

UNIT 1

Scattering

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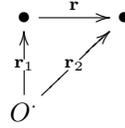
Scattering is such an important phenomenon that is used in high energy physics to understand the forces of the nature and the properties of the materials. In general, there are two types of scattering used in the scientific research. One type uses colliding beams of high energy particles to produce new particles. Looking at the by products of such collisions gives scientists insight into the fundamental forces of nature. The LHC (*Large Hadron Collider*) is the biggest examples for this kind of scattering, and it's very important. The other type is to scatter beams of particles, like neutrons, off a stationary material target. This type of experiment is used to understand the property of the target material. A prime example of this type is the SNS (*Spallation Neutron Source*) at Oak Ridge National Laboratory. It is one-of-a-kind facility provides the most intense pulsed neutron beams in the world for scientific research and industrial development.

Since we can consider the two colliding particle beams in the rest frame of one of the beams, studying these kinds of scattering phenomena is not as hard as it seems to be.

First of all, let me ask the question of whether two electrons will meet once they are directed to each other for collision. Since electrons are fundamental particles they are exact points and laws of classical mechanics cannot be used to answer this question. As an answer for this question we can say that there is a probability for these electrons to meet. Another question that begs an answer is: if electrons do not meet *how do they scatter then?* The Coulomb force causes the electrons to be deflected. On the other hand, for two particles attracting each other we can say that there is a certain possibility of these particles' positions therefore there is a finite possibility for these particles to find each other.

We are going to assume that what governs the force between each particle is the potential which only depends on the relative position $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ of the

particles.



where,

\mathbf{r} : distance between particle m_1 and m_2

\mathbf{r}_1 : distance of particle m_1 from the origin

\mathbf{r}_2 : distance of particle m_2 from the origin

In the center-of-mass reference frame of the two particles the problem will be reduced to the study of *the scattering of a single particle by the potential $V(\mathbf{r})$* . Therefore, the mass of the particles also will be reduced to a value of $\mu = \frac{m_1 m_2}{m_1 + m_2}$. This μ value is called the *effective* or *reduced* mass and it is the mass of the "relative particle".

In the rest frame of a scattering, in which there is a particle beam directed towards a target, we see the distribution of the particles on the detector.

1-Dimensional Case

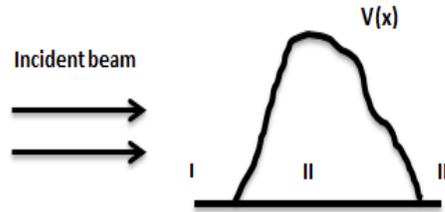


Figure 1: 1-d potential

Figure 1 shows the incident beam interacting with an arbitrary one dimensional potential. In case of interacting with a potential there will be transmitted and reflected beam of particles. As you may remember from the previous semester a square potential was given as an example for this type of scattering. For particles whose energy greater than zero there will be a continuous spectrum and the Schrodinger equation can be written as,

$$-\frac{\hbar^2}{2m}\varphi'' + V\varphi = E\varphi, \quad E > 0 \quad (1)$$

Since the spectrum is continuous solution of the Schrodinger equation for scattering potential gives a plane and non-normalizable wavefunction. It is,

$$\varphi_{inc} = Ae^{ikx}, \quad x \rightarrow -\infty \quad (2)$$

where $k = \frac{\sqrt{2mE}}{\hbar}$. The solutions for reflected and transmitted beam of particles are respectively,

$$\varphi_r = Be^{-ikx} \quad (3)$$

$$\varphi_t = Ce^{ikx} \quad (4)$$

The wave function incident in region I would be the sum of the wavefunctions which are incident and reflected.

$$\varphi_I = \varphi_{inc} + \varphi_r \quad (5)$$

The wavefunction transmitted in region III, where the potential ends, is,

$$\varphi_{III} = Ce^{ikx}, \quad x \rightarrow +\infty \quad (6)$$

The wavefunction is not a physical quantity therefore we cannot measure it in the experiments. What we measure in the experiments is the probability current. Probability current is defined as $\mathbf{J} = \frac{i\hbar}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi)$. There is a continuity equation for probability current and current density which gives the conservation law of probability current, \mathbf{J} . For this scattering case the probability current density, ρ , does not depend explicitly on time.

$$\frac{\partial\rho}{\partial t} + \frac{\partial J}{\partial x} = 0 \quad (7)$$

Once we do the calculation,

$$J = -\frac{i\hbar}{2m}\varphi^*\varphi'' + C.C. \quad (8)$$

$$J' = -i\frac{i\hbar}{2m}\varphi^*\varphi' - \frac{i\hbar}{2m}\varphi^*\varphi'' + C.C. \quad (9)$$

As you measure the physical quantities in the scattering process you stay away from the scattering potential therefore from the Schrodinger equation

$$\varphi'' = -\frac{2mE}{\hbar^2}\varphi \quad (10)$$

$$J' = -\frac{i\hbar}{2m}|\varphi'|^2 + C.C. = 0 \quad (11)$$

From equation (1.11) we can easily see that probability current, J , is conserved - i.e. it does not depend explicitly on x and it is just a number.

As $x \rightarrow -\infty$ there will be two contributions to the wavefunction, φ , i.e. one from incident beam of particles and one from reflected beam of particles. Therefore J becomes,

$$J = -i\frac{i\hbar}{2m}(A^*e^{-ikx} + B^*e^{ikx})ik(Ae^{ikx} - Be^{-ikx}) + C.C. = \frac{\hbar k}{m}(|A|^2 - |B|^2) \quad (12)$$

$$J_{inc} = \frac{\hbar k}{m} |A|^2, \quad J_r = \frac{\hbar k}{m} |B|^2 \quad (13)$$

As $x \rightarrow +\infty$ the only contribution comes from the transmitted probability current density.

$$J_t = \frac{\hbar k}{m} |C|^2 \quad (14)$$

Since J is a conserved quantity no matter how complicated the Schrodinger equation is the incident probability current is equal to the sum of the reflected probability current and the transmitted probability current.

$$J_{inc} = J_r + J_t. \quad (15)$$

If equation (1.15) is divided by J_{inc} then we obtain that

$$1 = \frac{J_r}{J_{inc}} + \frac{J_t}{J_{inc}}. \quad (16)$$

In the equation above the $\frac{J_r}{J_{inc}}$ value is called the reflection coefficient and denoted as R . The $\frac{J_t}{J_{inc}}$ value is called the transmission coefficient and denoted as T . Therefore,

$$R + T = 1 \quad (17)$$

The most interesting point of the scattering phenomenon is that the reflected particles are the scattered particles from the scattering potential. The number of reflected particles is about 10^{20} . Say we have a beam of particles which consists of N number of particles. The probability density, ρ , for such a beam is

$$\rho = |\varphi|^2 \quad \text{and} \quad \int \rho dx = 1 \quad (18)$$

If we measure a number of particles given a certain distance then,

$$\frac{\# \text{ of particles}}{\text{length}} = N\rho = \# \text{ density} \quad (19)$$

If the N number of particles are electrons with charge e then what you measure in the experiment is the charge density.

$$\text{charge density} = eN\rho \quad (20)$$

The *electrical current* is defined as the number of particles passing through a certain point in unit time. Therefore, the electrical current for this beam of particles is

$$\text{electrical current} = eNJ = \frac{\text{charge}}{\text{time}} \quad (21)$$

Since the electrical current is directly proportional to the probability current density, J , reflection and transmission coefficients can be written as the ratio of the reflected and transmitted currents to the incident current.

$$R = \frac{\text{reflected current}}{\text{incident current}} \quad \text{and} \quad T = \frac{\text{transmitted current}}{\text{incident current}}. \quad (22)$$

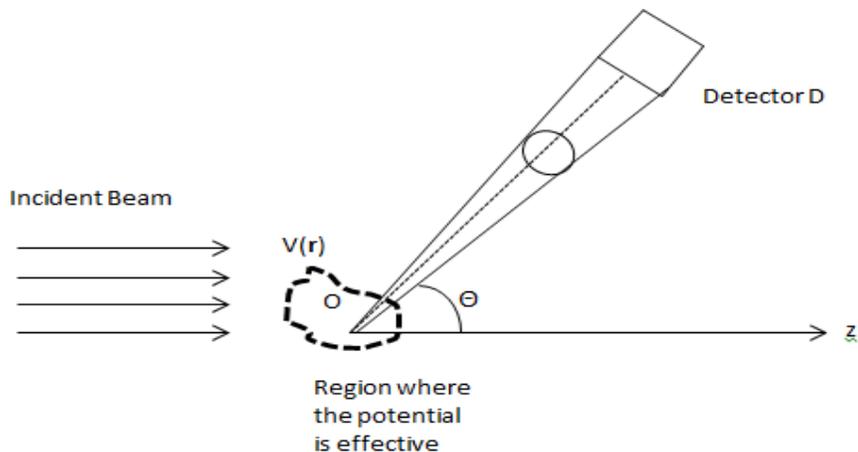


Figure 2: 3-d potential

3-Dimensional Case

In 3-d case we are going to introduce current density. To use the current density we need to introduce the concept of flux- the number of particles per unit time which traverse a unit surface perpendicular to direction of the beam. The flux of the incident particles beam is F_{inc} .

$$F_{inc} = \frac{\# \text{ of particles}}{(\text{area})(\text{time})} \quad (23)$$

$$\text{current density} = J = \frac{\text{charge}}{(\text{area})(\text{time})} = \frac{I}{\text{area}} \quad (24)$$

In Figure 2 a detector is placed far from the region under the influence of the potential. The number of particles, dn , scattered per unit time into the solid angle $d\Omega$ about the direction (θ, φ) is

$$dn = F_{inc} \sigma(\theta, \varphi) d\Omega \quad (25)$$

where $\sigma(\theta, \varphi)$ is the *differential scattering cross section* in the direction (θ, φ) . Scattering cross section is the coefficient of proportionality between dn and $F_{inc} d\Omega$. In other words, the scattering cross section is

$$\frac{\# \text{ of deflected particles/time}}{\text{incident flux}} \quad (26)$$

The scattering cross section has the dimension of area which is on the order of $\approx 10^{-24} \text{cm}^2$. Since 10^{-24}cm^2 is small the unit of barn is used.

$$1 \text{ barn} = 10^{-24} \text{cm}^2 \quad (27)$$

The total cross section is the integral over the solid angle, that is,

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} \quad (28)$$

The second term on the right-hand-side of the equation above is called the differential cross section and it is rather useful.

Now, let us find a simple expression for scattering cross section, σ . As far as the incident beam is concerned the wavefunction is $\varphi = Ae^{ikz}$, where $k = \frac{\sqrt{2mE}}{\hbar}$ and m is the reduced mass. For simplicity we set $A=1$, therefore the wavefunction for the incident beam is $\varphi = e^{ikz}$. On the other hand, reflected and transmitted wavefunctions are more complicated.

To find the scattered wavefunction we shall solve the Schrodinger equation. Since the detector is far from the scattering potential we can neglect the potential in the Schrodinger equation. Therefore,

$$-\frac{\hbar^2}{2m}\nabla^2\varphi = E\varphi \quad (29)$$

$$\nabla^2\varphi + k^2\varphi = 0 \quad (30)$$

We assume that there is a spherical symmetry and we shall use the spherical coordinates to solve the equation above.

$$\frac{1}{r}(r\varphi)'' + k^2\varphi = 0 \quad (31)$$

Let's denote $(r\varphi)$ as u , that is,

$$u'' + k^2u = 0 \quad \Rightarrow \quad u = e^{\pm ikr} \quad (32)$$

Since the particles are scattering we choose e^{ikr} as a solution for u . Therefore the generalized solution for the scattered wavefunction is,

$$\varphi = \frac{1}{r}e^{ikr}. \quad (33)$$

Figure 2 *does not* have spherical symmetry therefore we hope to manipulate φ in such a way as to arrive at an appropriate solution for φ . We therefore need to solve an equation that is a little more general,

$$\nabla^2\varphi + k^2\varphi = \rho \quad (34)$$

Where ρ will be something that I have to figure out if it means anything at all. If we have to solve Eq. (3) the solution is known because all one has to do is look to electrostatics for the necessary steps. And that will give me φ at r , that is,

$$\varphi(\vec{r}) = - \int d^3r' \rho(\vec{r}') G_{\pm}(\vec{r}, \vec{r}') \quad G_{\pm}(\vec{r}, \vec{r}') = - \frac{e^{ik|\vec{r}-\vec{r}'|}}{4\pi|\vec{r}-\vec{r}'|} \quad (35)$$

$G(\vec{r}, \vec{r}')$ is a Green's function, and $\varphi(\vec{r})$ is now a general solution to Eq. (3). So this Green function is the same as φ , the spherically symmetric case, so it must obey the Schrodinger equation.

$$\nabla^2 G_{\pm} + k^2 G_{\pm} = 0 \quad (36)$$

Have to be careful here because as $\vec{r} \rightarrow 0$ you get a singularity, so it's zero everywhere except exactly at the origin, therefore,

$$\nabla^2 G_{\pm} + k^2 G_{\pm} = \delta^3(\vec{r}) \quad (37)$$

Integrating Eq. (6),

$$\int d^3 r' (\nabla^2 G_{\pm} + k^2 G_{\pm}) = \int d^3 r' \delta^3(\vec{r}) \quad (38)$$

$$\int \vec{\nabla} G_{\pm} \cdot d\vec{S} + k^2 \int d^3 r G_{\pm} = 1 \quad (39)$$

And as the spherical volume element within the integral shrinks to zero Eq. (8) becomes one as it should.

$$1 + 0 = 1 \quad (40)$$

And now we understand how to solve Eq. (3), in general. But no matter what, we want to go far away from the scattering potential and we want to put the detector way out so it's not effected by what's happening. So we look at the behavior as $\vec{r} \rightarrow \infty$.

$$|\vec{r} - \vec{r}'| = \sqrt{r^2 + r'^2 - 2rr' \cos \beta} \approx r - r' \cos \beta \quad (41)$$

Where β is the angle between \vec{r} and \vec{r}' . If we go back to the expression for $\varphi(\vec{r})$ and use the approximation for $|\vec{r} - \vec{r}'|$,

$$\varphi(\vec{r}) = - \int d^3 r' \rho(\vec{r}') \frac{e^{ikr - ikr' \cos \beta}}{4\pi r} = - \frac{e^{ikr}}{4\pi r} \int d^3 r' \rho(\vec{r}') e^{-ikr' \cos \beta} \quad (42)$$

Notice the factor outside the integral it's a nice spherical wave traveling outward, and then there's the integral. What is this integral a function of? After integrating over r' this integral is going to be a function of \vec{r} , which has three component in spherical coordinates $f(r, \theta, \varphi)$. But because there is no r (the distance r not the vector \vec{r}) f will be a function of the angles only. So we have a nice spherical wave as it goes out but it's modulated as you go around the angles. We don't quite understand $\rho(\vec{r}')$ yet but at least we can write $\varphi(\vec{r})$ as,

$$\varphi(\vec{r}) = - \frac{e^{ikr}}{4\pi r} f(\theta, \varphi) \quad (43)$$

So this is our equation for the out going scattered wave. The entire wave function will be the combination of the incoming wave, e^{ikz} , and the outgoing wave.

$$\Phi = e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi) \quad (44)$$

The minus and factor of 4π were absorbed in the arbitrary function $f(\theta, \phi)$. This generalizes what we found in one dimension. Next, we're going to take a look at the probability current and try to generalize from one to three dimensions. Recall that the probability current and the gradient in spherical coordinates are given by,

$$\vec{J} = -\frac{i\hbar}{2m} \Phi^* \vec{\nabla} \Phi + C.C. \quad (45)$$

$$\vec{\nabla} = \frac{\partial}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \hat{\phi} \quad (46)$$

The incident current $\vec{J}_i = \frac{\hbar k}{m} \hat{z}$. Now the scattered wave, or the out going wave, it's going to have three components.

$$(J_{out})_r = -\frac{i\hbar}{2m} \frac{e^{-ikr}}{r} f^* f \left[\frac{ike^{ikr}}{r} - \frac{e^{ikr}}{r^2} \right] + C.C. = \frac{\hbar k}{m} \frac{|f|^2}{r^2} \quad (47)$$

$$(J_{out})_\theta = -\frac{i\hbar}{2m} \frac{1}{r^3} f^* \frac{\partial f}{\partial \theta} + C.C. \quad (48)$$

$$(J_{out})_\phi = -\frac{i\hbar}{2m} \frac{1}{r^3 \sin \theta} f^* \frac{\partial f}{\partial \phi} + C.C. \quad (49)$$

The currents are very complicated. So what can we do about it? Now remember we want to know what happens very far away from the scattering potential, as $r \rightarrow \infty$. That's where the detector is going to be and that's where I'm going to observe the currents. The angular components of the probability currents fall off like r^{-3} and we can forget about them. The current represents particles that come out so it has to be conserved. It's all coming out in the radial direction. The total out going current is given by integrating over a sphere.

$$I_{out} = \int J_r dS = \frac{\hbar k}{m} \int d\Omega |f|^2 \quad (50)$$

It turns out that I_{out} is a constant, no r dependence and only the solid angle. Which it needs to be because probability currents need to be conserved. Now we can build an expression for the scattering cross section.

$$\sigma = \frac{I_{out}}{J_{in}} = \int d\Omega |f|^2 \quad (51)$$

If we care about the distribution of particles then we need the differential cross section. You can see that the differential cross section is given precisely by the function f . This is a very important function because this is what we're going to be able to measure.

$$\sigma = \int d\Omega |f|^2 = \int d\Omega \frac{d\sigma}{d\Omega} \quad \rightarrow \quad \frac{d\sigma}{d\Omega} = |f|^2 \quad (52)$$

Where do we even find this $f(\Omega)$? We turn back to our old friend the Schrodinger equation. And when it is written in this way we can see that it's form is similar to that of Eq. (3). Except now we can see that ρ comes from φ itself.

$$\nabla^2 \varphi + k^2 \varphi = \frac{2m}{\hbar^2} V \varphi \quad k = \frac{\sqrt{2mE}}{\hbar} \quad (53)$$

If we can say $\rho = \frac{2m}{\hbar^2} V \varphi$ then we already know of the solution to Eq. (22). It is an integral equation and nobody can solve it.

$$\varphi(\vec{r}) = e^{ikz} + \frac{2m}{\hbar^2} \int d^3 r' G_+(\vec{r}, \vec{r}') V(\vec{r}') \varphi(\vec{r}') \quad (54)$$

But, if you can solve it you're going to get the function f . Well, like before we only care about what happens really far away at the detector. We have the right ρ now so f is therefore given by,

$$f(\theta, \phi) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3 r' e^{ik\vec{r}' \cdot \hat{r}} V(\vec{r}') \varphi(\vec{r}') \quad (55)$$

Now let's calculate this. To do so we need to use the Born approximation. Let $\varphi \approx e^{ikz}$. Then for Eq. (24),

$$f(\theta, \phi) \approx -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3 r' e^{ik\vec{r}' \cdot \hat{r}} V(\vec{r}') e^{ikz'} \quad (56)$$

And if we look in the direction of r we can write $kz' = \vec{k}_i \cdot \vec{r}'$. Which is the definition of the Fourier transform of V .

$$f_B = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3 r' e^{-i(\vec{k}_s - \vec{k}_i) \cdot \vec{r}'} V(\vec{r}') = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \tilde{V}(\vec{k}_s - \vec{k}_i) \quad (57)$$

We can improve our Born approximation through iterations.

$$\varphi_0 = e^{ikz} \quad (58)$$

$$\varphi_1 = e^{ikz} + \frac{2m}{\hbar} \int d^3 r' G_+(\vec{r}, \vec{r}') V(\vec{r}') e^{ikz'} \quad (59)$$

$$\varphi_2 = e^{ikz} + \frac{2m}{\hbar} \int d^3 r' G_+(\vec{r}, \vec{r}') V(\vec{r}') \varphi(\vec{r}') \quad (60)$$

Instead of having a plane wave let's try spherical wave. How do we find all solutions? Need to solve the equation $\nabla^2 \varphi + k^2 \varphi = 0$, and find the eigenvalues, of which will commute with a set of operators $\{H, L^2, L_z\}$.

$$\varphi_{klm} = R_{kl} Y_{lm}(\theta, \phi) \quad (61)$$

$$-\frac{\hbar^2}{2m} \frac{1}{r} (rR)'' + \frac{l(l+1)\hbar^2}{2mr^2} R = ER \quad \text{let } u = rR \quad (62)$$

$$-\frac{\hbar^2}{2m} u'' + \frac{l(l+1)\hbar^2}{2mr^2} u = Eu \quad (63)$$

Now as $r \rightarrow 0$ there is asymptotic behavior.

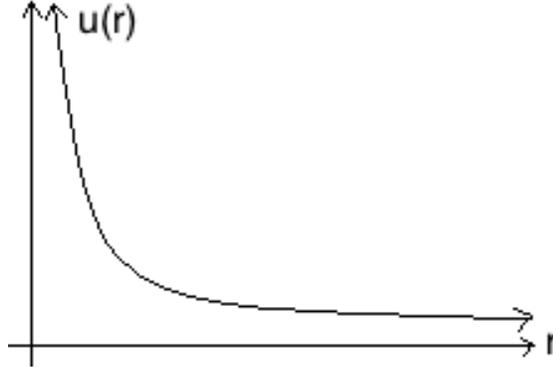


Figure 3: asymptotic behavior

Therefore,

$$-u'' + \frac{l(l+1)}{r^2} u = Eu \approx 0 \quad (64)$$

Solution of the differential equation above is done by writing $u = r^\lambda$ instead of u and then,

$$\lambda(\lambda+1) = l(l+1) \implies \lambda = -l \text{ or } l+1 \quad (65)$$

We choose the solution of $\lambda = l+1$ therefore the solution of this differential equation is r^{l+1} for $r \rightarrow 0$.

On the other hand, as $r \rightarrow \infty$, u becomes that of a free particle.

$$-\frac{\hbar^2}{2m} u'' = Eu \implies u = e^{\pm ikr} \quad (66)$$

We have found the general solution valid for a far away detector and the boundary conditions examined. For instance as $r \rightarrow 0$ we have found that u also goes to zero therefore $u \approx r^{l+1}$ and as $r \rightarrow \infty$ $u \approx e^{\pm ikr}$. Let us do an example about this kind of situation. We are going to examine them for different l and now we are going to start with the simplest case which is $l=0$.

- $l=0$

When we are far away from the potential there are two solutions and the most general solution is

$$u = A' e^{ikr} + B' e^{-ikr} \quad (67)$$

If we *Taylor expand* the function u it becomes

$$u = A' + B' + ik(A' - B')r + \dots \quad (68)$$

In the limit when r goes to zero we find that

$$A' = -B' \quad (69)$$

Using this relation between A' and B' we can write u as

$$u = A'(e^{ikr} - e^{-ikr}) = A \sin(kr) \quad (70)$$

then the radial part of the wavefunction which is R will be

$$R = A \frac{\sin(kr)}{r} \quad (71)$$

In this case it is very simple because l is zero and then to find the wavefunction we need to multiply this by spherical harmonics which is constant for $l = 0$. Now it can be seen that this radial wavefunction, R , is a mixture of incoming and outgoing waves which has to be in this way because we want a valid solution for everywhere so as $r \rightarrow 0$ this wavefunction needs to satisfy this condition as well. In case of the Hydrogen atom the radial part of the wavefunction needs to be normalized. But here we don't have normalization because the energy of the particles are greater than zero and we have a continuous spectrum therefore to normalize this radial wavefunction we are going to use the *delta function*. Let us write the inner product for the wavefunction.

$$I = \int d^3r \varphi_{k'0}^*(\vec{r}) \varphi_{k0}(\vec{r}) \quad (72)$$

If we separate this into radial and angular parts we find

$$I = \int_0^\infty dr u_k^*(r) u_{k'}(r) \int d\Omega |Y_{00}|^2 \quad (73)$$

Since spherical harmonics are normalized the second integral term will be equal to 1. Now to calculate the integral for the radial part let us substitute the value of $u = A \sin(kr)$ in the integral.

$$I = A_k^* A_{k'} \int_0^\infty dr \sin(kr) \sin(k'r) \quad (74)$$

To solve this integral we are going to write the sine functions in terms of exponentials.

$$I = A_k^* A_{k'} \int_0^\infty dr \frac{(e^{ikr} - e^{-ikr})}{2i} \frac{(e^{ik'r} - e^{-ik'r})}{2i} \quad (75)$$

$$I = \frac{A_k^* A_{k'}}{(2i)^2} \int_0^\infty dr [e^{i(k+k')r} - e^{-i(k-k')r} - e^{i(k'-k)r} + e^{-i(k+k')r}] \quad (76)$$

If we do change of variable from $r \rightarrow -r$ the first and the last terms in the integral will be the same except for their limits. For the last term the limit of the integral is going to be from $-\infty$ to zero.

$$I = \frac{A_k^* A_{k'}}{(2i)^2} \int_{-\infty}^\infty dr [e^{i(k+k')r} - e^{-i(k-k')r}] = 2\pi \frac{A_k^* A_{k'}}{(2i)^2} [\delta(k+k') - \delta(k-k')] \quad (77)$$

Since both k, k' are positive the first delta function goes to zero and the integral becomes

$$I = |A_k|^2 \frac{\pi}{2} \delta(k-k') \quad (78)$$

The normalization for a continuous spectrum will be equal to the delta function therefore the normalization constant, A_k , is

$$A_k = \sqrt{\frac{2}{\pi}} \quad (79)$$

This normalization constant is the same for the plane waves as well because $\langle k|k' \rangle = \delta(k-k')$.

- $l=1$

To calculate the wavefunction for the case of $l=1$ we are going to use the wavefunction we obtained for $l=0$ and we shall define the momentum operator, $P_+ = P_x + iP_y$. The momentum operator commutes with the Hamiltonian which means that they have the same eigenfunction. Let us apply the Hamiltonian and P_+ operator to the eigenfunction of the Hamiltonian.

$$H|\varphi\rangle = E|\varphi\rangle \quad (80)$$

$$HP_+|\varphi\rangle = P_+H|\varphi\rangle = EP_+|\varphi\rangle \quad (81)$$

Once we apply this momentum operator, P_+ , to the wavefunction for the case of $l=0$ we can find the wavefunction for the case of $l=1$.

$$P_+ \frac{\sin(kr)}{r} = -i\hbar \left(\frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right) \frac{\sin(kr)}{r} \quad (82)$$

The derivative of r with respect to x and y is respectively,

$$\frac{\partial r}{\partial x} = \frac{x}{r}, \quad \frac{\partial r}{\partial y} = \frac{y}{r} \quad (83)$$

Therefore,

$$P_+ \frac{\sin(kr)}{r} = -i\hbar \left(\frac{x+iy}{r} \right) \left(\frac{\sin(kr)}{r} \right)' \quad (84)$$

and

$$\frac{x+iy}{r} = \sin\theta e^{i\varphi} = (\text{constant}) Y_{11} \quad (85)$$

$$\varphi_{k11} = AY_{11}(\theta, \phi) \left[\frac{k \cos(kr)}{r} - \frac{\sin(kr)}{r^2} \right] \quad (86)$$

For $l = 1, m = -1, 0, 1$ therefore there are three wavefunctions and they are

$$-\varphi_{k11} = \varphi_{k10} \quad \text{and} \quad -\varphi_{k10} = \varphi_{k1-1} \quad (87)$$

- $l=2$

Let us apply the momentum operator, P_+ , for the second time to find the wavefunctions for the case of $l = 2$.

$$P_+^2 \frac{\sin(kr)}{r} = A' P_+ \frac{x + iy}{r} \left(\frac{\sin(kr)}{r} \right)' \quad (88)$$

Here one thing that you need to realize is that P_+ operator commutes with $(x+iy)$. Therefore,

$$P_+^2 \frac{\sin(kr)}{r} = A'(x + iy) P_+ \frac{1}{r} \left(\frac{\sin(kr)}{r} \right)' \quad (89)$$

$$P_+^2 \frac{\sin(kr)}{r} = A'(x + iy)^2 \frac{1}{r} \left(\frac{1}{r} \frac{\sin(kr)}{r} \right)' \quad (90)$$

As you look for different l 's you shall realize that there is a pattern which gives the wavefunction for a general l .

$$P_+^l \frac{\sin(kr)}{r} = A'(x + iy)^l \frac{1}{r} \left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{\sin(kr)}{r} = \varphi_{kl} \quad (91)$$

The term of $(x+iy)^l = r^l Y_{ll}$ and then if we define $\rho = kr$ then the equation above will become,

$$j_l(\rho) = (-\rho)^l \left(\frac{1}{\rho} \frac{d}{d\rho} \right)^l \frac{\sin \rho}{\rho}. \quad (92)$$

The functions which satisfy the equation above are called the *Spherical Bessel Functions*. The most general solution for the wavefunction written in terms of spherical Bessel functions is therefore,

$$\varphi_{klm} = A j_l(kr) Y_{lm}(\theta, \phi) \quad (93)$$

where $A = k \sqrt{\frac{2}{\pi}}$ is the same for every l .

The differential equation for the spherical Bessel function is the radial part of the Schrodinger equation.

$$\frac{1}{r} (rR)'' - \frac{l(l+1)}{r^2} R + k^2 R = 0 \quad (94)$$

$$j'' + \frac{2}{\rho} j' + \left[1 - \frac{l(l+1)}{\rho^2} \right] j = 0 \quad (95)$$

The asymptotic behaviour of the spherical Bessel functions which is important for physics as $r \rightarrow \infty$ is known.

$$r \rightarrow \infty; \quad j_l(kr) \approx \frac{\sin(kr - l\frac{\pi}{2})}{r} \quad (96)$$

Because of the sine function above j_l is a mixture of incoming and outgoing waves. Now, let us expand sine in exponentials

$$j_l(kr) \approx \frac{e^{i(kr - l\frac{\pi}{2})} - e^{-i(kr - l\frac{\pi}{2})}}{r} \quad (97)$$

$$j_l(kr) \approx \frac{e^{ikr}}{r} e^{-il\frac{\pi}{2}} - \frac{e^{-ikr}}{r} e^{il\frac{\pi}{2}} \quad (98)$$

If we take the first phase $e^{-il\frac{\pi}{2}}$ as a constant then the equation becomes

$$j_l(kr) \approx \frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r} e^{il\pi} \quad (99)$$

$e^{il\pi} = \pm 1$ so we obtain a phase difference between the first term in the equation above (the outgoing wave) and the second term (the incoming wave). This phase difference is fixed by the behaviour of the wavefunction where $r \rightarrow 0$. Generally near zero when there is a potential we cannot just go to zero and keep the same Schrodinger equation. In this type of situation what changes is this phase difference between the incoming and outgoing waves. Now we shall examine the behaviour of the wavefunction as $r \rightarrow 0$ to understand the physics. We know that as $r \rightarrow 0$ the wavefunction behaves like $r^{(l+1)}$. On the other hand, the spherical Bessel function's behaviour near $r \rightarrow 0$ is

$$j_l(kr) \approx (kr)^l \quad (100)$$

In figure 4, as $r \rightarrow 0$, j_l goes to zero as well. Where it starts picking up from zero is a number that is approximately l . Therefore, the larger l is, the more j_l stays at zero. The role that case plays in physics is that if $kr \lesssim l$ then the wavefunction $R \approx 0$. This means that the probability of finding a particle there is zero. Even if it is not exactly zero it will be very very small.

Now if we switch on a potential, for example a nuclear potential, whose range is $\lesssim \frac{l}{k}$ (shown in the figure above with the dashed lines) then the particles that you send for scattering shall not feel the potential because the probability of them being there is very very small. In other words, these particles will never see the potential. We know that $k = \frac{\sqrt{2mE}}{\hbar}$ therefore, it is directly proportional to the energy of the particles. The higher the energy, the smaller the ratio of $\frac{l}{k}$ which is the reason why we want to have high energy. With high energy you can go smaller distances.

l is a quantum number, so large l means that we are in the limit of classical physics. Let us consider the classical limit in more detail.

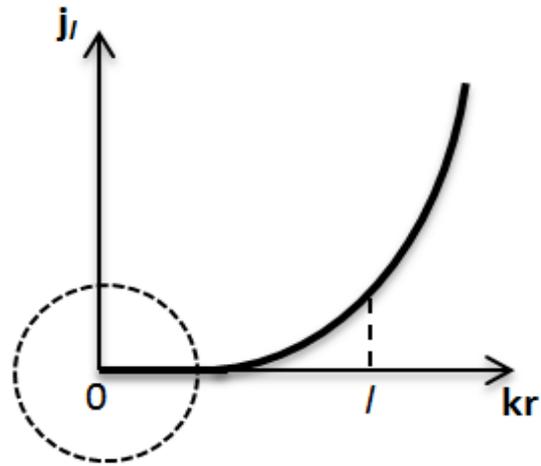


Figure 4: Plot of j_l vs. kr

CLASSICAL PHYSICS

Say we send a classical particle for scattering which has a momentum of \vec{p} as shown in figure 5. The distance b shown in the figure is called the *impact parameter* which is defined as the perpendicular distance between the path of a particle and the center of the scattering potential. The angular momentum of the particle is then,

$$L = pb = \hbar\sqrt{l(l+1)} \approx \hbar l \quad (101)$$

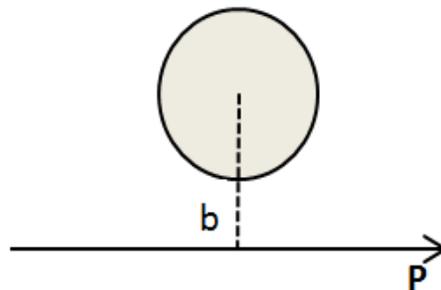


Figure 5: Scattering from a potential

The momentum of the particle and the angular momentum for large l where we are expecting to see the classical results are

$$p = \hbar k \quad \text{and} \quad L \approx \hbar l \quad (102)$$

respectively. Using these two equalities for the impact parameter we obtain

$$b = \frac{L}{p} = \frac{\hbar l}{\hbar k} = \frac{l}{k} \quad (103)$$

In quantum mechanical perspective we have found that if the range is $\lesssim \frac{l}{k}$ then the particle does not feel the potential. On the other hand, in classical perspective we also see that if the range of the potential is less than the ratio $\frac{l}{k}$ then the particle doesn't see the potential. Therefore, this case makes sense for both perspectives and this explains the physical meaning of this kind of wavefunctions.

Now let us assume that we have a central potential, $V(r)$. Then we still have a general solution which is

$$\varphi_{klm}(\vec{r}) = R_{kl}(r)Y_{lm}(\theta, \varphi) \quad (104)$$

We write $R = \frac{u_{kl}}{r}$ and then the wavefunction becomes

$$u'' + k^2 u - \left[\frac{l(l+1)}{r^2} + \frac{2mV}{\hbar^2} \right] u = 0 \quad (105)$$

We have solved this equation without any potential and we have found that the solution was spherical Bessel functions but now we have a potential. This equation becomes a one dimensional equation as r turns to be x . The limits for r is $0 \rightarrow \infty$ but for x is $-\infty \rightarrow \infty$. Fortunately we know the boundary condition for $r = 0$. This boundary condition says us that there is a wall at $r = 0$. so we can think of r from $-\infty \rightarrow \infty$ with a wall at $r = 0$. Therefore the potential will be complicated for $r > 0$ and infinite for $r < 0$. This way we can think of this case in one dimension. From the one dimensional point of view the scattering means reflection only. If we think of e^{ikr} as the incident wave and e^{-ikr} as the reflected wave then the wavefunction when you look at $r \rightarrow \infty$ is

$$u = Ae^{ikr} + Be^{-ikr} \quad (106)$$

When $r < 0$ then

$$u = 0 \quad (107)$$

Since the potential is infinite in $r < 0$ this means there is no transmission. Hence, the transmission coefficient, $T=0$ and since $R+T=0$, $R=1=|\frac{A}{B}|^2$. This simple argument tells us that

$$|A| = |B| \quad (108)$$

A and B are complex numbers so even though their norms are equal there will be a phase difference between them. If we set $A=1$ then

$$B = e^{i\beta} \quad (109)$$

New form of the wavefunction u is

$$u \approx e^{ikr} + e^{i\beta} e^{-ikr} \quad (110)$$

$$u \approx e^{-\frac{i\beta}{2}} e^{ikr} + e^{\frac{i\beta}{2}} e^{-ikr} \quad (111)$$

$$u \approx 2 \cos\left(kr - \frac{\beta}{2}\right) \quad (112)$$

This is the behaviour at infinity. We don't know β unless we solve the equation but we know how it should be. We can write the cosine in terms of sine.

$$u \approx 2 \sin\left(kr - \frac{\beta}{2} - \frac{\pi}{2}\right) \quad (113)$$

To compare this solution with that of no potential we can write

$$u \approx 2 \sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right) \quad (114)$$

In other words, the difference between having a potential and not having a potential is just a δ which is called the *phase shift* and δ in general will have an index of l and is a function of energy. It is very important to calculate the phase shift because it gives all of the information.

We have found the solution for particles coming from all directions. In experiments, instead of bombarding a target from every direction scientists send a beam on the target in one direction. But the solutions that we have found are the most general solutions and they form a complete set because they are the eigenfunctions of the Hamiltonian. We can write other solutions in terms of these general solutions' superposition. Hence, for any experimental arrangement you should be able to write it in terms of the eigenfunctions of Hamiltonian. In particular, the usual setup is to send the beam in z direction. It is a plane wave e^{ikz} . We can write this plane wave in terms of eigenfunctions of the Hamiltonian.

$$e^{ikz} = \sum_{l=0}^{\infty} \sum_{m=-l}^l a_{lm} \varphi_{klm}(\vec{r}) \quad (115)$$

The coefficients a_{lm} can be written as

$$a_{lm} = \int d^3r \varphi_{klm}^*(\vec{r}) e^{ikz} \quad (116)$$

Now we are going to write these a_{lm} in terms of spherical coordinates to calculate the integral.

$$\varphi_{klm}(\vec{r}) = C j_l(kr) Y_{lm}(\theta, \varphi) \quad \text{and} \quad e^{ikz} = e^{ikr \cos \theta} \quad (117)$$

$$a_{lm} = C^* \int d^3r e^{ikr \cos \theta} j_l(kr) Y_{lm}^*(\theta, \varphi) \quad (118)$$

Since the φ appears just in the last term of the integral above we can calculate the φ part separately.

$$\int_0^{2\pi} d\varphi Y_{lm}^*(\theta, \varphi) = P_l^m(\theta) \int_0^{2\pi} d\varphi e^{im\varphi} = 0 \text{ (unless } m = 0) \quad (119)$$

This simplifies the calculation and then

$$e^{ikz} = \sum_{l=0}^{\infty} C_l' j_l(kr) Y_{l0}(\theta) \quad (120)$$

$$e^{ikz} = \sum_{l=0}^{\infty} C_l j_l(kr) P_l(\cos \theta) \quad (121)$$

where you don't even need to sum till infinity since the first three or four terms suffice. For the purpose of normalization we can calculate the C_l' and C_l .

$$C_l' = i^l \sqrt{4\pi(2l+1)} \quad \text{and } C_l = i^l(2l+1). \quad (122)$$

where $i^l = e^{i\frac{\pi}{2}l}$.

It's nice to have the wave expressed in terms of the spherical harmonics because they are orthogonal functions. When you express the wave in terms of a sum you can see that the full wave is just the sum of partial waves. In practice, keeping only the first two or three terms is good enough. Depending on the value of l the partial waves will have different names. For instance, $l = 0$ is called the S wave and $l = 1$ is called the P wave, and so on.

So what is the wave function going to be after scattering from the potential? The incoming wave will turn into the outgoing wave, $e^{ikz} \rightarrow \varphi$, which is the sum of the incoming and outgoing wave $\varphi_{scattered}$. The entire wave will be,

$$\varphi = e^{ikz} + \varphi_s \quad (123)$$

In order to figure out the scattering cross section we need to determine the outgoing wave φ_s . To begin we look at the behavior of the wave very far away - because that's where we want to put the detector. The incoming partial wave is built with spherical Bessel functions, $j_l(kr)$, and we can expand this in the region where $r \rightarrow \infty$, where it becomes a sin function.

$$j_l(kr) \sim \frac{1}{2i} \left[\frac{e^{ikr}}{kr} e^{-il\frac{\pi}{2}} - \frac{e^{-ikr}}{kr} e^{il\frac{\pi}{2}} \right] \quad (124)$$

If we look at the total wave φ in the region $r \rightarrow \infty$ and there's gonna be a mixture of incoming and outgoing spherical waves again. And we introduced the phase shift δ_l which distinguishes the total wave from the incoming wave. The overall phase is arbitrary so we chose to put it with the first term.

$$\varphi \sim \frac{1}{2i} \left[\frac{e^{ikr}}{kr} e^{-il\frac{\pi}{2}} e^{2i\delta_l} - \frac{e^{-ikr}}{kr} e^{il\frac{\pi}{2}} \right] \quad (125)$$

That will be the behavior of the total wave and I know in general it'll behave like this. Really what I'm after is the outgoing wave, which will be the difference between the total and incoming waves. Therefore φ_s will take the form,

$$\varphi_s \sim \frac{e^{ikr}}{2ikr} e^{-il\frac{\pi}{2}} [e^{2i\delta_l} - 1] = \frac{e^{ikr}}{kr} \frac{1}{i^l} e^{i\delta_l} \sin \delta_l \quad (126)$$

We haven't really solved for anything yet. Just simplified our general expression for the outgoing wave to better see the behavior. So for each l there will be a different solution for the scattered wave. If I look at the entire wave, I just have to replace the j_l with the behavior of j_l at large r by this new behavior for φ_s .

$$e^{ikz} \rightarrow \frac{e^{ikr}}{kr} \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} e^{i\delta_l} \sin \delta_l Y_l(\theta) \quad (127)$$

So that's the expression for the outgoing wave, the entire outgoing wave. If you remember, this whole thing multiplying $\frac{e^{ikr}}{kr}$ we called it $f(\theta, \varphi)$ before. The entire sum is then this $f(\theta, \varphi)$ function.

$$e^{ikz} \rightarrow \frac{e^{ikr}}{kr} \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} e^{i\delta_l} \sin \delta_l Y_l(\theta) = \frac{e^{ikr}}{r} f(\theta, \varphi) \quad (128)$$

$$\Rightarrow f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} e^{i\delta_l} \sin \delta_l Y_l(\theta) \quad (129)$$

So if I somehow manage to calculate those δ_l 's I will be able to figure out the entire $f(\theta)$. Remember the cross section is given in terms of this function. Recall that $f(\theta)$ is sort of an amplitude because of the relation to the differential cross section. This is the quantity that I'm after because that's the experimental result that I'll be comparing things with.

$$\frac{d\sigma}{d\Omega} = |f|^2 \quad (130)$$

$$|f(\theta)|^2 = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} e^{i\delta_l} \sin \delta_l Y_l(\theta) \right|^2 \quad (131)$$

From this I can find the total cross section. I'll have to integrate the differential cross section over all the angles. Since the variable φ was constant I only need to integrate over θ .

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = \int d\Omega |f(\theta)|^2 = 2\pi \int_0^\pi d\theta \sin \theta |f(\theta)|^2 \quad (132)$$

I want to calculate the total cross section, so I'll plug in for $|f(\theta)|^2$ and remembering to keep track of the indices for $f^*(\theta)$ and $f(\theta)$.

$$\sigma = \frac{1}{k^2} \sum_{l,l'=0}^{\infty} \sqrt{4\pi(2l+1)} \sqrt{4\pi(2l'+1)} e^{-i\delta_l} e^{i\delta_{l'}} \sin \delta_l \sin \delta_{l'} \int d\Omega Y_l^*(\theta) Y_{l'}(\theta') \quad (133)$$

This integral we can do pretty easily because of the orthonormal nature of the spherical harmonics. It's a Kronecker delta function equal to one only when $l = l'$. So the total cross section boils down to a manageable expression in terms of the phases δ_l . And calculating the first few terms is usually good enough.

$$\sigma = \frac{1}{k^2} \sum_{l=0}^{\infty} 4\pi(2l+1) \sin^2 \delta_l \quad (134)$$

As an interesting aside, lets look at the function $f(\theta)$ when $\theta = 0$ and compare it to our expression for the total cross section when we look in the forward direction.

$$Y_l(0) = \sqrt{\frac{2l+1}{4\pi}} \quad (135)$$

$$f(\theta)|_{\theta=0} = \frac{1}{k} \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} e^{i\delta_l} \sin \delta_l Y_l(0) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} \sin \delta_l \quad (136)$$

Comparing this with the total cross section we see that σ has an extra factor of $\frac{4\pi}{k}$ and $\sin \delta_l$. This is a very general result and it even has it's own name, the *Optical Theorem*.

$$\sigma = \frac{4\pi}{k} \text{Im}f(0) \quad (137)$$

Example 1: Hard Sphere

We will now move on to do an example problem, scattering from a hard sphere. Hard sphere means anything you send in gets reflected. Modeled as an infinite potential wall at $r \leq r_0$.

$$V(r) = \begin{cases} 0 & \text{if } r > r_0 \\ \infty & \text{if } r \leq r_0 \end{cases}$$

So how do we solve this problem? We can actually solve it exactly. Remember that when $r > r_0$ we have a free particle and must solve the free Schrodinger equation. We already found it and lets call it $R_{k,l}(r)$, a spherical Bessel function.

$$R_{k,l}(r) = A j_l(kr) \quad A = \text{constant} \quad (138)$$

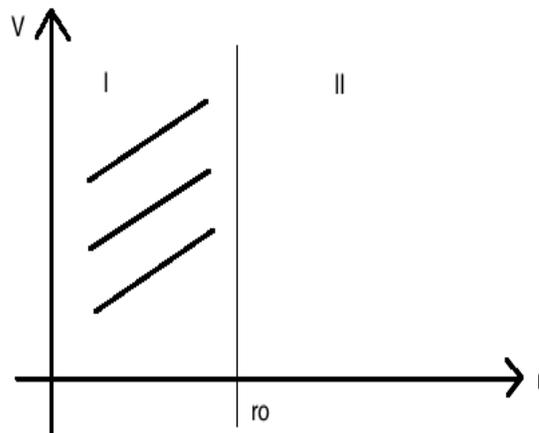


Figure 6: Hard sphere potential

Since we no longer have to worry about the behavior of the function at the origin we need to keep both pieces of the wave function. This other Bessel function we need is $n_l(kr)$. The n stands for Neumann.

$$R_{k,l}(r) = A j_l(kr) + B n_l(kr) \quad (139)$$

Next thing to do would be to apply the boundary conditions, and setting $A = 1$ because we arbitrarily can.

$$R_{k,l}(r = r_0) = 0 \quad \Rightarrow \quad \frac{B}{A} = \frac{j_l(kr_0)}{n_l(kr_0)} \quad (140)$$

So this completely determines the function but we want an expression for δ_l because this is what have expressions for. To do this we have to go far away $r \rightarrow \infty$.

$$\text{Definition of } \delta_l : \quad R_{k,l}(r) \sim \frac{1}{kr} \sin(kr - l\frac{\pi}{2} + \delta_l) \quad (141)$$

$$j_l(kr) \sim \frac{1}{kr} \sin(kr - l\frac{\pi}{2}) \quad (142)$$

$$n_l(kr) \sim -\frac{1}{kr} \cos(kr - l\frac{\pi}{2}) \quad (143)$$

$$\Rightarrow R_{k,l}(r) = A j_l(kr) + B n_l(kr) \sim \frac{A}{kr} \sin(kr - l\frac{\pi}{2}) - \frac{B}{kr} \cos(kr - l\frac{\pi}{2}) \quad (144)$$

That's the behavior of my wavefunction. When we compare this expression to that of the definition of δ_l I should get δ_l . Expanding the definition in terms of a trigonometric identity comparing the coefficients to match, then taking the ratio of $\frac{B}{A}$,

$$-\frac{B}{A} = \frac{\sin(\delta_l)}{\cos(\delta_l)} = \tan(\delta_l) = \frac{j_l(kr_0)}{n_l(kr_0)} \quad (145)$$

That's the solution I'm looking for. Let's look at it and try to figure out the behavior to find the cross section. Begin with the lowest value, $l = 0$. We can look up the spherical Bessel functions $j_0(\rho) = \frac{\sin(\rho)}{\rho}$ and $n_0(\rho) = -\frac{\cos(\rho)}{\rho}$, then the first phase shift.

$$\tan(\delta_0) = -\tan(kr_0) \quad \Rightarrow \quad \delta_0 = -kr_0 \quad (146)$$

Plugging this into the expression for the total cross section and keeping just the first term,

$$\sigma = \frac{1}{k^2} 4\pi \sin^2(kr_0) \quad (147)$$

When is this approximation good? Remember that k has to do with the energy of the beam. If I had a very low energy beam then $kr_0 \ll 1$ then $\sigma = 4\pi r_0^2$. So in the low energy limit the cross section becomes a constant. The lower the energy the better the approximation.

So let's make this problem a little more difficult. You never really have a hard sphere but you do have a potential well of finite depth. Such is life.

Example 2: Square Well

Outside the potential we have a free particle so the equation for $R_{k,l}(r)$ will be the same as that for the hard sphere. But now we do have to consider what happens for $r < r_0$. So when we are the region of the potential we'll have a new value for k and that'll be $k' = \frac{\sqrt{2m(E+V_0)}}{\hbar}$. So in the region of the potential, where the $n_l \rightarrow 0$,

$$R_{k,l}(r) = C j_l(k'r) \quad (148)$$

And outside the potential.

$$R_{k,l}(r) = A j_l(kr) + B n_l(kr) \quad (149)$$

Now we have to match the solutions at the boundary, including the derivatives.

$$A j_l(kr_0) + B n_l(kr_0) = C j_l(k'r_0) \quad (150)$$

$$A k j_l'(kr_0) + B k n_l'(kr_0) = C k' j_l'(k'r_0) \quad (151)$$

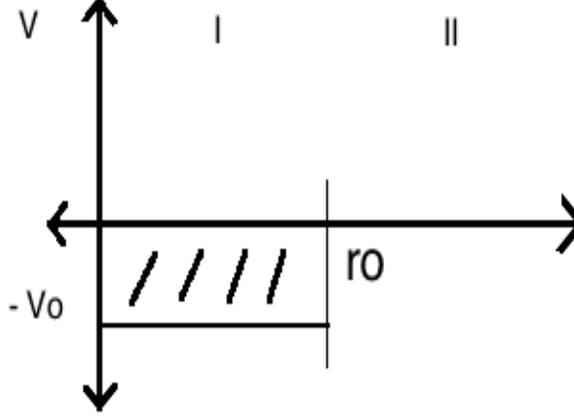


Figure 7: Potential step

Dividing the two equations and dividing through by A , and writing $-\frac{B}{A} = \tan(\delta_l)$,

$$\frac{j_l(kr_0) - \tan(\delta_l)n_l(kr_0)}{kj'_l(kr_0) - \tan(\delta_l)kn'_l(kr_0)} = \frac{j_l(k'r_0)}{k'j'_l(k'r_0)} \quad (152)$$

Now we only have one constant, δ_l and if we can solve this equation that will give me δ_l and that's all we need. So let's do the case when $l = 0$. Let $\rho = kr_0$ and $\rho' = k'r_0$, and using the Bessel functions from earlier. Plugging in and doing some algebra will give,

$$\left[\frac{\cos(\rho) \cos(\rho')}{\rho} + \frac{\sin(\rho) \sin(\rho')}{\rho'} \right] \tan(\delta_l) = \frac{\sin(\rho') \cos(\rho)}{\rho'} - \frac{\sin(\rho) \cos(\rho')}{\rho} \quad (153)$$

Then going to the low energy realm, $\rho \ll 1$. In this limit $\rho' \approx \frac{r_0}{\hbar} \sqrt{2mV_0}$ and $\rho \rightarrow 0$.

$$\left[\frac{\cos(\rho')}{\rho} \right] \tan(\delta_0) = \frac{\sin(\rho')}{\rho'} - \cos(\rho') \quad (154)$$

$$\Rightarrow \tan(\delta_0) = \rho \left[\frac{\tan \rho'}{\rho'} - 1 \right] \approx \sin(\delta_0) \approx \delta_0 \quad (155)$$

Now we can look into figuring out the first terms in the cross section and plugging in for $\rho = kr_0$.

$$\sigma = \frac{4\pi}{k^2} \delta_0^2 = 4\pi r_0^2 \left[\frac{\tan \rho'}{\rho'} - 1 \right]^2 \quad (156)$$

Again the cross section is a constant and this time it's less the four times the cross section. And how much less depends on the depth of the potential because of the dependence on ρ' . Looking at the behavior of the tangent function, it'll blow up as V_0 increases and then ρ' approaches $\frac{\pi}{2}$. Then,

$$V_0 < \frac{\pi^2 \hbar^2}{8mr_0^2} \quad (157)$$

If V_0 becomes as big as this number then the cross section blows up and there is lots of scattered particles. When this happens it's called a resonance. Is the cross section itself infinite? No, because we have made an approximation for the cross section when we wrote it. When ρ' is exactly $\frac{\pi}{2}$ a value may blow up but δ_0 will not be infinite because we take the tangent of δ_0 . That tells me the δ_0 will be precisely $\frac{\pi}{2}$. And if it's exactly $\frac{\pi}{2}$ I have to calculate the cross section again using the same formula.

$$\sigma = \frac{4\pi}{k^2} \quad (158)$$

So σ is not infinite but as $k \rightarrow 0$ the cross section becomes very, very large. The cross section is then large for low energies. So that means I have a resonance. Which is something we should be able to see in an experiment. Lots of particles coming out.

Lets now increase V_0 above this number. The tangent of ρ will begin to decrease and eventually you will get down to zero. If you keep increasing the potential there will be a point where $\tan(\rho') = \rho'$. If you solve that equation you'll find that $\rho' \approx 4.5$. At this point δ_0 will be exactly zero and the cross section will get a zero contribution from the first term, which is the most significant. So in practice, the other terms are going to contribute but they're going to contribute very little. If you do an experiment and you have a potential thats exactly at that value you'll see nothing.

This is a famous result that was obtained back in 1923 when people didn't know anything about quantum mechanics. They didn't have a wave equation, Schrodinger hadn't come up with it yet. So all of a sudden the experiment that they performed, which was the scattering of electrons by rare gasses, you detect nothing. They were wondering why you see nothing, and there was no explanation in terms of classical mechanics. It's a completely quantum mechanical effect, because it has to do with interference. It's only with interference that you can get absolutely nothing. This was a great mystery and is known as the Ramsauer-Townsend effect.

For $E < 0$ the zeroth order phase shift, which is the most important term in low energies, ρ , and ρ' values are respectively,

$$\tan \delta_0 = \rho \left(\frac{\tan \rho'}{\rho'} - 1 \right) \quad (159)$$

$$\rho = kr_0 = \frac{\sqrt{2mE}}{\hbar} r_0 \quad (160)$$

$$\rho' = k'r_0 = \frac{\sqrt{2m(E + V_0)}}{\hbar} r_0. \quad (161)$$

From the formula of the phase shift we can see that the resonance occurs when $\tan \rho'$ becomes infinite. In other words, the resonance occurs when ρ' takes the following values.

$$\rho' \approx \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots \quad (162)$$

At these points the cross section becomes large, not infinite. Now let us consider the values of V_0 that will cause the resonances.

Bound States

For the energy less than zero the spectrum will be discrete. For this kind of wavefunctions the solutions of the Schrodinger equation are

$$(I) \quad u''_I + k'^2 u_I = 0 \quad \Rightarrow \quad u_I = A \sin(k'r) + B \cos(k'r) \quad (163)$$

$$(II) \quad u''_{II} + k'^2 u_{II} = 0 \quad (164)$$

Since $E < 0$ say, $k = i\kappa$ where $\kappa = \frac{\sqrt{-2mE}}{\hbar}$ and is a real number. Therefore, u_{II} becomes,

$$u''_{II} - \kappa^2 u_{II} = 0 \quad \Rightarrow \quad u_{II} = C e^{\kappa r} + D e^{-\kappa r} \quad (165)$$

As $r \rightarrow \infty$ $u_{II} \rightarrow 0$ and once $r = 0$, $u_I = 0$. Therefore, coefficients B and C are zero. Using the continuity, these two solutions and their derivatives need to match at the boundary, that is, $r = r_0$.

$$A \sin(k'r_0) = D e^{-\kappa r_0} \quad (166)$$

$$k' A \cos(k'r_0) = -\kappa D e^{-\kappa r_0} \quad (167)$$

To cancel the coefficients A and D we divide by the two equations above and we obtain

$$\frac{1}{k'} \tan(k'r_0) = -\frac{1}{\kappa r_0} \quad (168)$$

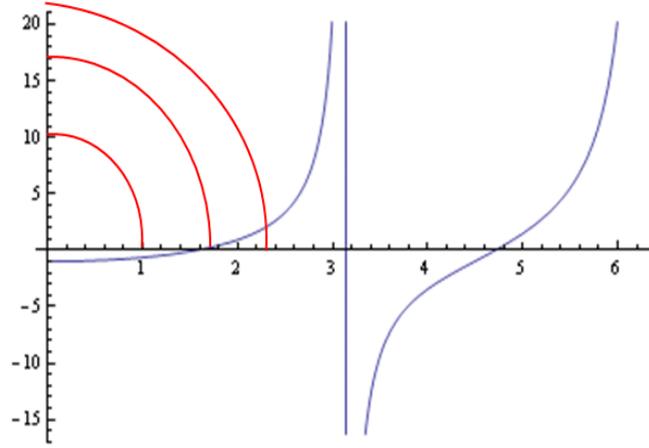
Once we solve this equation above we obtain the energy, E. We get discrete spectrum because the solution of this equation has finite number of solutions. To solve this equation we are going to use the graphical method and we are going to denote $k'r_0$ as x and κr_0 as y. Then the equation becomes,

$$\frac{1}{x} \tan(x) = -\frac{1}{y} \quad \Rightarrow \quad y = -x \cot x \quad (169)$$

If we look at the figure we see that one more function intersects with this graph.

$$x^2 + y^2 = \frac{2mV_0}{\hbar^2} r_0^2 \quad (170)$$

The circles in the figure changes according to the value of V_0 . For low V_0 values there is no intersection on the graphs. But there is one intersection where we

Figure 8: Plot of $k'r_0$ vs. κr_0

exactly get the *first bound state* for which $x = \frac{\pi}{2}$. We can continue in first bound state until drawing a circle intersecting with the second part of the graph and so on. Therefore,

$$x^2 + y^2 = \frac{2mV_0}{\hbar^2} r_0^2 = \left(\frac{\pi}{2}\right)^2 \quad (171)$$

$$V_0 < \frac{\hbar^2 \pi^2}{8mr_0^2} \quad \Rightarrow \quad \text{NO BOUND STATES!} \quad (172)$$

The values $\frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots$ are also the values for the resonance. This means that as V_0 changes, and there's a resonance, a new bound state has been added. This result relates the resonance, bound states and the cross section.

Absorption

We have been working on the elastic collisions so far but Nature does not work this way. We need to study inelastic scattering as well.

- Elastic Collisions:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0 \quad \Rightarrow \quad \text{Conserved current} \quad (173)$$

$$\frac{\partial \rho}{\partial t} = 0 \quad \Rightarrow \quad \text{No dependence on time} \quad (174)$$

$$\vec{\nabla} \cdot \vec{J} = 0 \quad \Rightarrow \quad \text{Conservation law} \quad (175)$$

where

$$\vec{J} = \frac{\hbar}{2mi} (\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*) \quad (176)$$

- Inelastic Collisions:

$$V = V_1 + iV_2 \quad (177)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t} \quad (178)$$

$$\frac{\partial\rho}{\partial t} = \psi\frac{\partial\psi^*}{\partial t} + C.C. \quad (179)$$

$$\frac{\partial\rho}{\partial t} = \frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + V|\psi|^2 + C.C.\right] \quad (180)$$

$$\frac{\partial\rho}{\partial t} = -\frac{\hbar}{2mi}\psi^*\nabla^2\psi + \frac{V_2}{\hbar}|\psi|^2 + C.C. \quad (181)$$

$$\frac{\partial\rho}{\partial t} = -\frac{\hbar}{2mi}\vec{\nabla}(\psi^*\vec{\nabla}\psi - \psi\vec{\nabla}\psi^*) + \frac{2V_2}{\hbar}|\psi|^2 \quad (182)$$

$$\frac{\partial\rho}{\partial t} = -\vec{\nabla} \cdot \vec{J} + \frac{2V_2}{\hbar}\rho \quad (183)$$

Since there is no time dependence,

$$\vec{\nabla} \cdot \vec{J} = \frac{2V_2}{\hbar}\rho \quad (184)$$

Using divergence theorem the total current is,

$$I = \int_S \vec{J} \cdot d\vec{S} = \int_V \vec{\nabla} \cdot \vec{J} d^3r = \int \frac{2V_2}{\hbar}\rho d^3r \quad (185)$$

We are interested in this situation because this appears in absorption. If there were no absorption then V_2 would be zero and there wouldn't be a term like I . Flux means the number of particles passing through a surface per time but they can both go out or come in. Therefore, I is the absorbed flux.

$$F_{abs} = -I \quad (186)$$

If we measure the entire cross section for the absorption it is,

$$\sigma_{abs} = \frac{F_{abs}}{J_{inc}} \quad (187)$$

We have already calculated the value of J_{inc} for incoming plane wave.

$$J_{inc} = \frac{\hbar k}{m} = Velocity \quad (188)$$

Then the absorbed cross section is calculated from

$$\sigma_{abs} = -\frac{2m}{\hbar^2 k} \int V_2 \rho d^3r = -\frac{m}{\hbar k} \int \vec{J} \cdot d\vec{S}. \quad (189)$$

To calculate this integral we will go through the same steps as the elastic scattering. First of all, we place the detector far away, that is, $r \rightarrow \infty$. The incoming wave is a plane wave which is e^{ikz} and it turns into the total φ ,

$$\varphi = \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} \left[\frac{e^{ikr}}{2ikr} e^{-il\frac{\pi}{2}} e^{2i\delta_l} - \frac{e^{-ikr}}{2ikr} e^{il\frac{\pi}{2}} \right] Y_{l0}(\theta) \quad (190)$$

As you go over the same procedure as in the elastic scattering part you get exactly the same answer. The crucial difference is that since the potential has the imaginary part the phase shift, δ_l , has an imaginary part. Hence we can write $\delta_l = \alpha_l + i\beta_l$. Since we know φ we can find J and the cross section.

$$\sigma_{abs} = -\frac{m}{\hbar k} \int J_r r^2 d\Omega = -\frac{mr^2}{\hbar k} \int J_r d\Omega \quad (191)$$

$$J_r = \frac{\hbar}{2mi} (\varphi^* \frac{\partial \varphi}{\partial r} - C.C.) \quad (192)$$

Let us calculate the partial differential of φ with respect to r .

$$\frac{\partial \varphi}{\partial r} = \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} \left[\left(\frac{e^{ikr}}{2r} - \frac{e^{ikr}}{2ikr^2} \right) e^{-il\frac{\pi}{2}} e^{2i\delta_l} + C.C.(\delta_l = 0) \right] Y_{l0}(\theta) \quad (193)$$

As $r \rightarrow \infty$ the term $\frac{e^{ikr}}{2ikr^2}$ may be ignored and let us call the coefficient as b_l .

$$\frac{\partial \varphi}{\partial r} = \frac{1}{2r} \sum_l b_l Y_{l0}(\theta) \quad (194)$$

For φ we already have an expression and if we take $\frac{1}{2r}$ out and write the rest as a coefficient, c_l , then,

$$\varphi = \frac{1}{2r} \sum_l c_l Y_{l0}(\theta) \quad (195)$$

Now we can calculate the absorption cross-section.

$$\sigma_{abs} = -\frac{mr^2}{\hbar k} \frac{\hbar}{2mi} \sum_{l,l'} \frac{1}{(2r)^2} \int d\Omega b_{l'} c_l^* Y_{l'0}^*(\theta) Y_{l0}(\theta) + C.C. \quad (196)$$

Since spherical harmonics are orthogonal this expression can be simplified.

$$\sigma_{abs} = -\frac{1}{8ki} \sum_l b_l c_l^* + C.C. \quad (197)$$

As expected you can see from the equation above the cross-section does not depend on r . The cross-section should not depend on where you put the detector. The flux has to be the same no matter where you are. We need to calculate the coefficient. To do this we are going to calculate the following expression.

$$b_l c_l^* - C.C. = \frac{8\pi(2l+1)}{ik} (e^{-4\beta_l} - 1) \quad (198)$$

Then the absorption coefficient is,

$$\sigma_{abs} = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)(1 - e^{-4\beta_l}). \quad (199)$$

If the phase shift due to absorption is zero then it is obvious from the equation that the absorption coefficient is zero. Remember when there is an elastic scattering we had a very similar expression for the cross-section. To remind, the φ and the scattering amplitude, $f(\theta)$, were

$$\varphi = \frac{e^{ikr}}{r} f(\theta) \quad (200)$$

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} e^{i\delta_l} \sin \delta_l Y_{l0}(\theta) \quad (201)$$

These two expressions are still the same for the inelastic scattering. But now we need to be careful because δ_l is not real anymore. Hence, we can write the terms with

$$e^{i\delta_l} \sin \delta_l = \frac{1}{2i} (e^{2i\delta_l} - 1) \quad (202)$$

Using the terms above the elastic scattering cross section becomes,

$$\sigma_{el} = \int d\Omega |f|^2 = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |e^{2i\delta_l} - 1|^2 \quad (203)$$

Now we don't have $\sin^2 \delta_l$ because δ_l is not real. For imaginary δ_l ,

$$|e^{2i\delta_l} - 1|^2 = |e^{2i\delta_l}|^2 + 1 - 2Re e^{2i\delta_l} = e^{-4\beta_l} + 1 - 2e^{-2\beta_l} \cos(2\alpha_l) \quad (204)$$

The total cross-section will be the sum of these cross-sections.

$$\sigma = \sigma_{abs} + \sigma_{el} \quad (205)$$

$$\sigma = \frac{2\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) [1 - e^{-2\beta_l} \cos(2\alpha_l)] \quad (206)$$

The last term in the sum above is $Re[1 - e^{2i\delta_l}]$ where,

$$S_l = e^{2i\delta_l} \quad (207)$$

S is called the *scattering matrix* and S_l is the eigenvalues of this scattering matrix.

Optical Theorem

Remember that the optical theorem relates the cross-section to the scattering amplitude in the forward direction. For the inelastic scattering case the optical theorem is,

$$f(0) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l} - 1) \quad (208)$$

$$\text{Im}f(0) = \frac{k}{4\pi} \sigma \quad (209)$$

This shows that the optical theorem is satisfied by the inelastic scattering case as well.