Quantum Scattering with Trajectories

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Abstract

We use the pilot wave formalism or Bohemian mechanics to calculate the trajectories of particles undergoing quantum scattering from a simple delta-shell potential. This example illustrates the connection between causal trajectories and the conventional quantum mechanical view of scattering. It also illustrates several important themes in time-dependent scattering theory, such as the significance of wave packets and their relation to experimentally measured cross sections.

1 Introduction

The classical scattering of particles is easy to visualize in terms of trajectories. In the usual picture, a bundle of parallel trajectories is sent along the polar axis toward a fixed scattering center. The particles are deflected, and beyond the range of the force, the trajectories again become straight lines radiating from the center. Thus there is a mapping between a particle’s initial distance from the axis or “impact parameter,” and its final polar scattering angle. The target can be regarded as an “archery target” with concentric circles of area $d\sigma(\theta)$. If a particle is directed at the circle labelled $d\sigma(\theta)$, it will scatter into solid angle $d\Omega(\theta)$.

In a quantum scattering experiment, the initial and final states resemble those just described, but the behavior of the particle in the vicinity of the target is hard to understand. Particles scatter, but differential cross sections display wave-like interference patterns. This is a subtle variant of the two-slit interference experiment, of course, but even this can be visualized partly in terms of trajectories: a particle propagates from the source to one of the two slits, and from there to the detection screen. The usual time-independent formalism makes scattering even more intangible: incident and scattered particles are represented by plane and spherical waves that presumably fill all space. Wave-particle duality is entirely sacrificed in favor of waves. Worse yet, these waves should interfere over all space. This completely unphysical effect is avoided by arbitrarily discarding the interference terms.

Quantum texts often acknowledge these problems and then present a more sophisticated time-dependent approach based on wave packets. The thrust of this argument is that the neglect of interference terms is justified, because the
incident and scattered packets do not overlap at large distances from the scattering center.\textsuperscript{1} The treatment has the feel of a mathematical proof in which various limiting procedures are employed. One concludes that interference can be neglected in the limit $r \to \infty$, without understanding what went on near the scattering center.

There is a way of formulating quantum mechanics that offers a third approach emphasizing particles rather than waves. The idea, variously called Bohmian mechanics, causal quantum mechanics, or pilot wave theory, was originally proposed by Louis deBroglie more than seventy years ago and periodically abandoned and rediscovered since then. Much of the current interest in the theory is due to John Bell who championed it throughout his career.\textsuperscript{2} It has been featured in Physics Today,\textsuperscript{3} and is the subject of two recent books\textsuperscript{4}

The theory is intriguing because of the way it resolves the usual paradoxes of quantum mechanics. For example, the two-slit interference experiment is explained as follows: a source emits a stream of particles, which follow smooth trajectories on their way to the detector. These trajectories are completely determined by their initial conditions, but they are very sensitive to these conditions. Any attempt to determine them would completely alter the trajectory. This is the uncertainty principle of course, but it arises in a completely “mechanical” way. Since we have no hope of determining the initial conditions of any one particle, we are forced to consider an ensemble of particles distributed according to the usual probability function $\rho(r, t) = |\psi(r, t)|^2$. In this way we obtain the probability distributions of ordinary quantum mechanics.

Why then are interference patterns observed? The particles move under the influence of a potential field that is derived from the Schrödinger equation. This field has wave-like properties, and it “guides” the particles along so that they are more likely to hit the detector in some regions and less likely in others. This is analogous to classical electrodynamics in which charged particles move in response to electric and magnetic fields calculated from Maxwell’s equations.

Much of the literature on pilot waves is of a philosophical nature arguing that it does (or does not) provide a conceptual framework for quantum mechanics that is superior to the usual Copenhagen interpretation. We do not wish to enter this controversy here. Our position is that pilot wave theory is mathematically consistent with quantum mechanics, yet it provides powerful tools for visualizing time-dependent processes. This is particularly true in the case of scattering. At the macroscopic level, the particles follow classical trajectories. The pilot wave formalism enables us to track these trajectories through the quantum regime.

The purpose of this article is two-fold: first to give a brief introduction to pilot wave theory as it pertains to scattering, and second, to describe a model

\textsuperscript{1}Except in the forward direction.
\textsuperscript{2}John Bell, \textit{Speakable and Unspeakable in Quantum Mechanics}
\textsuperscript{3}Sheldon Goldstein, \textit{Quantum Theory Without Observers – Part Two}, Physics Today, April 1998, pp 38-42
and “computational laboratory” that allows one to compute trajectories and cross sections for a wide range of scattering parameters.

The equations of motion in pilot wave theory are typically coupled non-linear differential equations that, except in a few simple cases, cannot be solved analytically. For this reason we base our model on the delta-shell potential, which yields exact closed-form solutions for the time-independent wave function and almost closed-form solutions (one remaining integration) for the time-dependent wave function. The rest is easily within the reach of modern computers and software, however, so simulations are not only physically insightful, they are useful instruction in a variety of theoretical and computational topics as well. We have written the code in MatLab \footnote{The MathWorks Inc} because of the many algorithms and graphic tools that are part of the MatLab package. It is used as a student project in our advanced computational physics laboratory at Oregon State University and is available for general use through our website.

We review the pilot wave formalism in Sec. 2 and conventional time-independent and time-dependent scattering theory in Sec. 3. In Sec. 4 we derive solutions to the Schrödinger equation for the delta-shell potential. In Sec. 5 we discuss computational details and present our results in various forms in Sec. 6. Sec. 7 is a brief summary.

2 Pilot wave theory: An introduction

In some sense, pilot wave theory is just a reformulation of quantum mechanics. It is based on the Schrödinger equation, and the pilot waves themselves are derived from the usual time-dependent wave functions. The wave functions are interpreted in terms of particle trajectories, but even this interpretation does not differ too much from conventional quantum mechanics.

The rules for deriving trajectories from wave functions are the following:

1. Solve the time-dependent Schrödinger equation using whatever potential is relevant to the problem. The usual rules of linear superposition apply.\footnote{The significance of operators is somewhat different, however.}

2. Take the wave function obtained in this way and decompose it as follows

\[ \psi(r, t) = R e^{iS/h} \]  

The new functions \( R \) and \( S \) are real functions of \( r \) and \( t \), and of course \( R > 0 \).

3. In ordinary quantum mechanics, we would be interested in \( R \) since \( R^2 = \psi^* \psi \). The new entity is the \( S \) function or guiding field. From it we obtain

the equations of motion,\textsuperscript{8}

\[ v(r, t) = \frac{dr}{dt} = \frac{1}{m} \nabla S(r, t) \quad (2) \]

4. Eq. (2) is a set of coupled first-order ordinary differential equations. The solution \( r(t) \) gives the position of the particle as a function of time. If we knew that the particle was at \( r(t_0) \) at time \( t_0 \) we could find the complete trajectory by numerically integrating Eq. (2). The trajectories determined in this way are smooth and unique in the following sense: any two particles occupying the same position \( r_0 \) at the same time \( t_0 \) have had and will have identical trajectories. For this reason, Bohmian trajectories must never cross in configuration space.

5. Start with an ensemble of particles randomly chosen with a probability distribution function

\[ \rho(r_0, t_0) = |\Psi(r_0, t_0)|^2 \quad (3) \]

Here \( \Psi \) is the initial wave function solution to the Schrödinger equation obtained in the first step above. Experiments performed subsequently will measure \( \rho(r, t) \).

This procedure, at first sight, seems completely mysterious or ad hoc. It is actually rooted in conventional quantum mechanics as well as classical hydrodynamics. This comes about because the usual probability current density is related to \( \mathbf{R} \) and \( S \) as follows

\[ j = \frac{i\hbar}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi) = \mathbf{R}\mathbf{v} \quad (4) \]

It is also easy to show that the density \( R \) obeys the continuity equation

\[ \nabla \cdot (R\mathbf{v}) + \frac{\partial R}{\partial t} = 0 \quad (5) \]

Thus \( R \) and \( \mathbf{v} \) can be interpreted as the density and velocity of a hydrodynamical flow of a compressible fluid. The trajectories are like the streamlines that are used to visualize this flow: a drop of fluid at \((r, t)\) has by virtue of its position a velocity \( v \), and it will follow the path along the streamline given by Eq. (2). Even if one does not believe that quantum particles follow deterministic trajectories, one can still adopt a “minimalist” position and say that the trajectories are just a way of visualizing the flow of quantum probability.

It is interesting to compare Eq. (2) with Newton’s second law of motion

\[ \frac{d^2r}{dt^2} = -\frac{1}{m} \nabla \phi(r, t) \quad (6) \]

\textsuperscript{8}There is an alternative formulation of Bohmian mechanics in which particles move under the influence of a force derived from the quantum potential, \( Q = -(\hbar^2/2m)\nabla^2 R/R \). In this formulation (2) appears as an equation of constraint. The approach above is much easier to use with numerical computation.
Eq. (6) defines a force field, or more properly, an acceleration field. A particle at \((r, t)\) has by virtue of its position, a certain acceleration. This acceleration comes about because of the potential \(\phi\) (due to gravity perhaps or electromagnetic interactions). Since this is a second order equation it requires two initial conditions, position and velocity, to determine the trajectory. Eq. (2), by contrast, defines a velocity field and fixes the subsequent motion with a single condition.

The potential \(\phi(r)\) in Eq. (6) is produced by matter that might be a great distance from \(r\). In classical language it represents “action at a distance.” The guiding field \(S\) in Eq. (2) comes from various sources, particularly the experimental apparatus, which, on the quantum scale, is also “distant matter.” In quantum language it embodies a “non-local hidden variable theory.” One significant difference is that \(\phi\) arises from mechanisms that are at least partly understood, the exchange of photons or gravitons for example, whereas \(S\) may or may not be produced by such mechanisms.

3 Scattering theory

The scattering of quantum particles from a fixed potential is covered in every introductory quantum text. The development begins with the following wave function.

\[
\psi = \frac{1}{(2\pi)^{3/2}} \left[ e^{ikr} + f(\theta) \frac{e^{ikr}}{r} \right] \tag{7}
\]

This is a solution to the time-independent free-particle Schrodinger equation in regions where \(r\) is so large the the “centrifugal” term, \(l(l+1)/r^2\), in the radial wave equation can be neglected. It represents an incident plane wave and an outgoing spherical scattered wave. The function \(f(\theta)\) is called the scattering amplitude. It is determined by the interaction of the incident wave with the potential. It contains the information that the scattered wave carries away from the interaction.

Next, one substitutes the second term of Eq. (7) into Eq. (3).

\[
j \propto |f|^2/r^2 \tag{8}
\]

This is interpreted as the flux of particles away from the target. The quantity that is actually measured is the differential cross section

\[
\frac{d\sigma}{d\Omega} = |f|^2 \tag{9}
\]

This argument is puzzling for two related reasons. One is never justified in calculating a probability from one term in a linear superposition. Otherwise there would be no such thing as interference. If the complete equation for \(\psi\) is

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9One could argue that the variables are not “hidden,” but completely manifest; nevertheless, this is the usual terminology. We should point out that Bell’s theorem on the impossibility of hidden variable theories does not apply to non-local theories of this sort.
substituted into Eq. (4) there appear interference terms proportional to $1/r$, which at macroscopic distances dominate the $1/r^2$ terms by typically thirteen orders of magnitude. The second difficulty is that Eq. (7) is a stationary state wave function. This would be appropriate for a bound state system in which nothing is happening. In a scattering experiment, by definition, something is happening; an incident particle is bouncing off of some other particle or scattering center.

The usual way around these difficulties is to use the solution of the time-dependent Schrödinger equation assuming that the initial state consists of a wave packet moving toward the scattering center. The scattering process then produces a spherical wave packet, i.e. an expanding spherical shell, and the incident packet continues undeflected. Some time after the scattering the two packets are separated, so that the interference terms are suppressed (except in the forward direction where the incident and scattered wave are still in contact). This is described mathematically as follows: Eq. (7) is replaced by the following time-dependent solution.

$$\Psi(r, t) = e^{i\omega k t} \Phi(r - ut, 0) + e^{i\omega k t} \frac{f(\hat{r})}{r} \Phi(r \hat{k} - ut, 0)$$

(10)

The function $\Phi(r - ut, 0)$ represents a wave packet centered at $r = ut$ moving with the group velocity $u = \hbar k/m$. At $t = 0$ the packet is centered at $r = 0$, which is the scattering center. The scattered spherical wave packet is $\Phi(r \hat{k} - ut, 0)$. The second term of Eq. (10) is substituted into Eq. (4) (arguing that the interference terms have been suppressed) and the entire expression integrated from $t = -\infty$ to $+\infty$. The resulting differential cross section is still given by Eq. (9).

As pointed out in the introduction, this is an argument about asymptotic quantities. In order to integrate trajectories through the scattering region, it is necessary to have time-dependent wave functions in the small $r$ region as well. This could present a formidable computational problem, since the trajectories themselves must be integrated numerically. For this reason we use the delta-shell potential in our simulations. This enables us to get exact time-independent wave functions and time-dependent wave packet solutions with a one-dimensional numeric integration. These steps are covered in the next two sections.

### 3.1 Time-Independent Wave Functions for the Delta-Shell Potential

The stationary-state wave equation can be written as follows:

$$\nabla^2 \psi_k(r) + k^2 \psi_k(r) = U(r) \psi_k(r)$$

(11)

\[10\] A poor approximation.

\[11\] I am using the notation from Kurt Gottfried, Quantum Mechanics, Vol I, Advanced Book Classics, Benjamin, 1989. Lower-case Greek letters are used for time-independent wave functions, upper-case letters for time-dependent wave functions.
where
\[
E = \frac{\hbar^2 k^2}{2m} \tag{12}
\]
\[
U(r) = \frac{2m}{\hbar^2} V(r) \tag{13}
\]

So long as the potential is spherically symmetric, \( \psi_k(r) \) can be expanded in Legendre polynomials
\[
\psi_k(r) = (2\pi)^{-3/2} \sum_{l=0}^{\infty} (2l + 1)^{l} A_l(k;r) P_l(\cos \theta) \tag{14}
\]
\( A_l(k;r) \) is a solution of the radial equation
\[
\left[ \frac{1}{r} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} - U(r) + k^2 \right] A_l(k;r) = 0. \tag{15}
\]
In regions where \( U(r) = 0 \), these solutions are the spherical Bessel functions, \( j_l(kr), n_l(kr), \) and \( h_l(kr) \). In particular, the incident plane wave (as in Eq. (7)) can be expanded
\[
\phi_k(r) = (2\pi)^{-3/2} e^{ik \cdot r} = (2\pi)^{-3/2} \sum_{l=0}^{\infty} (2l + 1)^{l} j_l(kr) P_l(\cos \theta), \tag{16}
\]
\( i.e. \ A_l(k;r) = j_l(kr). \)
The delta-shell potential is
\[
U(r) = -\lambda \delta(r - a). \tag{17}
\]

The corresponding wave functions must be linear superpositions of \( j_l(kr) \) and \( h_l(kr) \).
\[
\psi_k(r) = B_l(k)j_l(kr) + C_l(k)h_l(kr) \tag{18}
\]
\( j_l(kr) \) is regular at \( r = 0 \), and \( h_l(kr) \rightarrow e^{ikr}/r \) as \( r \rightarrow \infty. \) \( B_l \) and \( C_l \) can be determined by applying the appropriate boundary conditions at \( r = a. \) For \( a > r \) we have
\[
A_l(k;r) = j_l(kr) + ik\lambda a^2 A_l(k;a)j_l(ka)h_l(ka), \tag{19}
\]
and for \( r > a, \)
\[
A_l(k;r) = j_l(kr) + ik\lambda a^2 A_l(k;a)j_l(ka)h_l(ka). \tag{20}
\]
where
\[
A_l(k;a) = \frac{j_l(ka)}{1 - ik\lambda a^2 j_l(ka)h_l(ka)}. \tag{21}
\]
The first term on the right sides of Eq. (19) and Eq. (20), \( j_l(kr), \) gives the incident plane wave, the more complicated second term yields the scattered wave.
3.2 Time-Dependent Solutions

The time-dependent wave functions are obtained with the following argument: If there were no scattering potential, the incident particles could be described by a wave packet, $\Phi(r - ut, 0)$, moving in the $\hat{k}$ direction as described in connection with equation Eq. (10). At $t = 0$ it can be written as

$$\Phi(r, 0) = \int d^3q \chi(q) \phi_q(r)$$  \hspace{1cm} (22)

$\phi_q(r)$ is the usual plane wave function, Eq. (16), so the integral is just a fourier transform. $\chi(q)$ could be any function that produced a wave packet with the desired properties. We will use the gaussian

$$\chi(q) = \left(\frac{2\sigma^2}{\pi}\right)^{3/4} e^{-\sigma^2(k - q)^2}$$ \hspace{1cm} (23)

This has the advantage that it can be easily integrated.

$$\Phi(r, 0) = (2\pi\sigma^2)^{-3/4} e^{i\mathbf{k} \cdot \mathbf{r}} e^{-r^2/4\sigma^2}$$ \hspace{1cm} (24)

The width $\sigma$ is actually the half width of $|\Phi|^2$. The time-dependent wave function is found by integrating

$$\Phi(r, t) = \int d^3q \chi(q) \phi_q(r) e^{-i\omega_q t}$$ \hspace{1cm} (25)

with $\omega_q = \hbar k^2/2m$. This can be integrated exactly, but the following approximation will turn out to be valuable. We expand the frequency $\omega_q$ about $k$.

$$\omega_q = \omega_k + (q - k) \cdot u + \frac{\hbar}{2m}(q - k)^2$$ \hspace{1cm} (26)

where $u = \hbar k/m$ is the group velocity. The last term is of order $\Delta k/k$ compared with the second, and we neglect it.\(^{12}\)

$$-i\omega_q t \approx i\omega_k t - iq \cdot ut$$ \hspace{1cm} (27)

Then Eq. (25) becomes

$$\Phi(r, t) = e^{i\omega_k t} \int d^3q \chi(q) \frac{e^{iq \cdot (r - ut)}}{(2\pi)^{3/2}} = e^{i\omega_k t} \Phi(r - ut, 0)$$ \hspace{1cm} (28)

This is the first term in Eq. (10), a packet that moves to the right without change in shape along the direction of $\hat{k}$.

\(^{12}\)This term is responsible for the spreading of the packet. We assume that $\sigma$ is large enough that spreading is negligible over the time the collision occurs.
When the packet approaches the scattering center, the effect of the potential $U(r)$ becomes important. We obtain the complete wave function by simply replacing $\phi_q(r)$ in Eq. (25) with the complete solution of (10), $\psi_q(r)$.

$$\Psi(r, t) = \int d^3q \chi(q) \psi_q(r) e^{-i\omega_q t}$$ (29)

The only solution to Eq. (15) with outgoing wave boundary conditions in the asymptotic region is $h_l(kr)$, which in this limit is proportional to $e^{ikr}/r$ regardless of $l$. Therefore the scattered wave term in Eq. (28) becomes with the help of Eq. (27),

$$\Psi_{sc}(r, t) \rightarrow e^{i\omega_k t} \int \frac{d^3q}{(2\pi)^{3/2}} \chi(q) f(q \hat{r}, q) \frac{e^{iqr}}{r} e^{-i q \cdot u t}$$ (30)

Because of the form of $\chi(q)$ (Eq. (23)), the range of integration will be restricted to values of $q$ lying close to $k$. The range of integration is roughly $\Delta k \approx 1/\sigma$. It is plausible to assume that $f(q \hat{r}, q)$ doesn’t vary much in this interval, so it can be replaced by $f(k \hat{r}, k)$ and factored out of the integral. We use the same sort of argument to replace $qr \approx q \cdot kr$. Finally

$$\Psi_{sc}(r, t) \approx e^{i\omega_k t} f(k \hat{r}, k) \int \frac{d^3q}{(2\pi)^{3/2}} \chi(q) e^{iqr} \Phi(kr - ut, 0)$$ (32)

which is the second term in Eq. (10).

The approximations leading up to Eq. (32) are difficult to quantify. There is a more subtle concern in that the final result is independent of the choice of function, $\chi(q)$, used to represent the wave packet. How can scattering, which is the result of interference, be independent of the size and shape of the packets that are interfering? We address both concerns by deriving a more or less exact version of Eq. (32) for the delta-shell potential.

The integral Eq. (28) will be reduced to a one-dimensional numeric integration. First substitute Eq. (14) into Eq. (28) and use the approximation Eq. (27).

$$\Psi(r, t) = e^{i\omega_k t} \sum_l \int \frac{d^3q}{(2\pi)^{3/2}} \chi(q)(2l + 1)^{3/2} a_l(q; r) e^{-i q \cdot u t} P_l(\cos \theta q r)$$ (33)

This includes the incident wave packet, which has already been evaluated. (The expansion Eq. (16) is impractical for numerical computation because of its slow convergence.) We concentrate on the scattered wave function, $\Psi_{sc}(r, t)$, and separate out the angular integrations as follows.

$$\Psi_{sc}(r, t) = \left( \frac{\sigma^2}{2\pi} \right)^{3/4} \sum_l \int q^3 dq I_l(q, \hat{r}) \lambda a^2 (2l + 1)^{3/2} A_l(qa)$$

$$\times \left[ j_l(ka) h_l(kr) j_l(kr) h_l(ka) \right]$$
where
\[ I_1(q, \hat{r}) = \int d\Omega_q \exp[-\sigma^2(k - q)^2 - iq \cdot ut] P_l(\cos \theta_{rq}) \quad (34) \]
The upper term in brackets in Eq. (34) is valid for \( r > a \), the lower term for \( r < a \). We note that this equation refers, explicitly or implicitly, to three different angles: \( \theta_{rq} \) between \( r \) and \( q \), \( \theta_q \) between \( q \) and \( k \), and the actual scattering angle, \( \theta_r \). These are related by the addition theorem
\[ P_l(\cos \theta_{rq}) = \frac{4\pi}{2l+1} \sum_m Y_{l}^m(\theta_q, \varphi_q) Y_{l}^m(\theta_r, \varphi_r) \quad (35) \]
The angular integration can be done with the identity\(^\text{13}\)
\[ \int P_l(z)e^{\rho qz} dz = \frac{\rho^q z}{\rho q} \sum_{k=0}^{l} (-1)^k \frac{P_l^{(k)}(z)}{\rho^k q^k} \quad (36) \]
where \( z = \cos \theta_q \). In our case
\[ \rho = 2k\sigma^2 - iut \quad (37) \]
and \( P_l^{(k)}(z) \) is the \( k \)-th derivative of \( P_l \). The lower limit of the integral at \( z = -1 \) yields a term proportional to \( e^{-\rho q} \), which we neglect.

This last expression quantifies the approximation made by replacing \( \hat{q} \) with \( \hat{k} \) in the scattering amplitude in Eq. (30). Each successive term of the sum in Eq. (35) is reduced by the factor \( \rho q \approx 2\sigma^2 k^2 \). The usual approximation consists in keeping only the first term. The resulting integral is
\[ \Psi_{sc}(r) = \frac{\sigma^{3/2}}{\pi} \left( \frac{2}{\pi} \right)^{1/4} \frac{1}{\rho} \int q^2 dq \exp[-\sigma^2(k - q)^2 - iqut]e^{i\omega t} \times i\lambda a^2 \sum_l (2l + 1)j_l(qa) \left[ j_l(qa)h_l(qr) - j_l(qr)h_l(qa) \right] P_l(\cos \theta_r) \quad (38) \]
This formidable equation does indeed reduce to the second term in Eq. (10) in the limit \( r \to \infty \). It is straightforward to integrate numerically since the integrand is concentrated around the point \( q \approx k \). We integrate it using the trapezoid rule with 20 fixed steps between \( \pm 3\sigma \).

**4 Calculations**

In our simulation the scattering center is placed at the origin of the coordinate system with the \( z \) axis taken along the beam direction. The wave packet starts at some negative distance and moves along the \( z \) axis. The starting coordinates of the individual trajectories are chosen randomly with a distribution given by

|Φ(r, t₀)|² as explained previously. As time elapses, these particles are “carried along” by the incident wave packet. As the packet approaches the scattering center at \( z = 0 \), the interference terms divert some of the particles into the scattered packet, an expanding spherical shell.

The calculation is performed with dimensionless quantities. Distance is scaled by \( \bar{x} = 1/k \) and time by \( \bar{t} = m/\hbar k^2 \). Free particles then have a dimensionless velocity

\[
\frac{d(x/\bar{x})}{d(t/\bar{t})} = u = 1.
\]

There are three adjustable parameters at one’s disposal: the radius and strength of the potential and the size of the wave packet. The size parameter \( a \) in Eq. (17) can be related to physical size by \( a = 0.22 \tilde{a} \sqrt{T} \), where \( T \) is the energy of the projectile in units of MeV/c², and \( \tilde{a} \) is the range of the potential in fm. The calculations shown below use \( a = 3 \), which is the right order of magnitude for a 5 MeV/c² proton scattering from a complex nucleus with \( A = 100 \) or a 100 MeV/c² proton scattering from a single proton. The combination \( a \lambda \) is dimensionless and controls the strength of the interaction.

With these units Eq. (2) becomes

\[
v = \text{Im} \left( \frac{\nabla \Psi}{\Psi} \right)
\]

where

\[
\Psi(r, t) = \Phi(r - ut, 0) + \Psi_{\text{sc}}(r, t)
\]

Here \( \Phi \) is the incident wave packet calculated analytically from Eq. (28), and \( \Psi_{\text{sc}} \) is obtained from Eq. (38) by numeric integration. Eq. (40) defines a familiar computational problem, a set of coupled first-order differential equations with known initial conditions. The calculation is done in spherical components:

\[
\frac{\partial r}{\partial t} = \frac{\partial}{\partial r} S(r, \theta, t)
\]

\[
\frac{\partial \theta}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial \theta} S(r, \theta, t)
\]

We use the one-step Runge-Kutta low-order solver (ode23) that is part of the MathLab package.

### 4.1 Results: \( R \) and \( S \)

The conventional quantum mechanical view of scattering is embodied in the function \( R = |\Psi| \) in Eq. (1), whereas the pilot wave perspective is contained in \( S \). These are illustrated in Figure 1 and 2. The situation shortly after this has taken place is shown in Figure 1 and Figure 2. Figure 1 shows a “snapshot” of \( R \) at time \( t = 30 \) following a typical scattering event. The incident wave packet (truncated to make the scattered wave easier to see) is obvious centered at \( z = 30 \). The plot shows a slice through the scattered wave along the \( x-z \)
plane so that it appears like a donut. The packet width was chosen to be \( \sigma = 4 \), so the details could be seen clearly. There is a strong p-wave component to the scattering, which is evident in the shape of the packet.

Figure 2 shows the same instant from a pilot wave perspective. The \( S \) function can be visualized as a complicated surface: a sort of incline plane on which particles “slide” up in the direction of the local gradient. Incident particles slide up a flat plane with slope \( v_z = 1 \). Scattered particles slide up the inside of a cone with radial velocity \( v_r = 1 \). Both features are visible in this plot.

These plots depict an asymptotic condition, i.e. one in which Eq. (7) is approximately valid. The actual scattering takes place near \( t = 0 \). At this time \( S \) becomes extremely complicated as particles are channelled out of the incident wave packet and into the expanding spherical wave. None of these details are visible in \( R \).

4.2 Trajectories

A small sample of trajectories is plotted in Figure 3. The calculation was done for \( \lambda = 5 \) and \( \sigma = 6 \). The incident and forward scattered particles are clearly evident. Obviously the trajectories are not bouncing off the shell as they would in classical scattering, but rather swept around the sphere by the flow of current \( j \). One can discern “ripples” in the current just upstream from the scattering center, which are responsible for pushing the trajectories into the backward part of the outgoing wave.

4.3 The Significance of Cross Section

Even though the pilot wave approach describes scattering in terms of causal trajectories, the classical notion of an impact parameter is not relevant. The point is that the complete set of initial conditions for a trajectory consists not only of \( x_0 \) and \( y_0 \) (measured perpendicular to the scattering axis), but also \( z_0 \), the initial distance measured from the center of the wave packet. The differential cross section as it is usually defined in quantum mechanics is

\[
\frac{d\sigma}{d\Omega} = \frac{dN_{\text{sc}}/d\Omega}{dN_{\text{inc}}/dA}
\]

where \( dN_{\text{inc}} \) is the number of particles crossing the element of area \( dA \) normal to \( k \) in the incident beam, and \( dN_{\text{sc}} \) is the number of particle scattered into the solid angle \( d\Omega \). This assumes a configuration in which there are a vast number of scattering centers that cover a very small fraction of the cross sectional area of the beam. Our regime with a single scattering center and a relatively small wave packet\(^{14}\) cannot approach this limit. We can still assume that

\[
\frac{d\sigma}{d\Omega} \propto \frac{dN_{\text{sc}}}{d\Omega}
\]

\(^{14}\)The size of the wave packet is limited by computation time. The larger the packet, the smaller the fraction of particles that scatter out of the forward direction.
The constant of proportionality depends on the number of particles in the initial wave packet, the size of the packet, and the strength of the interaction. We will not attempt to calculate it, but we can still compare the DCS obtained by numerical experiments via (45) with the DCS obtained analytically from the asymptotic scattering amplitude using (9). A representative “experiment” is shown in Figure 4. The theoretical curve is normalized to the total number of events in the data sample. The fit is good ($\chi^2 = ????)$ except in the forward direction. The failure to reproduce the forward cross sections is an artifact of the small wave packets used in our calculation. The mechanism is as follows: after scattering, a “shear” develops between the incident packet (the first term on the right of Eq. (10)) and the the scattered packet (the second term). Particles that find themselves in this region after scattering are swept into the forward direction leaving a notch in the angular distribution. This is another way of saying that there is interference in the forward direction between the scattered and unscattered wave. This is a well-know phenomenon in other contexts. Here it happens at somewhat larger angles because of the relatively small size of the wave packet.

As mentioned above, there is a unique mapping between the starting location $(x_0, y_0, z_0)$ of the particle in the wave packet and the final scattering angle. The details of the mapping are quite complicated, but it is clear that most of the scattering takes place on the backward fringes of the wave packet. This can be understood roughly as follows: Scattering takes place in the interference region between the incident and scattered packets. This region doesn’t develop until the incident packet at least arrives at the scattering center. Particles that move through this region are those situated toward the back of the incident packet. It would thus seem that the shape of the angular distributions should depend sensitively on the shape of the wave packet. It is remarkable that despite this, the pilot wave formalism reproduces the differential cross sections using a gaussian packet that was chosen for no particular reason other than mathematical convenience. The shape of the distributions is independent of the size of the packet (except for the forward interference effect mentioned above), and presumably any other reasonable shape would work as well so long as the distribution of starting locations was consistent with $\rho = |\Phi|^2$.

5 Conclusions

We have obtained time-dependent wave functions for the delta-shell potential that are valid in the small-$r$ regime. We use these as input to the pilot-wave formalism to calculate scattering trajectories for a variety of scattering situations. These calculations illustrate the mechanics of causal trajectories as well as some important issues in time-dependent scattering theory, such as the role of the wave function in suppressing interference effects and the meaning of the differential cross section. Finally it provides an opportunity to explore some features of the potential model such as the variation of the cross section with energy, potential parameters, and angular momentum. The software package is...
available for general use at our website.