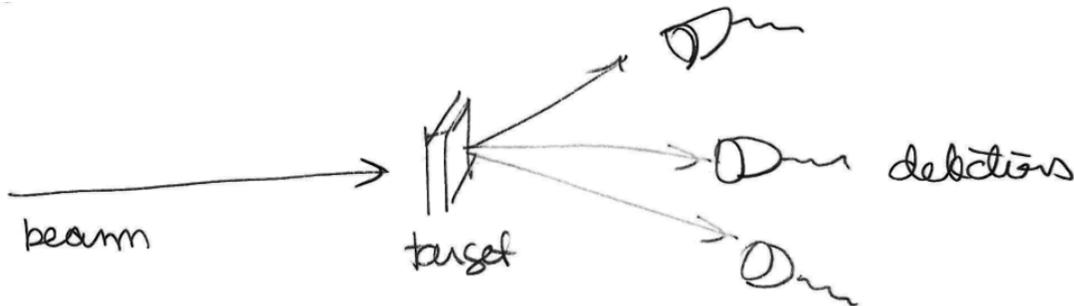


Chapter 7

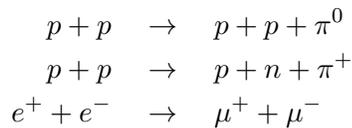
Scattering

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In high energy physics experiments a beam of particles hits a target composed of particles. By detecting the by-products one aims to study the interactions that occur during the collision.

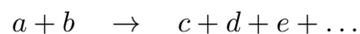


Collisions can be rather intricate. For example, the particles involved may be not elementary (protons) or they may be elementary (electrons and positrons)

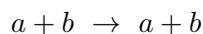


The final products may not be the same as the initial particles. Some particles may be created.

Here collisions are like reactions in which



We have *scattering* when the particles in the initial and final state are the same



The scattering is *elastic* if none of the particles internal states change in the collision¹. We will focus on *elastic scattering* of particles *without spin* in the *nonrelativistic approximation*.

We will also assume that the interaction potential is translational invariant, that is, $V(\mathbf{r}_1 - \mathbf{r}_2)$. It follows that in the CM frame the problem reduces, as we did for hydrogen atom, to scattering of a single particle of reduced mass off a potential $V(\mathbf{r})$. We will work with energy eigenstates and we will not attempt to justify steps using wave-packets.

7.1 The Schrödinger equation for elastic scattering

We are interested in energy eigenstates

$$H = \frac{\mathbf{p}^2}{2M} + V(\mathbf{r}) \quad (7.1.1)$$

$$\psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-\frac{iEt}{\hbar}} \quad (7.1.2)$$

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (7.1.3)$$



Figure 7.1: Potential is finite range, or vanishes faster than $\frac{1}{r}$ as $r \rightarrow \infty$

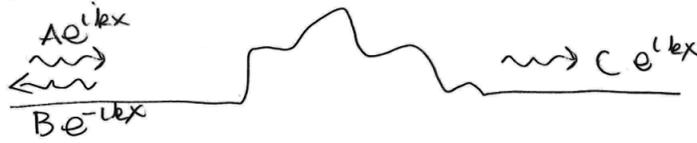
We will consider solutions with positive energy. The energy is the energy of the particle far away from the potential, $E = \frac{\hbar^2 k^2}{2M}$. The Schrödinger equation then takes the form

$$\left[-\frac{\hbar^2}{2M} (\nabla^2 + k^2) + V(\mathbf{r}) \right] \psi(\mathbf{r}) = 0 \quad (7.1.4)$$

Now we must set up the waves! Recall the 1D case. Physics dictates the existence of three waves: an incoming one, a reflected one, and a transmitted one. We can think of the reflected and transmitted waves as the scattered wave, the waves produced given the incoming wave. Setting up the waves is necessary in order to eventually solve the problem by looking into the details in the region where the potential is non-zero. When the potential has finite range the incoming and scattered waves are simple plane waves that are easily

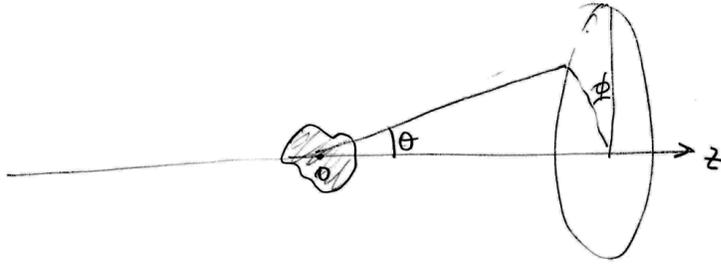
¹Frank-Hertz experiment involved inelastic collisions of electrons with mercury atoms in which the mercury atoms are excited.

written.



Equation (7.1.4) has an infinite degeneracy of energy eigenstates. When $V(\mathbf{r}) \equiv 0$, for example, $e^{i\mathbf{k}\cdot\mathbf{x}}$ for any \mathbf{k} such that $\mathbf{k}\cdot\mathbf{k} = k^2$ is a solution. Assume an incident wave moving towards $+\hat{z}$. Then the wavefunction will look like

$$\varphi(\mathbf{r}) = e^{ikz} \quad (7.1.5)$$



If we assume $V(\mathbf{r})$ has a finite range a , this $\varphi(\mathbf{r})$ satisfies (7.1.4) for any $r > a$. For $r < a$, however, it does not satisfy the equation; $\varphi(\mathbf{r})$ is a solution everywhere only if the potential vanishes.

Given an incident wave we will also have a scattered wave. Could it be an $\psi(\mathbf{r}) = e^{ikr}$ that propagates radially out?

$$(\nabla^2 + k^2) e^{ikr} \neq 0 \quad \text{fails badly for } r \neq 0!! \quad (7.1.6)$$

On the other hand

$$(\nabla^2 + k^2) \frac{e^{ikr}}{r} = 0 \quad \text{for } r \neq 0. \quad (7.1.7)$$

This is consistent with the radial equation having a solution $u(r) = e^{irk}$ in the region where the potential vanishes. Recall that the full radial solution takes the form $u(r)/r$.

Can the scattered wave therefore be $\frac{e^{ikr}}{r}$? Yes, but this is not general enough. We need to introduce some angular dependence. Hence our ansatz for the scattered wave is

$$\psi_s(\mathbf{r}) = f_k(\theta, \phi) \frac{e^{ikr}}{r} \quad (7.1.8)$$

We expect the intensity of the scattered wave to depend on direction and the function $f_k(\theta, \phi)$ does that. We will see that ψ_s is only a solution for $r \gg a$, arbitrarily far.

Both the incident and the scattered wave must be present, hence the wavefunction is

$$\psi(\mathbf{r}) = \psi_s(\mathbf{r}) + \varphi(\mathbf{r}) \simeq e^{ikz} + f_k(\theta, \phi) \frac{e^{ikr}}{r}, \quad r \gg a. \quad (7.1.9)$$

As indicated this expression is only true far away from the scattering center. We physically expect $f_k(\theta, \phi)$ to be determined by $V(\mathbf{r})$. $f_k(\theta, \phi)$ is called the *scattering amplitude*.

We now relate $f_k(\theta, \phi)$ to cross section!!

$$d\sigma = \frac{\left[\begin{array}{c} \# \text{ particles scattered per unit time} \\ \text{into solid angle } d\Omega \text{ about } (\theta, \phi) \end{array} \right]}{\left[\begin{array}{c} \text{flux of incident particles} = \frac{\# \text{ particles}}{\text{area} \cdot \text{time}} \end{array} \right]} \quad (7.1.10)$$

$d\sigma$ is called *differential cross section*, it's the area that removes from the incident beam the particles to be scattered into the solid angle $d\Omega$. Let us calculate the numerator and the denominator. First the denominator, which is the probability current:

$$\text{Incident flux in } e^{ikz} = \frac{\hbar}{m} \text{Im} [\psi^* \nabla \psi] = \frac{\hbar k}{m} \hat{z} \quad (7.1.11)$$

Intuitively, this can be calculated by multiplying the probability density $|e^{ikz}|^2 = 1$, by the velocity $\frac{p}{m} = \frac{\hbar k}{m}$. The result is again an incident flux equal in magnitude to $\frac{\hbar k}{m}$.

To calculate the numerator we first find the number of particles in the little volume of thickness dr and area $r^2 d\Omega$

$dn =$ number of particles in this little volume



$$dn = |\psi(\mathbf{r})|^2 d^3\mathbf{r} = \left| f_k(\theta, \phi) \frac{e^{ikr}}{r} \right|^2 r^2 d\Omega dr = |f_k(\theta, \phi)|^2 d\Omega dr \quad (7.1.12)$$

With velocity $v = \frac{\hbar k}{m}$ all these particles in the little volume will go cross out in time $dt = \frac{dr}{v}$, therefore the number of particles per unit time reads

$$\frac{dn}{dt} = |f_k(\theta, \phi)|^2 \frac{d\Omega dr}{\frac{dr}{v}} = \frac{\hbar k}{m} |f_k(\theta, \phi)|^2 d\Omega$$

Back in the formula for the cross section we get

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

hence

$$\text{Differential cross section: } \boxed{\frac{d\sigma}{d\Omega} = |f_k(\theta, \phi)|^2} \quad (7.1.13)$$

$$\text{Total cross section: } \boxed{\sigma = \int d\sigma = \int |f_k(\theta, \phi)|^2 d\Omega} \quad (7.1.14)$$

7.2 Phase shifts

Assume $V(\mathbf{r}) = V(r)$, so that we are dealing with a central potential. First recall the description of a free particle in spherical coordinates. With

$$V = 0, \quad E = \frac{\hbar^2 k^2}{2m}, \quad \psi(\mathbf{r}) = \frac{u_{E\ell}(r)}{r} Y_{\ell m}(\Omega) \quad (7.2.1)$$

the Schrödinger equation for $u_{E\ell}$

$$\begin{aligned} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \right) u_{E\ell}(r) &= \frac{\hbar^2 k^2}{2m} u_{E\ell}(r) \\ \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} \right) u_{E\ell}(r) &= k^2 u_{E\ell}(r). \end{aligned} \quad (7.2.2)$$

Now take $\rho = kr$, then (7.2.2) reads

$$\left(-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} \right) u_{E\ell}(\rho) = u_{E\ell}(\rho) \quad (7.2.3)$$

Since k^2 disappeared from the equation, the energy is not quantized. The solution to (7.2.3) is

$$u_{E\ell}(\rho) = A_\ell \rho j_\ell(\rho) + B_\ell \rho n_\ell(\rho) \quad \text{or} \quad u_{E\ell}(r) = A_\ell r j_\ell(kr) + B_\ell r n_\ell(kr) \quad (7.2.4)$$

where

$$\begin{array}{ll} j_\ell(\rho) \text{ is the spherical Bessel function} & j_\ell(\rho) \text{ is non singular at the origin} \\ n_\ell(\rho) \text{ is the spherical Neumann function} & n_\ell(\rho) \text{ is singular at the origin} \end{array}$$

Both have finite limits as $\rho \rightarrow \infty$

$$\rho j_\ell(\rho) \rightarrow \sin\left(\rho - \frac{\ell\pi}{2}\right) \quad (7.2.5)$$

$$\rho n_\ell(\rho) \rightarrow -\cos\left(\rho - \frac{\ell\pi}{2}\right) \quad (7.2.6)$$

Now, with the plane wave a solution, we must have

$$e^{ikz} = e^{ikr \cos \theta} = \sum_{\ell=0}^{\infty} a_\ell P_\ell(\cos \theta) j_\ell(kr) \quad (7.2.7)$$

for some coefficients a_ℓ . Using

$$Y_{\ell,0}(\theta) = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos \theta) \quad \text{and} \quad j_\ell(x) = \frac{1}{2i^\ell} \int_{-1}^1 e^{ixu} P_\ell(u) du \quad (7.2.8)$$

it can be shown that

$$e^{ikz} = \sqrt{4\pi} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} i^\ell Y_{\ell,0}(\theta) j_\ell(kr). \quad (7.2.9)$$

This is an incredible relation in which a plane wave is built by a linear superposition of spherical waves with all possible values of angular momentum! Each ℓ contribution is a *partial wave*. Each partial wave is an exact solution when $V = 0$.

We can see the spherical ingoing and outgoing waves in each partial wave by expanding (7.2.9) for large r :

$$j_\ell(kr) \rightarrow \frac{1}{kr} \sin\left(kr - \frac{\ell\pi}{2}\right) = \frac{1}{2ik} \left[\frac{e^{i(kr - \frac{\ell\pi}{2})}}{r} - \frac{e^{-i(kr - \frac{\ell\pi}{2})}}{r} \right] \quad (7.2.10)$$

Thus

$$e^{ikz} = \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} i^\ell Y_{\ell,0}(\theta) \frac{1}{2i} \left[\underbrace{\frac{e^{i(kr - \frac{\ell\pi}{2})}}{r}}_{\text{outgoing}} - \underbrace{\frac{e^{-i(kr - \frac{\ell\pi}{2})}}{r}}_{\text{incoming}} \right], \quad r \gg a \quad (7.2.11)$$

7.2.1 Calculating the scattering amplitude in terms of phase shifts

Recall 1D case



$$\varphi(x) = \sin(kx) = \frac{1}{2i} \left(e^{ikx} - \underbrace{e^{-ikx}}_{\text{ingoing}} \right) \quad \text{solution if } V = 0 \quad (7.2.12)$$

Exact solution

$$\psi(x) = \frac{1}{2i} \left(e^{ikx} e^{2i\delta_k} - \underbrace{e^{-ikx}}_{\substack{\text{same} \\ \text{ingoing} \\ \text{wave}}} \right) \quad \text{for } x > a \quad (7.2.13)$$

where the outgoing wave can only differ from the ingoing one by a phase, so that probability is conserved. Finally we defined

$$\psi(x) = \psi_s(x) + \varphi(x) \quad (7.2.14)$$

So do a similar transformation to write a consistent ansatz for $\psi(\mathbf{r})$. We have from (7.1.9)

$$\psi(\mathbf{r}) \simeq e^{ikz} + f_k(\theta) \frac{e^{ikr}}{r}, \quad r \gg a. \quad (7.2.15)$$

The incoming partial waves in the left-hand side must be equal to the incoming partial waves in e^{ikz} since the scattered wave is outgoing. Introducing the phase shifts on the outgoing waves of the left-hand side we get

$$\psi(\mathbf{r}) = \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} i^\ell Y_{\ell,0}(\theta) \frac{1}{2i} \left[\underbrace{\frac{e^{i(kr-\frac{\ell\pi}{2})} e^{2i\delta_\ell}}{r}}_{\text{outgoing}} - \underbrace{\frac{e^{-i(kr-\frac{\ell\pi}{2})}}{r}}_{\text{incoming}} \right] = e^{ikz} + f_k(\theta) \frac{e^{ikr}}{r}$$

The incoming partial waves in e^{ikz} cancel in between the two sides of the equation, and moving the outgoing partial waves in e^{ikz} into the other side we get

$$\frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} i^\ell Y_{\ell,0}(\theta) \frac{1}{2i} \underbrace{\left(e^{2i\delta_\ell} - 1 \right)}_{e^{i\delta_\ell} \sin \delta_\ell} \frac{e^{ikr} e^{-\frac{i\ell\pi}{2}}}{r} = f_k(\theta) \frac{e^{ikr}}{r} \quad (7.2.16)$$

$$= \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} Y_{\ell,0}(\theta) e^{i\delta_\ell} \sin \delta_\ell \frac{e^{ikr}}{r}, \quad (7.2.17)$$

where we noted that $e^{-\frac{i\ell\pi}{2}} = (-i)^\ell$ and $i^\ell (-i)^\ell = 1$. Therefore we get

$$\boxed{f_k(\theta) = \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} Y_{\ell,0}(\theta) e^{i\delta_\ell} \sin \delta_\ell.} \quad (7.2.18)$$

This is our desired expression for the scattering amplitude in terms of phase shifts.

We had

$$d\sigma = |f_k(\theta)|^2 d\Omega \quad (7.2.19)$$

and this differential cross section exhibits θ dependence. On the other hand for the full cross section the angular dependence, which is integrated over, must vanish

$$\begin{aligned} \sigma &= \int |f_k(\theta)|^2 d\Omega = \int f_k^*(\theta) f_k(\theta) d\Omega \\ &= \frac{4\pi}{k^2} \sum_{\ell, \ell'} \sqrt{2\ell+1} \sqrt{2\ell'+1} e^{-i\delta_\ell} \sin \delta_\ell e^{i\delta_{\ell'}} \sin \delta_{\ell'} \underbrace{\int d\Omega Y_{\ell,0}^*(\Omega) Y_{\ell',0}(\Omega)}_{\delta_{\ell\ell'}} \end{aligned}$$

Hence

$$\boxed{\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell.} \quad (7.2.20)$$

Now let us explore the form of $f(\theta)$ in the forward direction $\theta = 0$. Given that

$$Y_{\ell,0}(\theta) = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos \theta) \implies Y_{\ell,0}(\theta = 0) = \sqrt{\frac{2\ell+1}{4\pi}}$$

then

$$f_k(\theta = 0) = \frac{\sqrt{4\pi}}{k} \sum_{\ell=0}^{\infty} \sqrt{2\ell+1} \sqrt{\frac{2\ell+1}{4\pi}} e^{i\delta_\ell} \sin \delta_\ell = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) e^{i\delta_\ell} \sin \delta_\ell$$

Hence

$$\text{Im}(f(0)) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) e^{i\delta_\ell} \sin^2 \delta_\ell = \frac{1}{k} \frac{k^2}{4\pi} \sigma \quad (7.2.21)$$

Therefore we have found out a remarkable relation between the total elastic cross section and the imaginary part of the *forward* ($\theta = 0$) *scattering amplitude*. This relation is known as the *Optical theorem* and reads

$$\boxed{\sigma = \frac{4\pi}{k} \text{Im}(f(0))} \quad . \quad \text{Optical Theorem}$$

Let us consider ways in which we can identify the phase shifts δ_k . Consider a solution, restricted to a fixed ℓ

$$\psi(\mathbf{x})|_{\ell} = (A_{\ell} j_{\ell}(kr) + B_{\ell} n_{\ell}(kr)) Y_{\ell,0}(\theta) \quad x > a \quad (7.2.22)$$

If $B \neq 0$ then $V \neq 0$. As a matter of fact, if $V = 0$ the solution should be valid everywhere and n_{ℓ} is singular at the origin, thus $B_{\ell} = 0$.

Now, let's expand $\psi(\mathbf{x})|_{\ell}$ for large kr as in (7.2.10)

$$\psi(\mathbf{x})|_{\ell} \simeq \left[\frac{A_{\ell}}{kr} \sin\left(kr - \frac{\ell\pi}{2}\right) - \frac{B_{\ell}}{kr} \cos\left(kr - \frac{\ell\pi}{2}\right) \right] Y_{\ell,0}(\theta) \quad (7.2.23)$$

Define

$$\tan \delta_{\ell} \equiv -\frac{B_{\ell}}{A_{\ell}} \quad (7.2.24)$$

We must now confirm that this agrees with the postulated definition as a relative phase between outgoing and ingoing spherical waves. We thus calculate

$$\begin{aligned} \psi(\mathbf{x})|_{\ell} &\simeq \frac{1}{kr} \left[\sin\left(kr - \frac{\ell\pi}{2}\right) + \frac{\sin \delta_{\ell}}{\cos \delta_{\ell}} \cos\left(kr - \frac{\ell\pi}{2}\right) \right] Y_{\ell,0}(\theta) \\ &\simeq \frac{1}{kr} \sin\left(kr - \frac{\ell\pi}{2} + \delta_{\ell}\right) Y_{\ell,0}(\theta) \end{aligned} \quad (7.2.25)$$

$$\begin{aligned} &= \frac{1}{kr} \frac{1}{2i} \left[e^{i(kr - \frac{\ell\pi}{2} + \delta_{\ell})} - e^{-i(kr - \frac{\ell\pi}{2} + \delta_{\ell})} \right] Y_{\ell,0}(\theta) \\ &\simeq e^{-i\delta} \frac{1}{kr} \frac{1}{2i} \left[e^{i(kr - \frac{\ell\pi}{2} + 2\delta_{\ell})} - e^{-i(kr - \frac{\ell\pi}{2})} \right] Y_{\ell,0}(\theta) \end{aligned} \quad (7.2.26)$$

This shows that our definition of δ_k above is indeed consistent the expansion in (7.2.16). Finally we can read the phase shift from (7.2.25)

$$\psi(\mathbf{x})\Big|_{\ell} \simeq \frac{1}{kr} \sin\left(kr - \frac{\ell\pi}{2} + \delta_{\ell}\right) Y_{\ell,0}(\theta) \quad r \gg a \quad (7.2.27)$$

in the partial wave solution.

As an aside note that both the outgoing and ingoing components of a partial wave are separately acceptable asymptotic solutions obtained as:

- If $A_{\ell} = -iB_{\ell}$

$$\psi(\mathbf{x})\Big|_{\ell} \sim \left[i \sin\left(kr - \frac{\ell\pi}{2}\right) + \cos\left(kr - \frac{\ell\pi}{2}\right) \right] \frac{Y_{\ell,0}(\theta)}{kr} \sim \frac{e^{i(kr - \frac{\ell\pi}{2})}}{kr} Y_{\ell,0}(\theta) \quad (7.2.28)$$

- If $A_{\ell} = iB_{\ell}$

$$\psi(\mathbf{x})\Big|_{\ell} \sim \frac{e^{-i(kr - \frac{\ell\pi}{2})}}{kr} Y_{\ell,0}(\theta) \quad (7.2.29)$$

Each wave is a solution, but not a scattering one.

7.2.2 Example: hard sphere



$$V(r) = \begin{cases} \infty & r \leq a \\ 0 & r > a \end{cases} \quad (7.2.30)$$

Radial solution

$$R_{\ell}(r) = \frac{u}{r} = A_{\ell} j_{\ell}(kr) + B_{\ell} n_{\ell}(kr) \quad (7.2.31)$$

$$\psi(a, \theta) = \sum_{\ell} R_{\ell}(a) P_{\ell}(\cos \theta) \equiv 0 \quad (7.2.32)$$

The $P_{\ell}(\cos \theta)$ are complete, meaning that

$$0 = R_{\ell}(a) = A_{\ell} j_{\ell}(ka) + B_{\ell} n_{\ell}(ka) \quad \forall \ell \quad (7.2.33)$$

Recalling

$$\tan \delta_{\ell} \equiv -\frac{B_{\ell}}{A_{\ell}} = \frac{j_{\ell}(ka)}{n_{\ell}(ka)} \quad (7.2.34)$$

this implies all phase shifts are determined

$$\boxed{\tan \delta_{\ell} = \frac{j_{\ell}(ka)}{n_{\ell}(ka)}} \quad (7.2.35)$$

We can now easily compute the cross section σ , which, recalling (7.2.20) is proportional to $\sin^2 \delta_\ell$

$$\sin^2 \delta_\ell = \frac{\tan^2 \delta_\ell}{1 + \tan^2 \delta_\ell} = \frac{j_\ell^2(ka)}{j_\ell^2(ka) + n_\ell^2(ka)} \quad (7.2.36)$$

hence

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_\ell = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \frac{j_\ell^2(ka)}{j_\ell^2(ka) + n_\ell^2(ka)} \quad (7.2.37)$$

Griffiths gives you the low energy $ka \ll 1$ expansion

$$\sigma \simeq \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} \frac{1}{2\ell + 1} \left[\frac{2^\ell \ell!}{(2\ell)!} \right]^4 (ka)^{4\ell+2} \quad (7.2.38)$$

At low energy the dominant contribution is from $\ell = 0$

$$\sigma \simeq \frac{4\pi}{k^2} (ka)^2 = 4\pi a^2 \quad \begin{array}{l} \text{Full area of the sphere!} \\ \text{Not the cross section!} \end{array} \quad (7.2.39)$$

One more calculation!

$$i \tan \delta = \frac{e^{i\delta} - e^{-i\delta}}{e^{i\delta} + e^{-i\delta}} = \frac{e^{2i\delta} - 1}{e^{2i\delta} + 1} \implies e^{2i\delta} = \frac{1 + i \tan \delta}{1 - i \tan \delta} \quad (7.2.40)$$

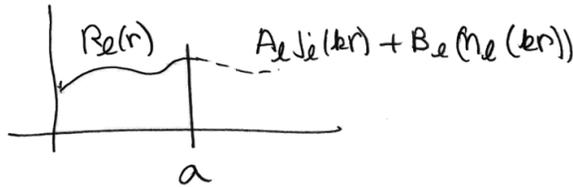
Therefore

$$e^{2i\delta_\ell} = \frac{1 + i \frac{j_\ell(ka)}{n_\ell(ka)}}{1 - i \frac{j_\ell(ka)}{n_\ell(ka)}} = \frac{n + ij}{n - ij} = \frac{i(j - in)}{-i(j + in)} \quad (7.2.41)$$

$$\boxed{e^{2i\delta_\ell} = \frac{j_\ell(ka) - in_\ell(ka)}{j_\ell(ka) + in_\ell(ka)}} \quad \begin{array}{l} \text{Hard sphere} \\ \text{phase shifts} \end{array} \quad (7.2.42)$$

7.2.3 General computation of the phase shift

Suppose you have a radial solution $R_\ell(r)$ known for $r \leq a$ ($V(r \geq a) = 0$). This must be matched to the general solution that holds for $V = 0$, as it holds for $r > a$:



At $r = a$ must match the function and its derivative

$$R_\ell(a) = A_\ell j_\ell(ka) + B_\ell n_\ell(ka) \quad (7.2.43)$$

$$aR'_\ell(a) = ka \left(A_\ell j'_\ell(ka) + B_\ell n'_\ell(ka) \right) \quad (7.2.44)$$

Let's form the ratio and define β_ℓ as the logarithmic derivative of the radial solution

$$\beta_\ell \equiv \frac{aR'_\ell(a)}{R_\ell(a)} = ka \frac{A_\ell j_\ell(ka) + B_\ell \eta'_\ell(ka)}{A_\ell j_\ell(ka) + B_\ell n_\ell(ka)} = ka \frac{j_\ell(ka) + \frac{B_\ell}{A_\ell} \eta'_\ell(ka)}{j_\ell(ka) + \frac{B_\ell}{A_\ell} n_\ell(ka)} = ka \frac{j_\ell(ka) - \tan \delta_\ell \eta'_\ell(ka)}{j_\ell(ka) - \tan \delta_\ell n_\ell(ka)} \quad (7.2.45)$$

In principle we can use eq. (7.2.45) to get $\tan \delta_\ell$, but let's push the calculation further to extract the phase shift from $e^{2i\delta_\ell}$

$$\begin{aligned} \beta_\ell &= ka \frac{j_\ell \cos \delta_\ell - \eta'_\ell \sin \delta_\ell}{j_\ell \cos \delta_\ell - n_\ell \sin \delta_\ell} = ka \frac{j_\ell (e^{i\delta_\ell} + e^{-i\delta_\ell}) + i\eta'_\ell (e^{i\delta_\ell} - e^{-i\delta_\ell})}{j_\ell (e^{i\delta_\ell} + e^{-i\delta_\ell}) + i n_\ell (e^{i\delta_\ell} - e^{-i\delta_\ell})} \\ &= ka \frac{e^{i\delta_\ell} (j_\ell + i\eta'_\ell) + e^{-i\delta_\ell} (j_\ell - i\eta'_\ell)}{e^{i\delta_\ell} (j_\ell + i n_\ell) + e^{-i\delta_\ell} (j_\ell - i n_\ell)} = ka \frac{e^{2i\delta_\ell} (j_\ell + i\eta'_\ell) + (j_\ell - i\eta'_\ell)}{e^{2i\delta_\ell} (j_\ell + i n_\ell) + (j_\ell - i n_\ell)} \end{aligned} \quad (7.2.46)$$

Solve for $e^{2i\delta_\ell}$

$$e^{2i\delta_\ell} = - \frac{ka(j_\ell - i\eta'_\ell) - \beta_\ell(j_\ell - i n_\ell)}{ka(j_\ell + i\eta'_\ell) - \beta_\ell(j_\ell + i n_\ell)} \quad (7.2.47)$$

which can be rewritten as

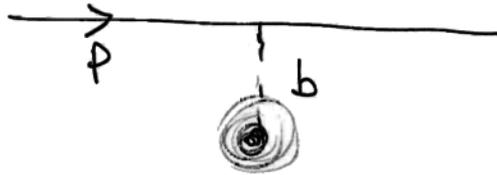
$$e^{2i\delta_\ell} = - \left(\frac{j_\ell - i n_\ell}{j_\ell + i n_\ell} \right) \left[\frac{\beta_\ell - ka \left(\frac{j_\ell - i\eta'_\ell}{j_\ell - i n_\ell} \right)}{\beta_\ell - ka \left(\frac{j_\ell + i\eta'_\ell}{j_\ell + i n_\ell} \right)} \right] \quad (7.2.48)$$

which we can also write as

$$e^{2i\delta_\ell} = \underbrace{e^{2i\xi_\ell}}_{\text{Hard sphere phase shift}} \left[\frac{\beta_\ell - ka \left(\frac{j_\ell - i\eta'_\ell}{j_\ell - i n_\ell} \right)}{\beta_\ell - ka \left(\frac{j_\ell + i\eta'_\ell}{j_\ell + i n_\ell} \right)} \right] \quad (7.2.49)$$

Phase shifts are useful when a few of them dominate the cross section. This happens when $ka < 1$ with a the range of the potential. So short range and/or low energy.

1. Angular momentum of the incident particle is $L = b \cdot p$ with b impact parameter and p momentum



$$L \simeq bp \quad \rightarrow \quad \hbar \ell \simeq b \hbar k \quad \rightarrow \quad b \simeq \frac{\ell}{k} \quad (7.2.50)$$

When $b > a$ there is no scattering

$$\frac{\ell}{k} > a \quad \boxed{\text{Expect no scattering for } \ell > ka} \quad (7.2.51)$$

Thus only values $\ell \leq ka$ contribute to σ .

2. Confirm the impact parameter intuition from partial wave expression. Consider the free partial wave $\sim j_\ell(kr)Y_{\ell,0}$. The impact parameter b_ℓ of such a wave would be estimated to be ℓ/k .

Recall that $j_\ell(kr)$ is a solution of the $V = 0$ radial equation with angular momentum ℓ and energy $\hbar^2 k^2 / (2m)$. Setting the effective potential equal to the energy:

$$\frac{\hbar^2 \ell(\ell+1)}{2mr^2} = \frac{\hbar^2 k^2}{2m} \quad (7.2.52)$$

we find that the turning point for the solution is at

$$k^2 r^2 = \ell(\ell+1). \quad (7.2.53)$$

Thus we expect $j_\ell(kr)$ to be exponentially small beyond the turning point

$$kr \leq \sqrt{\ell(\ell+1)} \simeq \ell \quad (7.2.54)$$

confirming that the wave is negligible for r less than the impact parameter $\ell/k!$

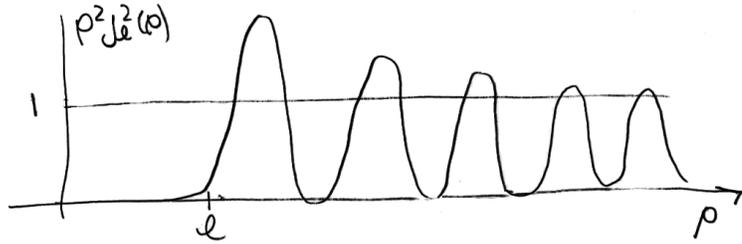


Figure 7.2: Plot of $\rho^2 J_\ell^2(\rho)$

7.3 Integral scattering equation

Some useful approximations can be made when we reformulate the time-independent Schrödinger equation as an integral equation. These approximations, as opposed to the partial waves method, allow us to deal with potentials that are not spherically symmetric. We consider the Schrödinger equation

$$\left[-\frac{\hbar^2}{2M} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad (7.3.1)$$

set the energy equal to that of a plane wave of wavenumber k and rewrite the potential in terms of a rescaled version $U(\mathbf{r})$ that simplifies the units:

$$E = \frac{\hbar^2 k^2}{2M} \quad \text{and} \quad V(\mathbf{r}) = \frac{\hbar^2}{2M} U(\mathbf{r}) \quad (7.3.2)$$

then the Schrödinger equation reads

$$[-\nabla^2 + U(\mathbf{r})] \psi(\mathbf{r}) = k^2 \psi(\mathbf{r}) \quad (7.3.3)$$

rewrite as

$$(\nabla^2 + k^2) \psi(\mathbf{r}) = U(\mathbf{r}) \psi(\mathbf{r}) \quad (7.3.4)$$

This is the equation we want to solve.

Let us introduce $G(\mathbf{r} - \mathbf{r}')$, a Green function for the operator $\nabla^2 + k^2$, i.e.

$$(\nabla^2 + k^2) G(\mathbf{r} - \mathbf{r}') = \delta^{(3)}(\mathbf{r} - \mathbf{r}') \quad (7.3.5)$$

Then we claim that any solution of the integral equation

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \int d^3 \mathbf{r}' G(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') \quad (7.3.6)$$

where $\psi_0(\mathbf{r})$ is a solution of the homogeneous equation

$$(\nabla^2 + k^2) \psi_0(\mathbf{r}) = 0 \quad (7.3.7)$$

is a solution of equation (7.3.4). Let's check that this is true

$$\begin{aligned} (\nabla_{\mathbf{r}}^2 + k^2) \psi(\mathbf{r}) &= (\nabla_{\mathbf{r}}^2 + k^2) \int d^3 \mathbf{r}' G(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') \\ &= \int d^3 \mathbf{r}' \delta^{(3)}(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') \\ &= U(\mathbf{r}) \psi(\mathbf{r}) \quad \checkmark \end{aligned} \quad (7.3.8)$$

To find G we first recall that

$$G(\mathbf{r}) \sim \begin{cases} \frac{C e^{\pm ikr}}{r} & \text{for } r \neq 0 & \text{as a matter of fact} & (\nabla_{\mathbf{r}}^2 + k^2) \frac{e^{\pm ikr}}{r} = 0 \quad \forall r \neq 0 \\ -\frac{1}{4\pi r} & \text{for } r \rightarrow 0 & \text{as a matter of fact} & \nabla^2 \left(-\frac{1}{4\pi r}\right) = \delta^3(\mathbf{r}) \end{cases} \quad (7.3.9)$$

Thus try

$$\boxed{G_{\pm}(\mathbf{r}) = -\frac{1}{4\pi} \frac{e^{\pm ikr}}{r}} \quad (7.3.10)$$

and we are going to refer to G_+ as the *outgoing wave* Green function and to G_- as the *ingoing wave* Green function.

Let's verify that this works, write G as a product: $G_{\pm}(r) = e^{\pm ikr} \left(-\frac{1}{4\pi r}\right)$, so that

$$\nabla^2 G_{\pm}(r) = \left(\nabla^2 e^{\pm ikr}\right) \left(-\frac{1}{4\pi r}\right) + e^{\pm ikr} \nabla^2 \left(-\frac{1}{4\pi r}\right) + 2 \left(\vec{\nabla} e^{\pm ikr}\right) \cdot \vec{\nabla} \left(-\frac{1}{4\pi r}\right) \quad (7.3.11)$$

Recall that

$$\nabla^2 = \nabla \cdot \nabla, \quad \nabla r = \frac{\mathbf{r}}{r}, \quad \nabla \cdot (f\mathbf{A}) = \nabla f \cdot \mathbf{A} + f \nabla \cdot \mathbf{A} \quad (7.3.12)$$

Therefore

$$\nabla e^{\pm ikr} = \pm ik \frac{\mathbf{r}}{r} e^{\pm ikr}, \quad \nabla^2 e^{\pm ikr} = \left(-k^2 \pm \frac{2ik}{r}\right) e^{\pm ikr} \quad (7.3.13)$$

then

$$\begin{aligned} \nabla^2 G_{\pm}(r) &= \left(-k^2 \pm \frac{2ik}{r}\right) e^{\pm ikr} \left(-\frac{1}{4\pi r}\right) + e^{\pm ikr} \delta^3(\mathbf{r}) + 2 \left(\pm ik e^{\pm ikr} \frac{\mathbf{r}}{r}\right) \cdot \left(\frac{\mathbf{r}}{4\pi r^3}\right) \\ &= -k^2 G_{\pm}(r) \mp \frac{2ik}{4\pi r} e^{\pm ikr} + \delta^3(\mathbf{r}) \pm \frac{2ik}{4\pi r} e^{\pm ikr} \\ &= -k^2 G_{\pm}(r) + \delta^3(\mathbf{r}) \quad \checkmark \end{aligned} \quad (7.3.14)$$

We will use

$$\psi_0(\mathbf{r}) = e^{ikz} \quad \text{and} \quad G = G_+ \quad (7.3.15)$$

Thus, with these choices, (7.3.6) takes the form

$$\psi(\mathbf{r}) = e^{ikz} + \int d^3\mathbf{r}' G_+(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') \quad (7.3.16)$$

where

$$G_+(\mathbf{r} - \mathbf{r}') = -\frac{1}{4\pi} \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \quad (7.3.17)$$

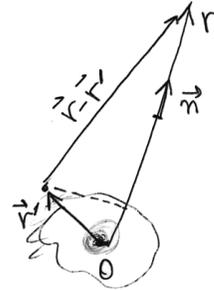
We now want to show that this is consistent with our asymptotic expansion for the energy eigenstates. For that we can make the following approximations

$$\text{For the } G_+ \text{ denominator:} \quad |\mathbf{r} - \mathbf{r}'| \simeq r \quad (7.3.18)$$

$$\text{For the } G_+ \text{ numerator:} \quad |\mathbf{r} - \mathbf{r}'| \simeq r - \mathbf{n} \cdot \mathbf{r}' \quad (7.3.19)$$

where

$$\mathbf{n} \equiv \frac{\mathbf{r}}{r}$$



In this way

$$G_+(\mathbf{r} - \mathbf{r}') = -\frac{1}{4\pi r} e^{ikr} e^{-ik\mathbf{n}\cdot\mathbf{r}'} \quad (7.3.20)$$

Thus

$$\psi(\mathbf{r}) = e^{ikz} + \left[-\frac{1}{4\pi} \int d^3\mathbf{r}' e^{-ik\mathbf{n}\cdot\mathbf{r}'} U(\mathbf{r}') \psi(\mathbf{r}') \right] \frac{e^{ikr}}{r} \quad (7.3.21)$$

The object in brackets is a function of the unit vector \mathbf{n} in the direction of \mathbf{r} . This shows that the integral equation, through the choice of G , incorporates both the Schrödinger equation and the asymptotic conditions. By definition, the object in brackets is $f_k(\theta, \phi)$, i.e.

$$f_k(\theta, \phi) = -\frac{1}{4\pi} \int d^3\mathbf{r}' e^{-ik\mathbf{n}\cdot\mathbf{r}'} U(\mathbf{r}') \psi(\mathbf{r}'). \quad (7.3.22)$$

Of course, this does not yet determine f_k as the undetermined wavefunction $\psi(\mathbf{r})$ still appears under the integral. The incident wave has the form of $e^{i\mathbf{k}_i\cdot\mathbf{r}}$ with \mathbf{k}_i the incident wave number, $|\mathbf{k}_i| = k$. For the outgoing wave we define $\mathbf{k}_s \equiv \mathbf{n}k$ (in the direction of \mathbf{n}), the scattered wave vector. The expression for $\psi(\mathbf{r})$ then becomes

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_i\cdot\mathbf{r}} + \left[-\frac{1}{4\pi} \int d^3\mathbf{r}' e^{-i\mathbf{k}_s\cdot\mathbf{r}'} U(\mathbf{r}') \psi(\mathbf{r}') \right] \frac{e^{ikr}}{r} \quad (7.3.23)$$

We will do better with the Born approximation.

7.3.1 The Born approximation

Consider the original integral expression:

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_i\cdot\mathbf{r}} + \int d^3\mathbf{r}' G_+(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \psi(\mathbf{r}') \quad (7.3.24)$$

Rewrite by just relabeling $\mathbf{r} \rightarrow \mathbf{r}'$

$$\psi(\mathbf{r}') = e^{i\mathbf{k}_i\cdot\mathbf{r}'} + \int d^3\mathbf{r}'' G_+(\mathbf{r}' - \mathbf{r}'') U(\mathbf{r}'') \psi(\mathbf{r}''). \quad (7.3.25)$$

Now plug (7.3.25) under the integral in (7.3.24) to get

$$\psi(\mathbf{r}) = e^{i\mathbf{k}_i\cdot\mathbf{r}} + \int d^3\mathbf{r}' G_+(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') e^{i\mathbf{k}_i\cdot\mathbf{r}'} + \int d^3\mathbf{r}' G_+(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \int d^3\mathbf{r}'' G_+(\mathbf{r}' - \mathbf{r}'') U(\mathbf{r}'') \psi(\mathbf{r}'') \quad (7.3.26)$$

Repeat the trick once more to find

$$\begin{aligned} \psi(\mathbf{r}) &= e^{i\mathbf{k}_i\cdot\mathbf{r}} + \int d^3\mathbf{r}' G_+(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') e^{i\mathbf{k}_i\cdot\mathbf{r}'} \\ &\quad + \int d^3\mathbf{r}' G_+(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \int d^3\mathbf{r}'' G_+(\mathbf{r}' - \mathbf{r}'') U(\mathbf{r}'') e^{i\mathbf{k}_i\cdot\mathbf{r}''} \\ &\quad + \int d^3\mathbf{r}' G_+(\mathbf{r} - \mathbf{r}') U(\mathbf{r}') \int d^3\mathbf{r}'' G_+(\mathbf{r}' - \mathbf{r}'') U(\mathbf{r}'') \int d^3\mathbf{r}''' G_+(\mathbf{r}''' - \mathbf{r}'') U(\mathbf{r}''') \psi(\mathbf{r}''') \end{aligned} \quad (7.3.27)$$

By iterating this procedure we can form an infinite series which schematically looks like

$$\psi = e^{i\mathbf{k}_i \cdot \mathbf{r}} + \int GUe^{i\mathbf{k}_i \mathbf{r}} + \int GU \int GUe^{i\mathbf{k}_i \mathbf{r}} + \int GU \int GU \int GUe^{i\mathbf{k}_i \mathbf{r}} + \dots \quad (7.3.28)$$

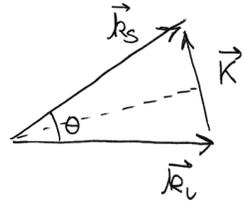
The approximation in which we keep the first integral in this series and set to zero all others is called the *first Born approximation*. The preparatory work was done in (7.3.23), so we have now

$$\psi^{\text{Born}}(\mathbf{r}) = e^{i\mathbf{k}_i \cdot \mathbf{r}} - \frac{1}{4\pi} \left(\int d^3\mathbf{r}' e^{-i\mathbf{k}_s \cdot \mathbf{r}'} U(\mathbf{r}') e^{i\mathbf{k}_i \cdot \mathbf{r}'} \right) \frac{e^{i\mathbf{k}_i \cdot \mathbf{r}}}{r} \quad (7.3.29)$$

hence

$$f_k^{\text{Born}}(\theta, \phi) = -\frac{1}{4\pi} \int d^3\mathbf{r} e^{-i\mathbf{K} \cdot \mathbf{r}} U(\mathbf{r}). \quad (7.3.30)$$

Here we defined the *wave-number transfer* \mathbf{K} :

$$|\mathbf{k}_i| = |\mathbf{k}_s|, \quad \mathbf{K} \equiv \mathbf{k}_s - \mathbf{k}_i \quad (7.3.31)$$


Note that we eliminated the primes on the variable of integration – it is a dummy variable after all. The *wave-number transfer* is the momentum that must be added to the incident one to get the scattered one. We call θ the angle between \mathbf{k}_i and \mathbf{k}_s (it is the spherical angle θ if \mathbf{k}_i is along the positive z -axis).

Note that

$$K = |\mathbf{K}| = 2k \sin \frac{\theta}{2} \quad (7.3.32)$$

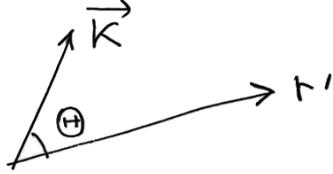
In the Born approximation the scattering amplitude $f_k(\theta, \phi)$ is simply the Fourier transform of $U(\mathbf{r})$ evaluated at the momentum transfer \mathbf{K} ! $f_k(\theta, \phi)$ captures some information of $V(\mathbf{r})$.

If we have a central potential $V(\mathbf{r}) = V(r)$, we can simplify the expression for the Born scattering amplitude further by performing the radial integration. We have

$$f_k^{\text{Born}}(\theta) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3\mathbf{r} e^{-i\mathbf{K} \cdot \mathbf{r}} V(\mathbf{r}). \quad (7.3.33)$$

By spherical symmetry this integral just depends on the norm K of the vector \mathbf{K} . This is why we have a result that only depends on θ : while \mathbf{K} is a vector that depends on both θ and ϕ , its magnitude only depends on θ . To do the integral think of \mathbf{K} fixed and let Θ be

the angle with \mathbf{r}

$$\begin{aligned}
 f_k(\theta) &= -\frac{m}{2\pi\hbar^2} \int_0^\infty 2\pi dr r^2 \int_{-1}^1 d(\cos \Theta) e^{-iKr \cos \Theta} V(r) \\
 &= -\frac{m}{\hbar^2} \int_0^\infty dr r^2 V(r) \frac{e^{-iKr} - e^{iKr}}{-iKr} = -\frac{m}{\hbar^2} \int_0^\infty dr r^2 V(r) \left(\frac{2 \sin(Kr)}{Kr} \right)
 \end{aligned}
 \tag{7.3.34}$$


hence

$$\boxed{f_k(\theta) = -\frac{2m}{K\hbar^2} \int_0^\infty dr r V(r) \sin(Kr)}
 \tag{7.3.35}$$

with $K = 2k \sin \frac{\theta}{2}$.

The Born approximation treats the potential as a perturbation of the free particle waves. This wave must therefore have kinetic energies larger than the potential. So most naturally, this is a good high-energy approximation.

Example: Yukawa potential Given

$$V(\mathbf{r}) = V(r) = \beta \frac{e^{-\mu r}}{r} \quad \beta, \mu > 0
 \tag{7.3.36}$$

from (7.3.35), one gets

$$f_k(\theta) = -\frac{2m\beta}{K\hbar^2} \int_0^\infty dr e^{-\mu r} \sin(Kr) = -\frac{2m\beta}{\hbar^2(\mu^2 + K^2)}.
 \tag{7.3.37}$$

We can give a graphical representation of the Born series. Two waves reach the desired point \mathbf{r} . The first is the direct incident wave. The second is a secondary wave originating at the scattering “material” at a point \mathbf{r}' . The amplitude of a secondary source at \mathbf{r}' is given by the value of the incident wave times the *density* $U(\mathbf{r}')$ of scattering material at \mathbf{r}' .

In the second figure again an incident wave hits \mathbf{r} . The secondary wave now takes two steps: the incident wave hits scattering material at \mathbf{r}'' which then propagates and hits scattering material at \mathbf{r}' , from which it travels to point \mathbf{r} .

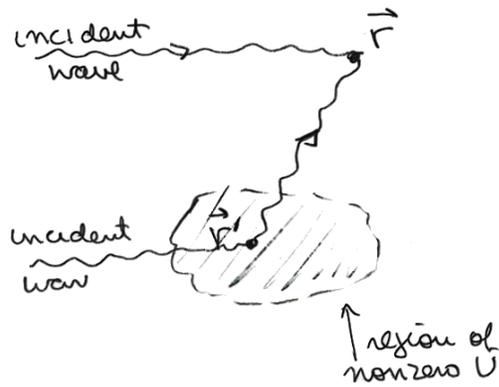


Figure 7.3: Pictorial view of Born approximation. Wave at \mathbf{r} is the sum of the free incident wave at \mathbf{r} , plus an infinite number of waves coming from the secondary source at \mathbf{r}' , induced by the incident wave.

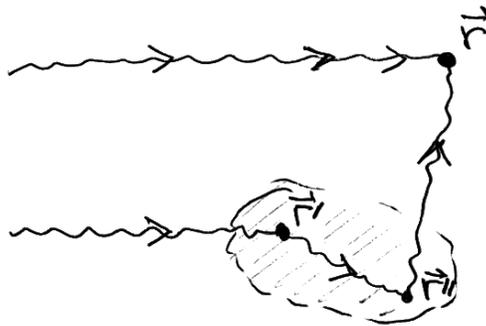


Figure 7.4: Pictorial view of second order Born term

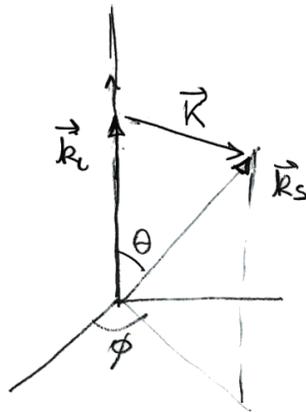


Figure 7.5: Given (θ, ϕ) and k (\sim energy), \mathbf{K} is determined.

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