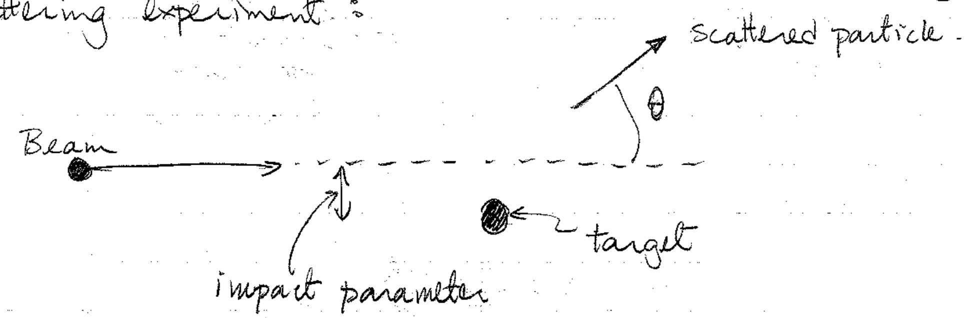
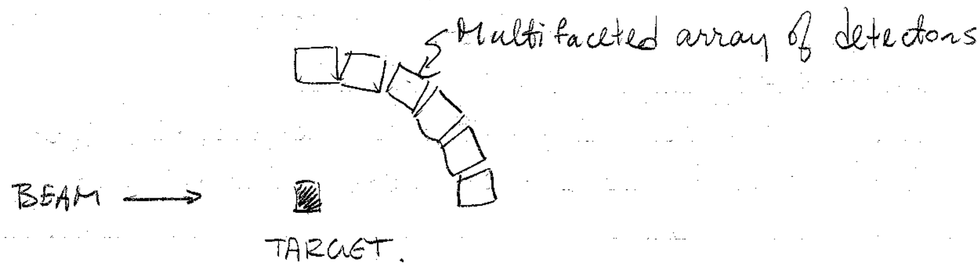
9. Theory of Scattering

Classical results:

In atomic and subatomic systems, often the only method of obtaining information is by performing a scattering experiment:



In early experimental work in both atomic & subatomic experiments, only one detector was used so that the relevant experimental quantity was the number of beam particles scattered into a particular angular region. More sophisticated experiments now measure many reaction products simultaneously



Time will limit our discussion to the 1 body distribution problem.

We introduce a quantity referred to as a differential cross section $\sigma(\theta, \varphi)$:

$$\Delta N \equiv J \, \sigma(\theta,\varphi) \, \Delta\Omega$$

ΔN = number of particles scattered into a solid angle $\Delta\Omega = \sin\theta \, \Delta\theta \, \Delta\varphi$ around an angle θ, φ. (per unit time)

J = flux of particles (# per unit area per unit time)

Equivalently,

$$\sigma(\theta,\varphi) = \frac{1}{J}\frac{dN}{d\Omega}$$

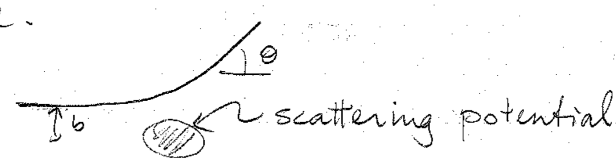
One will often see $\sigma(\theta,\varphi)$ written as $\frac{d\sigma(\theta,\varphi)}{d\Omega}$ for historical reasons.

Integrating over all angles gives:

$$N_{TOT} = J \underbrace{\int_{4\pi} \sigma(\theta,\varphi)\, d\Omega}_{\equiv \sigma_{TOT}\text{, the total cross section.}}$$

<u>Classical formulae</u>

In a classical, deterministic theory, one has a relationship between the impact parameter and the scattering angle.



We can write the classical expression as (assuming cylindrical symmetry, as we will do for the rest of this section)

$$dN = J \underline{\underline{dA}}$$ [this does not yet give $\sigma(\theta,\varphi)$; just says what dN is]

$$\text{classical area} = \int_0^{2\pi} d\varphi * b\,db = 2\pi b\,db.$$

$$\Rightarrow dN = J\,2\pi b\,db = J\,2\pi b \frac{db}{d\Omega} d\Omega = J \underbrace{\frac{b}{\sin\theta} \frac{db(\theta)}{d\theta}}_{\sigma(\theta)} d\Omega$$

<- using $d\Omega = 2\pi \sin\theta\, d\theta$

[There's actually a − sign buried in here since $\frac{db}{d\theta}$ is negative]

Knowing the potential then allows us to calculate the classical cross section. For example, in Coulomb scattering:

$$b = \frac{ZZ'e^2}{2E} \cot\frac{\theta}{2}.$$

$$\Rightarrow \frac{db}{d\theta} = \frac{ZZ'e^2}{2E}\left[\frac{-\sin\frac{\theta}{2}\sin\frac{\theta}{2}\cdot\frac{1}{2} - \cos\frac{\theta}{2}\cdot\cos\frac{\theta}{2}\frac{1}{2}}{\sin^2\frac{\theta}{2}}\right] = -\frac{ZZ'e^2}{4E\sin^2\frac{\theta}{2}}.$$

$$\Rightarrow \sigma(\theta) = -\frac{\frac{ZZ'e^2}{2E}\cot\frac{\theta}{2}}{\sin\theta}\left(-\frac{ZZ'e^2}{2E\sin^2\frac{\theta}{2}}\right)$$

$$= +\left(\frac{ZZ'e^2}{2E}\right)^2 \frac{1}{2} \cdot \frac{\cos\theta/2 \,/ \sin\theta/2}{2\sin\theta/2\,\cos\theta/2} \frac{1}{\sin^2\theta/2} = \left(\frac{ZZ'e^2}{4E}\right)^2 \frac{1}{\sin^4\frac{\theta}{2}}.$$

Where E is the incident energy. This is referred to as the Rutherford formula since it was used by Rutherford in the analysis of his scattering experiments of α + Au.

Note that

$$\int \sigma(\theta)\sin\theta\, d\theta \to \infty$$ for Coulomb scattering; the force is a long range one, in other words.

Quantum Mechanical

So much for classical results. We want to develop a quantum mechanical description of the scattering process. Let's look at the wavefunction:

$$-\left[\frac{\hbar^2\nabla^2}{2m} + V(r)\right]\psi = \epsilon\psi.$$

Now, the incoming wave is of the form $\psi \sim e^{ikz}$, assuming that it is along the z axis and using $E = \frac{\hbar^2 k^2}{2m}$.

After passing by the potential, the wave will be of the form

$$\psi \underset{r\to\infty}{\sim} \underbrace{e^{ikz}}_{\text{unscattered piece}} + \underbrace{f(\theta,\varphi)\frac{e^{ikr}}{r}}_{\text{scattered piece}}$$

unscattered piece

scattered piece. The $1/r$ takes care of relative (but not absolute) probability as $r\to\infty$.

Let's find a relationship between ψ and σ. The radial flux (i.e. flux in radial direction only) is given by

$$\underbrace{J_{inc} = -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*)}_{\text{from page 3-21}} = \frac{-i\hbar}{2m}\left[e^{-ikz}\frac{\partial}{\partial z}e^{ikz} - e^{ikz}\frac{\partial}{\partial z}e^{-ikz}\right] = -\frac{i\hbar}{2m}\,2ike^{0}$$

$$= \frac{\hbar k}{m}.$$

$$\left(= \frac{p}{m} = v\right).$$

The scattered flux is

$$J_{scatt} = \frac{-i\hbar}{2m}|f(\theta,\varphi)|^2\left[\left(\frac{e^{-ikr}}{r}\right)\frac{\partial}{\partial r}\frac{e^{ikr}}{r} - \frac{e^{ikr}}{r}\frac{\partial}{\partial r}\frac{e^{-ikr}}{r}\right]$$

$$= -\frac{i\hbar}{2m}|f(\theta,\varphi)|^2\left\{\frac{1}{r}\cdot\frac{ikr-1}{r^2} - \frac{1}{r}\frac{-ikr-1}{r^2}\right\} = -\frac{i\hbar}{2m}|f(\theta,\varphi)|^2\frac{2ik}{r^2}$$

$$J_{scatt} = \frac{\hbar k}{m} \frac{|f(\theta,\varphi)|^2}{r^2}$$

(Units may look screwy but they're ok. $\left|\frac{f}{r}\right|^2$ has units of density $\Rightarrow J \propto$ velocity × density = $\frac{\#}{\text{time} \cdot \text{area}}$)

Hence

$$dN = J_{scatt} \underbrace{(r^2 d\Omega)}_{\text{area subtended by solid angle}} \Rightarrow \frac{dN}{d\Omega} = \frac{\hbar k}{m} |f(\theta,\varphi)|^2 .$$

But

$$\sigma(\theta,\varphi) = \frac{1}{J_{inc}} \frac{dN}{d\Omega} = |f(\theta,\varphi)|^2 .$$

The quantity $f(\theta,\varphi)$ is obviously the central quantity in the scattering process and is defined as the scattering amplitude. There are several routes we can follow to find $f(\theta,\varphi)$

1. Solve Schrodinger equ. exactly! Very difficult in general and will not be pursued here.

2. Solve S.E. by approximation: Born series.

3. Recast into sum over partial waves and solve for phase shift.

We use route #2 first.

Born Series

We go back to the Schrodinger equation momentarily –

$$\left(-\frac{\hbar^2 \vec{\nabla}^2}{2m} + \lambda V\right)\psi = E\psi \qquad (1)$$

we now introduce λ in a perturbative sense.

This is a homogeneous equation in ψ, i.e. we can rewrite it as

$$\left(-\frac{\hbar^2\vec{\nabla}^2}{2m} + \lambda V - E\right)\psi = 0 \quad (2)$$

Suppose instead we define

$$u(\vec{r}) = \frac{2m}{\hbar^2}\lambda V(\vec{r})\,\psi(\vec{r})$$

and write,

$$-\left(\vec{\nabla}^2 + \frac{2mE}{\hbar^2}\right)\psi = -\frac{2m}{\hbar^2}\lambda V\psi = -u(\vec{r}) \quad (3)$$

If we now treat $u(r)$ as a "source" term, so to speak, then this equation is now inhomogeneous in ψ. What does this gain us? The general solution to (3) is of the form

$$\left.\begin{aligned} &(\vec{\nabla}^2 + k^2)\,\psi_i = 0 \quad (4) \\ + \quad &(\vec{\nabla}^2 + k^2)\,\psi_s = u \end{aligned}\right\} \text{add} \Rightarrow (\vec{\nabla}^2 + k^2)(\psi_i + \psi_s) = u(\vec{r})$$

where $k^2 = 2mE/\hbar^2$

(i.e. you can add to ψ_s a ψ_i satisfying $(\vec{\nabla}^2 + k^2)\psi_i = 0$)

Now, ψ_i satisfying (4) is $e^{i\vec{k}\vec{r}}$! So the form for ψ_s can be made to look like (i.e. $e^{ikz} = e^{i\vec{k}\cdot\vec{r}}$)

$$\psi_s \sim f(\theta,\phi)\frac{e^{ikr}}{r} \quad \text{as } r \to \infty.$$

In other words, recasting SE into the inhomogeneous form (3) gives us ψ in the asymptotic form that we want. Of course, we still have to solve (3).

The method of solution involves the introduction of a Green's function $G(\vec{r}, \vec{r}\,')$ satisfying

$$(\vec{\nabla}^2 + k^2)\, G(\vec{r}, \vec{r}\,') = \delta(\vec{r} - \vec{r}\,') \qquad (5)$$

Then $\psi_s(\vec{r}) = \int d\vec{r}\,'\, G(\vec{r}, \vec{r}\,')\, u(\vec{r}\,') \qquad (6)$

is the solution to (3): (Proof)

$$(\vec{\nabla}^2 + k^2)\,\psi_s = \int d\vec{r}\,' (\vec{\nabla}^2 + k^2)\, G(\vec{r}, \vec{r}\,')\, u(\vec{r}\,')$$

from (6) Does not depend on $\vec{r}\,'$

$$= \int d\vec{r}\,'\, \delta(\vec{r} - \vec{r}\,')\, u(\vec{r}\,') = u(\vec{r}) .$$

We have now formally written down a solution (6) for ψ_s, assuming that we can find a Green's function to satisfy (5). There are many forms for G which satisfy (5), so we impose the additional condition that ψ_s must have the asymptotic form

$$f(\theta, \varphi)\, e^{ikr}/r .$$

Then G has the form

$$G(\vec{r}, \vec{r}\,') = \frac{-1}{4\pi} \frac{e^{ik|\vec{r} - \vec{r}\,'|}}{|\vec{r} - \vec{r}\,'|}$$

$$\Rightarrow \psi(r) = \underbrace{e^{i\vec{k}\cdot\vec{r}}}_{\psi_i \text{ (same as } e^{ikz})} - \frac{2m\lambda}{4\pi\hbar^2} \int d\vec{r}\,' \frac{e^{ik|\vec{r} - \vec{r}\,'|}}{|\vec{r} - \vec{r}\,'|}\, \psi(\vec{r}\,')\, V(\vec{r}\,') \qquad (7)$$

Let's take stock of what we have done here.

1. We have recast the differential equation for ψ into an integral equation. We still have not found ψ explicitly.
2. The result converges only if $V(r)$ is not long range, i.e. $rV(r) \to 0$ as $r \to \infty$.
3. The real use of (7) is that it can generate an iterative sequence in λ:

$$\psi^{(0)} = e^{i\vec{k}\vec{r}}$$

$$\psi^{(1)} = e^{i\vec{k}\vec{r}} - \frac{2m\lambda}{4\pi\hbar^2}\int d\vec{r}\,' \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}\psi^{(0)}(\vec{r}\,')V(\vec{r}\,')$$

$$\vdots$$

$$\psi^{(n)} = e^{i\vec{k}\vec{r}} - \frac{2m\lambda}{4\pi\hbar^2}\int d\vec{r}\,' \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}\psi^{(n-1)}(\vec{r}\,')V(\vec{r}\,')$$

First Born Approximation

If λV is small, then $\psi^{(1)}$ may well be a reasonable approximation to the real ψ.

$$\psi^{(1)} = e^{i\vec{k}\cdot\vec{r}} - \frac{m\lambda}{2\pi\hbar^2}\int d\vec{r}\,' \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} e^{i\vec{k}\vec{r}\,'} V(\vec{r}\,').$$

To obtain the scattering amplitude, we only want the form of ψ at large $\vec{r}$. We use

$$|\vec{r}-\vec{r}\,'| = \left(r^2 - 2\vec{r}\cdot\vec{r}\,' + r'^2\right)^{1/2} = r\left(1 - 2\frac{\vec{r}\cdot\vec{r}\,'}{r^2} + O\left(\frac{r'}{r}\right)^2\right)^{1/2}$$

$$\simeq r - \frac{\vec{r}\cdot\vec{r}\,'}{r} \quad \text{for } r' \ll r$$

magnitude.

So that

$$\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|r-r'|} \rightarrow e^{-ik\frac{\vec{r}\cdot\vec{r}\,'}{r}} \, \frac{e^{ikr}}{r}.$$

Defining $\vec{k}\,' = k\frac{\vec{r}}{r}$ (i.e. it is a vector of length k pointing in the $\vec{r}$ direction)

we find

$$\psi^{(1)}(\vec{r}) \xrightarrow[r\to\infty]{} e^{i\vec{k}\cdot\vec{r}} - \frac{m\lambda}{2\pi\hbar^2}\frac{e^{ikr}}{r}\left[\int d\vec{r}\,' e^{i(\vec{k}-\vec{k}\,')\vec{r}\,'} V(\vec{r}\,')\right]$$

$\sim f(\theta,\varphi)$.

So, the first Born amplitude $f^{(1)}(\theta,\varphi)$ is

$$f^{(1)}(\theta,\varphi) = -\frac{m\lambda}{2\pi\hbar^2}\int d\vec{r}\,' e^{i(\vec{k}-\vec{k}\,')\vec{r}\,'} V(\vec{r}\,').$$

The difference in momenta is $\vec{K} = \vec{k} - \vec{k}\,'$ (or, the momentum transfer), so that we define

$$V(\vec{K}) = \int d\vec{r}\,' e^{i\vec{K}\cdot\vec{r}\,'} V(\vec{r}\,') \quad = \text{Fourier transform of } V(r).$$

Lastly, then

$$\sigma^{(1)} = \left(\frac{-m\lambda}{2\pi\hbar^2}\right)^2 |V(\vec{K})|^2.$$

Cross section, not series as in $\sigma = \sigma^{(0)} + \lambda\sigma^{(1)} \ldots$

Examples:

1. The coulomb problem works even though the potential is long ranged.

2. Gaussian potentials:

$$V = \lambda e^{-r^2/2\Delta^2} \leftarrow \text{(Weider is out by 2 in exp.)}$$

$$\Rightarrow V(K) = \int d^3r \, e^{i\vec{K}\cdot\vec{r}} e^{-r^2/2\Delta^2} = \int d^3r \, e^{-\frac{1}{2\Delta^2}\left[r^2 - 2\vec{r}\cdot i\vec{K}\Delta^2 + (iK\Delta^2)^2 - (iK\Delta^2)^2\right]}$$

$$= e^{-\frac{K^2\Delta^2}{2}} \underbrace{\int d^3r \, e^{-\frac{1}{2\Delta^2}(\vec{r} - i\vec{K}\Delta^2)^2}}_{\left(\sqrt{2}\Delta\int_{-\infty}^{\infty} d\xi \, e^{-\xi^2}\right)^3 = \left[\sqrt{2\pi}\,\Delta\right]^3}$$

$$\therefore V(K) = (2\pi)^{3/2}\Delta^3 e^{-\frac{K^2\Delta^2}{2}}$$

$$\Rightarrow \sigma^{(1)} = \left(\frac{m\lambda}{2\pi\hbar^2}\right)^2 (2\pi)^3 \Delta^6 e^{-K^2\Delta^2}$$

Lastly, expand $\vec{K}^2$ in terms of θ to get explicit θ dependence.

3. Partial Wave Analysis

Let's return to the general expression for the scattered wavefunction

$$\psi \sim e^{ikz} + \frac{f(\theta,\phi)e^{i\vec{k}\cdot\vec{r}}}{r}$$

Because angular momentum is conserved in a collision process, it is useful to express ψ in terms of angular momentum states. For example, let's expand

$$e^{ikz} = e^{ikr\cos\theta} = \sum_{\ell=0}^{\infty} a_\ell \underline{g_\ell(r)} P_\ell(\cos\theta).$$

← where this satisfies SE.

We solve for the functions $g_\ell(r)$ by using the orthogonality property of the Legendre polynomials: Multiply by $P_\ell(\cos\theta)$ & integrate

$$\sum_{\ell'} a_{\ell'} g_{\ell'}(r) \int P_{\ell'}(\cos\theta) P_\ell(\cos\theta)\, d\cos\theta = \int e^{ikr\cos\theta} P_\ell(\cos\theta)\, d\cos\theta$$

$$\text{LHS.} = \sum_{\ell'} a_{\ell'} g_{\ell'} \frac{2}{2\ell+1}\delta_{\ell\ell'} = \frac{2}{2\ell+1} a_\ell g_\ell$$

← [Normalized by $\int P_\ell \cdot P_{\ell'}\, du = \frac{2}{2\ell+1}\delta_{\ell\ell'}$]

$$\text{RHS.} = \int_{-1}^{+1} e^{ikru} P_\ell(u)\, du = \frac{1}{ikr}\int_{-1}^{1} \underbrace{(ikr\, e^{ikru})}_{f'} \underbrace{P_\ell(u)}_{g}\, du$$

← Integrate by parts.

[$\int (fg)' du = \int f'g\, du + \int f g'\, du$] →

$$= \frac{1}{ikr}\left\{ e^{ikru}P_\ell(u)\Big|_{-1}^{1} - \int_{-1}^{1} e^{ikru} P_\ell'(u)\, du \right\}$$

$$= \frac{1}{ikr}\left\{ e^{ikr}P_\ell(1) - e^{-ikr}P_\ell(-1) - \overline{\int_{-1}^{1} e^{ikru}P_\ell'(u)\, du} \right\}$$

This goes like 1/r compared to the first terms. So neglect as $r\to\infty$

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With our convention $P_\ell(1) = 1$
$P_\ell(-1) = (-1)^\ell$

$$\therefore \text{RHS} = \frac{1}{ikr}\left\{ e^{ikr} - \left(e^{i\pi}\right)^{\ell} e^{-ikr} \right\}.$$

$e^{i\pi} = \cos\pi + i\sin\pi = -1$

$$= \frac{1}{ikr}\, e^{\frac{i\pi\ell}{2}} \left\{ e^{ikr - i\pi\frac{\ell}{2}} - e^{-ikr + i\pi\frac{\ell}{2}} \right\}$$

$$= \frac{1}{ikr}\left[e^{\left(i\frac{\pi}{2}\right)}\right]^{\ell} 2i\sin\left(kr - \ell\frac{\pi}{2}\right)$$

$$= 2\,(i)^{\ell}\,(kr)^{-1} \sin\left(kr - \ell\frac{\pi}{2}\right).$$

$$\therefore a_\ell g_\ell(r) = (2\ell+1)\, i^{\ell}\, \frac{1}{kr}\sin\left(kr - \ell\frac{\pi}{2}\right).$$

Lastly,
$$e^{ikz} = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^{\ell} \underbrace{\left[\frac{1}{kr}\sin\left(kr - \ell\frac{\pi}{2}\right)\right]}_{\equiv g_\ell \text{, proportional to spherical Bessel functions.}} P_\ell(\cos\theta).$$

We can go through the same expansion for ψ as well, ending up with [calculate the $r \to \infty$ limit].

$$\psi(r,\theta) = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^{\ell}\, e^{i\delta_\ell}\, L_\ell(r)\, P_\ell(\cos\theta)$$

δ_ℓ is defined as the partial wave phase shift.

$L_\ell(r) = \frac{1}{kr}\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right).$

Lastly, substitute for ψ and e^{ikz} in $\psi = e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$ to obtain an expression for $f(\theta)$:

$$f(\theta) = \frac{1}{2ik}\sum_{\ell=0}^{\infty}(2\ell+1)\left(e^{2i\delta_\ell} - 1\right)P_\ell(\cos\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\, e^{i\delta_\ell}\sin\delta_\ell \times$$
$P_\ell(\cos\theta)$

This expression for $f(\theta)$ does not help a great deal in calculating a differential cross section:

$$\sigma(\theta) = \frac{1}{k^2}\left|\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\sin\delta_\ell P_\ell(\cos\theta)\right|^2$$

However, if we integrate $\int \sigma(\theta)d\Omega$ then the orthogonality property of the Legendre polynomials can be used to get rid of the cross terms in the partial wave sum:

$$\sigma_{TOT} = \int \sigma(\theta)d\Omega = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\sin^2\delta_\ell .$$

Example #1: Optical Theorem.

The expression for $f(\theta)$ shows that

$$\mathrm{Im}\, f(\theta=0) = \frac{1}{k}\sum_\ell (2\ell+1)\sin^2\delta_\ell$$

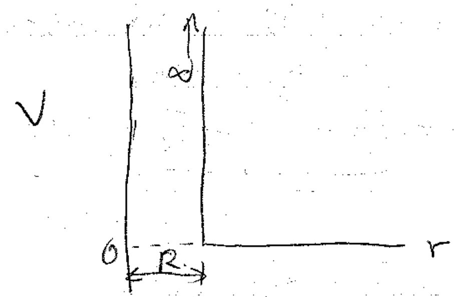
$$\Rightarrow \sigma_{TOT} = \frac{4\pi}{k}\mathrm{Im}\, f(\theta=0).$$

Example #2. S-wave scattering.

The strength of the partial wave expansion lies in the fact that for short range potentials, such as are found at the subatomic level, the number of partial waves of importance is limited:

$$\ell \lesssim \frac{pR}{\hbar}.$$

As an application, consider hard sphere scattering



Transforming the S.E. from ψ to $u(r)$ as was done previously, we have (for s-wave scattering)

$$u(r \leq R) = 0$$

$$\Rightarrow kR + \delta_0 = 0$$

$$\text{or} \quad \delta_0 = -kR .$$

Substituting for δ_0 in the cross section formula gives:

$$\sigma_{s,TOT} = \frac{4\pi}{k^2} (2 \times 0 + 1) \sin^2 kR$$

As $k \to 0$, this becomes

$$\sigma_{s,TOT} = \frac{4\pi}{k^2} k^2 R^2 = 4\pi R^2 .$$

This looks like a classical result (no $\hbar$) but it can't be since the classical limit is obtained for $E \gg V_0$. Further, the 4 indicates that we are looking at wavelength effects, since the classical result would be just πR^2.

Details of Hard Sphere potential

Go back to previous page where

$$\psi(r,\theta) = \sum_{\ell=0}^{\infty} (2\ell+1)\, i^{\ell}\, e^{i\delta_\ell}\, \underline{\underline{L_\ell(r)}}\, P_\ell(\cos\theta)$$

$$L_\ell = \frac{1}{kr}\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right).$$

Now, take only the $\ell=0$ solution for this equation:

$$\psi^0(r,\theta) = (1)(1)\, e^{i\delta_0}\, \frac{1}{kr}\sin(kr+\delta_0)(1)$$

[This looks like the $\frac{u(r)}{r}$ - type solutions considered before on pg 5-9 for a particle in a spherical well].

Since the wavefunction must vanish at $r=R$,

$$\delta_0 = -kR$$

$$\Rightarrow \psi^0 = \frac{1}{kr}(\sin kr - kR)$$

Substitute into the cross section expression $\quad \sigma = \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\sin^2\delta_\ell$

$$\rightarrow \sigma_0 = \frac{4\pi}{k^2}\sin^2(kR)$$