Quantum Theory of Scattering

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Contents

1 Scattering in one dimension

We begin by discussing the basic set up of potential scattering problems in one dimension.

1.1 Probability currents, Reflection and Transmission

• Consider the scattering of (say) electrons off a molecule. The scattering centre (molecule) is localized. Far away from the molecule, the electrons feel almost no force. In one dimension, this means the potential due to the molecule $V(x) \to 0$ as $x \to \pm\infty$. In such scattering problems, we are primarily interested in understanding the structure of the molecule. The electrons are called test particles, they are used to determine the nature of the molecular forces. We do so by firing in electrons of definite energy 'from infinity' in one direction towards the molecule (say from $x = -\infty$). Then, based on how the electrons are scattered, in various directions, we try to infer what $V(x)$ is. Or, if we know $V(x)$, then we can predict how the electrons will scatter.

• We seek the energy eigenstates of the 1-dimensional SE $-(\hbar^2/2m)\psi'' + V(x)\psi(x) = E\psi(x)$ with $V(x) \to 0$ as $x \to \pm\infty$. For large $|x|$ the SE reduces to that for a free particle, $\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x)$. If $E < 0$, the wave function would have to decay exponentially at $\pm\infty$ and would not represent a scattering state. So suppose $E \geq 0$, and let $k = \frac{\sqrt{2mE}}{\hbar} \geq 0$. Then asymptotically,

$$\psi(x) \to Ae^{ikx} + Be^{-ikx} \text{ as } x \to -\infty, \quad \text{and} \quad \psi(x) \to Ce^{ikx} + De^{-ikx} \text{ as } x \to \infty. \tag{1}$$

To physically interpret $A, \cdots, D$ we compute the corresponding probability current densities $j = \frac{\hbar}{2mi}\left(\psi^*\psi' - \psi^{*\prime}\psi\right)$

$$\begin{aligned}
j_A &= \frac{\hbar k}{m}|A|^2, \text{ rightward probability current at } x = -\infty \\
j_B &= -\frac{\hbar k}{m}|B|^2, \text{ leftward probability current at } x = -\infty \\
j_C &= \frac{\hbar k}{m}|C|^2, \text{ rightward probability current at } x = \infty \\
j_D &= -\frac{\hbar k}{m}|D|^2, \text{ leftward probability current at } x = \infty
\end{aligned} \tag{2}$$

Exercise: *Show that the probability current as $x \to -\infty$ is the sum $j(x \to -\infty) = j_A + j_B$ and similarly $j(x \to -\infty) = j_C + j_D$.* We say that A is the amplitude of the incoming wave from the left, D the amplitude of the incoming wave from the right, B the amplitude of the outgoing wave on the left and C the amplitude of the outgoing wave on the right. These interpretations are seen to be reasonable if we introduce the harmonic time dependence of energy eigenstates $e^{-i\omega t}$ where $E = \hbar\omega$. Then we have $Ae^{i(kx-\omega t)}$ which represents a right moving wave in the vicinity of $x = -\infty$. Similarly, $Be^{-i(kx+\omega t)}$ represents a left-moving wave at $x = -\infty$, etc.

• For definiteness, suppose particles are sent in from $x = -\infty$ at momentum $\hbar k$, and no particles are sent in from $x = +\infty$. This set up requires $D = 0$. B is called the amplitude of the REFLECTED wave and C is called the amplitude of the TRANSMITTED wave.

• Of particular interest: relative probability current of reflection per unit incoming probability current

$$R = \frac{|j_B|}{|j_A|} = \frac{|B|^2}{|A|^2} = \text{ 'Reflection coefficient'} \tag{3}$$

Similarly, the transmission coefficient is defined as the relative probability of transmission

$$T = \frac{|j_C|}{|j_A|} = \frac{|C|^2}{|A|^2} = \text{ 'Transmission coefficient'} \tag{4}$$

One of the goals of scattering problems is to find these reflection and transmission coefficients (for a given potential) since they can be measured experimentally (e.g. experimentally, R is the ratio of number of particles back scattered to the number of particles sent in per unit time). Of course, we are also interested in finding the allowed scattering energy eigenvalues E, just as we wanted to find the bound state energy levels. However, unlike bound states, typically there is no restriction on the allowed energies of scattering scattering states (they form a continuous spectrum for $E > 0$). Nevertheless, R and T will depend on the energy E. E.g. If the energy of the incoming electrons is very high, most are likely to pass through the molecule and get transmitted, only a few may be reflected.

1.2 Scattering states for a Dirac delta potential

• For the attractive $V(x) = -g\delta(x)$ potential, let us study the scattering problem for an incoming probability current from the left. The solutions of the SE in the regions $x < 0$ and $x > 0$ are

$$\psi(x < 0) = Ae^{ikx} + Be^{-ikx}, \qquad \psi(x > 0) = Ce^{ikx}. \tag{5}$$

We must now impose continuity of $\psi(x)$ at $x = 0$ and discontinuity of ψ' across $x = 0$ by an amount determined as follows. We integrate the SE from $-\epsilon$ to ϵ for small $\epsilon > 0$ to get

$$-\frac{\hbar^2}{2m}(\psi'(0^+) - \psi'(0^-)) - g\psi(0) = E\int_{-\epsilon}^{\epsilon}\psi(x)dx. \tag{6}$$

As $\epsilon \to 0$, the integral on the right vanish due to continuity of ψ. These two conditions will allow us to determine B, C in terms of A, leaving $E \geq 0$ undetermined. In other words, there are scattering eigenstates for all non-negative energies.

• In more detail, continuity at $x = 0$ implies $A + B = C$. In addition,

$$\psi'(0^+) - \psi'(0^-) = -\frac{2mg}{\hbar^2}\psi(0) \;\Rightarrow\; ik(C - A + B) = -\frac{2mg}{\hbar^2}(A + B) \tag{7}$$

We can solve for B, C in terms of A and the wave number k. In fact it is convenient to introduce a dimensionless measure of the strength of the attractive potential $\gamma = \frac{mg}{\hbar^2 k}$. γ is small if the coupling g is weak or the energy E (or k) is large. We find

$$B = \frac{i\gamma A}{1 - i\gamma}, \qquad C = \frac{A}{1 - i\gamma}. \tag{8}$$

In terms of these, the reflection and transmission probabilities are

$$R = \frac{|B|^2}{|A|^2} = \frac{\gamma^2}{1+\gamma^2}, \quad T = \frac{|C|^2}{|A|^2} = \frac{1}{1+\gamma^2}, \qquad \gamma = \frac{mg}{\hbar^2 k} \tag{9}$$

The particles must either be reflected or transmitted, there is nowhere else for them to go. Indeed, we find that $T + R = 1$. With probability one, the particles are either reflected or transmitted.

• Furthermore, $T \to 0$ if $k \to 0$ or $g \to \infty$. Particles of very low energies are not transmitted. Such particles are reflected $R(\gamma \to \infty) = 1$. On the other hand, high energy projectiles tend to be transmitted $T(\gamma \to 0) = 1$. Plot T and R as a function of energy (or γ). What is the critical energy at which there is an equal probability for the particle to be reflected as to be transmitted?

• If we had a repulsive delta-function potential $-g\delta(x), g < 0$, then the sign of γ changes. But the reflection and transmission coefficients are unchanged, being functions only of γ^2. In particular, despite the repulsive force, the particle injected from $x = -\infty$ has a finite probability to penetrate the potential barrier and emerge on the right. This is the classically forbidden phenomenon of quantum mechanical tunneling. A repulsive delta function potential is like a short-range repulsive barrier. Classically, a particle of any finite energy would have been reflected.

• Tunneling is the phenomenon by which a particle can have a non-zero probability of being found beyond a barrier despite having an energy less than the height of the barrier. If the barrier is very high or very wide (when appropriately compared to the energy of the particle), the transmission probability across the barrier is small.

• Tunneling is a wave phenomenon and does not have a simple explanation in terms of particle trajectories. It has been experimentally observed and used to explain several phenomena. E.g. decay of nuclei by emission of α particles. The alpha particle does not have enough energy to classically escape from the nuclear potential. But it occasionally does so, on account of the non-zero tunneling probability. When two conductors are separated by a thin layer of insulator and a current is injected, there can be a current across the insulator due to tunneling. Scanning tunneling microscopes employ tunneling to permit atomic resolution imaging.

1.3 Scattering against a rectangular barrier/well and tunneling

• We consider scattering from the left against a rectangular barrier of width $2a$ modeled by the repulsive potential $V(x) = V_0 > 0$ for $|x| < a$ and zero otherwise. We seek scattering energy eigenstates $E > 0$.

• For $|x| > a$, the equation for stationary states is $\psi'' = -k^2\psi$ where $\hbar k = \sqrt{2mE} \geq 0$. Thus we have a wave Ae^{ikx} incident from the left, a reflected wave Be^{-ikx} and a transmitted wave Fe^{ikx}.

• For $|x| < a$, $\psi'' = \kappa^2\psi$ where $\hbar^2\kappa^2 = 2m(V - E) \geq 0$. So $\psi(|x| < a) = Ce^{\kappa x} + De^{-\kappa x}$.

• Now we must impose continuity of ψ, ψ' at $x = \pm a$.

$$\begin{aligned} x = -a \qquad & Ae^{-ika} + Be^{ika} = Ce^{-\kappa a} + De^{\kappa a}, \qquad ikAe^{-ika} - ikBe^{ika} = C\kappa e^{-\kappa a} - D\kappa e^{\kappa a}. \\ x = a \qquad & Ce^{\kappa a} + De^{-\kappa a} = Fe^{ika}, \qquad C\kappa e^{\kappa a} - D\kappa e^{-\kappa a} = ikFe^{ika} \end{aligned} \tag{10}$$

A, B, C, D, E, F are 6 unknowns. We can choose $A = 1$ to normalize the incoming probability current from the left. The above 4 equations will determine B, C, D, F in terms of the energy $E \geq 0$ which remains arbitrary.

• In more detail, we use the b.c. at $x = a$ to express C, D (which do not appear in the reflection and transmission coefficients) in terms of F

$$C = \frac{F\,(\kappa + ik)}{2\kappa} e^{(ik-\kappa)a}, \quad D = \frac{F\,(\kappa - ik)}{2\kappa} e^{(ik+\kappa)a}. \tag{11}$$

Putting these in the b.c. at $x = -a$ we get

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= \frac{F}{\kappa} e^{ika} \left[\kappa \cosh(2\kappa a) - ik \sinh(2\kappa a)\right] \\ Ae^{-ika} - Be^{ika} &= \frac{F}{ik} e^{ika} \left[ik \cosh(2\kappa a) - \kappa \sinh(2\kappa a)\right]. \end{aligned} \tag{12}$$

Adding we get

$$\frac{A}{F} = \frac{1}{2} e^{2ika} \left[2\cosh(2\kappa a) + i \sinh(2\kappa a) \frac{(\kappa^2 - k^2)}{\kappa k}\right] \tag{13}$$

The transmission coefficient is the absolute square

$$T^{-1} = |A/F|^2 = \cosh^2(2\kappa a) + \frac{1}{4} \sinh^2(2\kappa a) \frac{(\kappa^2 - k^2)^2}{\kappa^2 k^2} \tag{14}$$

Now $\cosh^2 = 1 + \sinh^2$ and $1 + \frac{(\kappa^2 - k^2)^2}{4\kappa^2 k^2} = \frac{(\kappa^2 + k^2)^2}{4\kappa^2 k^2}$. Moreover, $\kappa^2 = \frac{2m}{\hbar^2}(V_0 - E)$ and $k^2 = \frac{2mE}{\hbar^2}$. So

$$\frac{1}{T} = 1 + \sinh^2(2\kappa a)\left\{\frac{(\kappa^2 + k^2)^2}{4\kappa^2 k^2}\right\} = 1 + \frac{1}{4}\frac{V_0^2}{E(V_0 - E)}\sinh^2(2\kappa a). \tag{15}$$

This non-zero transmission coefficient is again a quantum tunneling effect. As $E \to 0$ $T^{-1} \to \infty$, so there is no transmission for $E = 0$. On the other hand, if $E \to V_0$, i.e., the energy is just equal to the barrier height, then using $\sinh x \approx x$ for small x,

$$\frac{1}{T} \to 1 + \frac{2m}{\hbar^2} V_0 a^2 > 1. \tag{16}$$

So the transmission coefficient is less than one even if the energy of the incoming wave is equal to the height of the barrier.

• We can get T for $E > V_0$ by putting $l^2 = 2m(E - V)/\hbar^2$ and $\kappa = il$ in the above formula and use $\sinh(ix) = i \sin x$:

$$\frac{1}{T} = 1 + \frac{1}{4}\frac{V^2}{E(E - V)}\sin^2(2la), \qquad E > V_0. \tag{17}$$

As $E \to \infty$ we see that $T \to 1$ and there is complete transmission as we would expect. Interestingly, we also have $T = 1$ when $2la = n\pi$ for $n = 1, 2, \ldots$ where l is the wave number in the region of the barrier $|x| < a$. If we call $\lambda = 2\pi/l$ the wave length in the region of the barrier, then this condition for reflectionless transmission is $n\frac{\lambda}{2} = 2a$, i.e., an integer number of half-wavelengths must fit in the region of the barrier. The barrier is transparent at certain specific energies!

• We can also get the transmission coefficient for scattering over a finite square well by putting $V_0 \to -V_{well}$. Then

$$\frac{1}{T} = 1 + \frac{1}{4}\frac{V^2}{E(E + V_{well})}\sin^2(2la), \quad l^2 = 2m(E + V_{well})/\hbar^2. \tag{18}$$

Again we have reflectionless transmission if an integer number of half wavelengths fit inside the well. This condition is familiar to us since it also determines the energy levels of the infinite square well.

• Scattering by a finite square well can be used to model the scattering of electrons by atoms. The well represents the attraction between the nucleus and the incident electron. The above transparent scattering at the energy corresponding to $\frac{\lambda}{2} = 2a$ has been observed (Ramsauer effect).

1.4 Scattering matrix in one dimension

• Suppose the potential from which we scatter is localized: $V(x) \to 0$ sufficiently fast as $x \to \pm\infty$. We seek scattering eigenstates of the Schrodinger operator (time-independent Schrodinger equation)

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x) = \frac{\hbar^2 k^2}{2m}\psi(x) \tag{19}$$

The asymptotic behavior of the wave function must be of the form

$$\psi(x) \to \begin{cases} Ae^{ikx} + Be^{-ikx} & as \;\; x \to -\infty \\ Ce^{ikx} + De^{-ikx} & as \;\; x \to +\infty \end{cases} \tag{20}$$

A, D represent the incoming amplitudes from $\pm\infty$ while B, C are the amplitudes of scattered plane waves to $\pm\infty$. An aim of scattering theory is to predict the 'scattering amplitudes' $B(k), C(k)$ given the incoming amplitudes A and D[1], the potential and incoming wave number k, by solving the Schrödinger eigenvalue problem.

• What is more, on account of the linearity of the equation, these quantities must be linearly related. Let S be the 2×2 matrix such that

$$\begin{pmatrix} B \\ C \end{pmatrix} = S(k) \begin{pmatrix} A \\ D \end{pmatrix} \tag{21}$$

S is called the scattering matrix. It takes the amplitudes of the incoming plane waves and transforms them into the outgoing plane waves. The matrix elements of S depend on k, the wave number of the incoming waves as well as on the potential. Moreover, S is a unitary matrix, as we will see shortly.

• To find the $S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix}$ matrix, we need to find its columns (the images of the basis vectors)

$$S \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} S_{11} \\ S_{21} \end{pmatrix}, \quad \text{and} \quad S \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} S_{12} \\ S_{22} \end{pmatrix}. \tag{22}$$

But these we recognize are the scattering problems considered before $A = 1, D = 0$ is scattering of a unit amplitude wave from the far left. So $S_{11} = B/A = r$ and $S_{21} = C/A = t$ are the reflected and transmitted amplitudes for this situation. $A = 0, D = 1$ is the scattering of a unit amplitude wave from the far right. So S_{12} and S_{22} are the transmitted and reflected amplitudes for this situation. Thus, if we know the reflected and transmitted amplitudes for the unit scattering problems from the left and right, we can synthesize the S-matrix. Moreover, if $V(x)$ is even, the transmitted amplitude for unit scattering from the left must be the same as the transmitted amplitude for unit scattering from the right and $S = \begin{pmatrix} r & t \\ t & r \end{pmatrix}$.

• Unitarity of S is the statement that $\langle Su, Sv \rangle = \langle u, v \rangle$ for any pair of vectors u and v. In more detail, $u = \begin{pmatrix} A \\ D \end{pmatrix}$ and $v = \begin{pmatrix} A' \\ D' \end{pmatrix}$ can be any two vectors representing the incoming amplitudes. Then unitarity $SS^\dagger = S^\dagger S = I$ is the statement that inner products (lengths and angles) are preserved:

$$\left\langle \begin{pmatrix} A \\ D \end{pmatrix}, \begin{pmatrix} A' \\ D' \end{pmatrix} \right\rangle = \left\langle S \begin{pmatrix} A \\ D \end{pmatrix}, S \begin{pmatrix} A' \\ D' \end{pmatrix} \right\rangle \quad \text{or} \quad A^* A' + D^* D' = B^* B' + C^* C' \tag{23}$$

To get an idea of why this is true, let us consider first the condition of preservation of norms $\langle u, u \rangle = \langle Su, Su \rangle$ which is the condition $|A|^2 + |D|^2 = |B|^2 + |C|^2$. We recognize this as the conservation of probability current density as shown below.

[1] A, D can be regarded as the two constants of integration of the second order ODE.

• The probability current density (which is proportional to the Wronskian of ψ^* and ψ)

$$j(x,t) = \frac{\hbar}{2mi}\left(\psi^* \partial_x \psi - \partial_x \psi^* \psi\right) \tag{24}$$

is shown to be independent of x, $\frac{\partial j}{\partial x} = 0$ by use of the Schrödinger eigenvalue equation. For an eigenstate, $\rho = |\psi|^2$ is time-independent. So the conservation law $\rho_t + j_x = 0$ becomes $j_x = 0$. So

$$j(-\infty) = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) = j(\infty) = \frac{\hbar k}{m}\left(|C|^2 - |D|^2\right) \quad \Rightarrow \quad |A|^2 + |D|^2 = |B|^2 + |C|^2. \tag{25}$$

This shows the diagonal elements of $SS^\dagger$ are 1 (in any basis). See the hw problem for the rest.

• More generally, to show that $A^*A' + D^*D' = B^*B' + C^*C'$, consider two scattering eigenstates ψ_1, ψ_2 of the Schrödinger eigenvalue problem in a real potential with the same energy E and asymptotics

$$\psi_1(x) \to \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{as } x \to -\infty \\ Ce^{ikx} + De^{-ikx} & \text{as } x \to +\infty \end{cases}, \quad \psi_2(x) \to \begin{cases} A'e^{ikx} + B'e^{-ikx} & \text{as } x \to -\infty \\ C'e^{ikx} + D'e^{-ikx} & \text{as } x \to +\infty. \end{cases} \tag{26}$$

Since $V(x)$ is real, ψ_1^* is also an eigenstate with energy E. We construct the Wronskian

$$W(\psi_1^*, \psi_2)(x) = \psi_1^*(x)\psi_2'(x) - \psi_1^{*'}(x)\psi_2(x). \tag{27}$$

We check that the Wronskian is a constant $W'(x) = 0$ and therefore equate its asymptotic values

$$W(-\infty) = 2ik(A^*A' - B^*B') = W(\infty) = 2ik(C^*C' - D^*D') \tag{28}$$

and conclude that $A^*A' + D^*D' = B^*B' + C^*C'$. In other words, S is unitary.

• Let us look at an example, scattering against a delta-potential well $V(x) = -g\delta(x)$. In this case, for scattering of a unit amplitude plane wave from the left we found that the reflected amplitude is $r = B/A = \frac{i\gamma}{1-i\gamma}$ and the transmitted amplitude is $t = \frac{1}{1-i\gamma}$ where $\gamma = \frac{mg}{\hbar^2 k}$. Thus we find the S-matrix for scattering against a delta well

$$S = \frac{1}{1-i\gamma}\begin{pmatrix} i\gamma & 1 \\ 1 & i\gamma \end{pmatrix}. \tag{29}$$

Check that S is unitary.

• The S-matrix contains all the information about the scattering problem. It allows us to predict the amplitudes of the outgoing waves given any configuration of incoming waves. In particular, we can find the reflection and transmission coefficients from S, $T = |t|^2 = |S_{12}|^2$ and $R = |r|^2 = |S_{11}|^2$.

• Moreover, the S-matrix also encodes information about the bound states ('waves' that decay exponentially at infinity). In general, the bound state energies are given by $E = \hbar^2 k^2/2m$ for each pole k of the S-matrix that lies on the positive *imaginary* k-axis. In the above example, it has a pole in the upper half of the complex k plane at $k = \frac{img}{\hbar^2}$, which corresponds to the energy of the single bound state $E = \frac{\hbar^2 k^2}{2m} = -\frac{mg^2}{2\hbar^2}$.

• Why should poles of the S-matrix on the upper half of the imaginary axis correspond to bound states? Let us give a heuristic argument. For a bound state, there is nothing coming in from

$\pm\infty$. So we will take $A = D = 0$ and suppose $\psi \to Be^{-ikx}$ as $x \to -\infty$ and $\psi \to Ce^{ikx}$ as $x \to \infty$. Moreover, for a bound state, we want the wave function to decay (exponentially) as $x \to \pm\infty$. This will be the case if $k = i\kappa$ with $\kappa > 0$ so that $\psi \to Be^{\kappa x}$ as $x \to -\infty$ and $\psi \to Ce^{-\kappa x}$ as $x \to \infty$. This argument also indicates why the S-matrix cannot have poles in the lower half of the complex k plane. These exponentially decaying waves describe a bound particle trying to explore what lies beyond the classically allowed region without quite propagating out of the well. They are the quantum analogs of evanescent waves/fields (exponentially decaying and not carrying an energy current), say in optics, observed on the 'other side' when light is reflected from a boundary.

• The scattering matrix is unitary, so its eigenvalues are complex numbers of unit magnitude, though they need not be complex conjugates of eachother. For an even potential $S = \begin{pmatrix} r & t \\ t & r \end{pmatrix}$ is a complex symmetric matrix. Unitarity is the pair of conditions $|r|^2 + |t|^2 = 1$ and $rt^* + tr^* = 0$. The eigenvectors of S are $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ with eigenvalues $r + t$ and $r - t$ respectively. Unitarity ensures that $r + t = e^{i\delta_1}$ and $r - t = e^{i\delta_2}$ are complex numbers of unit magnitude. These eigenvectors correspond to incoming amplitudes that scatter to outgoing amplitudes which differ from the incoming ones by a multiplicative phase. δ_1 and δ_2 can be called phase shifts since they encode the shifts in the phases of the incoming amplitudes, due to scattering.

$$S \begin{pmatrix} 1 \\ 1 \end{pmatrix} = (r+t) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = e^{i\delta_1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad S \begin{pmatrix} 1 \\ -1 \end{pmatrix} = (r-t) \begin{pmatrix} 1 \\ -1 \end{pmatrix} = e^{i\delta_2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{30}$$

Asymptotic amplitudes which are eigenvectors of the S-matrix scatter in particularly simple ways with just a change in the asymptotic phase. E.g. the eigenvector $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ corresponds to the situation where plane waves of equal amplitude are incident from both sides of the scatterer. However, the asymptotic amplitudes which are eigenstates of the S-matrix are usually not the most convenient incident amplitudes from an experimental viewpoint, where we send a beam from one side. The situation is worse in three dimensions, where again, we send in plane waves from one side, though the eigenstates of the S-matrix correspond to spherical waves imploding on the target!

2 Scattering in three dimensions: differential scattering cross section

• We are interested in scattering by a (spherically symmetric) potential $V(r)$ which vanishes sufficiently fast as $r \to \infty$. This is two-body scattering after passage to the relative coordinate r. Scattering eigenstates must satisfy the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(r)\psi(\vec{r}) = E\psi(\vec{r}). \tag{31}$$

Interesting examples of scattering potentials are (1) Coulomb $V(r) = \frac{\alpha}{r}$, as in Rutherford scattering of positively charged α-particles by a positively charged nucleus; (2) Screened coulomb $V(r) = \frac{\alpha e^{-\mu r}}{r}$ which is usually relevant when the charge of the scattering center is screened by opposite nearby charges, as in a medium; and (3) hard sphere $V(r) = V_0\theta(r < a)$ as when atoms collide. In most of these situations, we only have access to the particles/waves that are sent in and come out, far from the scattering center. The aim of scattering is to predict the angular distribution of the scattered particles (as $r \to \infty$), given how the particles are sent in (and with what energy). For simplicity, the incoming particles are usually directed at the scattering center in a single collimated beam of fixed energy.

• For scattering in 3d, the S-matrix is infinite dimensional. Since $V \approx 0$ for large r, the incoming and out-going waves are asymptotically free particle energy eigenstates. We can choose any convenient basis for them. E.g. we could send in plane waves with any wave vector $\vec{k}_{in} = k\hat{n}$ pointing radially inward, so the incoming states are labeled by inward directed unit vectors. For outgoing states we could again use plane waves, now with outward directed wave vectors $\vec{k}_{out} = k\hat{n}'$. The magnitude of the wave vector is the same for elastic scattering. Then the S-matrix relates the incoming amplitudes to the outgoing amplitudes, and in particular, $S(\hat{n}', \hat{n})$ gives the amplitude for an outgoing wave vector pointing along $\hat{n}'$ if the incoming wave vector was pointing along $\hat{n}$. Unlike the situation in 1d, where the S-matrix was 2×2, here the S-matrix has a continuously infinite number of rows and columns (each labeled by points on a sphere). We will not pursue the problem of determining the S-matrix directly. Instead we will repeat what we did in 1d, i.e., consider the standard scattering problem of predicting the outgoing amplitudes given that there is a plane wave incident on the target from the left. But in essence this determines the S-matrix, since the columns of the S-matrix are the outgoing amplitudes in the plane wave basis for each possible radial direction of incoming plane wave, just as we found in one dimension.

• The free particles in the incoming collimated beam are modeled by plane waves with wave vector $\vec{k}$. For a spherically symmetric $V(r)$ we can take the incoming wave vector $\vec{k} = k\hat{z}$ to be along $\hat{z}$ without loss of generality. If A is a constant with dimensions of $L^{-3/2}$,

$$\psi_{in}(\vec{r}) = Ae^{i\vec{k}\cdot\vec{r}} = Ae^{ikz} = Ae^{ikr\cos\theta}. \tag{32}$$

The scattered wave function asymptotically for large r is again that of a free particle. However, the direction of linear momentum is not conserved (translation invariance is broken by the presence of a scattering center located around $r = 0$). The scattered wave is not an eigenstate of linear momentum. In fact, we should expect a scattered wave that is roughly a spherical wave, but whose amplitude is more in the forward direction $\hat{z}$ ($\theta \approx 0$) and varies as θ is increased up to π (back-scattered direction $-\hat{z}$).

• To find the general form the scattered wave function ψ_{sc} can take, we must solve (for large r) the free particle SE for energy eigenvalue $E = \hbar^2k^2/2m$ where k is the magnitude of the incoming wave vector. Let us recall how this is done

$$\left(\frac{p_r^2}{2m} + \frac{L^2}{2mr^2}\right)\psi = \frac{\hbar^2k^2}{2m}\psi \quad \text{where } p_r = -i\hbar\frac{1}{r}\partial_r r \quad \Rightarrow \quad p_r^2\psi = -\hbar^2\frac{1}{r}\frac{\partial^2 r\psi}{\partial r^2}.$$

We proceed by separation of variables and seek a solution in the product form $\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$. Separation of variables leads to the pair of equations

$$L^2Y = l(l+1)\hbar^2Y \quad \text{and} \quad -\frac{\hbar^2}{2m}\frac{1}{r}(rR)'' + \frac{\hbar^2 l(l+1)}{2mr^2}R = \frac{\hbar^2k^2}{2m}R. \tag{33}$$

We already know the eigenfunctions of L^2 are $Y_{lm}(\theta,\phi)$. In terms of $u = rR$, the radial equation becomes

$$-\frac{\hbar^2}{2m}u'' + \left(\frac{\hbar^2 l(l+1)}{2mr^2} - \frac{\hbar^2k^2}{2m}\right)u(r) = 0. \tag{34}$$

For very large r[2], the angular momentum term is subdominant compared to the energy eigenvalue term and we get $-u'' = k^2 u$, so $u(r) = a e^{irk} + b e^{-ikr}$ or

$$R_{kl}(r) = \frac{a e^{ikr}}{r} + \frac{b e^{-ikr}}{r}, \quad \text{as} \quad r \to \infty \tag{35}$$

So to leading order in this crude approximation, as $r \to \infty$, the radial wave function is independent of l and consists of a superposition of an outgoing and incoming spherical wave. Since the scattered wave must be outgoing, $b = 0$. The general solution of the free particle eigenvalue problem can be written as a linear combination of separable eigenstates with the same energy

$$\psi(r, \theta, \phi) = \sum_{lm} c_{lm} R_{kl}(r) Y_{lm}(\theta, \phi) \tag{36}$$

As $r \to \infty$ $R_{kl}(r)$ is independent of l, so the scattered wave can be written as

$$\psi_{sc}(r, \theta, \phi) = a \frac{e^{ikr}}{r} \sum_{lm} c_{lm} Y_{lm}(\theta, \phi) \tag{37}$$

But $a \sum_{lm} c_{lm} Y_{lm}(\theta, \phi)$ just represents an arbitrary function of θ and ϕ which we denote $A f(\theta, \phi)$. Thus for large r, the scattered wave may be written as

$$\psi_{sc}(\vec{r}) = A \frac{e^{ikr}}{r} f(\theta, \phi) \quad \text{or} \quad \psi(\vec{r}) = A e^{ikr\cos\theta} + A \frac{e^{ikr}}{r} f(\theta, \phi). \tag{38}$$

This asymptotic form of the wavefunction is called the scattering boundary condition or Sommerfeld radiation boundary condition. It is a boundary condition in the sense that it says there is no incoming wave from infinity (except for the incident plane wave). In fact it can be regarded as a definition of $f(\theta, \phi)$. $f(\theta, \phi)$ is called the scattering amplitude; it has dimensions of length and we will discuss its physical meaning shortly.

• Before doing so let us improve the above argument by not throwing away the centrifugal repulsion term involving angular momentum. Let us work out the simultaneous eigenstates of energy and angular momentum for the free particle. These are $R_l(r) Y_{lm}(\theta, \phi)$. In terms of $u = rR$ and $\rho = kr$, the radial equation becomes the spherical Bessel equation

$$-\frac{d^2 u_l(\rho)}{d\rho^2} + \frac{l(l+1)}{\rho^2} u_l = u_l \tag{39}$$

The solutions are expressed in terms of the spherical Bessel and spherical Neumann functions

$$R_l(\rho) = a_l j_l(\rho) + b_l n_l(\rho) \tag{40}$$

For $l = 0$, $j_0(\rho) = \frac{\sin\rho}{\rho}$ and $n_0(\rho) = -\frac{\cos\rho}{\rho}$. By a method of Infeld, j_l, n_l for $l = 1, 2, 3, \ldots$ can be obtained from j_0, n_0 by applying a raising operator, which raises the value of l without changing the energy $\hbar^2 k^2/2m$. This is explored in the problem set. While j_l are finite at $\rho = 0$, n_l diverge at $\rho = 0$. To see this we return to the radial equation

$$-\frac{\hbar^2}{2m} u''(r) + \frac{l(l+1)}{2mr^2} u = \frac{\hbar^2 k^2}{2m} u(r) \tag{41}$$

[2] r large compared to the incoming wavelength $2\pi/k$, more precisely, $kr \gg l(l+1)$. Actually, this is an over simplification and is strictly valid only for $l = 0$. Even for large r, $R(r)$ depends on l in a manner that we will derive soon.

For small r the energy eigenvalue term may be ignored compared to the centrifugal repulsion to get

$$-u'' + \frac{l(l+1)}{r^2}u = 0 \quad \text{for} \ \ r \to 0. \tag{42}$$

We put the guess $u \sim r^\alpha$ in this equation and get a quadratic equation for α

$$\alpha(\alpha - 1) = l(l+1) \tag{43}$$

with solutions $\alpha = l+1$ and $\alpha = -l$. Thus for small r the two solutions behave like $u_l \propto r^{l+1}$ and $u_l \propto r^{-l}$, or in terms of $R = u/r$, the two solutions behave like $j_l \propto \rho^l$ and $n_l \propto \rho^{-l-1}$. Including the proportionality constants,

$$j_l(\rho) \to \frac{\rho^l}{(2l+1)!!} = \frac{2^l\, l!\, \rho^l}{(2l+1)!} \quad \text{and} \quad n_l(\rho) \to \frac{(2l-1)!!}{\rho^{l+1}} = \frac{(2l)!}{2^l\, l!\, \rho^{l+1}} \quad \text{as} \ \ \rho \to 0. \tag{44}$$

Here $(2l+1)!! = (2l+1)(2l-1)(2l-3)\cdots 5\cdot 3\cdot 1$. However both n_l and j_l contain radially ingoing and outgoing parts and both are polynomials in $\sin\rho$, $\cos\rho$ and $\frac{1}{\rho}$. On the other hand, the linear combinations (spherical Hankel functions of first and second kinds) $h_l^{\pm}(\rho) = j_l(\rho) \pm i n_l(\rho)$ are purely outgoing and purely incoming for all ρ. For example, as $\rho \to \infty$

$$h_l^+(\rho) \to \rho^{-1} e^{i\rho}(-i)^{l+1} \quad \text{and} \quad h_l^-(\rho) \to \rho^{-1} e^{-i\rho} i^{l+1}. \tag{45}$$

Similarly, the asymptotic behavior of the spherical Bessel and Neumann functions are

$$j_l(\rho) \to \rho^{-1}\sin(\rho - l\pi/2) \quad \text{and} \quad n_l(\rho) \to -\rho^{-1}\cos(\rho - l\pi/2) \tag{46}$$

So we can write an energy $E = \hbar^2 k^2/2m$ eigenstate of the free particle hamiltonian as a linear combination of separable angular momentum eigenstates with the same energy

$$\psi(r,\theta,\phi) = \sum_{lm} d'_{lm} R_l(kr) Y_{lm}(\theta,\phi) \tag{47}$$

In particular, the scattered wave must admit such an expansion far from the scattering center where $V \approx 0$. However, the scattering b.c. says that there must not be any incoming spherical wave, so the expansion can only involve the outgoing spherical Hankel functions

$$\psi_{sc}(r,\theta,\phi) = \sum_{lm} d_{lm} h_l^+(kr) Y_{lm}(\theta,\phi) \tag{48}$$

For large kr we use the asymptotic behavior of the spherical Hankel function $h_l^+ \to (-i)^{l+1} e^{i\rho}/\rho$ to get

$$\psi_{sc} \to a\frac{e^{ikr}}{r}\sum_{lm} c_{lm} Y_{lm}(\theta,\phi), \quad \text{where} \quad a c_{lm} = \frac{(-i)^{l+1} d_{lm}}{k}. \tag{49}$$

We conclude that the asymptotic behavior of the scattered wave is a spherical wave modulated by a largely arbitrary function $f(\theta,\phi)$ called the scattering amplitude

$$\psi_{sc}(r,\theta,\phi) = A\frac{e^{ikr}}{r} f(\theta,\phi) \tag{50}$$

To understand the physical meaning of f, we compute the probability current density (for large r) of the incoming and scattered waves (the two don't interfere since the incoming beam is assumed to be collimated in a pipe along the z-axis[3]. More precisely, for any fixed angle $\theta \neq 0, \pi$, we can always choose r sufficiently large so that the point r, θ, ϕ is located outside the beam pipe both in the back and forward scattering directions)

$$\vec{j} = \frac{\hbar}{2mi}\left(\psi^* \nabla \psi - \nabla \psi^* \psi\right) \tag{51}$$

If $d\vec{S}$ is an infinitesimal surface area vector, then $\vec{j} \cdot d\vec{S}$ is the current across dS and can be interpreted as the number of particles crossing infinitesimal area $d\vec{S}$ per unit time.

• The probability current density of the incident wave Ae^{ikz} is $\vec{j}_{inc} = \frac{\hbar k |A|^2}{m}\hat{z}$. The unit cross-sectional area vector in the direction of the incident beam is $\hat{z}$, so $\vec{j}_{inc} \cdot \hat{z} = |A|^2 \hbar k/m$ is interpreted as the number of particles crossing unit cross-sectional area of the incoming beam per unit time.

• For the scattered wave $\psi_{sc}(r) = A f(\theta, \phi)\frac{e^{ikr}}{r}$, one first checks that for large r,

$$\nabla \psi \to A f(\theta, \phi) \frac{\partial}{\partial r}\left(\frac{e^{ikr}}{r}\right)\hat{r} + \mathcal{O}\left(\frac{1}{r^2}\right) \quad \text{using} \quad \nabla = \hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial \theta} + \frac{\hat{\phi}}{r \sin\theta}\frac{\partial}{\partial \phi} \tag{52}$$

Then one finds

$$\vec{j}_{sc} \to \frac{|A|^2 \hbar k |f|^2}{m} \frac{\hat{r}}{r^2} \quad \text{as} \quad r \to \infty. \tag{53}$$

Let us find the scattered probability flux across an infinitesimal area element $d\vec{S} = \hat{r} r^2 d\Omega$ pointing radially outward. Here $d\Omega = \sin\theta \, d\theta \, d\phi$. The scattered probability density current crossing $d\vec{S}$ per unit time (loosely, the number of scattered particles crossing $d\vec{S}$ per unit time) is

$$\vec{j}_{sc} \cdot d\vec{S} = \frac{\hbar k |A|^2 |f|^2}{m} \, d\Omega \tag{54}$$

The scattering amplitude f is not a probability amplitude, $|f|^2$ does not integrate to 1 in general, see below. Note that the scattered flux is zero if $f = 0$, which is the case if $V = 0$. This does not mean that particle number is not conserved in the absence of a potential. In the absence of a potential, there is no scattered wave at all, the incoming plane wave just passes through and all the particles come out with $\theta = 0$ in the form of a plane wave.

• We see that the scattered flux is proportional to the incident flux $\frac{\hbar k |A|^2}{m}$ We define the ratio to be the cross-section for scattering into the angular region $d\Omega$ in the vicinity of $\Omega = (\theta, \phi)$

$$d\sigma(\Omega) = \frac{\vec{j}_{sc} \cdot d\vec{S}}{\vec{j}_{inc} \cdot \hat{z}} = |f|^2 \, d\Omega \tag{55}$$

$d\sigma$ is proportional to the angular element $d\Omega$, so we define the ratio to be the so-called differential scattering cross section

$$\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2 \tag{56}$$

$\frac{d\sigma}{d\Omega} d\Omega = |f|^2 d\Omega$ is the number of particles scattered into the angular region $d\Omega$ per unit time per unit incident flux. So $f(\theta, \phi)$ is the amplitude for *scattering* in the angular direction defined by θ, ϕ. The differential scattering cross section $\frac{d\sigma}{d\Omega} = |f|^2$ has dimensions of an area.

[3] Though the pipe is narrow, it is wide enough so that the largest impact parameters of the incoming particles usually exceeds the range of the potential $V(r)$, which is usually very localized.

• Classically, $d\sigma/d\Omega$ is the cross sectional area of the incident beam through which incoming particles must pass in order to be *scattered* into the angular region $d\Omega$.

• The total scattering cross-section is defined as the integral of the differential scattering cross section over all directions

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int |f(\theta, \phi)|^2 \sin\theta \, d\theta \, d\phi. \tag{57}$$

σ has dimensions of area. The total cross section σ can be thought of as the total effective cross-sectional area (normal to the incident beam) presented by the scattering potential. If $V = 0$, the scattering x-section vanishes, there are no scattered particles, yet particle number is conserved since there is an undeflected incoming beam that passes through.

• An aim of scattering theory is to determine the differential scattering cross section, given the potential V. This is called the direct scattering problem. This is the problem we will address. For this, it suffices to find the scattering amplitude $f(\theta, \phi)$, which will depend on the potential V, energy of the incoming waves, m and $\hbar$. In fact, for a spherically symmetric potential, we have cylindrical symmetry about the z-axis of the incoming beam, so $f(\theta, \phi) = f(\theta)$ must be independent of ϕ.

• There is another interesting problem, the inverse scattering problem, whose aim is to reconstruct the potential given the scattering data (i.e., the differential scattering cross section or scattering amplitudes). This is a much harder problem, but is of great practical importance in fields such as tomography (medical imaging CAT (computed axial tomography), PET (positron emission tomography) scans, seismic imaging, oil exploration etc.)

3 Partial wave expansion

• As mentioned, direction of linear momentum is not conserved in the scattering process, but angular momentum is conserved for a spherically symmetric potential. This suggests we can decompose the scattering problem into different angular momentum sectors labeled by l. Roughly, the component parts of the wave function corresponding to different values of angular momentum quantum number l are the 'partial waves'. The overall strategy is simple: solve the Schrödinger eigenvalue problem in the potential $V(r)$ with the above scattering boundary condition and determine the scattering amplitude $f(\theta)$. The partial wave expansion is an approach to find $f(\theta)$ as a sum over over partial amplitudes of increasing l. Truncating the partial wave expansion after the first few partial waves provides a good approximation especially for low energy scattering, i.e. where the wavelength $2\pi/k$ of the incoming beam is large compared to the range of the scattering potential a: $ka \ll 1$.

3.1 Partial wave amplitudes

• For a spherically symmetric potential $f(\theta, \phi) = f(\theta)$, so we may expand the scattering amplitude

$$f(\theta) = \sum_l (2l+1) \, a_l \, P_l(\cos\theta) \tag{58}$$

in spherical harmonics with $m = 0$: $Y_{l0}(\theta) = \frac{1}{\sqrt{4\pi}}\sqrt{2l+1} P_l(\cos\theta)$. The factor $(2l+1)$ is conventional and for later convenience. So to find the scattering amplitude, it suffices to find the (generally complex) *partial wave amplitudes* a_l. a_l have dimensions of length. In many scattering problems, a good approximate cross section is got by retaining just the first few a_l. The differential cross section is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \sum_{l,l'=0}^{\infty} a_l^* a_{l'} (2l+1)(2l'+1) P_l^*(\cos\theta) P_{l'}(\cos\theta). \tag{59}$$

The total scattering cross section is simpler due to orthogonality of Legendre polynomials

$$\int_{-1}^{1} P_l(x) P_{l'}(x) dx = \frac{2}{2l+1}\delta_{ll'}. \tag{60}$$

Thus the partial wave expansion for the total cross section is

$$\sigma = \sum_{ll'} a_l^* a_{l'} (2l+1)(2l'+1) \int_0^{2\pi} d\phi \int_0^{\pi} P_l(\cos\theta) P_{l'}(\cos\theta)\ \sin\theta\ d\theta = 4\pi \sum_{l=0}^{\infty} (2l+1)|a_l|^2. \tag{61}$$

Note that we have merely chosen to parametrize the angular distribution of scattered amplitudes $f(\theta,\phi)$ as a sum of partial wave amplitudes a_l of definite angular momentum. The problem of direct scattering is to find a_l. We will do this by solving the SE in the presence of the potential and then read off the a_l by considering the asymptotic behavior of the wave function.

3.2 Phase shifts

• In fact, it is physically revealing and more economical to express these partial wave amplitudes a_l, in terms of certain scattering phase shifts δ_l given by[4]

$$a_l = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l}\sin\delta_l}{k} \tag{62}$$

This is similar to the situation in 1d where we could express the (complex) scattered amplitudes (B, C) for eigenstates of the S-matrix in terms of phase shifted incoming amplitudes (A, D). Moreover these phases $e^{i\delta_{1,2}}$ were the eigenvalues of the S-matrix. In 3d, the eigenstates of the S-matrix are the spherical harmonics and we have an infinite number of phase shifts δ_l labelled by angular momentum quantum number l. The eigenvalues of the S-matrix are the phases $e^{2i\delta_l}$. To extract the scattering phase shifts, we first need to know the phases of the wave function in the absence of scattering, i.e., the asymptotic phases of the incoming plane wave

• However, the incoming plane wave Ae^{ikz} is not a state of definite angular momentum. Nevertheless, it is a free particle eigenstate. Moreover, the angular momentum (L^2) eigenstates $R_{kl}(r)Y_{lm}(\theta,\phi)$ of the free particle form a complete set and we should be able to expand $e^{ikr\cos\theta}$ as a linear combination of them. Since $e^{ikr\cos\theta}$ is independent of ϕ, we only need the $m=0$ spherical harmonics, the Legendre polynomials $P_l(\cos\theta)$ and since $e^{ikr\cos\theta}$ is finite at $r=0$, we don't need the spherical Neumann functions $n_l(kr)$. Thus for some coefficients c_l we must have

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} c_l\, j_l(kr)\, P_l(\cos\theta). \tag{63}$$

[4] It is not clear at present why the complex number a_l can be expressed with modulus and phase related in this particular manner. This form will be shown to be a consequence of probability and angular momentum conservation.

Multiplying by $P_{l'}(\cos\theta)$ and integrating with respect to $\cos\theta$ using the orthogonality of Legendre polynomials, it turns out with some more work, that $c_l = i^l(2l+1)$ (see problem set). Thus we expressed the incoming plane wave as a linear combination of spherical waves of various angular momenta

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta). \tag{64}$$

The point of this expansion is that in a spherically symmetric potential, angular momentum is conserved, so spherical waves of definite angular momentum scatter independently and in a simple manner.

• Let us look at the behavior of these component spherical waves for large r. Using the asymptotic behavior $j_l(kr) \sim \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2}\right)$, we get for large kr,[5]

$$e^{ikr\cos\theta} \to \sum_{l=0}^{\infty} \frac{i^l(2l+1)P_l(\cos\theta)}{kr}\sin\left(kr - \frac{l\pi}{2}\right) = \sum_l \frac{(2l+1)P_l(\cos\theta)}{2ikr}\left[e^{ikr} - (-1)^l e^{-ikr}\right]. \tag{65}$$

So the incident plane wave is a superposition of imploding and exploding spherical waves of all angular momenta l, with the specific phases given above. Notice that the coefficients of the imploding and exploding spherical wave have the same absolute magnitude and only differ by the phase $-(-1)^l$. As is explained below, this feature is a consequence of conservation of probability. If the magnitudes of the coefficients were different there would be a net accumulation/deficit of probability at $r=0$ which is not the case for a plane wave that is just 'passing through'.

• If $V=0$, this plane wave would not be modified and is the complete solution of the Schrödinger eigenvalue problem. Comparing Ae^{ikz} with the scattering b.c. the scattering amplitude $f=0$ if $V=0$.

• In the presence of a spherically symmetric potential, the spherical waves for different values of l scatter independently due to conservation of angular momentum. For example, if the incoming wave only had $l=0$, the outgoing wave would also be an S-wave.

• Summarizing, we have merely re-written the scattering boundary condition as a sum of partial waves of definite angular momentum. The scattering b.c. is the statement that the scattering eigenstate wave function for large r must be of the form

$$\psi(\vec r) \to A\left[e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right] = A\sum_l (2l+1)P_l(\cos\theta)\left[\frac{e^{ikr}-(-1)^l e^{-ikr}}{2ikr} + \frac{a_l e^{ikr}}{r}\right] \quad \text{for large } r. \tag{66}$$

We write this a sum of radially incoming and outgoing waves:

$$\psi(\vec r) \to A\sum_l (2l+1)P_l(\cos\theta)\left[A_l\frac{e^{ikr}}{r} + B_l\frac{e^{-ikr}}{r}\right] \quad \text{where} \quad B_l = \frac{-(-1)^l}{2ik} \;\&\; A_l = a_l + \frac{1}{2ik}. \tag{67}$$

While A_l receives contributions both from the incident and scattered waves, B_l depends only on the incident wave. A is the same old constant with dimensions of $L^{-3/2}$.

[5] Use $e^{\pm il\pi/2} = (\pm i)^l$. We could also work with the spherical Hankel functions $h_l^{\pm}(\rho) = j_l(\rho) \pm i n_l(\rho)$ which have the virtue of being purely outgoing and incoming spherical waves. For large ρ, $h_l^{\pm}(\rho) \to \rho^{-1}e^{\pm i\rho}(\mp i)^{l+1}$.

• Remarkably, conservation of probability and angular momentum imply that A_l must have the same absolute magnitude as B_l. This puts constraints on the form of the partial wave amplitudes a_l allowing us to express them in terms of phase shifts δ_l.

• For a real potential, the probability current density $j = \frac{\hbar}{2mi}(\psi^* \nabla \psi - \nabla \psi^* \psi)$ for an *eigenstate* of the Schrödinger operator is divergence-free $\nabla \cdot \vec{j} = 0$ since $\frac{\partial \rho}{\partial t} = 0$. In other words, $\int j \cdot d\vec{s} = 0$ over any closed surface. In particular, $\int \vec{j} \cdot d\vec{s} = 0$ for a spherical surface at $r = \infty$. For the above ψ, as $r \to \infty$

$$\vec{j} \to \frac{\hbar k |A|^2 \hat{r}}{m r^2} \sum_{ll'} (2l+1)(2l'+1) P_l(\cos\theta) P_{l'}(\cos\theta) \left[A_l^* A_{l'} - B_l^* B_{l'} \right] \tag{68}$$

Using the spherical area element $d\vec{s} = \hat{r} r^2 \sin\theta \, d\theta \, d\phi$ we get

$$\int \vec{j} \cdot d\vec{s} = \frac{4\pi \hbar k |A|^2}{m} \sum_l (2l+1) \left[|A_l|^2 - |B_l|^2 \right] = 0. \tag{69}$$

Conservation of probability implies $\sum_l (2l+1) \left(|A_l|^2 - |B_l|^2 \right) = 0$. Conservation of angular momentum means there cannot be leakage of probability current between distinct angular momentum sectors. Thus, conservation of probability plus conservation of angular momentum implies that $|A_l| = |B_l|$ for each l. Thus even in the presence of a potential, the amplitude of the outgoing spherical wave A_l can differ from the amplitude of the ingoing spherical wave B_l, only by a multiplicative phase. By convention,

$$A_l = \frac{e^{2i\delta_l}}{2ik} \quad \text{while} \quad B_l = \frac{-(-1)^l}{2ik}. \tag{70}$$

δ_l is called the l^{th} partial wave phase shift, it is real and defined modulo π. In other words, the asymptotic solution of the Schrödinger eigenvalue problem must be of the form

$$\psi(r,\theta) \to A \sum_l \frac{(2l+1) P_l(\cos\theta)}{2ikr} \left[e^{2i\delta_l} e^{ikr} - (-1)^l e^{-ikr} \right]. \tag{71}$$

Note that this is the total wave function. In particular, the coefficient $e^{2i\delta_l}$ of the exploding wave includes contributions both from ψ_{inc} and ψ_{sc}, but the coefficient of the imploding wave arises entirely from ψ_{inc}.

• The phases of the outgoing partial waves in the total wave function have been shifted by $2i\delta_l$ compared to the un-scattered outgoing waves in e^{ikz}. It is also convenient to write this as

$$\psi(r,\theta) \to A \sum_{l=0}^{\infty} \frac{i^l (2l+1) P_l(\cos\theta)}{kr} e^{i\delta_l} \sin\left(kr - \frac{l\pi}{2} + \delta_l \right). \tag{72}$$

Comparing with the expansion of $e^{ikz} = \sum_l i^l (2l+1) P_l j_l$ where $j_l \to \frac{\sin(kr - l\pi/2)}{kr}$, we see that the effect of the potential on the total wavefunction is to shift the phase of the sine function by δ_l and $\times$ it by $e^{i\delta_l}$.

• We may also state this in terms of the radial wave function. When $V = 0$, the radial wave function had the asymptotic behavior

$$R_l(kr) \propto \frac{\sin\left(kr - \frac{l\pi}{2} \right)}{kr} \quad \text{for} \quad kr \gg 1. \tag{73}$$

In the presence of a potential, it has the phase-shifted asymptotic behavior

$$R_l(r) \propto \frac{\sin\left(kr - \frac{l\pi}{2} + \delta_l\right)}{kr} \quad \text{for} \quad kr \gg 1. \tag{74}$$

• From (67) and (70) the partial wave amplitudes a_l are related to the phase shifts δ_l by

$$\frac{e^{2i\delta_l}}{2ik} = a_l + \frac{1}{2ik} \quad \Rightarrow \quad a_l = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l}\sin\delta_l}{k}. \tag{75}$$

Having exploited conservation of probability (unitarity) and angular momentum to replace the complex partial wave amplitudes a_l by the real phase shifts δ_l, we write the partial wave expansion for the scattering amplitude and differential cross section as

$$\begin{aligned} f(\theta) &= \sum_{l=0}^{\infty}(2l+1)a_l P_l(\cos\theta) \\ \Rightarrow \frac{d\sigma}{d\Omega} &= |f|^2 = \frac{1}{k^2}\sum_{l,l'}(2l+1)(2l'+1)e^{-i(\delta_l-\delta_{l'})}\sin\delta_l\sin\delta_{l'}P_l(\cos\theta)P_{l'}(\cos\theta). \end{aligned} \tag{76}$$

Integrating, the total cross section becomes

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \equiv \sum_l \sigma_l. \tag{77}$$

The partial x-sections are all non-negative and in particular, σ is bounded below by the S-wave x-section $\sigma \geq \sigma_0$. We also get the so-called 'unitarity bound' on the 'partial cross sections':

$$\sigma_l \leq \frac{4\pi}{k^2}(2l+1). \tag{78}$$

The unitarity bound is saturated iff the phase shifts are odd multiples of $\pi/2$. So to find the cross section, it suffices to find the scattering phase shifts δ_l, which are dimensionless real quantities depending on the potential and the incoming wave number k. To do so, we must solve the Schrödinger eigenvalue problem in the given potential. Soon, we will do this in some examples.

• More advanced treatments show that for an attractive potential $V(r) < 0$ in 3d, if the S-wave phase shift is small, then it is positive and for a repulsive potential it is negative. Roughly, this is because in a repulsive potential, the particle slows down and is able to accumulate less phase shift while in an attractive potential, it speeds up and accumulates more phase shift compared to a free particle. We will see this in some examples. The quantum mechanical phase shift is related to Wigner's time-delay.

3.3 Semiclassical estimate of relative sizes of phase shifts

• Let us get a rough semi-classical estimate for which phase shifts can be significantly different from zero. Suppose we scatter classical particles of momentum p from a potential that is negligible for $r > a$. Then for impact parameters $b > a$ there is negligible scattering/deflection.

The magnitude of angular momentum[6] $L = pb$ is proportional to b. So for fixed energy of incoming particles (or fixed momentum p), there will be no scattering if L is too large, i.e. $L > pa$. Semi-classically we write $L = \hbar\sqrt{l(l+1)} \approx \hbar l$ and $p = \hbar k$ and find that partial waves with $l > ka$ suffer no phase shift.

• For very low energy scattering, $ka \ll 1$ and the only partial wave that can have a non-zero phase shift is the $l = 0$ S-wave. The corresponding scattering amplitude is

$$f(\theta) = \frac{1}{k}\sum_l (2l+1)P_l(\cos\theta)e^{i\delta_l}\sin\delta_l \to \frac{e^{i\delta_0}\sin\delta_0}{k} \tag{79}$$

In particular, for S-wave scattering, the scattering amplitude is spherically symmetric. The incoming wave e^{ikz} contains all angular momenta l. But at low energies, only its S-wave part was scattered, leading to a spherically symmetric outgoing wave with a phase shift.

• A parameter that is often used to characterize the scattering at low energies is the (S-wave) scattering length α defined as

$$\alpha = -\lim_{k\to 0} f(\theta). \tag{80}$$

As we argued above, at low energies (k small) δ_l for $l \geq 1$ vanish and S-wave scattering dominates. The scattering length α is independent of θ, it is a real parameter with length dimensions, but it can be positive or negative. Often a positive scattering length arises for a repulsive potential and a negative scattering length for an attractive potential as we will see in the examples.

3.4 Optical theorem

An immediate consequence of writing the total cross section in terms of the phase shifts is the optical theorem. It relates the total cross section to the imaginary part of the forward scattering amplitude. By forward scattering we mean scattering in the direction $\theta = 0$.

$$f(\theta) = \sum_l (2l+1)P_l(\cos\theta)\frac{e^{i\delta_l}\sin\delta_l}{k} \quad\Rightarrow\quad \Im f(0) = \frac{1}{k}\sum_l (2l+1)\sin^2\delta_l \quad\Rightarrow\quad \sigma = \frac{4\pi}{k}\Im f(0). \tag{81}$$

Here we used $P_l(1) = 1$, which follows from the Rodrigues formula by successive differentiation

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l(x^2-1)^l}{dx^l}. \tag{82}$$

The optical theorem can be thought of as a consequence of unitarity of the S-matrix. The possibility of writing the scattering amplitude in terms of real phase shifts was, after all, contingent on the conservation of probability.

[6] Angular momentum is defined with respect to an origin. We have been using the scattering center $r = 0$ as the origin. However, angular momentum of the projectile is more easily computed with respect to a point ($\mathbf{s}$ in the $-\hat{z}$ direction) far to the left along the beam pipe, since there, the momentum is known to be in the $\hat{z}$ direction. It turns out that the two angular momenta are equal, as we check now. Suppose the incoming particle far to the left has momentum $\mathbf{p}$ directed along $\hat{z}$ at a point $\mathbf{r}$. We write $\mathbf{r} = \mathbf{s} + \mathbf{b}$ where $\mathbf{b}$ is a 'vertical' vector with magnitude equal to the impact parameter. Thus $\mathbf{L}_{\text{origin}} = \mathbf{r}\times\mathbf{p} = \mathbf{s}\times\mathbf{p} + \mathbf{b}\times\mathbf{p} = \mathbf{b}\times\mathbf{p}$ as $\mathbf{p}$ and $\mathbf{s}$ are anti-parallel.

• The optical theorem implies that if the scattering amplitude is real, the total cross section must be zero. If there is non-trivial scattering, the amplitude f cannot be a real function. Moreover, its imaginary part must be +ve in the forward direction. The optical theorem and differential cross section $d\sigma/d\Omega = |f|^2$ together give information on both the real and imaginary parts of f in the forward direction.

• The optical theorem traces its origin to light scattering in inhomogeneous media (such as the sky) studied by Wolfgang von Sellmeier and Lord Rayleigh (1871). There is an analogy between quantum mechanical wave equations and those in wave optics with the potential roughly playing the role of refractive index.

4 Example: Infinitely hard sphere scattering

This could be used to model scattering of atoms by atoms, where the nuclei strongly repel electrostatically when brought nearby but do not feel much of a force when far apart due to the neutrality of atoms. An infinitely hard sphere refers to a repulsive spherical barrier given by the potential

$$V(r) = \begin{cases} \infty & \text{for } r \le a \\ 0 & \text{for } r > a. \end{cases} \tag{83}$$

Classically, the cross section is the cross sectional area seen by a projectile, i.e., $\sigma_{cl} = \pi a^2$. Classically, if the impact parameter $\ge a$, the particle passes undeflected, while if it is less than a, it is deflected according to the law of reflection.

• In QM, the dimensionless quantity ka is a measure of the size of the obstacle relative to the wavelength of the incident wave. Our aim is to find the phase shifts and thereby determine the cross section. The phase shifts δ_l are dimensionless and we will express them in terms of ka. To do so, we must solve the Schrödinger eigenvalue problem for the free particle in the exterior of the hard sphere and impose the scattering boundary condition as $r \to \infty$ (which defines the phase shifts) and the Dirichlet boundary condition $\psi(r = a) = 0$ on the surface of the sphere.

• The solution of the free particle Schrödinger eigenvalue problem outside the hard sphere is given by $\psi = \sum_{lm} c_{lm} R_l(r) Y_{lm}(\theta, \phi)$ where

$$-\frac{1}{r}(rR_l)'' + \left[\frac{l(l+1)}{r^2} - k^2\right] R_l = 0, \quad \text{for } r > a \tag{84}$$

The radial function must be a linear combination of spherical Bessel and Neumann functions

$$R_l(r) = \alpha_l\, j_l(kr) + \beta_l\, n_l(kr). \tag{85}$$

Imposing $\psi(r = a) = 0$ gives

$$R(a) = 0 \quad \Rightarrow \quad -\frac{\beta_l}{\alpha_l} = \frac{j_l(ka)}{n_l(ka)}. \tag{86}$$

The scattering b.c. at $r = \infty$ which serves to define the phase shifts is

$$\psi \quad \to \quad A \sum_l (2l+1) P_l(\cos\theta) \frac{i^l e^{i\delta_l}}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$$

$$= \quad A\sum_l (2l+1)P_l(\cos\theta)\frac{i^l e^{i\delta_l}}{kr}\left[\sin\left(kr-\frac{l\pi}{2}\right)\cos\delta_l + \cos\left(kr-\frac{l\pi}{2}\right)\sin\delta_l\right] \quad \text{or}$$

$$R_l(r) \quad \propto \quad \frac{1}{kr}\sin(kr-\frac{1}{2}l\pi+\delta_l) \propto \frac{1}{kr}\left[\sin\left(kr-\frac{l\pi}{2}\right)\cos\delta_l + \cos\left(kr-\frac{l\pi}{2}\right)\sin\delta_l\right]. \quad (87)$$

We must compare this with the behavior of the wave function as $r\to\infty$,

$$R_l(r) = \alpha_l\, j_l(kr) + \beta_l\, n_l(kr) \to \frac{1}{kr}\left[\alpha_l \sin\left(kr-\frac{l\pi}{2}\right) - \beta_l\cos\left(kr-\frac{l\pi}{2}\right)\right] \quad (88)$$

We get

$$-\frac{\beta_l}{\alpha_l} = \frac{\sin\delta_l}{\cos\delta_l} = \tan\delta_l \quad (89)$$

Now combining with the b.c. at $r=a$ we get a formula for the phase shifts in terms of the physical parameters of the problem k and a

$$\tan\delta_l = \frac{j_l(ka)}{n_l(ka)} \quad \Rightarrow \quad \delta_l = \arctan\frac{j_l(ka)}{n_l(ka)}. \quad (90)$$

The partial wave amplitudes $a_l = \frac{e^{i\delta_l}\sin\delta_l}{k}$ follow as a consequence.

• To understand this result, let us first consider the S-wave phase shift $l=0$ in which case $j_0(\rho)=\sin\rho/\rho$ and $n_0(\rho)=-\cos\rho/\rho$. For this repulsive potential, the S-wave phase shift is *negative*:

$$\delta_0 = \arctan(-\tan ka) = -ka \qquad \mod \pi. \quad (91)$$

The S-wave partial wave amplitude is $a_0 = -k^{-1}e^{-ika}\sin ka$.

• The partial x-sections are $\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l$ and the total x-section is the sum of these non-negative partial x-sections. Thus the S-wave scattering x-section is

$$\sigma_0(k) = \frac{4\pi}{k^2}\sin^2 ka \quad (92)$$

So the S-wave x-section is maximal at the longest wavelengths (low energy, ka small)

$$\sigma_0(k\to 0) = 4\pi a^2 \quad (93)$$

and decreases with growing wave number. In fact, at long wavelengths, the S-wave x-section is equal to the surface area of the hard sphere. So the total x-section (as $k\to 0$) is at least as big as the area of the sphere. Contrast this with the classical x-section which is equal to πa^2, the x-sectional area of the hard sphere. So for low energy scattering, the target in wave mechanics looks bigger than for classical particle scattering.

• Moreover the S-wave x-section oscillates within a decreasing envelope as k increases. Interestingly, σ_0 vanishes if $ka = n\pi$. The target is transparent at these energies within the S-wave approximation.

• When is the S-wave approximation good? i.e., when can we ignore the other phase shifts? S-wave scattering dominates at low energies or large incident wavelengths compared to the miniscule size of the obstacle. For a small obstacle $ka \ll 1$ and[7]

$$\tan\delta_l = \frac{j_l(ka)}{n_l(ka)} \to -\frac{2^{2l}(l!)^2}{(2l)!(2l+1)!}(ka)^{2l+1} \quad (94)$$

[7] We use the behaviors for small ρ: $j_l(\rho)\to\frac{2^l l!}{(2l+1)!}\rho^l = \frac{\rho^l}{(2l+1)!!}$ and $n_l(\rho)\to -\frac{(2l)!}{2^l l!}\frac{1}{\rho^{l+1}} = -\frac{(2l-1)!!}{\rho^{l+1}}$.

So as $ka \to 0$, $\tan\delta_l \to 0$ for $l = 1, 2, 3 \ldots$. So the P,D,F ... wave phase shifts all vanish for very low energy scattering. The S-wave phase shift alone can have a non-zero low energy limit. At low energies, even though the incoming plane wave had all angular momentum components, only its S-wave component gets non-trivially scattered producing a spherically symmetric scattered wave, while higher angular momentum components pass the minuscule obstacle unaffected. The higher angular momentum components of ψ_{inc}, $j_l(\rho) \propto \rho^l$ are suppressed near $\rho = 0$ and do not feel the effects of the obstacle.

• Using the above phase shifts we can construct the scattering amplitude

$$f(\theta) = \frac{1}{k} \sum_l (2l+1) P_l(\cos\theta) e^{i\delta_l} \sin\delta_l \tag{95}$$

In particular, at low energies ($k \to 0$) $\delta_l = 0$ for $l \geq 1$ and this implies the (S-wave) scattering length is equal to the radius of the obstacle a:

$$\alpha = -\lim_{k\to 0} f(\theta) = -\lim_{k\to 0} \frac{e^{-ika}\sin(-ka)}{k} = a \tag{96}$$

For a repulsive potential, the S-wave scattering length is usually positive.

5 Finite spherical well: S-wave scattering

• See Liboff for example. Let us consider low wave number scattering against a finite spherical well. This could be used to model scattering of an electron against an atom. The nuclear attraction is effective only within the atom and is effectively screened outside the neutral atom. So we take

$$V(r) = \begin{cases} -V & \text{for } r < a \\ 0 & \text{for } r \geq a. \end{cases} . \tag{97}$$

At low energies $ka \ll 1$, it is adequate to truncate the partial wave expansion after the $l = 0$ term and consider S-wave scattering. The aim is to solve the Schrödinger eigenvalue problem in the S-wave sector and read off the S-wave phase shift δ_0 by comparing with the scattering boundary condition. In the S-wave sector $\psi(\vec r) = R(r) Y_{00}$ and we only need consider $l = 0$. In the interior of the well, the radial eigenvalue equation for $u = rR$ is

$$-\frac{\hbar^2}{2m} u'' - Vu = \frac{\hbar^2 k^2}{2m} u \quad \Rightarrow -u'' = k'^2 u \;\text{ where }\; k'^2 = k^2 + \frac{2mV}{\hbar^2}. \tag{98}$$

So $R(r < a) = r^{-1}(A \sin k'r + B \cos k'r)$. Since the wave function must be regular at $r = 0$, $B = 0$.

• Outside the well, we have the free particle SE $-u'' = k^2 u$ with solution $u = c_1 \sin kr + c_2 \cos kr$ which can be written as

$$R(r > a) = \frac{B}{r} \sin(kr + \varphi) \tag{99}$$

Comparing with the scattering boundary condition which defines the phase shift, $R(r) \sim \sin(kr - l\pi/2 + \delta_0)$, we conclude that $\varphi = \delta_0$ is just the S-wave phase shift. To find δ_0 we need to impose the continuity of the wave function ψ and its gradient $\nabla\psi$ across the surface $r = a$. Since $\psi = RY_{00}$, we must impose continuity of R and R'. Continuity of R (or u) gives

$$A \sin k'a = B \sin(ka + \delta_0) \tag{100}$$

Continuity of R' upon using continuity of R gives

$$Ak' \cos k'a = Bk \cos(ka + \delta_0) \tag{101}$$

Taking a quotient, we get a relation between δ_0 and the physical parameters of the problem:

$$k' \cot k'a = k \cot(ka + \delta_0(k)) \quad \text{where} \quad k'^2 = k^2 + \frac{2mV}{\hbar^2} \tag{102}$$

In principle, this transcendental equation expresses δ_0 as a function of incident wave number k, V and a. In what follows we find δ_0 approximately in some regimes. These approximations could easily fail and one must check the conclusions for consistency.

• We first consider the case where δ_0 is small. Since ka is also small, in this case, we can approximate $\cot(ka + \delta_0) \approx (ka + \delta_0)^{-1}$ and get[8]

$$\delta_0^{\text{approx}}(k) = ka \left(\frac{\tan k'a}{k'a} - 1 \right) \quad \text{when } \delta_0 \text{ and } ka \text{ are small.} \tag{103}$$

Note that when the energy is small compared to the depth of the well $E \ll V$, we may write

$$k'a = a\sqrt{\frac{2mV}{\hbar^2}} \sqrt{1 + \frac{\hbar^2 k^2}{2mV}} \approx \frac{a}{\hbar}\sqrt{2mV} \left(1 + \frac{E}{2V} + \cdots \right) \quad \text{where } E = \frac{\hbar^2 k^2}{2m}. \tag{104}$$

So that for small ka *and* small E/V, we have

$$\delta_o^{\text{approx}}(k) \approx ka \left[\frac{\tan\left[\frac{a}{\hbar}\sqrt{2mV}\left(1 + \frac{E}{2V}\right)\right]}{\frac{a}{\hbar}\sqrt{2mV}\left(1 + \frac{E}{2V}\right)} - 1 \right]. \tag{105}$$

• Let us compute the S-wave scattering amplitude f and cross section σ_0 for small ka and small δ_0:

$$f(\theta) = \sum_l (2l+1) P_l a_l \approx a_0 = \frac{1}{k} e^{i\delta_0} \sin\delta_0 \tag{106}$$

• When $\delta_0 \ll 1$ we approximate $e^{i\delta_0} \approx 1$ and $\sin\delta_0 \approx \delta_0$ to get

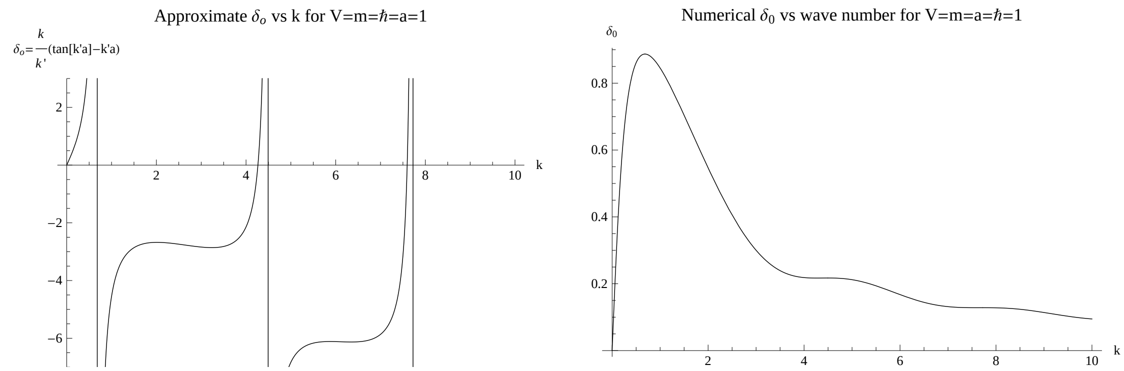
$$f(\theta) \approx a \left(\frac{\tan k'a}{k'a} - 1 \right) \quad \text{and} \quad \sigma_0 \approx 4\pi |a_0|^2 \approx \frac{4\pi\delta_0^2}{k^2} \approx 4\pi a^2 \left(\frac{\tan k'a}{k'a} - 1 \right)^2. \tag{107}$$

As expected, the S-wave scattering amplitude is spherically symmetric. An interesting feature of this approximate S-wave cross section is that it vanishes at energies satisfying the transcendental relation $k'a = \tan k'a \pmod{\pi k'/k}$. At those energies, the target appears transparent to S-waves! Note that at these energies $\delta_0 = 0$ so we are allowed to use our approximate formula for small δ_0 *provided* ka is also small.

• The S-wave scattering length for small δ_0 is obtained from the low energy limit of $f(\theta)$

$$\alpha \approx -\lim_{k\to 0} f(\theta) = a \left(1 - \frac{\tan a\sqrt{\frac{2mV}{\hbar^2}}}{a\sqrt{\frac{2mV}{\hbar^2}}} \right). \tag{108}$$

[8] Note that $g(x) = \tan x - x$ satisfies $g(0) = 0$ and $g'(x) = \tan^2 x \geq 0$, so $\tan x \geq x$ for $0 \leq x \leq \pi/2$. Thus δ_0 is guaranteed to be positive (as is often the case for an attractive potential) for the energy range $0 \leq \sqrt{\frac{2m(E+V)a^2}{\hbar^2}} \leq \pi/2$.



(a) (b)

Figure 1: (a) Approx. S-wave phase shift $\delta_0^{\text{approx}} = ka\left(\frac{\tan k'a}{k'a} - 1\right)$ (valid for small ka and small δ_0) versus k for $V = a = m = \hbar = 1$. For small $k < \frac{1}{2}$ or so, δ_0^{approx} is small (and positive in this case), and the approximation may be relied upon. δ_0^{approx} diverges at the potential S-wave resonances $k'a = (2n+1)\pi/2$, where the formula cannot be trusted. But periodically, δ_0^{approx} vanishes (mod π) signaling possible transparency to S-wave scattering. Near such k the formula may be trusted provided ka is small. However, the first such possibility for these parameters occurs only at $ka \approx 1.3$ which is not small compared to 1. So this δ_0^{approx} cannot a priori be trusted near these 'higher zeros' of δ_0 (mod π). (b) Numerical solution of transcendental equation for δ_0 for same $V, m, a, \hbar$. S-wave phase shift does show some local maxima roughly where expected from δ_0^{approx}. It does not vanish anywhere, though the phase shift has local minima. δ_0^{approx} can only be trusted for small k for these parameters.

For $0 \leq a\sqrt{\frac{2mV}{\hbar^2}} \leq \pi/2$, i.e., if the well is not too deep, this scattering length is negative, as is often the case for an attractive potential. Note that this is only an approximate scattering length and is valid only when the S-wave phase shift δ_0 is small.

• The above approximate phase shift $\delta_0^{\text{approx}}(k)$ most dramatically fails to be reliable at those k where the tangent function blows up, i.e., when $k'a \approx (2n+1)\pi/2$. At those energies, δ_0 is not small and we need to go back and solve $k'\cot k'a = k\cot(ka + \delta_0)$ without assuming δ_0 is small. In fact near such values ($k'a = (2n+1)\pi/2$), $\cot k'a = 0$ and so $\sin(ka + \delta_0) \approx \pm 1$ which means $\sin(\delta_0) \approx \pm 1$ if $ka \ll 1$. So if ka is small *and* $k'a$ is near an odd multiple of $\pi/2$, the S-wave scattering phase shift reaches a peak of $\pi/2$ modulo π where the S-wave scattering cross section saturates the unitarity bound

$$\sigma_0^{\text{unitarity bound}} = \frac{4\pi}{k^2}\sin^2\delta_0 = \frac{4\pi}{k^2} \tag{109}$$

When the S-wave x-section goes through a maximum it is called an S-wave resonance (even if it does not saturate the unitarity bound). The target looks very large at resonant energies. It is as if the incoming particle gets nearly trapped bouncing around the potential well, before eventually escaping to infinity. Note that in atomic scattering, infinity just means a few atomic diameters, by which time the potential would have died out. Also, the time ($\sim 10^{-10}$s) particles spend in the vicinity of the scattering center can be very small compared to human time scales.

• The case of low energy scattering by a repulsive finite spherical barrier $V > 0$ for $r < a$ is also interesting. See the problem set. In the interior region $r < a$, we have $E < V$ so k' is replaced by $i\kappa$ where $\hbar^2\kappa^2/2m = V - E$. The S-wave cross section for low energy scattering is

$$\sigma = 4\pi a^2 \left(\frac{\tanh \kappa a}{\kappa a} - 1\right)^2 . \quad (110)$$

When the barrier becomes infinitely high $V \to \infty$ $\kappa \to \infty$ and $\tanh \kappa a \to 1$. We recover the S-wave cross section $\sigma = 4\pi a^2$ for scattering by a hard sphere.

6 Born series and approximation in potential scattering

• Consider the wave mechanical treatment of scattering of non-relativistic particles of mass m against a potential $V(\mathbf{r})$ that vanishes for large $|\mathbf{r}|$. We suppose that free particles (with wave amplitude Ae^{ikz}) come in along the z-axis from $-\infty$ and scatter. Scattered particles are detected at large $r = |\mathbf{r}|$ at the angular location specified by the polar and azimuthal angles θ and ϕ. The scattered wave amplitude is expressed as $f(\theta,\phi)e^{ikr}/r$ for large r. $f(\theta,\phi)$ is called the scattering amplitude. The differential cross section is given by $d\sigma/d\Omega = |f|^2$ and the total cross section is $\sigma = \int |f|^2 d\Omega$ where $d\Omega = \sin\theta d\theta d\phi$ is the element of solid angle. σ with dimensions of area may be thought of as the total effective cross-sectional area (normal to the incident beam) presented by the scattering potential. $d\sigma$ is the average number of particles scattered into the angular region $d\Omega$ per unit time per unit incident flux of particles. The incident flux across unit area of the beam is $\mathbf{j}_{inc} \cdot \hat{z}$ where $\mathbf{j}$ is the probability current density.

• Max Born's approximation to find the scattering amplitude $f(\theta,\phi)$ is useful especially when the scattering potential $V(\vec r)$ is weak compared to the energy of the incoming wave $\hbar^2k^2/2m$. In such a situation, the scattered wave is expected to be small compared to the incoming plane wave. So it is useful in the regime of high energies while the partial wave approximation is useful at low energies. Loosely, the Born series is an expansion in powers of the potential V, treated as a perturbation to the kinetic term. V need not be spherically symmetric.

6.1 Integral form of the Schrödinger equation and Green's function for the Helmholtz operator

• The starting point for the Born series is a rewriting of the Schrödinger eigenvalue problem as an integral equation. We begin by writing

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec r)\psi = \frac{\hbar^2k^2}{2m}\psi \quad \Rightarrow \quad \left(\nabla^2 + k^2\right)\psi = \frac{2mV}{\hbar^2}\psi. \quad (111)$$

$\nabla^2 + k^2$ is the Helmholtz operator and if the rhs $\frac{2mV}{\hbar^2}\psi$ had been a source $\chi(\vec r)$ independent of $\psi(\vec r)$, this would be the inhomogeneous Helmholtz equation. Recall that the general solution of an inhomogeneous linear equation $A\psi = \chi$ is given by the sum of a particular solution and the general solution of the homogeneous equation $A\psi = 0$. Though the SE is in fact a homogeneous equation, it pays to think of it as an inhomogeneous Helmholtz equation and treat the rhs $\frac{2mV}{\hbar^2}\psi$ as a small source.

• The idea is to try to invert the operator $\nabla^2 + k^2$ and take it to the rhs. However, $\nabla^2 + k^2$ is not invertible, as it is 'many to one', it has zero eigenvalues. Indeed, it has a large null space consisting of all free particle eigenstates: $(\nabla^2 + k^2)\psi_0 = 0$, e.g., the plane waves $\psi_0(\vec r) = e^{i\vec l\cdot\vec r}$

for *any* vector $\vec{l}$ whose length is $|\vec{l}| = k$. These plane waves span the zero eigenspace of the Helmholtz operator (though we could just as well use angular momentum eigenstates of the free particle with energy $\hbar^2 k^2/2m$).

• Though it isn't invertible, we may be able to find a 'right inverse' in the sense of a 'Green's function' $G(r,r')$ satisfying (here ∇ is the gradient in $\vec{r}$ as opposed to the gradient ∇' in $\vec{r}'$)

$$\left(\nabla^2 + k^2\right) G(\vec{r}, \vec{r}') = \delta^3(\vec{r} - \vec{r}'). \tag{112}$$

But such a Green's function is not unique. However, any two Green's functions $G^{(1)}, G^{(2)}$ for the Helmholtz operator differ by a solution ψ_0 of the homogeneous Helmholtz equation

$$\left[\nabla^2 + k^2\right] \left(G^{(1)}(\vec{r}, \vec{r}') - G^{(2)}(\vec{r}, \vec{r}')\right) = 0 \quad \Rightarrow G^{(1)}(\vec{r}, \vec{r}') - G^{(2)}(\vec{r}, \vec{r}') = \psi_0(r) \tag{113}$$

We will find a Green's function for the Helmholtz operator shortly. The virtue of having one is that it in effect provides a 'particular solution' of the inhomogeneous Helmholtz equation. In more detail, we may write the 'general solution' of the SE as

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int G(\vec{r}, \vec{r}') \frac{2mV(\vec{r}')}{\hbar^2} \psi(\vec{r}')\, d^3r' \tag{114}$$

where $\psi_0(\vec{r})$ is any solution of $(\nabla^2 + k^2)\psi = 0$, i.e., a free particle energy eigenstate. It is easily checked that this ψ satisfies the SE. However, it is not an explicit solution since ψ appears both on the left and right sides. Nevertheless, it is an integral equation for ψ which looks a bit like the scattering boundary condition if we take $\psi_0 = e^{ikz}$! So we should expect the integral expression on the rhs to tend to the scattered wave for large r.

• We can iterate this expression to get the Born series, which gives a formal solution of the SE:

$$\begin{aligned}\psi(r) \;\; &= \;\; \psi_o(r) + \int G(r,r') \frac{2mV(r')}{\hbar^2} \psi_o(r')\, dr' + \iint G(r,r') \frac{2mV(r')}{\hbar^2} G(r',r'') \frac{2mV(r'')}{\hbar^2} \psi_o(r'')\, dr'\, dr'' \\ &\quad + \iiint G(r,r') \frac{2mV(r')}{\hbar^2} G(r',r'') \frac{2mV(r'')}{\hbar^2} G(r'',r''') \frac{2mV(r''')}{\hbar^2} \psi_o(r''')\, dr'\, dr''\, dr''' + \cdots\end{aligned} \tag{115}$$

• We still have to find a Green's function for the Helmholtz operator, i.e., any one solution of

$$\left(\nabla^2 + k^2\right) G(\vec{r}, \vec{r}') = \delta^3(\vec{r} - \vec{r}'). \tag{116}$$

We will select a solution that is appropriate to the scattering problem. A priori $G(r,r')$ is a function of six coordinates and it is daunting to find a solution of this partial differential equation that involves derivatives in three of them r, θ, ϕ. However, on account of the translation invariance ($\vec{r} \to \vec{r} + \vec{b}$) of the Helmholtz operator, we choose to look for a Green's function that depends only on the translation-invariant vector $\vec{r} - \vec{r}'$. So we have gone from 6 to 3 variables. Furthermore, on account of the rotation invariance of the Helmholtz operator[9], we choose to look

[9]By rotation-invariance we mean that if $\vec{r}' = (x', y', z') = R\vec{r}$ for a rotation R applied to $\vec{r} = (x,y,z)$, then the formula for the Laplacian $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + \frac{\partial^2}{\partial z'^2}$ is unchanged. It is good to check this first in two dimensions, where $x' = cx - sy$ and $y' = sx + cy$ for $s = \sin\alpha$ and $c = \cos\alpha$ where α is the angle of (counter-clockwise) rotation. Just as translation-invariance is manifest in Cartesian coordinates, rotation-invariance is manifest in spherical polar coordinates. Suppose the rotation is by a counter-clockwise angle α about some axis. Let us choose our coordinate system so the axis of rotation is the z-axis. Then under such a rotation $(r,\theta,\phi) \mapsto (r,\theta,\phi+\alpha)$. Now the laplacian is $\nabla^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$. The formula for this differential operator is clearly unchanged under $\phi \to \phi + \alpha$. Thus the Laplacian is rotation invariant.

for a Green's function that depends only on the rotation invariant quantity $s = |\vec{s}| = |\vec{r} - \vec{r}'|$. This reduces the above partial differential Helmholtz operator to an ordinary differential operator. $G(s)$ must satisfy[10]

$$\frac{1}{s}\frac{d^2 sG(s)}{ds^2} + k^2 G(s) = \delta^3(\vec{s}). \tag{117}$$

Let us first consider the case $s > 0$ where this is a homogeneous linear ODE $(sG)'' + k^2 sG = 0$. The general solution is $G(s) = \frac{Ae^{iks}}{s} + \frac{Be^{-iks}}{s}$. However, we choose $B = 0$ since we will be interested in the outgoing scattered wave. To find A, we look at the behavior for small s, where $G(s) \to \frac{A}{s}$ independent of k. So to find A, it suffices to consider the case $k = 0$. For $k = 0$, it is easy to show that

$$\nabla^2 \left(\frac{1}{r}\right) = -4\pi\delta^3(\vec{r}) \tag{118}$$

For $r \neq 0$, this is immediate since $\nabla^2 r^{-1} = \frac{1}{r}(rr^{-1})'' = 0$. To check that it is correct also at $r = 0$ we integrate over the interior of a unit sphere and use Stokes theorem:

$$\int \vec{\nabla} \cdot \vec{\nabla}\frac{1}{r}\, d^3r = \int_{S^2} \vec{\nabla}\frac{1}{r} \cdot \hat{r} r^2 d\Omega = \int -\frac{\hat{r}}{r^2} \cdot \hat{r} r^2 d\Omega = -4\pi. \tag{119}$$

So we conclude that $A = -\frac{1}{4\pi}$. Thus we have found one Green's function for the Helmholtz operator

$$G(s) = -\frac{1}{4\pi}\frac{e^{iks}}{s} \quad \text{or} \quad G(\vec{r} - \vec{r}) = -\frac{1}{4\pi}\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|}. \tag{120}$$

A Green's function is not unique, we can add to this $G(s)$ any solution of the homogeneous equation and get another Green's function. However, for the problem of interest, $G(s)$ is most appropriate, as it satisfies the scattering b.c.

- To summarize, we have written the Schrödinger eigenvalue problem as an integral equation

$$\psi(r) = \psi_0(r) - \frac{1}{4\pi}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|}\,\frac{2mV(\vec{r}')}{\hbar^2}\psi(\vec{r}')\, d^3r' \tag{121}$$

and iterated it to obtain the Born series (115).

6.2 Born approximation

So far we have not made any approximation. Now we apply this to the scattering problem by choosing $\psi_0(r) = e^{i\vec{k}\cdot\vec{r}}$ to be the incoming plane wave with $\vec{k} = k\hat{z}$. Notice that successive terms in the Born series involve higher powers of the potential. We suppose that the potential is weak so that the total wave function does not differ much from the incoming plane wave and truncate the Born series after one iteration. This gives the first Born approximation

$$\psi(r) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|}\,\frac{2mV(\vec{r}')}{\hbar^2}e^{i\vec{k}\cdot\vec{r}'}\, d^3r' + \mathcal{O}(V^2). \tag{122}$$

[10]For $G(\vec{r}, \vec{r}') = G(\vec{r} - \vec{r}')$, we can re-cast the derivatives w.r.to $\vec{r}$ as derivatives with respect to $\vec{s}$ since $\frac{\partial G(x-x')}{\partial x} = \frac{\partial G(x-x')}{\partial (x-x')}$.

To find the scattering amplitude, we must extract the asymptotic behavior for large r and compare with the scattering boundary condition

$$-\frac{1}{4\pi}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}\,\frac{2mV(\vec{r}')}{\hbar^2}e^{i\vec{k}\cdot\vec{r}'}\;d^3r' \to f(\theta,\phi)\frac{e^{ikr}}{r}. \tag{123}$$

To extract the large r behavior of the integral, we assume that the potential is localized around $\mathbf{r}=0$, so that the integral over $\vec{r}'$ receives non-trivial contributions only for small r'. So we may assume that $r \gg r'$ inside the integral. The simplest possibility is to take $|\vec{r}-\vec{r}'|\approx r$. Within this crude approximation the scattering amplitude is independent of θ and ϕ (below $\vec{k}=k\hat{z}$ for a plane wave incident from the left)

$$f_{crude}(\theta,\phi) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\tilde{V}\left(-\vec{k}\right) \quad \text{where}\ \ \tilde{V}\left(\vec{k}\right) = \int V(\vec{r}')e^{-i\vec{k}\cdot\vec{r}'}\;d^3r'. \tag{124}$$

Though too crude, it indicates that the scattering amplitude is proportional to the Fourier transform of the potential, which we will see is a general feature of the Born approximation.

• To do justice to the first Born approximation and extract the angular dependence of the scattering amplitude, we need a better approximation for $|\vec{r}-\vec{r}'|$. We write

$$|\vec{r}-\vec{r}'|^2 = r^2-2\vec{r}\cdot\vec{r}'+r'^2 = r^2\left(1-2\frac{\vec{r}\cdot\vec{r}'}{r^2}+\frac{r'^2}{r^2}\right) \;\Rightarrow\; |\vec{r}-\vec{r}'| = r\left(1-2\frac{\vec{r}\cdot\vec{r}'}{r^2}+\frac{r'^2}{r^2}\right)^{\frac{1}{2}} = r-\hat{r}\cdot\vec{r}'+\mathcal{O}\left(\frac{r'^2}{r^2}\right).$$

Using $|\vec{r}-\vec{r}'|\approx r-\hat{r}\cdot\vec{r}'$ in the first Born approximation, we get[11]

$$\psi(r) \approx e^{i\vec{k}_i\cdot\hat{r}} - \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{e^{ikr}}{r}\int V(\vec{r}')e^{-i(\vec{k}_f-\vec{k}_i)\cdot\vec{r}'}d^3r' \tag{125}$$

where we defined $\vec{k}_i=\vec{k}$ for the incoming wave vector and an[12] outgoing wave vector $\vec{k}_f=k\hat{r}$ in the direction defined by θ,ϕ. From this we can read off the scattering amplitude

$$f(\theta,\phi) = f(\hat{k}_f) = f(\hat{r}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\tilde{V}(\vec{k}_f-\vec{k}_i) = -\frac{m}{2\pi\hbar^2}\tilde{V}\left(\vec{q}\right). \tag{126}$$

This is the first Born approximation for the scattering amplitude and is valid even if V isn't spherically symmetric. The vector $\vec{q}=\vec{k}_f-\vec{k}_i$ is called the momentum transfer. The main result of the Born approximation is that the scattering amplitude $f(\hat{r})$ is proportional to the Fourier transform of the potential with respect to the momentum transfer $\vec{q}=k\hat{r}-\vec{k}$.

• The Born approximation gives a solution to the direct scattering problem valid at high energies. In treating the potential term in the Hamiltonian $H=\frac{p^2}{2m}+V$ as a perturbation, V has been assumed to be small compared to the free particle energy, which is the energy of the incoming

[11] In the denominator we use the crude approximation $|\vec{r}-\vec{r}'|\approx r$. This is because $|\vec{r}-\vec{r}'|^{-1}\approx\frac{1}{r}\left(1-\frac{\hat{r}\cdot\vec{r}'}{r}\right)^{-1}\approx \frac{1}{r}\left(1+\frac{\hat{r}\cdot\vec{r}'}{r}+\cdots\right)\approx\frac{1}{r}+\frac{\hat{r}\cdot\vec{r}'}{r^2}$. The 2^{nd} term is $\sim r^{-2}$ for $r\to\infty$ and wouldn't contribute to $f(\theta,\phi)$, which is the coefficient of $\frac{e^{ikr}}{r}$ for large r.

[12] $\vec{k}_f=k\hat{r}$ is not the wave vector of a plane wave. The outgoing wave is a spherical wave. $\hat{k}_f$ is just a convenient notation for the unit vector $\hat{r}$ in the direction in which we are interested in finding $f(\theta,\phi)$. But it is a reasonable notation, since in an experiment, we would detect a outgoing scattered free particle at angular location θ,ϕ with momentum $\hbar\vec{k}_f$.

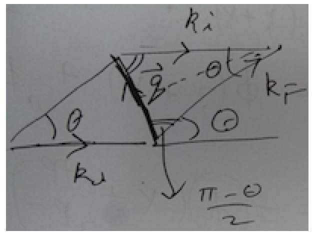


Figure 2: Momentum transfer $\mathbf{q}$.

particle in the beam. This is what allows us to replace $\psi(\vec{r}')$ under the integral by the free particle $\psi_0(\vec{r}')$.

• The Born approximation also gives a partial result in inverse scattering: a way to extract the potential if the scattering amplitude is known.

• In the limit of zero momentum transfer $\vec{q} \to 0$, the Born scattering amplitude simplifies. In this limit, the scattering amplitude is spherically symmetric and sensitive only to the integral of the potential:

$$f_{\vec{q}\to 0}(\hat{r}) = -\frac{m}{2\pi\hbar^2}\tilde{V}(0) = -\frac{m}{2\pi\hbar^2}\int V(\vec{r}')d^3r'. \tag{127}$$

6.3 Born approximation for spherically symmetric potential

• For a spherically symmetric potential, the Born approximation for the scattering amplitude may be simplified. If $\vec{k} = k\hat{z}$ and $\vec{k}_f = k\hat{r}$, then from the isosceles triangle, the momentum transfer $\vec{q} = \vec{k}_f - \vec{k}_i$ is seen to have a magnitude $q = 2k\sin\frac{\theta}{2}$. To evaluate the Fourier transform of the potential

$$\tilde{V}(\vec{q}) = \int e^{-i\vec{q}\cdot r'} V(r')r'^2 dr' \sin\theta' d\theta' d\phi' \tag{128}$$

we pick the $\hat{z}'$ axis to point in the direction of $\vec{q}$ so that $\vec{q}\cdot\vec{r}' = qr'\cos\theta'$ and get

$$\tilde{V}(q) = \int V(r')e^{-iqr'\cos\theta'} r'^2 \sin\theta' dr' d\theta' d\phi' \tag{129}$$

We can perform the θ' integral by the substitution $t = \cos\theta'$

$$\int_0^\pi e^{-iqr'\cos\theta'} \sin\theta' d\theta' = \int_{-1}^1 e^{-iqr't} dt = \frac{2\sin qr'}{qr'} \tag{130}$$

Thus the Fourier transform of a spherically symmetric potential is rotationally invariant in momentum space as well

$$\tilde{V}(\vec{q}) = \tilde{V}(q) = \frac{4\pi}{q}\int_0^\infty V(r')\, r'\, \sin qr'\, dr' \tag{131}$$

Thus the scattering amplitude in the first Born approximation is

$$f(\theta,\phi) = -\frac{2m}{\hbar^2 q}\int_0^\infty V(r)\, r\, \sin qr\, dr \quad \text{where } q = 2k\sin\frac{\theta}{2}. \tag{132}$$

6.4 Rutherford scattering

• In the case of Rutherford scattering of charge q_1 against charge q_2, the potential is $V(r) = \frac{q_1 q_2}{4\pi\epsilon_0 r}$, and

$$\tilde{V}(q) = \frac{q_1 q_2}{\epsilon_0 q}\int_0^\infty \sin qr\; dr = \frac{q_1 q_2}{\epsilon_0 q^2}\int_0^\infty \sin\rho\; d\rho \tag{133}$$

However, the dimensionless oscillatory integral appearing above is not absolutely convergent. In the absence of additional (physical) input we could assign any numerical value to it. However aside from this numerical constant, if we put $q = 2k\sin\theta/2$, we see that the cross section $|\frac{m}{2\pi\hbar^2}\tilde{V}(q)|^2$ resembles the Rutherford cross section. We have already encountered difficulties with the Coulomb potential in that its total scattering cross section is infinite classically. The Coulomb potential does not die off fast enough as $r \to \infty$ for us to be able to legitimately treat the incoming and scattered particles as free. This is reflected in the above ambiguity in defining the Fourier transform of the Coulomb potential. However, in many physical situations, the Coulomb potential is screened beyond a screening length. So we can treat the Coulomb potential as the $\mu \to 0$ limit of a screened Coulomb (or Yukawa) potential

$$V(r) = \alpha\frac{e^{-\mu r}}{r} \quad \text{where} \quad \alpha = \frac{q_1 q_2}{4\pi\epsilon_0}. \tag{134}$$

μ^{-1} is called the screening length. For $r > \mu^{-1}$, the Coulomb potential is effectively screened by the exponential damping factor. For the Yukawa potential, we find

$$\tilde{V}(q) = \frac{4\pi}{q}\int_0^\infty \frac{\alpha e^{-\mu r}}{r}\, r\,\sin qr\; dr = \frac{4\pi\alpha}{\mu^2+q^2}. \tag{135}$$

Putting $\alpha = q_1 q_1/4\pi\epsilon_0$ in the limit $\mu \to 0$ we get for the Coulomb potential

$$\tilde{V}(q) \to \frac{q_1 q_2}{\epsilon_0}\frac{1}{q^2}. \tag{136}$$

Putting $q = 2k\sin(\theta/2)$ we get the limiting scattering amplitude in the Born approximation

$$f(\theta,\phi) \approx -\frac{2m}{\hbar^2}\frac{q_1 q_2}{4\pi\epsilon_0}\frac{1}{q^2} = -\frac{q_1 q_2}{16\pi\epsilon_0 E}\frac{1}{\sin^2\theta/2} \tag{137}$$

where $E = \hbar^2 k^2/2m$. The differential cross section for Coulomb scattering in the Born approximation is found to match Rutherford's result from classical mechanics

$$\frac{d\sigma}{d\Omega} = |f|^2 \approx \left(\frac{q_1 q_2}{16\pi\epsilon_0 E}\right)^2 \frac{1}{\sin^4\theta/2}. \tag{138}$$

Scattering in the forward direction dominates, but there is significant scattering through wide angles as well, as found in Rutherford's alpha scattering experiment.

7 Classical approach to Rutherford scattering cross section

• Scattering of alpha particles against gold atoms (by Geiger, Marsden and Rutherford in 1909-1911) was instrumental in identifying the nuclear model of the atom where a heavy positive charge is concentrated at a point-like nucleus with light electrons surrounding it.

• Suppose the beam of incoming particles has an intensity/flux of $\mathcal{F}$ particles per unit time per unit area normal to the beam. After scattering, we want to find dN, the number of particles entering solid angle $d\Omega$ per unit time. dN is the rate at which particles should be detected by a detector covering solid angle $d\Omega$. This should be proportional to the incoming flux, so $dN = \mathcal{F} d\sigma$ where $d\sigma$ is an area. $d\sigma$ may be interpreted as the area normal to the beam through which the particles must pass so that they are scattered into $d\Omega$. The ratio $\frac{d\sigma}{d\Omega}$ is called the differential scattering cross section.

• Suppose charge q_1 of mass m and energy E scatters off point charge q_2 fixed at the origin with repulsive Coulomb potential $V = \frac{q_1 q_2}{4\pi r}$. Rutherford's differential scattering cross section is

$$\frac{d\sigma}{d\Omega} = \left(\frac{q_1 q_2}{16\pi E \sin^2 \frac{\theta}{2}} \right)^2 \tag{139}$$

where θ is the (polar) scattering angle $\theta = 0, \pi$ for forward/back scattering.

• Let us recall how this formula is obtained. Consider particles coming in through an annulus with impact parameters between b and $b+db$ and any azimuthal angle ϕ. They will be scattered by angles between θ and $\theta+d\theta$ and therefore correspond to $d\Omega = 2\pi \sin\theta d\theta$. Now $dN = 2\pi b db \mathcal{F}$ is the product of the area of the annulus and the incident flux. Divide by $\mathcal{F}$ to get $d\sigma$ and divide by $d\Omega$ to get $\frac{d\sigma}{d\Omega} = -\frac{b}{\sin\theta}\frac{db}{d\theta}$. The minus sign is because larger impact parameters imply smaller scattering angles.

• By integrating the energy equation $E = \frac{1}{2}mv^2 = \frac{1}{2}m\dot{r}^2 + \frac{L^2}{2mr^2} + V(r)$ in a repulsive Coulomb potential, one obtains the following relation between impact parameter and scattering angle $1 + \frac{4b^2}{a^2} = \mathrm{cosec}^2(\theta/2)$. Differentiate to get the Rutherford differential cross section

$$\frac{8b}{a^2} db = -2\sin^{-3}(\theta/2)\cos(\theta/2)\frac{1}{2}d\theta \quad \Rightarrow \quad -\frac{db}{d\theta} = \frac{\cos(\theta/2)}{\sin^3(\theta/2)}\frac{a^2}{8b}. \tag{140}$$

• To derive the relation between b and θ we use Newton's 2nd law. In fact we only need to integrate once if we use conservation of energy $E = \frac{1}{2}m\dot{r}^2 + \frac{l^2}{2mr^2} + \frac{q_1 q_2}{4\pi r}$. If v is the initial speed of the projectile (say coming in from the left), then its (conserved) angular momentum and energy are $l = mvb$ and $E = \frac{1}{2}mv^2$. So we may eliminate l in favor of b: $l^2/2m = Eb^2$. Since we are interested in the angular deviation of the orbit rather than its time dependence, we parametrize the orbit by $r(\phi)$ instead of $\mathbf{r}(t)$, where ϕ is the polar angle in the plane of the trajectory measured with respect to the direction of the projectile source. The orbit equation simplifies if we use $u = 1/r$ in place of r. Thus $\dot{r} = r'(\phi)\dot{\phi}$ and $l = mr^2\dot{\phi}$ give

$$\dot{r} = -u'(\phi)\frac{l}{m} \quad \Rightarrow \quad \frac{1}{2}m\dot{r}^2 = \frac{l^2}{2m}u'(\phi)^2 = Eb^2 u'(\phi)^2. \tag{141}$$

and the conservation of energy becomes $Eb^2 u'(\phi)^2 = E - Eb^2u^2 - \frac{q_1 q_2}{4\pi}u$. Defining the length $a = \frac{q_1 q_2}{4\pi E}$ which is the (hypothetical) radial distance at which the Coulomb energy equals the total projectile energy[13]

$$d\phi = \frac{b du}{\sqrt{1 - b^2u^2 - au}} \tag{142}$$

[13] Except in the case of zero impact parameter, the projectile does not actually get as close as a since it never comes to rest if the angular momentum is non-zero

Now the projectile comes in from $r = \infty$ with $\phi = 0$, reaches a point of closest approach where $r = r_{min} = 1/u_{max}$ [$\dot{r} = 0$, the mid-point of the trajectory, with $\phi = \phi_0$. u_{max} is the positive root of the quadratic under the square-root sign, $u_{max} = \left(\sqrt{a^2 + 4b^2} - a\right)/2b^2$] and eventually scatters off to $r = \infty$ reaching an asymptotic $\phi = 2\phi_0$. Draw a diagram! The scattering angle is $\theta = \pi - 2\phi_0$. The integral can be done by completing the square and a trigonometric substitution using $\int \frac{dx}{\sqrt{1-x^2}} = \arcsin x$,

$$\phi_0 = \int_0^{u_{max}} \frac{b\, du}{\sqrt{1 - au - b^2u^2}} = \frac{\pi}{2} - \arcsin \frac{1}{\sqrt{1 + 4b^2/a^2}} \quad \Rightarrow \quad \sin^2(\theta/2) = \frac{1}{1 + 4b^2/a^2}. \tag{143}$$

This is the advertised relation between impact parameter and scattering angle for Coulomb scattering, which leads to the Rutherford cross section.

• Physical remarks on Rutherford cross section formula.

• (1) The Coulomb field has a long range (though the scatterer is point-like). Particles with large impact parameters (small scattering angles) contribute significantly to the total cross section $\sigma = \int (d\sigma/d\Omega) 2\pi \sin\theta d\theta$. In fact, strictly speaking, the total cross section for Coulomb scattering is infinite due to a divergence at $\theta = 0$. This means there is scattering even for large impact parameters b, though the scattering angle decreases with b.

• (2) The charges need not have the same sign, the potential could be attractive or repulsive, since the cross section only depends on the square of each of the charges.

• (3) The cross section falls off as $1/E^2$ with increase in energy. This is a characteristic feature of scattering of point charges at high energies, since the energy is the only dimensional parameter in the problem[14] with which to construct a quantity with dimensions of area (particle masses are small compared to sufficiently large E and there is no length scale from the dimensions of the point particles). For instance, the cross section for e^+e^- annihilation to any final state has been measured from MeV to 100s of GeV center of mass energies (see fig. 5.3, p.145 in Perkins 4th Ed.). It shows an overall $1/E^2$ fall off with localized peaks corresponding to resonances (e.g. the $q\bar{q}$ vector mesons) like $\rho(d\bar{d} - u\bar{u}, 776MeV), \omega(d\bar{d} + u\bar{u}, 783MeV), \phi(s\bar{s}, 1019MeV), J/\psi(c\bar{c}, 3.1GeV), \Upsilon(b\bar{b}, 9.5GeV)$ and the weak gauge bosons Z^0 (91 GeV), W^+W^- (160 GeV) etc. The scalar mesons π^0 and η^0 can also appear as resonances in e^+e^- annihilation, but they are suppressed due to the need for two photon processes unlike the single photon intermediary which is adequate in the above cases.

• (4) Rutherford scattering cross section depends on θ, it is not isotropic. There is non-trivial scattering for large impart parameters. In other words, different incoming angular momenta $L = mvb$ of the projectile scatter differently but non-trivially. This is to be contrasted with a very short range potential (like a delta function or a Yukawa potential $e^{-r/\xi}/r$ with ξ much less than the impact parameter or de Broglie wavelength of incoming matter waves), where S-wave ($L = 0$) scattering dominates, and there is no scattering for larger impact parameters $b \gg \xi$, and $d\sigma/d\Omega$ is independent of θ.

• (5) Though the differential cross section decays monotonically as θ goes from 0 to π (back scatter), there is still significant scattering through large angles. The fall-off would be much

[14] A 'scale invariant' potential like the Coulomb potential $q_1q_2/4\pi r$ does not introduce any length scale of its own. Other potentials may have a length scale ξ associated with them, in which case the formula for the cross section could depend on both E and ξ. An example of non-point-like particle scattering is hadron-hadron scattering, hadrons have a size a of order a Fermi and at high energies, the cross section approaches a constant, roughly the classically expected value of $\pi(2a)^2$.

faster if the repulsive charge isn't concentrated at a point, but spread all over the atom. This was the experimental signal favoring Rutherford's nuclear model of the atom over J J Thomson's 'plum pudding' model.

• (6) The same Rutherford formula arises in non-relativistic QM in the first Born approximation (which is valid at high (non-relativistic) energies). If $E = \hbar^2 k^2/2m$ is the initial and final kinetic energy (elastic scattering, the electron just changes direction), then the magnitude of transferred momentum $\mathbf{q} = \vec{k}_f - \vec{k}_i = k\hat{r} - k\hat{z}$ is $q = 2k\sin(\theta/2)$ since

$$q^2 = (k\hat{r} - k\hat{z})^2 = 2k^2(1-\cos\theta) = 4k^2\sin^2(\theta/2) \tag{144}$$

The Born scattering amplitude $f(\theta,\phi)$ is proportional to the Fourier transform[15] of the potential, $f(\theta,\phi) \approx -\frac{2m}{4\pi\hbar^2}\tilde{V}(q)$ where

$$\tilde{V}(\mathbf{q}) = \int V(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r} \quad \text{and} \quad V(r) = \frac{q_1 q_2}{4\pi r} \quad \Rightarrow \quad \tilde{V}(q) = \frac{q_1 q_2}{q^2} \tag{145}$$

And the cross section is the square of the scattering amplitude

$$f(\theta,\phi) \approx -\frac{2m}{4\pi\hbar^2}\tilde{V}(q) \approx -\frac{2m}{4\pi\hbar^2}\frac{q_1 q_2}{q^2} = -\frac{q_1 q_2}{16\pi E}\frac{1}{\sin^2\theta/2} \quad \Rightarrow \quad \frac{d\sigma}{d\Omega} = |f|^2 \approx \left(\frac{q_1 q_2}{16\pi E \sin^2\theta/2}\right)^2. \tag{146}$$

• (7) In a relativistic treatment using Feynman diagrams in QED, scattering between a pair of charges is (at leading order) due to exchange of a virtual photon. For example, one may consider electron muon scattering or electron proton scattering (so that one of the particles is much heavier than the other and we may ignore its recoil, just as in the α-gold nucleus case.) The calculation is more involved (dealing with Dirac spinors), but the answer, Mott's formula (see for e.g. Griffiths 2nd ed., p.255), bears a resemblance to Rutherford's formula (and reduces to it in the non-relativistic limit $p \ll mc$). Assuming both particles have charge of magnitude e,

$$\left[\frac{d\sigma}{d\Omega}\right]_{\text{Mott}} = \left(\frac{e^2}{16\pi(p^2/2m)\sin^2(\theta/2)}\right)^2 \left[1 + \frac{p^2}{m^2c^2}\cos^2(\theta/2)\right]. \tag{147}$$

p is the magnitude of the lab frame momentum of the electron, m its mass and θ the scattering angle. In the non-relativistic approximation $p^2/2m$ is simply the kinetic energy E of the incoming electron.

[15] The FT can be got from knowledge that the electrostatic potential for a point charge e, $\phi = e/4\pi r$ satisfies Poisson's equation $-\nabla^2\phi = \rho = e\delta^3(\mathbf{r})$ since $E = -\nabla\phi$ and $\nabla\cdot E = \rho$. Fourier expanding $\phi(r) = \int \tilde{\phi}(q) e^{i\mathbf{q}\cdot\mathbf{r}}[dq]$ and $\nabla^2\phi(r) = -\int q^2\tilde{\phi}(q)e^{i\mathbf{q}\cdot\mathbf{r}}[dq]$. Using $\delta^3(\mathbf{r}) = \int e^{i\mathbf{q}\cdot\mathbf{r}}[dq]$ Poison's equation gives $\tilde{\phi}(q) = -e/q^2$ if $\phi(r) = -e/4\pi r$.