 + 11.52425 |
| 5   | 0.68799 – i0.30506              | -0.65940 + 11.29164 | -0.50155 + i0.05523                | -0.87486 + 11.52425 |
| 10  | -0.61098 + i0.07836             | -0.89552 + 11.53816 | -0.89552 + 11.53816                | -0.89552 + 11.53816 |
| 20  | -0.61098 + i0.07836             | -0.89552 + 11.53816 | -0.89552 + 11.53816                | -0.89552 + 11.53816 |
| 30  | -0.61173 + i0.07971             | -0.89552 + 11.53816 | -0.89552 + 11.53816                | -0.89552 + 11.53816 |

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