A shadow of the repulsive Rutherford scattering in the fixed-target and the center-of-mass frame

Petar Žugec\textsuperscript{1} and Ivan Topić\textsuperscript{2}

\textsuperscript{1} Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia
\textsuperscript{2} Archdiocesan Classical Gymnasium, Zagreb, Croatia

E-mail: pzugec@phy.hr

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Abstract

The paper explores the shadow of the repulsive Rutherford scattering—the portion of space entirely shielded from admitting any particle trajectory. The geometric properties of the projectile shadow are analyzed in detail in the fixed-target frame as well as in the center-of-mass frame, where both the charged projectile and the charged target cast their own respective shadows. In both frames the shadow is found to take an extremely simple paraboloidal shape. In the fixed-target frame the target is precisely at the focus of this paraboloidal shape, while the focal points of the projectile and target shadows in the center-of-mass frame coincide. In the fixed-target frame the shadow takes on a universal form, independent of the underlying physical parameters, when expressed in properly scaled coordinates, thus revealing a natural length scale to the Rutherford scattering.

Keywords: Rutherford scattering, shadow, fixed-target frame, center-of-mass frame

Supplementary material for this article is available online

1. Introduction

Rutherford scattering—a scattering of electric charges due to the Coulomb interaction, whether it be attractive or repulsive—is one of the most famous concepts in physics. The series of historical experiments by Geiger and Marsden \cite{1–3}, demonstrating some unexpected properties in the scattering of \(\alpha\)-particles by thin metal foils, has led to the discovery of the atomic nucleus by Rutherford \cite{4} and the subsequent birth of nuclear physics. Today Rutherford scattering is a regular subject in all textbooks on classical mechanics and introductory nuclear physics, and
the basis of several experimental techniques such as Rutherford backscattering spectrometry [5] and elastic recoil detection analysis [6].

Throughout most educational sources, undergraduate or otherwise, the fact that repulsive Rutherford scattering casts a shadow seems to be little known—as if it were entirely forgotten, neglected or ignored. At best, it is only tacitly recognized, whenever a plot such as the one from figure 1 is presented, showing several stacked trajectories for a charged projectile moving through a Coulomb field of a stationary target. Clearly, there is an isolated portion of space admitting no trajectories due to their deflection in a Coulomb field, which can be considered as a proverbial shadow of the repulsive scattering. The attractive scattering of opposing charges shows no such feature, as the trajectories of a projectile of any initial energy may be continuously brought closer to a target, until they bend entirely around it, sweeping out the entire geometric space.

The reality of this shadow is not only of great educational value, as a motivation for some beautiful calculations and insights, but also plays an important role in low-energy ion scattering spectroscopy [7, 8]. It may already be intuited from figure 1 that the shape of the shadow in the fixed-target frame might be parabolic, that is paraboloidal when considered in a three-dimensional space. Indeed, the paraboloidal shape is obtained even in small-angle scattering (i.e. high projectile energy) approximation [9], leading to the correct value of the paraboloid stiffness parameter (its leading coefficient). This result is often quoted, and its use is justified by the fact that for low-energy ions not much would be gained by the exact result, as the screening of the ‘naked’ nuclear potential plays a far greater role than the nature of approximation [10].

However, rarely is the form of this shadow treated accurately, or analyzed in detail as a subject in its own right, even in a fixed-target frame, let alone in any other reference frame. One example is a mechanics textbook by Sommerfeld, where the topic appears as a supplemental problem I.12, with a short guideline on how to obtain the correct solution [11]. Further examples include succinct works by Adolph et al [12] and Warner and Huttar [13], all these efforts being decades apart. In the review paper by Burgdörfer the paraboloidal shadow form is also quickly obtained, but relying on the properties of the Coulomb continuum wavefunctions [14]. Interestingly, Samengo and Barrachina [15] consider the incident projectile trajectories from a point source, finding in that case the hyperboloidal shadow. At the same time, they recover the more familiar paraboloidal shape in the limit $R \to \infty$, with $R$ as the initial projectile–target distance. Most of these works make a point of this easily accessible topic being forgotten [12].
generally unknown [13] and commonly omitted from the standard textbooks [15]. Nothing much seems to have changed to this day.

We aim to give the subject our full attention and the detailed treatment it deserves, with the intent of rekindling the general interest in it as a worthy educational topic. In this work we analyze the geometric shape of the Rutherford scattering shadow, as it appears in the fixed-target and the center-of-mass frame. A transition to the laboratory frame (where the target is at rest only at the initial moment, i.e. when the projectile is just put into motion) or any other comoving frame (moving with a constant velocity relative to the center-of-mass frame) is much more involved than it may seem at the first glance and will be the subject of a separate work.

We will treat the scattering kinematics non-relativistically, which is a common enough approach. There is a myriad of sources offering some form of derivation of the classical trajectories within the Coulomb field, of which we cite only a few classics [16–19]. The trajectories are usually determined within the context of the two-body Kepler problem, i.e. assuming the gravitational potential, while the chapters on Rutherford scattering typically focus on the scattering cross-section. Quite often the problem is approached from the onset with the assumption of a large disparity between the masses, such that one body or particle (e.g. a star or the target nucleus) is much heavier than the other (e.g. a planet or the charged projectile). The obvious advantage of this approach is that the fixed-target frame also corresponds (at least approximately) both to the center-of-mass and the laboratory frame. As we are interested in each of these frames in its own right, we will follow the more general approach, making no specific assumptions about the masses involved.

Since the fixed-target frame of a finite-mass target is accelerated (as the target will recoil from the incoming projectile), a savvy reader might pose a legitimate question: is the force that the target exerts upon the projectile in such frame purely electrostatic? Or is there also a radiative component to the target’s electromagnetic field, even in the frame where it stays at rest, due to its acceleration in an outside inertial frame? The question is, in fact, entirely nontrivial and has indeed been the subject of a long-standing debate. The paradox has since been resolved and we know now that the electric field of a charge at rest is indeed purely electrostatic even in an accelerated frame [20]. Therefore, we are entirely justified in assuming a pure electrostatic force between the finite-mass particles in a fixed-target frame, which will serve as a starting point for a transition into any other reference frame.

This paper is accompanied by a supplementary note, expanding upon the main material presented herein.

2. Coulomb trajectories

Let us consider the Coulomb force \( \mathbf{F}_{t-p} \) exerted upon the projectile by the charged target:

\[
\mathbf{F}_{t-p} = \frac{Z_p Z_r e^2}{4\pi\epsilon_0} \frac{\mathbf{r}_p - \mathbf{r}_t}{|\mathbf{r}_p - \mathbf{r}_t|^3},
\]

where \( Z_p \) and \( Z_r \) are the projectile and target charge, respectively, in units of the elementary charge \( e \); \( \epsilon_0 \) is the vacuum permittivity; and \( \mathbf{r}_p \) and \( \mathbf{r}_t \) are the particle and target position-vectors.

For each particle Newton’s second law, in combination with the third one (\( \mathbf{F}_{t-p} = -\mathbf{F}_{p-t} \)), states

\[
m_p \ddot{\mathbf{r}}_p = \mathbf{F}_{t-p},
\]

\[
m_t \ddot{\mathbf{r}}_t = -\mathbf{F}_{t-p},
\]
with \( m_p \) and \( m_t \) as the projectile and target mass, respectively. By introducing the center-of-mass position \( \mathbf{R} \):

\[
\mathbf{R} \equiv \frac{m_p \mathbf{r}_p + m_t \mathbf{r}_t}{m_p + m_t} \tag{4}
\]

and summing (2) and (3):

\[
m_p \ddot{\mathbf{r}}_p + m_t \ddot{\mathbf{r}}_t = (m_p + m_t) \ddot{\mathbf{R}} = \mathbf{0}, \tag{5}
\]

one immediately obtains the equation of motion for the center of mass: \( \ddot{\mathbf{R}} = \mathbf{0} \), clearly showing that in the absence of the additional external forces the system as the whole cannot accelerate, which is to say that the linear momentum of the isolated system is conserved. By subtracting the acceleration terms from (2) and (3) and defining the target–relative projectile position \( \mathbf{r} \):

\[
\mathbf{r} \equiv \mathbf{r}_p - \mathbf{r}_t, \tag{6}
\]

one obtains the second equation of motion:

\[
\ddot{\mathbf{r}} = \left( \frac{1}{m_p} + \frac{1}{m_t} \right) \mathbf{F}_{r-p} = \frac{Z_p Z_t e^2}{4\pi\varepsilon_0 \mu r^2} \hat{\mathbf{r}}, \tag{7}
\]

where the common definition of the reduced mass \( \mu \):

\[
\frac{1}{\mu} \equiv \frac{1}{m_p} + \frac{1}{m_t} \tag{8}
\]

has been used, together with the vector norm \( r = |\mathbf{r}| \) and the corresponding unit direction \( \hat{\mathbf{r}} = \mathbf{r}/r \).

In parameterizing the projectile trajectory we will make use of the cylindrical coordinates \( \rho \) and \( z \), alongside their spherical counterparts \( r \) and \( \theta \). Figure 2 clearly illustrates their relation. In that, the direction of the \( z \)-axis corresponds to the projectile’s initial direction of motion (i.e. its initial velocity). Assuming that the projectile has been put into motion as a free particle of initial speed \( v_0 \) and with the impact parameter \( \varrho_0 \)—from the negative side of the \( z \)-axis, at an infinite distance from the target \( (\theta_0 = \pi) \)—for the initial conditions we can write

\[
\mathbf{r}(\theta_0 = \pi) = \varrho_0 \hat{\rho} + \lim_{z_0 \to -\infty} (z_0) \hat{z},
\]

\[
\dot{\mathbf{r}}(\theta_0 = \pi) = v_0 \hat{z}. \tag{9}
\]

Section A of the supplementary note derives a solution to the equation of motion (7) under these conditions. Introducing the following shorthand:

\[
\chi = \frac{Z_p Z_t e^2}{4\pi\varepsilon_0 \mu v_0^2} \tag{11}
\]

the solution for the relative coordinate may be expressed as

\[
r(\theta; \varrho_0) = \frac{\varrho_0^2}{\sqrt{\chi^2 + \varrho_0^2 \sin[\theta - \arctan(\chi/\varrho_0)] - \chi}}. \tag{12}
\]
Figure 2. Geometric parameters used for describing the projectile trajectory (full line). The target-relative projectile position $\mathbf{r}$ is described both by the spherical coordinates $r$ and $\theta$, and their cylindrical counterparts $\rho$ and $z$. Due to the axial symmetry the azimuthal angle $\varphi$ bears no relevance to the problem.

It is well known that for the repulsive interaction, i.e. for $\chi > 0$ (12), defines a hyperbolic trajectory. By construction, one of its asymptotes is parallel to the $z$-axis, at a distance $\varrho_0$ from it. The other asymptote is defined by the famous scattering angle $\vartheta$ from a fixed-target frame, which is easily determined from (12) as the angle for which the expression diverges, i.e. the denominator vanishes, leading to

$$\vartheta = 2 \arctan \frac{\chi}{\varrho_0}. \tag{13}$$

This also means that some particular angle $\theta$ may be reached only by those trajectories whose scattering angle is further on ($\vartheta < \theta$). Evidently, those are the trajectories whose impact parameter satisfies $\varrho_0 > \chi / \tan(\theta/2)$.

It should be noted that (12) has a universal shape, independent of all the underlying physical parameters borne by $\chi$, when expressed in the scaled, dimensionless coordinates $\bar{r} = r / \chi$ and $\bar{\varrho}_0 = \varrho_0 / \chi$:

$$\bar{r} = \frac{\bar{\varrho}_0^2}{\sqrt{1 + \bar{\varrho}_0^2 \sin[\theta - \arctan(1/\bar{\varrho}_0)] - 1}}, \tag{14}$$

which will have the same repercussions upon the later results. This allows us to intuit that there is a natural length scale to the Rutherford scattering, which is a notion that will only be reinforced further on, and repeatedly so.

3. Fixed-target frame

The target-relative position $\mathbf{r}$, as defined by (6), immediately implies the fixed-target frame. In other words, for the absolute positions it holds by definition $\mathbf{r}^{(\text{fix})}_t = \mathbf{0}$ and thus $\mathbf{r}^{(\text{fix})}_p = \mathbf{r}$. In order to determine the geometric shape of the shadow we pose the following question: under a particular angle $\theta$, which trajectory passes closest to the target? In other words, for a given $\theta$, which impact parameter $\varrho_0$ minimizes the distance $r(\theta; \varrho_0)$? The answer is, of course, to be
found by finding the zero of the derivative in respect to $\varrho_0$:

$$\frac{dr(\theta; \varrho_0)}{d\varrho_0} \bigg|_{\varrho_0} = \frac{\varrho_0 \sin \theta - 2\chi (1 + \cos \theta)}{\varrho_0^3} r^2(\theta; \varrho_0) = 0. \tag{15}$$

This is satisfied by a vanishing numerator, yielding the sought impact parameter:

$$\tilde{\varrho}_0(\theta) = \frac{2\chi \tan \frac{\theta}{2}}{\chi}. \tag{16}$$

Returning this value to (12), we find that under an angle $\theta$ the trajectory with an impact parameter $\tilde{\varrho}_0$ comes closest to the target, at the distance

$$r[\theta; \tilde{\varrho}_0(\theta)] = \frac{2\chi}{\sin^2 \frac{\theta}{2}}. \tag{17}$$

Since $r[\theta; \tilde{\varrho}_0(\theta)]$ determines the shadow boundary, it is the solution to our problem: it represents the shadow equation in spherical coordinates. However, to make shadow shape more evident, we express its cylindrical coordinate $\rho$ (see figure 2):

$$\rho(\theta) = r[\theta; \tilde{\varrho}_0(\theta)] \sin \theta = \frac{4\chi}{\tan \frac{\theta}{2}}, \tag{18}$$

as well as its $z$-coordinate:

$$z(\theta) = r[\theta; \tilde{\varrho}_0(\theta)] \cos \theta = 2\chi \left( \frac{1}{\tan^2 \frac{\theta}{2}} - 1 \right). \tag{19}$$

Eliminating the term $\tan(\theta/2)$ from the previous two equations, the following connection is obtained:

$$z(\rho) = \frac{\rho^2}{8\chi} - 2\chi, \tag{20}$$

which is the shadow equation in the cylindrical coordinates, and the main result of this paper. Evidently, in the fixed-target frame—as suggested by an example from figure 1—all the projectile trajectories of a given energy form a paraboloidal shadow. As portended by (14), the shadow features a universal shape in scaled coordinates $\bar{z} = z/\chi$ and $\bar{\rho} = \rho/\chi$, such that: $\bar{z} = \bar{\rho}^2/8 - 2$, thus confirming the notion that there is a natural length scale to the Rutherford scattering. In addition, it is easily determined from the paraboloid’s leading coefficient that the focal distance $f$ between the shadow focus and its vertex equals $f = 2\chi$, exactly corresponding to its free parameter. Therefore, in the fixed-target frame the target is precisely at the shadow focus.

Figure 3 shows shadow shapes for several arbitrary values $\chi$, i.e. for several values of the initial projectile energy. From (11) it is clear that the increase in the initial energy—i.e. in the initial relative speed $v_0$—means a decrease in $\chi$. The shadows are perfectly in accordance with expectations: not only do the projectiles of higher energy (lower $\chi$) manage to come closer to the central target (as governed by the free parameter $-2\chi$), they are also less easily deflected than the projectiles of lower energy, meaning a stiffer paraboloid (as governed by the leading coefficient $1/8\chi$).

Section B of the supplementary note offers some additional observations in regard to (13), (16) and (18).
Figure 3. Shadow examples in a fixed-target frame for several values of $\chi$, with $\chi_0$ as the arbitrary length scale. The charged target is shown by a central dot, which is precisely at the focus of each paraboloidal form. The shadow approaches the target and becomes stiffer as the initial energy of the projectile increases ($\chi$ decreases).

4. Center-of-mass frame

In order to make a transition from a fixed-target frame into any other frame, we invert the definitions of $R$ and $r$ from (4) and (6), thus obtaining

$$r_p = R + \frac{m_t}{m_p + m_t}r,$$  \hspace{1cm} (21)

$$r_t = R - \frac{m_p}{m_p + m_t}r.$$  \hspace{1cm} (22)

By definition, the center-of-mass position in the center-of-mass frame is the origin of the coordinate frame: $R^{(cm)} = 0$. Thus, introducing the shorthand

$$\eta_{pt} \equiv \frac{m_{pt}}{m_p + m_t}$$  \hspace{1cm} (23)

we immediately obtain both the particle and target trajectories:

$$r_p^{(cm)} = \eta_t r,$$  \hspace{1cm} (24)

$$r_t^{(cm)} = -\eta_t r.$$  \hspace{1cm} (25)

As the projectile’s position vector in the center-of-mass frame is only scaled by the factor $\eta_t$ relative to the position in the fixed-target frame, the definition of the angle $\theta$ stays the same. The only effect upon the projectile trajectory is a decreased radial distance to the center of
mass \( r_p^{(\text{cm})} = \eta_p r \), leading to the minimization condition:

\[
\left. \frac{d}{d\varrho_0} r_p^{(\text{cm})}(\theta; \varrho_0) \right|_{\varrho_0} = \eta_p \left. \frac{d}{d\varrho_0} r(\theta; \varrho_0) \right|_{\varrho_0} = 0. \tag{26}
\]

As the minimization procedure is unaffected in regard to (15), the same minimizing value \( \tilde{\varrho}_0(\theta) \) from (16) is obtained. It is only that the minimum projectile distance from the origin of the center-of-mass frame is scaled by a factor \( \eta_p \) when compared to that from (17), with the same factor propagating into the cylindrical coordinates from (18) and (19), so that

\[
\rho_p(\theta) = \frac{4\eta_p \chi}{\tan \frac{\theta}{2}}, \tag{27}
\]

\[
z_p(\theta) = 2\eta_p \chi \left( \frac{1}{\tan^2 \frac{\theta}{2}} - 1 \right). \tag{28}
\]

For brevity and clarity we have dropped the explicit frame designation (cm). Eliminating again the term \( \tan(\theta/2) \) from the previous two equations, we arrive at the shadow equation in the center-of-mass frame:

\[
z_p(\rho_p) = \frac{\rho_p^2}{8\eta_p \chi} - 2\eta_p \chi. \tag{29}
\]

Since \( \eta_p < 1 \), the paraboloid vertex is closer to the origin of the coordinate frame (as determined by the free parameter \( -2\eta_p \chi \)), while the paraboloid shape is stiffer than in the fixed-target frame (as determined by the leading coefficient \( 1/8\eta_p \chi \)). Both effects are due to the fact that the origin is no longer the target itself, but rather the center of mass. Being somewhere in between the two particles, both the origin and the \( z \)-axis of the coordinate frame are at each point along the particle trajectory brought closer to the projectile, when compared to the fixed-target frame, thus constricting the shadow profile.

In the center-of-mass frame the target is in motion, in an entirely symmetric manner to the projectile, so it also casts its own shadow. Its exact shape is easily deduced from the projectile shadow, as at any moment we may interchange the roles of the target and the projectile by a simple change in indices: \( p \leftrightarrow t \). Additionally taking into account that the target shadow points in the opposite direction to the projectile shadow (along the negative direction of \( z \)-axis), we may immediately write

\[
z_t(\rho_t) = -\frac{\rho_t^2}{8\eta_p \chi} + 2\eta_p \chi. \tag{30}
\]

Examining the focal distances \( f_{p,t} \) of the projectile and target shadows from (29) and (30), we invariably find \( f_{p,t} = 2\eta_p \chi \), meaning that the focal points of both shadows are at the origin of the selected coordinate frame. Therefore, in the center-of-mass frame the two foci coincide, i.e. the same focus is shared between the two shadows.

If we were to examine the effect of varying masses upon the shadow form, it would not do to naively keep \( \chi \) constant, while varying only the ratios \( \eta_{p,t} \) from products \( \eta_{p,t} \chi \) appearing in (29) and (30). This is because the term \( \chi \) itself, as defined by (11), inherits the mass dependence via a reduced mass, so that the products \( \eta_{p,t} \chi \):

\[
\frac{\eta_{p,t} \chi}{\mu} \propto \frac{m_p + m_t}{m_p m_t} \frac{m_p}{m_p + m_t} = \frac{1}{m_{p,t}}. \tag{31}
\]
are dependent only on the mass of a single particle. Therefore, in the center-of-mass frame the projectile and target shadows are determined solely by their own masses, being entirely independent of the other particle’s mass. This needs to be held in mind, as it is in striking opposition with what the expression \( \eta_t, p, \chi \) deceptively suggests: that the shadow form should not only be sensitive to both masses, but that it should also be more directly determined by the mass of the ‘wrong’ particle.

In the sense of (31), figure 3 may also be interpreted as a comparison of projectile shadows in the center-of-mass frame for varying projectile masses, if the labels \( \chi_i \) are replaced by the projectile mass dependence \( m_i = m_0 / i \) (\( m_0 \) being some arbitrary reference value).

Finally, it is again interesting to take note of the shadow form in the appropriately scaled coordinates. In fact, the projectile shadow from (29) takes on exactly the same universal form \( \bar{z}_p, \rho_p \) of (20) when expressed in scaled coordinates \( z_p, \rho_p / \eta_t, \chi \). However, in order to reach the same form for the target shadow, its coordinates should be scaled by a different factor: \( \bar{z}_t, \rho_t / \eta_t, \chi \). Therefore, scaling all coordinates by a unique factor \( \chi \) (or any constant, but parameter-invariant multiple of it) remains the most sensible choice. The price is that in the center-of-mass frame there is no parameter-independent universal form for both the projectile and target simultaneously. Rather, with \( \bar{z}_{pt} = z_p / \chi \) and \( \bar{\rho}_{pt} = \rho_p / \chi \) we have to contend with two separate forms: \( \bar{z}_p = \bar{\rho}_p^2 / 8 \eta_t - 2 \eta_t \) and \( \bar{z}_t = -\bar{\rho}_t^2 / 8 \eta_p + 2 \eta_p \), where the ‘most generalized’ shadow shapes still depend on the relation between the two masses, but only on them. However, the advantage of this approach is that the length scale \( \chi \) is revealed not only as the most natural between the two particles (i.e. for both of them simultaneously), but also between multiple frames.

5. Quantum-mechanical case

We present a short overview of the quantum-mechanical scattering and the appearance of the scattering shadow within such framework. A starting point is, of course, a Schrödinger equation for the joint particle-target system under a repulsive Coulomb interaction. After a typical separation of variables such that the motion of the center of mass is decoupled from the relative motion, the equation for the relative motion reads

\[
\left(-\frac{\hbar^2}{2\mu} \nabla^2 + \frac{Z_p Z_t e^2}{4\pi \epsilon_0 r}\right) \psi_k(r) = E_k \psi_k(r),
\]

as a quantum-mechanical counterpart to the classical equation of motion (7). Just like Newton’s equation, Schrödinger’s equation for relative motion features a reduced mass \( \mu \). Since the relative vector \( r \) is still the same as in (6)—its origin being at the target position—one has to contend with two separate forms: \( \bar{z}_p = \bar{\rho}_p^2 / 8 \eta_t - 2 \eta_t \) and \( \bar{z}_t = -\bar{\rho}_t^2 / 8 \eta_p + 2 \eta_p \), where the ‘most generalized’ shadow shapes still depend on the relation between the two masses, but only on them. However, the advantage of this approach is that the length scale \( \chi \) is revealed not only as the most natural between the two particles (i.e. for both of them simultaneously), but also between multiple frames.

\[
\lim_{k \to +\infty} \psi_k(r) \propto e^{ik r}
\]
Introducing (33) and (34) into (32) in the limit $r \to \infty$, a well-known parameterization of energy remains: $E_k = \hbar k^2 / 2\mu = \mu v_0^2 / 2$. With this, (32) may be rewritten using the definition of $\chi$ from (11):

$$
\left( \nabla^2 + k^2 - \frac{2\chi k^2}{r} \right) \psi_k(r) = 0.
$$

The solution to this Schrödinger equation, satisfying the boundary condition from (33), is well known [21]:

$$
\psi_k(r) = e^{-\pi \chi k^2 / 2} \Gamma(1 + i\chi k) e^{ik \cdot r} M[-i\chi k, 1, i(kr - k \cdot r)],
$$

where $\Gamma$ is the conventionally defined gamma function and $M$ is Kummer’s confluent hypergeometric function, otherwise denoted as $_1F_1$. The wavefunctions from (36) are normalized such that:

$$
\int \psi_k^*(r) \psi_k(r) \, dV = (2\pi)^3 \delta(k - k').
$$

As opposed to classical mechanics, where all trajectories are strictly excluded from the shadow zone, in quantum mechanics we would always expect the wavefunction tunneling into this classically forbidden region of space. The question that naturally arises is whether the wavefunction exhibits any recognizable features at all, that would allow us to identify the appearance of the classical shadow. In the general case, its precise position could hardly be pinpointed from the Coulomb continuum wavefunction, as the quantum shadow is diffuse. However, we can make some observations in the opposite direction: knowing the classical shadow, we can analyze the wavefunction behavior in its vicinity. Burgdörfer notices: ‘A (smoothed) caustic appears also in the corresponding quantum scattering wavefunction as an (anti) nodal surface. The locus of the caustic is, in fact, most conveniently derived from the nodal structure of Coulomb continuum wavefunctions. Nodal surfaces are given by the argument of the hypergeometric function (…)’ (quotation from [14]). In this rather ingenious insight, we only caution against the use of the term ‘(anti) nodal’, as it might suggest that the shadow appears at some extremum related to the wavefunction—presumably the extremum of modulus $|\psi_k(r)|$—which we will soon disprove. A more appropriate term would be ‘level surfaces’ (‘equipotentials’), which are indeed defined by the constancy of the argument of the confluent hypergeometric function from (36):

$$
kr - k \cdot r = C.
$$

For $k$ defined as in (34), equation (37) reduces to $k(\sqrt{z^2 + p^2} - z) = C$. Solving for $z$ yields

$$
z(p) = \frac{k}{2C} p^2 - C \frac{2k}{2k} = \frac{p^2}{8(C/4k)} - 2(C/4k)
$$

for the shape of level surfaces of $|\psi_k(r)|$ (but not of $\psi_k(r)$ itself, due to the extra $e^{ik \cdot r}$ factor). This has the same form as (20), allowing us to determine the shadow-related value of constant $C$ as

$$
C_{\text{shadow}} = 4\chi k
$$

and, indeed, to recognize the classical scattering shadow as a particular level surface in the quantum-mechanical probability density of the incoming projectile.

Figure 4 shows an example of the modulus $|\psi_k(r)|$ of the wavefunction from (36) for $\chi k = 1$, in a plane containing the $z$-axis, where the target rests at $r = 0$. One can readily appreciate by eye the fact that the level surfaces are parabolic, as shown by (38). The thick black line indicates the level surface corresponding to the shadow caustic—i.e. where, along the wavefunction, the classical shadow appears—clearly proving that it is not related to any extremal (antinodal)
Figure 4. Modulus of the projectile’s Coulomb continuum wavefunction for a repulsive Rutherford scattering in the fixed-target frame, in a plane containing the z-axis, with the target at $r = 0$. The relevant wavefunction features are governed by the confluent hypergeometric function $M[-i\chi k, 1, i\chi k(\sqrt{\bar{\rho}^2 + \bar{z}^2} - 3)]$, with $\bar{z} = z/\chi$ and $\bar{\rho} = \rho/\chi$, and here selected $\chi k = 1$. The thick black line shows the classical shadow caustic, beyond which the wavefunction clearly exhibits quantum-mechanical tunneling.

The portion of the wavefunction bounded by this caustic (below the thick black line) shows a clear case of quantum-mechanical tunneling into the classically forbidden zone.

The fact that the classical scattering shadow may indeed be identified within the quantum-mechanical description indicates that we might again perform the appropriate coordinate scaling—such that $\bar{z} = z/\chi$ and $\bar{r} = r/\chi$—and express the wavefunction as

$$\psi_k(r) = e^{-\pi \chi k^2/2} \Gamma(1 + i\chi k) e^{i\chi k(\bar{r} - \bar{z})} M[-i\chi k, 1, i\chi k(\bar{r} - \bar{z})],$$

where we used, for simplicity, the convention $k = \hat{z}k$ from (34). This reveals that, while the shape of the scattering shadow still remains scale-invariant, the details of the wavefunction still depend on $k$, but in such a way that—alongside the length scale $\chi$—there appears another, dimensionless scale $\chi k$, otherwise known as the Sommerfeld parameter. But how can that be, considering that in the classical mechanics all the spatial aspects of the Coulomb trajectories from (14) are scaled only by $\chi$? How can another scale be admitted in quantum mechanics, since—by the correspondence principle—at some point both the classical and quantum description must coincide? The answer lies in the temporal aspects of the scattering, of which the purely geometrical expression (14) has been devoided. For the same spatial scaling $\chi$, the projectile speed—entering $k$ through (34)—may still be varied. Thus, the time the projectile spends in a given portion of space still depends on its speed. In consequence, so do the details of the wavefunction, governing the probability density $|\psi_k(r)|^2$ of finding the projectile at a given point. This probabilistic interpretation, in combination with the correspondence principle applied to the projectile trajectories displayed in figure 1, also allows us to understand why the highest antinode in $|\psi_k(r)|$ appears just before the shadow, prior to tunneling. It is for two reasons: for $z/\chi \lesssim -1$ the projectiles are slowest just around the scattering shadow (see section C of the supplementary note), while for $z/\chi \gtrsim -1$ the trajectories pile around the shadow caustic (see figure 1), both effects...
increasing the probability of finding the projectiles at the edge of the classically forbidden zone.

Wavefunction dependence upon $\chi k$ is further exemplified by figure 5, showing the modulus $|\psi_k(r)|$ along the central axis $\rho = 0$, passing through a target at $z = 0$, for different values of $\chi k$. The position of the classical shadow caustic—now corresponding to its vertex—is shown by the vertical line. There is no single point at which all the wavefunctions intersect, as might be falsely inferred from this specific display.

Figure 5 allows us to make some additional interesting observations. Since at $\rho = 0$ it holds: $r = |z|$, for $z \geq 0$ the confluent hypergeometric function from (40) reduces to $M(-i\chi k, 1, 0) = 1$, so $|\psi_k(r)|$ is indeed constant there, as suggested by the figure. At the first glance it might be confusing why this value is not 0 at $z = 0$, where the target lies. In other words, how can Schrödinger’s equation from (32) or (35) be satisfied by a nonvanishing wavefunction at the point where the repulsive potential diverges? As figure 5 shows, the wavefunction at $z = 0$, while continuous, is not smooth—its gradient $\nabla \psi_k(r)$ is discontinuous, so that its Laplacian $\nabla^2 \psi_k(r)$ diverges, canceling the divergence from the potential energy in Schrödinger’s equation. Finally, figure 5 also indicates that by increasing $\chi k$ the wavefunction behavior around the shadow caustic becomes sharper and sharper. This suggests that if one were to investigate the limit $\chi k \to \infty$ of a very strong repulsion and/or a very slow projectile—$\lim_{\chi k \to \infty} |\psi_k(r)| \propto \lim_{\chi k \to \infty} |M(-i\chi k, 1, i\chi k \xi)|$ with, in our case, $\xi = (r - z)/\chi$—one would expect a sharp drop at $\xi = 4$, in accordance with (39). This specific result could then be extended to a case of finite $\chi k$ and taken as an agreed-upon value determining the shadow caustic even in the case of a diffuse shadow. This is how the scattering shadow can be determined self-consistently from the wavefunction itself, without reference to the classical mechanics.

6. Conclusion

We have explored the geometry of the repulsive Rutherford scattering, finding the exact shape of the scattering shadow in the fixed-target and the center-of-mass frame. In both frames the projectile shadow has a simple paraboloidal shape. The difference between frames is, of course,
reflected in the different values of the paraboloids’ coefficients, i.e. in their stiffness and the distance of their vertices from the origin of the coordinate frame. In that, the projectile shadow in the center-of-mass frame is stiffer and closer to the origin than its counterpart from the fixed-target frame. Since the motion of the target in the center-of-mass frame is—in mathematical form—symmetrical to the motion of the projectile, the target also casts a paraboloidal shadow in the same frame, such that the two shadows intersect. It was found that the target is precisely at the shadow focus in the fixed-target frame, while in the center-of-mass frame the focal points of the projectile and target shadow coincide with the center of mass itself. A somewhat surprising finding is that the shadow parameters in the center-of-mass frame depend only on the mass of the particle casting the shadow, rather than the ratio of masses as might at first be expected. The Rutherford scattering is revealed to feature a natural length scale $\chi$, determined by the physical parameters of the system. A quantum-mechanical treatment of the repulsive Rutherford scattering was addressed and the scattering shadow was also observed appearing in a Coulomb continuum wavefunction. Unlike the sharply defined classical shadow, quantum mechanics yields a diffuse shadow caustic, due to the wavefunction tunneling into a classically forbidden zone. Alongside the length scale $\chi$, in quantum mechanics another relevant scale appears: the dimensionless Sommerfeld parameter $\chi k$. A sharp shadow caustic is recovered in the limit $\chi k \to \infty$. The transition of the scattering shadow to the laboratory frame—wherein the target is at rest only at the initial moment, subsequently being recoiled by the approaching projectile—is much more involved and will be the subject of future work.

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ORCID iDs

Petar Žugec © https://orcid.org/0000-0001-6933-3100

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