

Understanding Quantum Scattering in the Pilot Wave Formalism

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1 Prologue

Quantum mechanics is beset by paradoxes, perhaps the greatest of which is that it works at all. Within this one paradox are many sub-paradoxes. The two-slit interference experiment is an example: massive particles make interference patterns just as light waves do, but the particles themselves are indivisible point-like objects. To account for the phenomenon one must somehow believe that the *possibility* that a particle *might* have gone through one slit interferes, constructively or destructively, with the possibility that it might have gone through the other.

Quantum scattering is another sub-paradox in the same genre. Particle accelerators accelerate particles and detectors mark their passing, but their distributions resemble interference patterns. The many manifestations of a single particle passing to the right of a scattering center, we are told, interfere with those of the same particle passing to the left.

There is a way of formulating quantum mechanics that has had some success resolving these conundrums. 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. The theory works by abandoning wave-particle duality. There are waves and there are particles, but they are separate entities. Particles pursue deterministic trajectories under the influence of a potential, not unlike particles in classical electro-magnetism. The potential itself arises from the dark mills of quantum mechanics and is ultimately non-local and spooky. The theory is controversial in that it implies that the conventional Copenhagen interpretation of quantum mechanics is wrong. It appeals to people (like myself) who think it is wrong anyway.

Much of the current interest in the theory is due to John Bell who championed it throughout his career.¹ Bell regarded it as, if not the ultimately correct interpretation of quantum mechanics, at least the prototype of such an interpretation. It has been featured in *Physics Today*,² and is the subject of a recent book, *The Quantum Theory of Motion* by Peter Holland.³ Pilot wave theory has become, if not mainline physics, at least a semi-respectable cottage industry.

Pilot wave theory has an additional virtue even if one disregards its philosophical implications: the theory is not wrong. It gives the same results as conventional quantum mechanics in those situations where they can be directly compared, but in a way that is conceptually and non-trivially different. I am tempted to say that quantum mechanics *should* be like this. Whether it actually is is a separate question.

Pilot wave theory explains the two-slit interference experiment as follows: the source emits a stream of particles, electrons let's say, and these particles follow smooth trajectories on their way to the detector. The trajectories are completely deterministic; if we knew exactly the initial conditions of any particle we could calculate its exact path through the system. The trajectories are very sensitive to these conditions however. 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.

Why then is the interference pattern observed? The particles move under the influence of a potential field that is derived from the Schrodinger 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 the electric and magnetic fields that are calculated using Maxwell's equations.

Quantum scattering, in a subtle way, is even more puzzling. The two-slit device automatically localizes the particles. The slits can be regarded as microscopic quantum sources. Particle accelerators, on the other hand, are mammoth devices. It is not clear how and on what scale the localization takes place. Elementary scattering theory treats the process in a time-independent way. The incident particles are represented by a plane wave that fills all space. One avoids the bizarre consequences of this assumption by ignoring them.

¹John Bell, *Speakable and Unsayable in Quantum Mechanics*

²Sheldon Goldstein, *Quantum Theory Without Observers – Part Two*, *Physics Today*, April 1998, pp 38-42

³*The Quantum Theory of Motion*, Peter Holland, Cambridge University Press, 1993

There is a more respectable approach to scattering theory in which the plane wave is replaced by wave packets. The packets are assumed to be much larger than the range of the interaction but smaller than macroscopic sizes. This avoids the formal problems inherent in the time-independent approach,⁴ but at the expense of introducing two new difficulties: one conceptual and one mathematical. The conceptual difficulty is this: accelerators produce particles, not packets. The packets seem not to correspond to anything in the “real world.”⁵ The mathematical treatment deals with “asymptotic” behavior: the differential cross section is derived from the properties of the wave packet after it has spread far beyond the scattering center. The connection between the interaction region and the asymptotic region is made with some rather vague approximations, however.⁶ It is hard to avoid the impression that the differential cross section, which can be measured, must somehow depend on the exact nature of the wave packet, which is a mathematical fiction.

This project addresses a very specific question: is the wave packet formalism an adequate representation of quantum scattering? To put it another way: are the asymptotic results of scattering theory independent of the microscopic details of the wave packets? I really don’t know the complete answer to this question. The best I can say is that, in some situations, yes. The complete answer will require much more research, partly because there are so many details to think about, and partly because the calculations require a lot of computing time to get accurate results. You are invited to participate in this research. Please let me know what you learn.

The equations of motion in pilot wave theory are typically coupled nonlinear differential equations that cannot be solved analytically. This is probably one reason why the theory was not accepted more readily. The calculations are easily within the reach of modern computers and software, however, so simulations such as this exercise are topical as well as useful instruction in a variety of theoretical and computational topics. I have written the code in MATLAB 6⁷ because of the many algorithms and graphic tools that are part of the MATLAB package.

⁴These will be explained presently.

⁵Unlike the slits, which are demonstrably real.

⁶In fact, there are situations in which the approximations are known to be invalid.

⁷The MathWorks Inc

2 Pilot Wave Theory

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

Let's make this more concrete by explaining in a few rules how to derive trajectories from wave functions.

1. Solve the time-dependent Schrodinger equation using whatever potential is relevant to the problem. The usual rules of linear superposition apply.⁸
2. Take the wave function obtained in this way and decompose it as follows

$$\psi(\mathbf{x}, t) = Re^{iS/\hbar} \quad (1)$$

The new functions R and S are real functions of \mathbf{x} 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. From it we obtain the equations of motion

$$\mathbf{v} = \frac{d\mathbf{x}}{dt} = \frac{1}{m} \nabla S(\mathbf{x}, t) \quad (2)$$

4. Equation (2) is a set of coupled first-order ordinary differential equations. The solution $\mathbf{x}(t)$ gives the position of the particle as a function of time. If we knew that the particle was at $\mathbf{x}(t_0)$ at time t_0 we could find the complete trajectory by numerically integrating (2). (Finding analytic solutions is a hopeless task except in the case of a few "toy" problems.) The trajectories determined in this way are unique and smooth.

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

$$\mathbf{j} = \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi) = R\mathbf{v} \quad (3)$$

⁸The significance of operators is somewhat different, however.

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

$$\nabla \cdot (R\mathbf{v}) + \frac{\partial R}{\partial t} = 0 \quad (4)$$

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 (\mathbf{x},t) has by virtue of its position a velocity \mathbf{v} , and it will follow the path along the streamline given by the solution of (2). Even if one does not believe that quantum particles follow deterministic trajectories (and this is certainly not the usual interpretation) 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 (2) with Newton’s second law of motion

$$\frac{d^2\mathbf{x}}{dt^2} = -\frac{1}{m}\nabla\phi(\mathbf{x},t) \quad (5)$$

Equation (5) defines a force field, or more properly, an acceleration field. A particle at (\mathbf{x},t) has by virtue of its position, a certain acceleration. This acceleration comes about because of the potential ϕ (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. Equation (2), by contrast, defines a *velocity* field and fixes the subsequent motion with a single condition.

Equation (5) bothered physicists for two centuries because of the mysterious nature of ϕ . How could the sun, for example, move the earth 96 million miles away when there was nothing in between but empty space? This was called “action at a distance,” and it seemed no better than believing that the earth was moved along by angels! We now know that potentials are a consequence of deeper theories involving the exchange of particles such as photons or gravitons. Pilot waves are also an action at a distance theory. The S function comes about because of mysterious non-local quantum mechanical interactions with other particles and with the experimental apparatus. Even if it is not the ultimate reality behind quantum mechanics, it may be a useful step toward some more complete theory.

3 Scattering Theory

3.1 A Few Basics

The scattering of quantum particles from a fixed potential is covered in every introductory quantum text. The development invariably goes like this; the

following wave function “looks like” it might be relevant to scattering.

$$\psi \propto e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\frac{e^{ikr}}{r} \quad (6)$$

More specifically, it 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, $e^{i\mathbf{k}\cdot\mathbf{r}}$, 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.

The second step is to substitute the *second* term of (6) into (3). One easily finds

$$\mathbf{j} \propto |f|^2/r^2 \quad (7)$$

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

$$\frac{d\sigma}{d\Omega} = |f|^2 \quad (8)$$

This argument is wrong 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 ψ is substituted into (3) there appear interference terms proportional to $1/r$, which at macroscopic distances dominate the $1/r^2$ terms by typically thirteen orders of magnitude.⁹ The second difficulty is that (6) 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 Schrodinger 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

⁹A poor approximation.

still in contact). This is described mathematically as follows: Equation (6) is replaced by the following time-dependent solution.

$$\Psi(\mathbf{r}, t) = e^{i\omega_k t} \Phi(\mathbf{r} - \mathbf{v}_k t, 0) + e^{i\omega_k t} \frac{f(\hat{\mathbf{r}})}{r} \Phi(r\hat{\mathbf{k}} - \mathbf{v}_k t, 0) \quad (9)$$

The function $\Phi(\mathbf{r} - \mathbf{v}_k t, 0)$ represents a wave packet centered at $\mathbf{r} = \mathbf{v}_k t$ moving with the group velocity $\mathbf{v}_k = \hbar\mathbf{k}/m$. At $t = 0$ the packet is centered at $\mathbf{r} = 0$, which is the scattering center. The scattered spherical wave packet is $\Phi(r\hat{\mathbf{k}} - \mathbf{v}_k t, 0)$ where $\hat{\mathbf{k}}$ is a unit vector in the \mathbf{v}_k direction. The second term of (9) is substituted into (3) (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 (8).

The argument is semi-quantitative at best. True, the interference terms vanish at large distances, but it is not clear what they are doing inside the packets during the scattering process. The usual derivation requires various approximations, particularly some assumptions about the size of the wave packet. This point is puzzling. Why should the physical results depend on something so artificial as a wave packet? Real accelerators, after all, produce particles, not packets.

Despite this, scattering theory works. Equation (8) together with all the procedures that have been developed for calculating f seem to describe the real world. The purpose of this project is to develop some insight into how and in what circumstances the wave packet formalism works. We are open to the possibility that wave functions are not a valid description of the scattering process and that some other formalism is required. Our approach is to calculate the pilot wave functions R and S using a wave packet approach that does not require the approximation $r \rightarrow \infty$. The physical content of these functions can be exhibited in various ways, both by calculating particle trajectories and by visualizing the functions directly.

3.2 More Theory

In order to describe the model used in this project, it is necessary to summarize the techniques used to find scattering solutions of Schrodinger's equation. This material is covered in most quantum texts. I have found the treatment in Gottfried's *Quantum Mechanics* particularly helpful.¹⁰

The wave equation can be written as follows:

$$(\nabla^2 + k^2)\psi(\mathbf{r}) = U(r)\psi(\mathbf{r}) \quad (10)$$

¹⁰Kurt Gottfried, *Quantum Mechanics, Vol I*, Advanced Book Classics, Benjamin, 1989

where

$$E = \frac{\hbar^2 k^2}{2m} \quad (11)$$

$$U(r) = \frac{2m}{\hbar^2} V(r) \quad (12)$$

Scattering problems are best solved using a Green's function that has the right asymptotic boundary conditions "built in to it." The Green's function for (10) is defined by the following equation:

$$(\nabla^2 + k^2)G_k(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (13)$$

The solution is well known from classical as well as quantum scattering.

$$G_k(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \quad (14)$$

This expression looks simple, but it is ambiguous because of the singularity at $\mathbf{r} = \mathbf{r}'$. In fact it is this ambiguity that makes it possible to construct Green's functions with the right asymptotic boundary conditions. One exploits this opportunity by writing G_k as a fourier transform in complex k space and choosing the integration contour appropriately.

The simplest solution to (10) is

$$\psi(\mathbf{r}) = \int G_k(\mathbf{r}, \mathbf{r}')U(r')\psi(\mathbf{r}')d^3r' \quad (15)$$

We are free to add to this any solution to the homogeneous equation

$$(\nabla^2 + k^2)\phi = 0 \quad (16)$$

This is the natural way to take into account the unscattered wave

$$\phi_k(\mathbf{r}) = (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (17)$$

since this would be the solution to (10) in the absence of a potential. The general solution is therefore

$$\psi(\mathbf{r}) = \phi_k(\mathbf{r}) + \int G_k(\mathbf{r}, \mathbf{r}')U(r')\psi(\mathbf{r}')d^3r' \quad (18)$$

This is the basic integral equation of scattering theory. Its solutions will have the form

$$\psi(\mathbf{r}) = \phi_k(\mathbf{r}) + \psi_{\text{sc}}(\mathbf{r}) \quad (19)$$

The last term is called the “scattered wave.”

There are various techniques for solving an equation like (18). We will use the method of separation of variables. Solutions of (16) can be written as sums over “partial waves.”

$$\phi_{\mathbf{k}}(\mathbf{r}) = \sum_{l=0}^{\infty} R_l(k; r) P_l(\cos \theta) \quad (20)$$

The Legendre polynomials are functions of θ , the angle between \mathbf{k} and \mathbf{r} . The radial functions, $R_l(k; r)$, satisfy

$$\left[\frac{1}{r} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 \right] R_l(k; r) = 0 \quad (21)$$

The solutions of (21) are the spherical Bessel functions, j_l , n_l and h_l . Their asymptotic behavior is important. As $\rho \rightarrow \infty$

$$\begin{aligned} j_l(\rho) &\rightarrow \frac{1}{\rho} \sin\left(\rho - \frac{\pi l}{2}\right) \\ n_l(\rho) &\rightarrow -\frac{1}{\rho} \cos\left(\rho - \frac{\pi l}{2}\right) \\ h_l(\rho) &\rightarrow \frac{1}{i^{l+1} \rho} e^{i\rho} \end{aligned}$$

Only j_l is regular at $\rho = 0$. It can be used to construct plane wave functions as follows:

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta) \quad (22)$$

This formula is important theoretically, but it is not of much use for computation: it converges very slowly for large r . The complex function h_l is the obvious choice to represent outgoing spherical waves.

The Green’s function (14) can be expanded using these functions.

$$G_{\mathbf{k}}(|\mathbf{r} - \mathbf{r}'|) = \sum_{lm} Y_{lm}(\hat{\mathbf{r}}) Y_{lm}(\hat{\mathbf{r}}') G_{\mathbf{k}}^{(l)}(r; r') \quad (23)$$

This expansion will enable us to reduce the three-dimension equation (18) to a one-dimensional equation in the variable r as we shall see presently. It can be shown that

$$G_{\mathbf{k}}^{(l)}(r; r') = -ik j_l(kr_{<}) h_l(kr_{>}) \quad (24)$$

The notation $r_{<} (r_{>})$ means r or r' , whichever is smaller (larger).¹¹

¹¹Students of electro-magnetism will recognize this as a “patchwork” Green’s function. See J. D. Jackson, *Classical Electrodynamics*, Wiley, Sec. 3.9

3.3 The Model

There are very few potentials for which (18) can be solved exactly, and most of these are quite unrealistic. It can be solved numerically, but an analytic solution would allow us to do numerical experiments quickly without being concerned with the complications of this very non-trivial integral equation. The issue of precision is especially important. The equations of motion that govern the particle trajectories must be solved numerically. When these trajectories pass close to the scattering center they become nearly unstable. Small errors in the calculations can have large effects on their subsequent paths.

Fortunately there is a potential for which we can obtain exact and interesting solutions. This is the delta-shell potential

$$U(r) = -\lambda\delta(r - a) \quad (25)$$

Here a is the diameter of the shell, and λ is a parameter that determines the strength of the potential. (A negative λ makes the potential repulsive, a positive λ , attractive.) The potential is zero inside and outside the sphere, but the wave functions in the two regions satisfy different boundary conditions. The wave function outside must decrease like $1/r$ as $r \rightarrow \infty$, whereas the wave function inside must be at least regular at $r = 0$. The two solutions must be continuous at $r = a$. This leads to the following wave function, which should be compared with (20).

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} \frac{2l+1}{\sqrt{8\pi^3}} i^l A_l(k; r) P_l(\cos \theta) \quad (26)$$

The functions $A_l(k; r)$ are obtained from the radial wave equation.

$$\left[\frac{1}{r} \frac{d}{dr} r^2 \frac{d}{dr} - \frac{l(l+1)}{r^2} - U(r) + k^2 \right] A_l(k; r) = 0 \quad (27)$$

The curious normalization in (26) is chosen so that if $U = 0$ and $A_l(k; r) = j_l(kr)$, then from (22)

$$\psi(\mathbf{r}) \rightarrow (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}}$$

Substituting (23), (22), and (26) into (18), we get the radial equation that was anticipated in the previous section:

$$A_l(k; r) = j_l(kr) + \int_0^\infty G_k^{(l)}(r; r') U(r') A_l(k; r') r'^2 dr' \quad (28)$$

Our delta-shell potential makes this integration trivial and reduces (28) to an algebraic equation. For $a > r$,

$$A_l(k; r) = j_l(kr) + ik\lambda a^2 A_l(k; a) j_l(kr) h_l(ka), \quad (29)$$

and for $r > a$,

$$A_l(k; r) = j_l(kr) + ik\lambda a^2 A_l(k; a) j_l(ka) h_l(kr). \quad (30)$$

The constants $A_l(k; a)$ are obtained by solving (29) or (30) with $r = a$

$$A_l(k; a) = \frac{j_l(ka)}{1 - ik\lambda a^2 j_l(ka) h_l(ka)} \quad (31)$$

This potential might describe, in a very rough way, the surface of a nucleus. Much more important is the fact that the solutions have all the mathematical properties one would expect from a more realistic potential. For example they exhibit bound states and resonant scattering states. The analytic properties of the scattering amplitude are all consistent with the results of more general scattering theory.

The solution to (18), $\psi_k(\mathbf{r})$, is a time-independent wave function, which is inadequate for reasons already explained. The time-dependent wave function is obtained with the following argument. If there were no scattering potential, the incident wave packet, $\Phi(\mathbf{r} - \mathbf{v}_k t, 0)$, would move in the $\hat{\mathbf{k}}$ direction as described in connection with equation (9). At $t = 0$ it can be written as

$$\Phi(\mathbf{r}, 0) = \int d^3q \chi(\mathbf{q}) \phi_q(\mathbf{r}) \quad (32)$$

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

$$\chi(\mathbf{q}) = \left(\frac{2\sigma^2}{\pi}\right)^{3/4} e^{-\sigma^2(\mathbf{k}-\mathbf{q})^2} \quad (33)$$

This has the advantage that it can be easily integrated.

$$\Phi(\mathbf{r}, 0) = (2\pi\sigma^2)^{-3/4} e^{i\mathbf{k}\cdot\mathbf{r}} e^{-r^2/4\sigma^2} \quad (34)$$

The parameter σ is called the ‘‘width’’ of the gaussian.¹² The time-dependent wave function is found by integrating

$$\Phi(\mathbf{r}, t) = \int d^3q \chi(\mathbf{q}) \phi_q(\mathbf{r}) e^{-i\omega_q t} \quad (35)$$

¹²More precisely, σ is the half width of $|\Phi|^2$.

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

$$\omega_q = \omega_k + (\mathbf{q} - \mathbf{k}) \cdot \mathbf{v}_k + \frac{\hbar}{2m} (\mathbf{q} - \mathbf{k})^2$$

where $\mathbf{v}_k = \hbar \mathbf{k}/m$ is the group velocity. The last term in ω_q is of order $\Delta k/k$ compared with the second, and we neglect it.¹³ Then (35) becomes

$$\Phi(\mathbf{r}, t) = e^{i\omega_k t} \int d^3q \chi(\mathbf{q}) \frac{e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{v}_k t)}}{(2\pi)^{3/2}} = e^{i\omega_k t} \Phi(\mathbf{r} - \mathbf{v}_k t, 0) \quad (36)$$

This is the first term in (9), a packet that moves to the right along the direction of $\hat{\mathbf{k}}$.

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 $\phi_q(\mathbf{r})$ in (32) with the complete solution of (18), $\psi_q(\mathbf{r})$.

$$\Psi(\mathbf{r}, t) = \int d^3q \chi(\mathbf{q}) \psi_q(\mathbf{r}) e^{-i\omega_q t} \quad (37)$$

This automatically satisfies the time-dependent Schrodinger equation, since $\psi_q(\mathbf{r})$ is a time-independent solution with energy eigenvalue $\hbar\omega_q$. Unfortunately, this last equation cannot be integrated exactly, even if one is lucky enough to have an exact expression for $\psi_q(\mathbf{r})$. It can be shown however, that $\Psi(\mathbf{r}, t)$ reduces to (9) in the limit $r \rightarrow \infty$. This argument appears in all the standard texts. We outline it here because we will use the same technique to obtain an approximate solution to (37) for small r .

Our solution to the delta-shell potential for $r > a$, (26) and (30), has the form of an incident plane wave and an outgoing scattered wave consisting of an infinite sum of terms proportional to $h_l(kr)$. (Of course, all solutions to (18) have this property outside the range of the potential.) Because of the asymptotic form of $h_l(kr)$ the scattered wave term in (37) becomes, in the limit $r \rightarrow \infty$

$$\psi_{\text{sc}}(\mathbf{r}, t) \rightarrow \int \frac{d^3q}{(2\pi)^{3/2}} \chi(\mathbf{q}) f(q\hat{\mathbf{r}}, \mathbf{q}) \frac{e^{ikq}}{r} e^{-i\omega_q t} \quad (38)$$

The function f contains an infinite series of terms proportional to $P_l(\cos \theta)$ where θ is the angle between \mathbf{q} and $\hat{\mathbf{r}}$, but it does not depend on r .

¹³This term is responsible for the spreading of the packet. We assume that σ is large enough that spreading is negligible over the time the collision occurs.

Because of the form of $\chi(\mathbf{q})$ (equation (33)), 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 $f(q\hat{\mathbf{r}}, \mathbf{q})$ doesn't vary much in this interval, so it can be replaced by $f(k\hat{\mathbf{r}}, \mathbf{k})$ and factored out of the integral.¹⁴ This leaves the integrand with a complex phase $\varphi = qr - \omega_q t$. We expand the frequency ω_q about \mathbf{k} as before. Then

$$\varphi \approx \omega_k t + qr + \mathbf{q} \cdot \mathbf{v}_k t$$

Since the values of \mathbf{q} lie close to \mathbf{k} , we can replace $qr \approx \mathbf{q} \cdot \hat{\mathbf{k}}r$ so that

$$\varphi \approx \omega_k t + \mathbf{q} \cdot (\hat{\mathbf{k}}r - \mathbf{v}_k t)$$

With all these approximations then

$$\begin{aligned} \psi_{\text{sc}}(\mathbf{r}, t) &\approx \frac{e^{i\omega_k t}}{r} f(k\hat{\mathbf{r}}, \mathbf{k}) \int \frac{d^3 q}{(2\pi)^{3/2}} \chi(\mathbf{q}) e^{i\mathbf{q} \cdot (\hat{\mathbf{k}}r - \mathbf{v}_k t)} \\ &\approx \frac{e^{i\omega_k t}}{r} f(k\hat{\mathbf{r}}, \mathbf{k}) \Phi(\hat{\mathbf{k}}r - \mathbf{v}_k t, 0), \end{aligned} \quad (39)$$

which is the second term in equation (9).

We will be especially interested in trajectories that pass close to the scattering center where this asymptotic expansion is not appropriate. We can get a better approximation by noting that $\psi_{\text{sc}}(\mathbf{r})$ has the form

$$\psi_{\text{sc}}(\mathbf{r}) = \sum_l C_l h_l(kr) P_l(\cos \theta).$$

The constants C_l are determined by (26), (30), and (31), but their exact form does not concern us here. The radial functions have the form

$$h_l(\rho) = \frac{g_l(\rho)}{i^{l+1}} \frac{e^{i\rho}}{\rho}$$

where $g_l(\rho)$ is an l 'th order polynomial in powers of $1/\rho$. Consequently

$$\psi_{\text{sc}}(\mathbf{r}) = \frac{e^{ikr}}{r} \sum_l \frac{C_l}{i^{l+1} k} g_l(kr) P_l(\cos \theta) \quad (40)$$

In the limit $\rho \rightarrow \infty$, $g_l(\rho) \rightarrow 1$. Comparison with (6) shows that

$$f_k(\cos \theta) \rightarrow \sum_l \frac{C_l}{i^{l+1} k} P_l(\cos \theta) \quad (41)$$

¹⁴There are important circumstances in which this is not true. This comes about when there are sharp resonant states. See Gotfried Section 16

We don't need to make this approximation, however, because we have an exact solution for $\psi_{\text{sc}}(\mathbf{r})$. This enables us to define a "generalized scattering amplitude," $\tilde{f}(\mathbf{r}, \mathbf{k})$, which is a function of the magnitude of r as well as its direction.

$$\tilde{f}(\mathbf{k}, \mathbf{r}) = \sum_l \frac{C_l}{i^{l+1} k} g_l(kr) P_l(\cos \theta) \quad (42)$$

We can now repeat the derivation of (9) with $\tilde{f}(\mathbf{k}, \mathbf{r})$ replacing $f_k(\cos \theta)$. The result is exact (up to $r = a$) in the sense that it does not involve any large- r approximations. It is still approximate in the sense that we have replaced \mathbf{q} with \mathbf{k} in equations (36) and (39). The error due to this replacement can be made arbitrarily small by making the the wave packet much larger than the scattering center.

3.4 Units and Dimensions

There are two lengths that are fundamental to the scattering process. The first of these is the size of the particles that are scattering. In nuclear and particle physics these sizes are on the order of 1 fermi = 10^{-13} cm. Nucleons and charged pions whose size can actually be measured by electron scattering have radii of roughly 1.4 fm. Complex nuclei typically have radii equal to $1.4 A^{1/3}$ fm, where A is the atomic number. Evidently the nucleons pack together like hard spheres.

Quantum scattering theory attempts to model these complex structures using potentials. A simple example is the Yukawa potential,

$$U(r) = V \frac{e^{-\alpha r}}{\alpha r}$$

In this potential V represents the strength, and $1/\alpha$ the range of the potential, or equivalently, the size of the scattering center. Unfortunately, even this simple function leads to a time-independent Schrodinger equation that is impossible to solve analytically. For this reason we have adopted the delta-shell potential

The other fundamental length is the wavelength of the incident particle. A plane wave in quantum mechanics is $\phi \sim e^{ikx}$, so the natural variable to represent this length is the inverse of the wave number $k = p/\hbar$. To get a feeling for the numbers involved, think of a proton with a mass of 938 MeV/ c^2 . If $k = 1 \text{ fm}^{-1}$, the corresponding kinetic energy is 4.6 MeV. This is an easy energy to achieve, even with relatively primitive accelerators. (At this energy the proton is moving about 20% the speed of light, a complication we do not consider here.)

These two lengths can be thought of in analogy with optical microscopes. In order to resolve an object of size ℓ it is necessary to use light with a wavelength $\lambda \leq \ell$. In order to study the internal structure of a nucleon, it is necessary to use higher energy probe particles with smaller k^{-1} . The motivation for building higher energy accelerators is basically this, to study the internal structure of particles with higher resolution.

There are two other sizes that are not fundamental, but rather peculiar to this calculation. The first of these is the size of the wave packet, σ . The previous discussion of approximations highlights the fact that the momentum spread in the packet, $\Delta k/k$, must be small enough to allow the replacement $\mathbf{q} \rightarrow \mathbf{k}$. For gaussian wave functions, $\Delta x \Delta k = 1/2$, so $\Delta k \approx 1/2\sigma$. The packet must also be substantially larger than the scattering center, so $\sigma > a$.

The potential strength parameter, λ , has units of inverse length. Its significance will be discussed in the next section.

There are no fundamental units of time in scattering theory. This is almost a truism, since scattering calculations are often done in a time-independent formalism. Wave packets introduce a fundamental velocity, the group velocity $v = \hbar k/m$, but the packets reach the detectors eventually, we don't much care when. We can take advantage of this fact to simplify the calculations. We introduce a unit of distance $x_o = 1/k$, and a unit of time $t_o = x_o/v$; t_o is obviously the time required for a free particle to travel the distance $1/k$. It is as close as we can come to a fundamental unit of time; but numerically, (assuming k is measured in fm's)

$$t_o = 1.58 \times 10^{-23} k^{-2} \text{sec},$$

an inconceivably small unit. If we agree to measure all distances in units of x_o and time in units of t_o , however, the dimensionless velocity

$$u = \frac{d(x/x_o)}{d(t/t_o)}$$

is unity for all free particles.

We can simplify the programming even further by noticing that all distance variables like r appear in the equations multiplied by k . Likewise the potential range a is always multiplied by k or λ . The size of the wave packet σ gets multiplied by k . As a consequence, there are only three independent pieces of information that can be input to the program, the dimensionless numbers ka , σk , and λa . All of the output can be expressed in dimensionless ratios such as x/x_o and t/t_o .

You can take advantage of this in one of two ways. The easiest is to set $k = 1$ and remember that a , σ , and λ must be in units of k^{-1} . For

example, $a = 2$ means that the fundamental length, k^{-1} is half the size of the scattering center. The other way is to inter k in units of inverse fermi's (or nautical miles, whatever your favorite unit of distance). Then a , σ , and λ must be in the same units. Distance and time will be rescaled in the output and on the plots so that $dr/dt = 1$.

3.5 Properties of the Potential

The time-independent wave function for the delta-shell potential has some interesting properties that are investigated in Gottfried's book.¹⁵ I will summarize them without any proofs.

1. There are bound state solutions for positive λ . These have negative energy in general. Pilot wave trajectories are not well suited to bound state problems, which are really steady state phenomena. Just for the record, however, if $\lambda a = 2l_o + 1$, there is a bound state of angular momentum l_o with energy zero. As λa increases beyond $2l_o + 1$, the state becomes more tightly bound. There are bound states for all values of $l < l_o$.
2. In the limit $|\lambda a| \rightarrow \infty$ the shell becomes impenetrable: particles inside can't get out and particles outside can't get in. In this limit there can be positive energy bound states inside the sphere.
3. The total scattering cross section can be calculated from phase shifts using the general formula

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l.$$

When $\delta_l = \pi/2$ one says that there is an l -wave *resonance* at the corresponding energy. At this energy the cross section will have a maximum value given by $4\pi(2l+1)/k^2$ (in addition to contributions from other partial waves.)

The delta-shell potential produces a complicated set of resonances. Gottfried works out the properties of the s-wave resonances in some detail. It turns out that there are two kinds, sharp resonances and broad resonances. Broad resonances appear near $ka = \pi/2, 3\pi/2, 5\pi/2, \dots$ and sharp resonances near $ka = \pi, 2\pi, 3\pi, \dots$. The number of resonances is roughly $\lambda a/\pi$.

¹⁵Op. cit. Section 15

4. In the vicinity of the sharp resonances, the amplitude varies so rapidly with energy that the approximation of replacing \mathbf{q} with \mathbf{k} in (36) and (39) is no longer valid. This interesting regime is treated in Section 16 of Gottfried's book.

4 Running the Software

The program is written in MATLAB 6. This is a collection of programming tools intended to be “all things to all people.” The language itself looks superficially like Fortran and is optimized for fast, large scale numerical calculations. Its unique feature is the ability to do matrix calculations with very compact abstract notation and to dynamically re-size matrices as the calculation proceeds. Except for these features (which are maddeningly non-intuitive) the language is easy to learn and fun to use. I have relied on the text, *Mastering Matlab 6*.¹⁶ The on-line help facility will tell all you need to know about specific commands and functions.

I have made no attempt to write a user interface. Think of the program as a “test bed,” which you can rewire to do many different experiments. This requires that you learn some MATLAB and understand how the program works. Here are some important things to know. The main routine is called `Pshift`. It would be helpful to have the listing in hand while we go over some details.

Variables declared “global” are common to all subroutines. They are like “common” variables in Fortran except that they must keep the same name wherever they appear. They are used here to communicate the various parameters to the rest of the program. Change them here and you change them everywhere.

The “turnoff” and “stopclock” variables were originally used for debugging, but they are useful to get a feeling for various parts of the calculation in isolation. `turnoff1` controls the incident wave. Set `turnoff1=0` to see what happens if the scattered wave appears (as if by magic) without any interference from in incident wave. If you just set `turnoff2=0`, you get the incident wave without scattering. `turnoff3=0` replaces the gaussian wave packets with plane wave and spherical wave solutions. Finally, `stopclock=0` gives the paradoxical situation of trajectories propagating through a time-independent wave function.

The next lines let you change k , σ (called `sigma0`), the range of the potential a (called `a0`), and λ (called, surprise, `lambda`). The number of

¹⁶*Mastering Matlab 6*, D. Hanselman and B. Littlefield, Prentice Hall, 2001

trajectories integrated through the potential is given by `nX0s`.

The next section of code integrates trajectories through the scattering process. The center of the wave packet moves from the point $z_o = tstart * u$, goes through the scattering center $z = 0$ at $t = 0$, and continues to $z = tfinish * u$. The initial conditions for the trajectories are contained in the arrays `X0` and `Z0`. These are generated with a gaussian distribution of width σ about the center of the wave packet. There is a table of ten starting locations in the code. These are useful if you want to check the reproducibility of the calculations under various circumstances.¹⁷

The equations of motion can be solved numerically by a variety of different algorithms. Look for the statement `[T,R]=ode23(...` MATLAB has a suite of seven different solvers for this sort of problem. See the Help menu under “ODE” for more details. The statement `options=odeset(...` allows you to adjust the integration tolerances. I have written my own solver called `MyOde`. It is crude algorithm using a fixed step size. The issue of integration routines is discussed further in the last section.

The following four plots, figure(1) through figure(4), are self-explanatory. Figure 4 is a 3-d plot with coordinates x , z , and t . You can “pick it up” and rotate it. The initial and final points on the trajectories are saved in arrays and written to a file named `Results.doc`. It contains the initial coordinates `X0` and `Z0`, the final coordinates `Xsave` and `Zsave`, the distance from this point to the origin `Rsave`, and the final scattering angle `Thetasave`. There is a simple program `Pplot` that reads this file and histograms the results. There is no user interface. You can change the code to plot whatever you like.

The last section produces time dependent plots of the various pilot wave functions. Figure 5 is a gradient plot (or quiver plot in Matlab terminology) of the S function. The arrows point in the direction of ∇S . Contour lines of constant S are superimposed. Figure 6 is a surface plot of S , and 7 is a plot of R . The plots are first produced for time $t = tmin$. The program then goes into pause mode to give you a chance to study the plots. Press any key, and the program steps on to $t = tmin + \Delta t$, etc.¹⁸ Note that while in the pause mode the CPU is running at 100%.¹⁹ This makes it difficult to get things done and makes the computer vulnerable to hang-ups.²⁰

¹⁷The random number generator generates a different sequence of numbers each time the program is run.

¹⁸The meaning of this time unit was explained previously.

¹⁹Doing nothing is hard work. You can always interrupt MatLab by pressing Ctrl-c.

²⁰Matlab makes it easy to make movies of sequences of plots like these. Try it if this sort of thing appeals to you. You can even add music!

We conclude this section with two technical notes, the first about the S function. S is really an angle, so from a mathematical point of view it is infinitely multiple-valued. So far as the physical interpretation is concerned, however, it is unique. For example, if $\psi = e^{ikx}$ then $S = \hbar kx$ and $\nabla S = \mathbf{p}$. On the other hand, if we try to calculate S numerically, for example, $S = \hbar \ln \psi/i$, we get an S that flip-flops between $-\pi$ and $+\pi$. MatLab provides the function `unwrap` that smooths out these jumps. It only works in one dimension, however. Unwrapping in two dimensions is an interesting computational problem. The algorithm I have written is not 100% successful. Occasionally you will see jagged cliffs in the S plots. They are probably not due to the physics you are investigating. Also note that the gradients are calculated analytically. They are not angles and do not suffer from this problem.

The second point has to do with dimensionality. The formalism is three dimensional in the sense that the full 3-d Schrodinger equation is used. The starting coordinates are all chosen in the x - z plane, however. Since there is no spin, the scattering stays in the same plane. In this sense the calculation is 2-d, and there is no φ angle. This is only of concern in interpreting the differential cross section. For example, a constant scattering amplitude would give a constant $d\sigma/d\Omega$ in the full 3-d formalism. In this calculation it produces a constant $d\sigma/d\theta$.

5 Running the Program Again for the First Time

The program is ready to run. If you are using the Physics Department network, copy the folder `PacketScattering` into your own directory. Open MATLAB with the command `matlab &`, and set the Current Directory (in the upper right corner of the MATLAB window) to the directory into which you have copied the source files. Type `Pshift` at the MATLAB prompt.

The program is set to generate 100 trajectories with a potential radius $a = 1$ and a packet width $\sigma = 2$. It first generates the four trajectory plots, then draws the three time-dependent plots as explained above. Press any key and the program will redraw the last three plots with t incremented by 1. You can terminate at any point by pressing Ctrl-c.

Figure 4 is easy to interpret. It shows the trajectories just as you would draw them. You can look at this plot with your browser without running the program. It is in the directory as file `Trajectories.jpg`. Notice the clear separation between the forward or unscattered particles and those for which you would calculate a differential cross section.

Figure 5 is a combination contour plot and quiver plot. The colored lines are contours of equal S . The arrows are proportional to ∇S . Of course the arrows *should* always be perpendicular to the contours. This is not always the case for several reasons. The gradient is calculated analytically at discrete points on a grid. The contour lines are drawn on the same grid using some smoothing and interpolation algorithm. If S changes rapidly in a small region, the contours and arrows can get out of alignment. Also the horizontal and vertical scales of the plot are not the same so the angles are distorted slightly. Notice that at first the arrows point “upstream” corresponding to incident unscattered particles. When $t \approx 0$ a complicated interference region develops close to the origin. At later times the outgoing spherical wave appears as the incident packet moves out of the picture.

Figure 6 shows S as a surface in a 3-d plot. Remember that the magnitude of S has no dynamical significance. It’s the slope that counts. Particles, unlike water, always flow up hill, so a plane wave looks like an incline plane and a spherical wave like a cone.²¹

Finally, Figure 7 shows R as a function of time. Of course, R is the square root of the usual quantum mechanical probability function, so this is a more conventional view of scattering. Watch for the development of the outgoing spherical wave. (In this view it looks like a donut.) Notice that the spherical wave “turns on” around $t = 0$. This is an important point. The time-independent solution, equation (6), implies that the incoming and outgoing waves interfere over all space and consequently over all time as well. The time-dependent solution automatically insures that the scattered wave doesn’t develop until the wave packet reaches the target.²² The last frame is available as a .jpg file. Look for `Wave packet.jpg`.²³

The `Pshift` program automatically writes (overwrites actually) the file `Results.doc` as described in Section 4. The program `Pplot` reads the file and histograms the results. Just type `Pplot` at the prompt.

²¹It may be surprising that a wave packet solution produces a flat S . For a free particle, at least, the packet shape is contained in R and the dynamics are in S . Think of it like this; the packet is a block that slides with constant velocity up the incline S plane!

²²To be consistent we should use a wave packet for the target as well. This point is discussed at length in Goldberger and Watson, *Collision Theory*, Wiley 1964. It turns out to have no effect on the final solution.

²³MATLAB can export graphics in many different formats. Consult *Mastering MATLAB* for details.

6 Think and Do

After you have run the program and experimented with some of the adjustable parameters, you might want to conduct some independent investigations. Here is a list of suggested experiments or projects to work on. Some of these are really physics research, others are more oriented toward computation. Take your pick.

1. What does quantum scattering really look like in a completely time independent formalism? This question was investigated extensively in the 70's using the impenetrable sphere potential.²⁴ You can model this by setting `stopclock=0`. The following claims have been made: (1) There is no scattering at macroscopic distances, *i.e.* all trajectories are eventually swept forward into the beam. (2) It is still possible to make sense of the total cross section (not, of course, the differential cross section). (3) Trajectories with very small impact parameters “crawl” around the surface of the sphere and become surface waves. (4) There is a vacuum region directly in front of the sphere just as there would be in the flow of a compressible fluid. Most of these results were obtained analytically, often with some semi-classical approximation. See if you can verify them numerically.
2. Scattering really comes about because of complicated interference between the incident and scattered wave. See how simple scattering would be without this interference. First set `turnoff2=0`. Watch the wave packet in Figure 7 move across the screen without change of shape. The gradient plot consists of straight lines. Look at the scattered wave by setting `turnoff1=0`.

For the remainder of these experiments keep all the turnoffs and stop-clock set equal to one.

3. Matlab has many sophisticated graphics features. You might, for example, make movies of some scattering process. I would be interested in seeing the time development of the trajectories in Figure 4. The point is that particles travel at different speeds through the scattering region. This seems to violate the conservation of energy; after all, the conventional potential is zero outside the sphere. The reason for this apparent violation is that there is an additional effective potential

²⁴H. J. Korsch and R. Mohlenkamp, J. Phys. B:Atom. Molec. Phys., Vol. 11, No 11, 1978 and references therein

acting outside the sphere. The pilot wave formalism, in fact, can be thought of as a classical Hamilton-Jacobi mechanics problem with a potential $V + Q$ where V is the usual potential that appears in the Schrodinger equation, and Q , the “quantum potential”

$$Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}$$

4. Study the behavior of the trajectories. Elementary texts often portray scattering in terms of an impact parameter. According to this view, the scattering center looks like an archery target. If you hit the red circle the particle will scatter into the angle $\Delta\theta$. This is all wrong, at least in this formalism.²⁵ The scattering angle depends on the incident particle’s position, both transverse and longitudinal, with respect to the center of the wave packet. This effect is well known in the context of one dimensional scattering.²⁶ So far as I know it has not been investigated in three dimensions. There is a feature in `Pplot` that makes a map of the starting points of the trajectories, color coded according to their final scattering angle. Typically, those particles that start out near the front of the packet are more likely to scatter through small angles or perhaps not scatter at all. Can you say anything more about this? Can you explain how this comes about?²⁷
5. All this brings me to the central question. Is quantum scattering really independent of the size (and other details) of the wave packet? With this program you can set the size to be anything you like to study the effects.
6. Is it possible to make sense of the differential cross section when there is only one scattering center? Is it independent of the size of the packet?
7. All the above exercises should be done, at least at first, using the delta-sphere potential. You are welcome to try your hand at phase shifts. The information necessary to do this is contained in the appendix. This is not exactly “kosher”, because the phase shift formalism is based on the asymptotic solution and is not expected to be meaningful near $r = 0$. Nonetheless, the results could be interesting. What is the

²⁵As T. S. Elliot put it, “Man can not bear too much reality.”

²⁶C. Dewdney and B. J. Hiley, *Found. Phys.*, **12**, 27-48.

²⁷If so, will you explain it to me?

effect, for example, of a resonant partial wave? Inelastic scattering can be represented phenomenologically with complex phase shifts. What does inelastic scattering look like in this formalism? (This is another virgin research topic.)

8. I have written a routine called `MyODE` that integrates the equations of motion using a primitive algorithm with fixed step size. This is a deliberate swindle. More sophisticated algorithms get into trouble at isolated regions where the phase cancellations are particularly delicate. My routine avoids this by “goose stepping” through the potential. It gives results that are qualitatively reasonable; I make no claims about its precision. MATLAB provides seven different integration routines, all with different algorithms. You could make a project studying how well they perform. One way to do this is to integrate forwards and then backwards to see if, in the words of T. S. Elliot, “In our end is our beginning.”²⁸

7 APPENDIX A— File List

The following files must be present in the same directory to run the programs: `fshell`, `Fvec`, `gradS`, `jfile`, `modulus`, `MyOde`, `Pplot`, and `Pshift`. MatLab automatically links the files when you enter `Pshift` on the console.

There are two additional files, `Trajectories.jpg` and `Wave Packet.jpg`. These are picture files intended for promotional purposes. Open them with your browser.

8 APPENDIX B— Using Phase Shifts

You can run the program with phase shifts rather than the delta-shell potential. Simply change line 14 in `fshell` from `phaseshifts=0` to `phaseshifts=1`. You can enter your own phase shifts at line 105. The format is `d=[d0, d1, d2, ...]`. `di` is the phase shift for the *i*-th partial wave. The program currently has a single resonant p-wave phase shift.

²⁸Four Quartets