April 5

Identification of the Scattering Amplitude

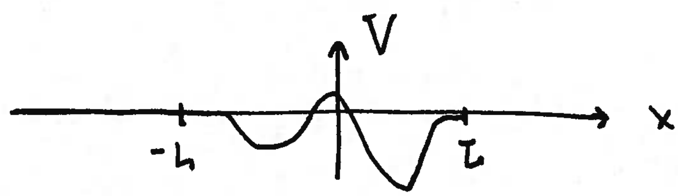
In the previous lecture, I described the scattering of a quantum-mechanical particle from a potential in general terms. The brute-force method for computing the results of a scattering process would involve solution of a time-dependent partial differential equation. I claimed that there was an easier method. In this lecture, I will explain that this calculation can be reduced to the analysis of the time-independent Schrödinger equation. The basic tool for this analysis will be the wavepackets that I described at the end of the previous lecture.

The method is easiest to explain for scattering in 1 dimension. Consider the Hamiltonian

$$H = \frac{p^2}{2m} + V(x)$$

where

$$V(x) = 0 \quad \text{for} \quad |x| > L$$



Not much can happen in this system; the quantum particle can either be reflected from the potential or transmitted through it. I will develop a formalism to compute the probability of reflection or transmission.

We can find solutions of the Schrödinger equation with fixed energy. In the region $-L < x < L$, these solutions are complicated, but it is easy to solve the Schrödinger equation for $x < -L$ and for $x > L$. In these regions, the solutions are just plane waves

$$\varphi_k(x) = e^{\pm ikx} \qquad E = \frac{k^2}{2m}$$

The Schrödinger equation may have eigenfunctions with $E < 0$, bound states, but in the regions outside $-L < x < L$, only eigenfunctions with $E > 0$ extend to infinity. Bound state wavefunctions fall of exponentially outside this region.

A general solution of the time-independent Schrödinger equation with $E > 0$ has the form

$$A_k e^{ikx} + B_k e^{-ikx}$$

for $x < -L$ and

$$C_k e^{ikx} + D_k e^{-ikx}$$

for $x > L$. Since we are solving a second-order ordinary differential equation, we obtain a unique solution if we apply two boundary conditions. I will choose $A_k = 1$, $D_k = 0$. This choice is called "outgoing boundary conditions", for reasons that will be clear shortly. We can write the solution as

$$\varphi_k(x) = \begin{cases} e^{ikx} + R(k)\, e^{-ikx} & x < -L \\ T(k)\, e^{ikx} & x > L \end{cases}$$

with more complicated behavior in the region $-L < x < L$.

I would now like to use this solution to analyze the problem of scattering of a wavepacket that is set up far to the left of the potential and moves across it to the right. Start from

$$\psi(x) = \int \frac{dk}{2\pi}\, e^{-ikx_0} (4\pi\Delta)^{\frac{1}{4}} e^{-\frac{\Delta}{2}(k-k_0)^2} \varphi_k(x)$$

where $x_0 \ll -L - \sqrt{\Delta}$. I claim that this is a wavepacket of size $\sqrt{\Delta}$ localized near x_0. To check this, first evaluate the integral in the region $x < -L$. To do this, put in the above form for $\varphi_k(x)$ and perform the integrals as we did at the end of the previous lecture. The term e^{ikx} gives

$$\psi(x) = \frac{1}{(\pi\Delta)^{1/4}} e^{ik_0(x-x_0)} \exp\left[-\frac{1}{2\Delta}(x-x_0)^2\right]$$

For the term with $R(k)$, if Δ is very large (if the initial momentum or energy is very well defined), we can approximate

$$R(k) \approx R(k_0)$$

Then this term gives a reflected Gaussian centered at $-x_0$ or $|x_0|$, far to the right.

$$R(k_0) \frac{1}{(\pi\Delta)^{1/4}} e^{ik_0(-x-x_0)} \exp\left[-\frac{1}{2\Delta}(x+x_0)^2\right]$$

However, our analysis is valid only for $x < -L$, and so only the part of this Gaussian that extends into the region $x < -L$ is correctly calculated. If we take x_0 to lie far to the left, we can make the contribution from this second Gaussian as small as we wish.

There is a nice way to understand this cancellation of the second term that extends to the other regions. If $x_0 \ll -L$, the factor

$$e^{-ikx_0}$$

is a rapidly oscillating phase factor in the dk integral. Unless it is compensated, the integral over k will annihilate any contribution. In the expression we are dealing with here, the first term of $\varphi_k(x)$ gives the factor

$$e^{ik(x-x_0)}$$

which does compensate the phase near $x = x_0$, but the second term has only the factor

$$e^{-ikx - ikx_0}$$

which does not compensate the phase for any $x < 0$. A similar argument shows that there are no significant contributions to the integral if x is near 0 or if $x > 0$. Notice that, if the coefficient D_k were nonzero, we would have a phase factor

$$e^{-ik(x+x_0)}$$

with slow variation near $x = -x_0 > 0$. The choice of outgoing boundary conditions, with $D_k = 0$ removes this possibility. Then the initial condition is a wavepacket of size $\sqrt{\Delta}$ localized near $x = x_0$.

$$\psi(x) \approx \frac{1}{(\pi \Delta)^{1/4}} e^{ik_0(x-x_0)} \exp\left[-\frac{1}{2\Delta}(x-x_0)^2\right]$$

Next, turn on the time-dependence of this solution by replacing

$$\varphi_k(x) \longrightarrow \varphi_k(x)\, e^{-i\frac{k^2}{2m}t}$$

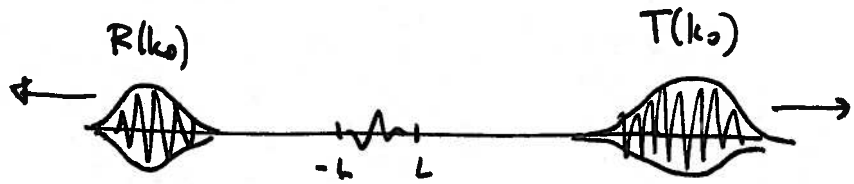
Using the integrals done at the end of the last lecture, we can calculate the time-dependent wavefunction in both asymptotic regions. For $x \ll -L$, we find

$$\psi(x,t) \simeq \left(\frac{\Delta}{\pi\Delta^2}\right)^{1/4} e^{ik_0(x-x_0)} e^{-ik_0^2/2m\, t} \exp\left[-\frac{1}{2\Delta}\left(x-x_0-\frac{k_0}{m}t\right)^2\right]$$
$$+ R(k_0)\left(\frac{\Delta}{\pi\Delta^2}\right)^{1/4} e^{ik_0(-x-x_0)} e^{-ik_0^2/2m\, t} \exp\left[-\frac{1}{2\Delta}\left(-x-x_0-\frac{k_0}{m}t\right)^2\right]$$

For $t < |x_0|/(k_0/m)$, this is a wavepacket moving in from the left. But, for $t \gg |x_0|/(k_0/m)$, the first term moves off to the right and becomes irrelevant to this region of x, while, in the second term, the center of the Gaussian moves into the appropriate region. The solution becomes a wavepacket of amplitude $R(k_0)$ moving to the left. For $x \gg L$, we find

$$\psi(x,t) \simeq \left(\frac{\Delta}{\pi\Delta^2}\right)^{1/4} e^{ik_0(x-x_0)} e^{-ik_0^2/2m\, t} \cdot T(k_0) \cdot \exp\left[-\frac{1}{2\Delta}\left(x-x_0-\frac{k_0}{m}t\right)^2\right]$$

This is essentially zero for $t < |x_0|/(k_0/m)$. For $t \gg |x_0|/(k_0/m)$, the wavepacket emerges into the region $x > L$, and the solution becomes a wavepacket with amplitude $T(k_0)$ moving to the right. The final picture at late times is



The "outgoing boundary conditions" thus correspond to a situation in which a definite wavepacket comes in from the left and an arbitrary linear combination of wavepackets, determined by the potential, exits in both directions.

The initial wavefunction describes *one quantum particle.* The final state should be interpreted as a wavefunction that gives probabilities for this particle to be transmitted or reflected. The probabilities are given by computing the norm of each piece of the wavefunction. From the discussion in the previous lecture, each of the component wavefunctions is normalized. Then we can immediately see that the part of the wavefunction to the left has norm

$$\int_{x<0} dx \, |\psi(x,t)|^2 = |R(k_0)|^2$$

and the part of the wavefunction to the right has the norm

$$\int_{x>0} dx \, |\psi(x,t)|^2 = |T(k_0)|^2$$

These are the probabilities for reflection and tranmission. Because the overall norm of the Schrödinger wavefunction is conserved,

$$|R(k)|^2 + |T(k)|^2 = 1$$

thus, the probabilities sum to 1, as they must.

It is instructive to work out the reflection and transmission probabilities explicitly at least for one example. A simple case is that of a repulsive delta-function potential

$$V(x) = A\,\delta(x)$$

Here, the asymptotic regions contain all points different from $x = 0$. The eigenfunctions of H are

$$\varphi_k(x) = \begin{cases} e^{ikx} + R_k \, e^{-ikx} & x<0 \\ T_k \, e^{ikx} & x>0 \end{cases}$$

with some matching conditions linking the wavefunctions with $x < 0$ and $x > 0$. We can find the matching conditions by integrating the Schrödinger equation

$$\left[-\frac{1}{2m}\frac{d^2}{dx^2} + V(x)\right]\varphi_k(x) = E\varphi_k(x)$$

over a small interval from $x = -\epsilon$ to $x = +\epsilon$. This gives

$$-\frac{1}{2m}\int_{-\epsilon}^{\epsilon} dx\ \frac{d^2\varphi_k}{dx^2} + A\varphi_k(0) = \mathcal{O}(\varepsilon)$$

or

$$-\frac{1}{2m}\left[\frac{d\varphi_k}{dx}(x=\epsilon) - \frac{d\varphi}{dx}(x=-\varepsilon)\right] = -A\varphi_k(0)$$

The wavefunction $\varphi_k(x)$ is thus *continuous* at $x = 0$ with a *discontinuous first derivative.* Thus

$$1 + R_k = T_k$$

$$-\frac{1}{2m}\, ik\left[T_k - (1 - R_k)\right] = -AT_k$$

It is easy to solve these equations, and we find

$$R_k = -\frac{A}{A - ik/m} \qquad T_k = -i\frac{k/m}{A - ik/m}$$

Notice that, automatically,

$$|R_k|^2 + |T_k|^2 = 1$$

The reflection probability $|R_k|^2$ is

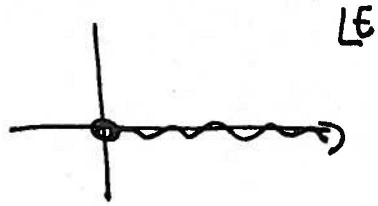
$$|R_k|^2 = \frac{A^2}{A^2 + (k/m)^2}$$

This is 1 at $k = 0$ and decreases monotonically as the energy is increased.

It is interesting to write the reflection coefficient as a function of the energy E,

$$\mathcal{R} = -\frac{A}{A - i\sqrt{2E/m}}$$

and to consider this as a function of E as a complex variable. R_k is an analytic function of E with a square root branch cut extending from 0 to ∞.



Physical values of E correspond to $E > 0$. Later in the course, I will discuss this analytic structure carefuly and argue that the physical region is the axis $E > 0$ *above the branch cut.* To analytically continue the expression for R_k to the rest of the complex E plane, we follow the behavior of $\sqrt{E}$. This function is real and positive above the cut, equal to $i\sqrt{|E|}$ on the negative real axis, and equals $-\sqrt{|E|}$ just below the cut. The analytic function R_k is nonsingular in the whole plane.

However, the same analysis can be applied to the case of an *attractive* delta-function potential

$$V(x) = -B\,\delta(x)$$

The algebra is the same, and we find

$$R = -\frac{B}{B + i\sqrt{2E/m}}$$

Notice that, in this case, the reflection coefficient has a *pole* on the negative E axis, since the denominator vanishes at

$$\sqrt{\frac{2E}{m}} = iB \qquad \text{or} \qquad E = -\frac{mB^2}{2}$$

The significance of this pole is quite interesting. The attractive delta-function potential (and, actually *any* attractive potential in 1 dimension) has a bound state. We can solve for the bound state by writing

$$E_b = -\frac{\kappa^2}{2m}$$

and, solving for the wavefunction away from $x = 0$,

$$\varphi(x) = \begin{cases} a_L e^{\kappa x} & x < 0 \\ a_R e^{-\kappa x} & x > 0 \end{cases}$$

and then applying the matching conditions

$$a_L = a_R \qquad -\frac{1}{2m}(-\kappa)\cdot 2 = +B$$

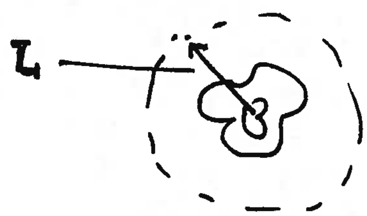
The result is that there is a solution for

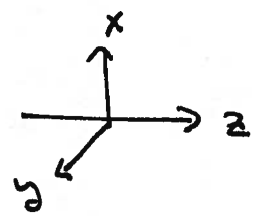
$$\kappa = mB \qquad E_b = -\frac{mB^2}{2}$$

which agrees precisely with the position of the pole found above.

It is amazing that the scattering amplitude, which involves only calcuations for $E > 0$, through the magic of analytic continuation, knows all about the bound state problem at $E < 0$. We will see more examples of this as the course proceeds.

This argument in 1 dimension has a somewhat more subtle generalization to 3 dimensions. To set up the problem, picture a potential in 3 dimensions that is nonzero inside a sphere of radius L.





Outside the sphere, the Schrödinger equation is that of a free particle. We would like to solve the time-independent Schrödinger equation for this problem with a set of boundary conditions appropriate for the relation to scattering. I claim that we can impose the following as "outgoing boundary conditions" for $|\vec{x}| \gg L$:

$$\varphi_k(\vec{x}) = e^{ikz} + \frac{f_k(\theta,\phi)}{r} e^{ikr} + \mathcal{O}\left(\frac{1}{r^2}\right)$$

where $r = |\vec{x}|$. The first term will represent the incoming wavepacket. The second term will represent the scattered wave, with an arbitrary coefficient that is a function of the angles θ and ϕ. This coefficient $f_k(\theta, \phi)$ is called the *scattering amplitude.* The factor of $1/r$ is needed, as we will see, for probability conservation. I will defend this choice of boundary conditions at the end of the lecture by presenting a perturbation series solution for the wavefunction in which every term has the above asymptotic form for $r \gg L$.

I will now explain that this asymptotic form gives the solution to the time-dependent problem in which a wave packet comes in from the left and scatters from the potential, with part of the wave packet missing the target and simply continuing forward while another part is scattered into other directions. To see this, I will start from the wavepacket initial condition

$$\psi(x) = \frac{1}{\sqrt{D^2}} \int \frac{dk}{2\pi} (4\pi\Delta)^{1/4} e^{ik(x-x_0)} e^{-\frac{\Delta}{2}(k-k_0)^2}$$

This is a one-dimensional wavepacket in z of the same form as those we studied earlier in the lecture. We would like the initial values of the momenta k_x, k_y to be very close to zero. To arrange this, we would like the wavepacket to be *constant* in the $\hat{x}$ and $\hat{y}$ directions. For definiteness, I will consider the wavepacket to be confined to a very large box of size $D \gg L$ in the transverse directions. The normalization condition for the box gives the factor $1/\sqrt{D^2}$ in the above equation. It is not difficult to check by examining the phases that, if the factor e^{ikz} is replaced by the above asymptotic form of the Schrödinger wavefunction, the additional terms give no significant contribution if $x_0 \ll -L - \sqrt{\Delta}$. Then then expression

$$\psi(\vec{x}) = \frac{1}{\sqrt{D^2}} \int \frac{dk}{2\pi} (4\pi\Delta)^{1/4} e^{-ikz_0} e^{-\frac{\Delta}{2}(k-k_0)^2} \varphi_k(\vec{x})$$

is a Gaussian wavepacket well localized near z_0 far to the left.

To turn on the time-dependence of the wavefunction, replace

$$\varphi_k(\vec{x}) \longrightarrow \varphi_k(\vec{x})\, e^{-i\frac{k^2}{2m}t}$$

Now we can evaluate $\psi(\vec{x}, t)$ in the asymptotic region for general values of t. For $t \gg |x_0|/(k_0/m)$, the first time of φ_k gives a wavepacket that moves off to the right. This the piece of the wavepacket that misses the target. We should ignore it. The second term of φ_k gives a wavepacket

$$\frac{f_k(\theta,\phi)}{r} \frac{1}{\sqrt{D^2}} \left(\frac{\Delta}{\pi\Delta^2}\right)^{1/4} e^{ik_0(r-z_0)} e^{-i\frac{k^2}{2m}t} \exp\left[-\frac{1}{2\Delta}\left(r - z_0 - \frac{k_0}{m}t\right)^2\right]$$

that moves in the radial direction. Since $r > 0$, this term is negligible for $t < |x_0|/(k_0/m)$, but for $t \gg |x_0|/(k_0/m)$, it is a physical outgoing wavefunction with amplitude $f_k(\theta, \phi)$. The normalization of this piece of the wavefunction is

$$\int dr\, r^2 d^2\Omega \left|\frac{f_k(\theta,\phi)}{r}\right|^2 \frac{1}{D^2} \left(\frac{\Delta}{\pi\Delta^2}\right)^{1/2} \left|\exp\left[-\frac{1}{\Delta}\left(r - z_0 - \frac{k_0}{m}t\right)^2\right]\right|^2$$

Notice that the factors of r cancel. The wavepacket is normalized in 1 dimension, so this integral becomes

$$\int d^3x \; |\psi(x,t)|^2 = \frac{1}{D^2} \int d^2\Omega \; |f_k(\theta,\phi)|^2$$

This is the total probability for the quantum particle in the initial wavepacket to scatter from the potential.

We can easily related this expression to the scattering cross section. The rate of scattering is given by dividing the scattering probability by the time T that it takes the wavepacket to cross through the scattering center. That time is of the order of $\sqrt{\Delta}/(k_0/m)$, but anyway, it will cancel out in a moment. The flux of particles incident on the target is

$$\Phi = \frac{(1 \text{ particle})}{D^2 \cdot T}$$

Then the cross section is

$$\sigma = \frac{\text{rate of scattg}}{\text{flux}} = \frac{\frac{1}{T}\frac{1}{D^2} \int d^2\Omega \, |f_k(\theta,\phi)|^2}{\frac{1}{D^2 T}}$$

which gives

$$\sigma = \int d^2\Omega \; |f_k(\theta,\phi)|^2$$

At the energy $E = k^2/2m$, the differential cross section is

$$\frac{d\sigma}{d^2\Omega} = |f_k(\theta,\phi)|^2$$

The scattering amplitude, defined from the asymptotic expansion of the time-independent Schrödinger wavefunction with outgoing boundary condition, is indeed very simply related to the scattering cross section.

To complete this argument, I need to defend the choice of boundary conditions that I imposed on the Schrödinger wavefunction. I will argue this by constructing a formal solution to the Schrödinger equation as a perturbation theory in powers of the potential V. This expansion, which will be valid at least when the potential is weak, will manifestly have the chosen boundary conditions.

Let us, then, analyze the equation

$$\left[-\frac{1}{2m}\nabla_x^2 + V(x)\right]\varphi_k(x) = E\,\varphi_k(x)$$

with $E = k^2/2m$. We can reorganize the equation as

$$\left[-\nabla_x^2 - k^2\right]\varphi_k(x) = -2m\,V(x)\,\varphi_k(x)$$

where $\nabla_x^2 = (\partial/\partial\vec{x})^2$. Now look for a solution of the form $(\vec{k}_0 = k\hat{z})$

$$\varphi_k(x) = e^{i\vec{k}_0\cdot\vec{x}} + \varphi_k^{(1)}(x) + \varphi_k^{(2)}(x) + \cdots$$

where $\varphi_k^{(n)}(x)$ is of order V^n when V is small. The leading term is a solution to

$$\left[-\nabla_x^2 - k^2\right]\varphi(x) = 0$$

Up to order V^1, then, the equation reads

$$\left[-\nabla_x^2 - k^2\right] \varphi_k^{(1)}(x) = -2m V(x)\, e^{i\vec{k}_0\cdot\vec{x}}$$

Similarly, if we wish to solve the equation to order V^2, we need also to solve

$$\left[-\nabla_x^2 - k^2\right] \varphi_k^{(2)}(x) = -2m V(x)\, \varphi_k^{(1)}(x)$$

and so forth.

There is a systematic way to solve these equations. You are familiar with this from electrostatics, where you studied the Laplace equation

$$-\nabla_x^2 \phi(x) = \rho(x)$$

where the source term on the right-hand side is the distribution of charges. To solve this equation, we first find the solution to the simpler equation

$$-\nabla_x^2 G(x,y) = \delta^{(3)}(\vec{x}-\vec{y})$$

and then write

$$\phi(x) = \int d^3y\; G(x,y)\, \rho(y)$$

The function $G(x,y)$ is called the *Green's function* associated with the operator on the left. It is straightforward to check that the formal solution given is indeed a solution

$$-\nabla_x^2 \phi(\vec{x}) = \int d^3y \, [-\nabla_x^2 G(\vec{x},\vec{y})] \, \rho(\vec{y})$$

$$= \int d^3y \, \delta(\vec{x-y}) \, \rho(\vec{y}) = \rho(\vec{x})$$

The Green's function for the Laplace equation is simply the Coulomb potential of a point charge

$$G(x,y) = \frac{1}{4\pi |\vec{x-y}|}$$

Then the solution of the Laplace equation is given by

$$\phi(\vec{x}) = \int d^3y \, \frac{1}{4\pi|\vec{x-y}|} \, \rho(\vec{y})$$

which you will immediately recognize. I should point out that this formula gives the solution of the Laplace equation for which $\phi(\vec{x}) to 0$ as $\vec{x} \to infty$. We imposed this boundary condition on the solution by imposing the boundary condition on $G(x,y)$ when we solved the equation for the Green's function.

We can apply the same method to the Schrödinger equation above. We need to find the Green's function $G(x,y)$ that satisfies

$$(-\nabla_x^2 - k^2) \, G(x,y) = \delta^{(3)}(\vec{x-y})$$

I claim that the solution is

$$G(x,y) = \frac{1}{4\pi r} e^{ikr} \qquad r = |\vec{x-y}|$$

I will prove this at the beginning of the next lecture. In principle, the exponent could have been $\pm kr$, or we could have had any linear combination of these exponentials. The solution I have written imposes outgoing boundary conditions.

With this Green's function, we can immediately write the solution for $\varphi_k^{(1)}$ as

$$\varphi_k^{(1)}(\vec{x}) = \int d^3y \, \frac{1}{4\pi|\vec{x}-\vec{y}|} e^{ik|\vec{x}-\vec{y}|} \left(-2mV(\vec{y})\right) e^{i\vec{k}_0\cdot\vec{y}}$$

Similarly, for each successive term in the perturbation series

$$\varphi_k^{(n+1)}(x) = \int d^3y \, \frac{1}{4\pi|\vec{x}-\vec{y}|} e^{ik|\vec{x}-\vec{y}|} \left(-2mV(\vec{y})\right) \varphi_k^{(n)}(\vec{y})$$

When we carry out the integrals, we will note that the values of $\vec{y}$ are bounded by $|\vec{y}| <$, since the potential is nonzero only in that region. Thus, if we take the limit $r = |\vec{x}| \to \infty$, each term has the limiting form

$$\frac{1}{4\pi|x-y|} e^{ik|x-y|} \to \frac{1}{4\pi r} e^{ikr}$$

Thus, every term in the perturbation series has the form

$$\frac{1}{r} e^{ikr} \cdot F(\theta,\phi) + O\left(\frac{1}{r^2}\right)$$

and satisfies the outgoing boundary conditions in the form that I postulated above.