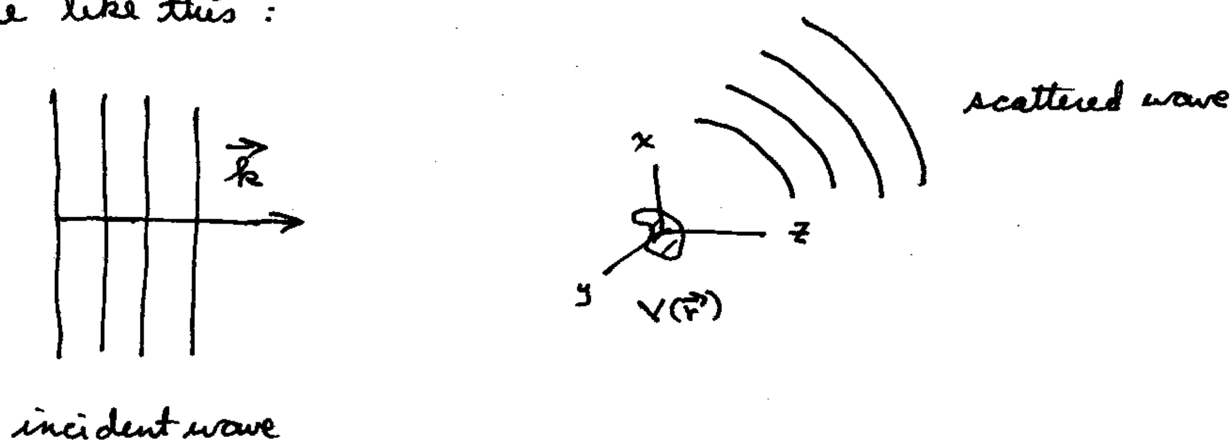
2/14/08

Now scattering theory. Will concentrate on potential scattering of spinless particles in 3D. The potential is $V(\vec{r})$, which need not be rotationally invariant. We will treat central force scattering, $V(\vec{r}) = V(r)$, later, as a special case. We assume $V(\vec{r}) \to 0$ fast enough as $|\vec{r}| \to \infty$; thus, at large $|\vec{r}|$, the solutions are approximately free-particle solutions. Later we quantify what "fast enough" means.

We imagine launching a beam of particles of fixed momentum $\vec{p} = \hbar \vec{k}$ at the scatterer. We describe the beam by a plane wave $e^{i\vec{k}\cdot\vec{r}}$, although this is unphysical and unrealistic in several respects. As the beam enters the region where $V(\vec{r})$ has an effect, the plane wave fronts are bent and the wave is scattered. We get a picture like this:



We wish to solve the Schrödinger eqn in the potential $V(\vec{r})$,

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

for positive energy $E > 0$. The energy eigenvalue E is related in a simple way to the wave vector $\vec{k}$ of the incident wave, which we assume is launched far enough away from the scatterer that $V(\vec{r})$ is negligable at the launch point. Then

$$E = \frac{\hbar^2 k^2}{2m},$$

the free-particle relation. The spectrum is continuous for $E>0$, and the energy eigenfunctions are not normalizable. Each energy $E>0$ is also highly degenerate, since the experimenter can vary the direction of $\vec{k}$ without changing E, and generate a continuous family of linearly independent solutions. (Only two in 1D, since there are two sides to launch the wave from.) There are also solutions of the Schrödinger equation for given E that do not correspond to anything that is easy to set up experimentally. We will have to distinguish the solutions we are interested in by the <u>boundary conditions</u> they satisfy.

Our first task is to identify the <u>asymptotic form</u> of the solution $\psi(\vec{r})$ of the Sch. eqn., that is, what does it look like at large $|\vec{r}|$. We do this partly by guessing and partly by physical intuition. We define the <u>incident wave</u> by

$$\psi_{inc}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$$

It is a free particle solution ~~by~~ but not a solution in the presence of the potential $V(\vec{r})$. We let $\psi(\vec{r})$ be the <u>exact</u> solution of the Schrödinger equation we are interested in, and we define the <u>scattered wave</u> by

$$\psi_{sc}(\vec{r}) = \psi(\vec{r}) - \psi_{inc}(\vec{r}).$$

At large $|\vec{r}|$ the scattered wave should be approximately a free-particle solution, out there $(V(\vec{r}) \to 0)$ and it should consist of ~~wave~~ spherical wave fronts radiating outward. The probability density $|\psi_{sc}|^2$ should go as $\frac{1}{r^2}$, since this is what happens to the density of a classical stream of particles radiating away from a small region of space (it is just conservation of particles). This leads to the functional form,

$$\psi_{sc}(\vec{r}) \sim \frac{e^{ikr}}{r} f(\theta,\phi)$$

where $\sim$ means that the leading asymptotic form for large $|\vec{r}|$ is shown, that is, the LHS equals the RHS plus terms that go to 0 more rapidly as $|\vec{r}| \to \infty$ than the terms shown (in this case, more rapidly than $1/r$). Altogether, we obtain

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

A more rigorous derivation of this result follows from an asymptotic analysis (large $|\vec{r}|$) of the Schrödinger equation, which shows that this is the correct asymptotic form of the solution as long as the potential dies off faster than $1/r$. The Coulomb potential and modified Coulomb potentials (only the asymptotic form is at issue here) do not satisfy this criterion, and in fact the asymptotic form of $\psi(\vec{r})$ in those potentials is more complicated than indicated above. For now we assume that $V(\vec{r}) \to 0$ faster than $1/r$. We will treat the Coulomb potential as a special case later.

The function $f(\theta,\phi)$, which gives the angular dependence of the scattered wave, is called the <u>scattering amplitude</u>. It is in general complex. A good deal of scattering theory is devoted to determining the scattering amplitude, since it bears a simple relation to the differential cross-section. To explore this we compute the fluxes associated with the incident and scattered waves. The probability flux in QM is

$$\vec{J} = \psi^* \left(\frac{-i\hbar}{2m} \nabla\psi \right) + \text{c.c.}$$

$$= \frac{\hbar}{m} \operatorname{Im}(\psi^* \nabla\psi).$$

Computing this for the incident wave we find

$$\vec{J}_{inc} = \frac{\hbar \vec{k}}{m} = \frac{\vec{p}}{m} = \vec{v},$$

the velocity of the incident beam. This is the same as a classical beam with 1 particle/vol., what we have here in this case since $|\psi_{inc}|^2 = 1$. As for the scattered flux, we compute the gradient in spherical coordinates,

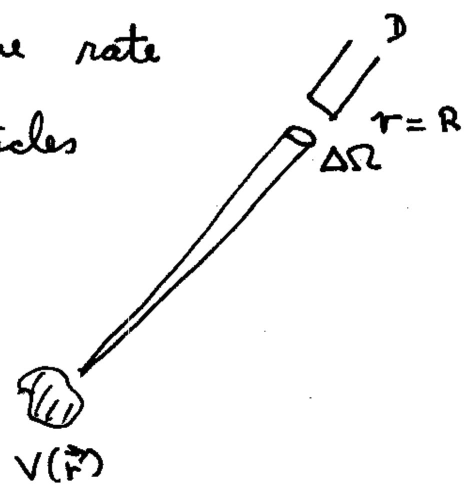
$$\nabla \psi_{sc} = \left(\hat{r}\frac{\partial}{\partial r} + \frac{\hat{\theta}}{r}\frac{\partial}{\partial \theta} + \frac{\hat{\phi}}{r\sin\theta}\frac{\partial}{\partial \phi} \right) \frac{e^{ikr}}{r} f(\theta,\phi)$$

$$= ik\hat{r}\frac{e^{ikr}}{r} f(\theta,\phi) + O\left(\frac{1}{r^2}\right).$$

One term dominates the others; it $\to 0$ as $1/r$, same as ψ_{sc} itself (which itself is only an asymptotic form). Thus,

$$\vec{J}_{sc} \sim \frac{\hbar k}{m}\hat{r}\frac{|f(\theta,\phi)|^2}{r^2}.$$

Now suppose we have a detector D at a large distance $r = R$ from the scatterer that intercepts small solid angle $\Delta\Omega$ relative to the scatterer. Then the rate w at which particles are intercepted by the detector is given by



$$w = \int_{\substack{\text{aperture}\\ \text{of detector}}} \vec{J}_{sc} \cdot d\vec{a} \,.$$

But $d\vec{a} = R^2 \, d\Omega \, \hat{r}$, so

$$w = \frac{\hbar k}{m} R^2 \Delta\Omega \, \frac{|f(\theta,\phi)|^2}{R^2} = v \, \Delta\Omega \, |f(\theta,\phi)|^2 .$$

But we should write $w \to \frac{dw}{d\Omega} \Delta\Omega$, and then use definition of the cross section,

$$\frac{dw}{d\Omega} = |J_{inc}| \frac{d\sigma}{d\Omega}$$

to get

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

A nice simple result. This is why there is great interest in computing $f(\theta,\phi)$.

2/14/08

Now we specialize to central force scattering, in which $V(\vec{r}) \to V(r)$. There are quite a few special considerations for this important special case. The main simplification for central force scattering is that the ~~wave~~ Schrödinger equation is separable in spherical coordinates, and has solutions of the form,

$$\psi(\vec{r}) = R(r)\, Y_{\ell m}(\Omega).$$

The radial wave fn $R(r)$ depends on ℓ and also on E or k $\left(E = \frac{\hbar^2 k^2}{2m}\right)$, so sometimes we may write ~~$R_{\ell E}$~~ $R_\ell(r)$ or $R_{\ell,E}(r)$, etc. The radial wave eqn. is

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_\ell}{dr}\right) + \left[\frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r)\right] R_\ell(r) = E\, R_\ell(r),$$

or, by rearranging,

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_\ell}{dr}\right) + k^2 R_\ell(r) = \left[\frac{\ell(\ell+1)}{r^2} + W(r)\right] R_\ell(r),$$

where

$$W(r) = \frac{2m}{\hbar^2} V(r).$$

As usual with radial wave equations, we may substitute

$$R_\ell(r) = \frac{u_\ell(r)}{r},$$

so that

$$u_\ell''(r) + k^2 u_\ell(r) = \left[\frac{\ell(\ell+1)}{r^2} + W(r)\right] u_\ell(r).$$

2/14/08

First consider case of free particle ($W(r)=0$). The R-eqn. is easier to solve in this case, and the gen'l solution is a linear comb. of the 2 types of spherical Bessel functions, $j_\ell(kr)$ and $n_\ell(kr)$:

$$R_{\ell,k}(r) = A\, j_\ell(kr) + B\, n_\ell(kr).$$

Of these, however, $n_\ell \to \infty$ as $r \to 0$, so it is not acceptable, and we just have the j_ℓ solution:

$$R_\ell(r) = j_\ell(kr).$$

Thus we may now write down the most general free particle solution of energy $E>0$ in 3D as a linear combination of spherical waves,

$$(\text{free}) \quad \psi(\vec{r}) = \sum_{\ell m} A_{\ell m}\, j_\ell(kr)\, Y_{\ell m}(\Omega).$$

There is a great deal of degeneracy because of the freedom in the choice of the coefficients $A_{\ell m}$.

In particular, the plane wave $e^{i\vec{k}\cdot\vec{r}}$ can be expanded in terms of radial solutions. The expansion is

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{\ell m} i^\ell\, j_\ell(kr)\, Y^*_{\ell m}(\hat{k})\, Y_{\ell m}(\hat{r}).$$

To derive this one must get involved with the normalization and phase conventions of special functions. This expansion is derived in Sakurai's book, and will not be repeated here.

By the way, note the asymptotic form of the j_ℓ:

$$j_\ell(kr) \sim \frac{\sin(kr - \ell\pi/2)}{kr}, \quad \text{when } kr \gg \ell.$$

Now take the case of nonzero potential $V(r)$. If we can solve the radial eqn. for $R_{\ell,k}(r)$, then we can write down the most general soln of the Sch. eqn with $E>0$,

$$(\text{any } V(r)): \qquad \psi(\vec{r}) = \sum_{\ell m} A_{\ell m}\, R_{\ell,k}(r)\, Y_{\ell m}(\Omega).$$

We can't solve for the $R_\ell(r)$ exactly without knowing $V(r)$ and doing some work, but we can say something about the asymptotic form. Look at the u eqn,

$$u_\ell'' + k^2 u_\ell = \left[\frac{\ell(\ell+1)}{r^2} + W(r)\right] u_\ell$$

If r is large then [ ] is small, assuming $W(r) \to 0$ as $r \to \infty$, so as a first approx. let's neglect it. Then solution is

$$u_\ell(r) = e^{\pm ikr}$$

To find a correction, let's write

$$u_\ell(r) = e^{g(r) \pm ikr},$$

where $g(r)$ is to be determined. Substituting this into the exact u eqn, we find

$$g'' + g'^2 \pm 2ikg' = \frac{\ell(\ell+1)}{r^2} + W(r)$$

2/14/08

Now if $W(r)$ falls off faster than centrifugal potential, then the centrifugal potential dominates, while if slower, then $W(r)$ dominates. So let's assume

$$W(r) \sim \frac{a}{r^p}$$

$a =$ const.
$p =$ power,
$1 < p \le 2$

To find a solution for g, assume a power law,

$$g(r) \sim \frac{b}{r^s}$$

b, s constants to be determined. Then

$$g' \sim -\frac{sb}{r^{s+1}}, \qquad g'^2 \sim \frac{s^2 b^2}{r^{2s+2}}, \qquad g'' \sim \frac{s(s+1)\,b}{r^{s+2}}.$$

Thus the term in g' dominates, and we have

$$\pm 2ikg' \sim \frac{a}{r^p},$$

$$\pm 2ikg = -\frac{1}{p-1}\,\frac{a}{r^{p-1}} \to 0 \quad \text{as} \quad r \to \infty.$$

Thus the correction $g \to 0$,

$$u_\ell = e^{g(r) \pm ikr} = e^{g(r)}\, e^{\pm ikr} \sim e^{\pm ikr}.$$

~~So the~~ But in the case $W(r) = \frac{a}{r}$ (Coulomb), we have

$$\pm 2ikg' \sim \frac{a}{r},$$

$$\pm 2ikg \sim a \ln(kr)$$

$$g \sim \mp \frac{ia}{2k} \ln(kr)$$

$$u_\ell(r) = e^{\pm i\left(kr - \frac{a}{2k}\ln(kr)\right)}.$$

2/14/08

Conclusion: The Coulomb potential gives rise to long range, logarithmic phase shifts that do not $\to 0$ as $r \to \infty$.

For other, shorter range potentials, the asymptotic form is

$$u_\ell(r) = e^{\pm ikr} \qquad (2 \text{ lin. indep. solns.}),$$

that is

$$R_\ell(r) = \frac{A \sin kr + B \cos kr}{kr}, \qquad \text{gen'l. lin. comb.}$$

Since radial wave eqn. is real, we can choose $R_\ell(r) = $ real, hence A, B above $=$ real. Can rewrite this as

$$R_\ell(r) = C \, \frac{\sin(kr + \phi_\ell)}{kr}$$

where ϕ_ℓ is a phase shift. We normalize $R_\ell(r)$ by setting $C = 1$.

For the free particle, the asymptotic phase shift is $-\ell\pi/2$, so let's write

$$\phi_\ell = -\frac{\ell\pi}{2} + \delta_\ell,$$

so that δ_ℓ is the phase shift in the asymptotic form of $R_\ell(r)$ for potential $V(r)$, relative to the free particle phase shift. Thus,

$$R_\ell(r) \sim \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr}.$$

The phase shift δ_ℓ contains the effects of the potential, as seen in the asymptotic form of the radial wave function.

At this point we have the expansion of the incident plane wave in spherical waves,

$$\psi_{inc}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{lm} i^l \, j_l(kr) \, Y^*_{lm}(\hat{k}) \, Y_{lm}(\hat{r}),$$

and we can also expand the exact solution in terms of spherical waves,

$$\psi(\vec{r}) = 4\pi \sum_{lm} i^l \, A_{lm} \, R_l(r) \, Y_{lm}(\hat{r}),$$

where $R_l(r)$ is the exact solution of the radial equation including the potential V, and where we have split off a factor $4\pi i^l$ from the (as yet unknown) expansion coefficients A_{lm} to make the expansion look similar to the one for $\psi_{inc}(\vec{r})$.

By imposing physical boundary conditions it turns out we can express the coefficients A_{lm} in terms of the phase shifts δ_l in the asymptotic form of the $R_l(r)$. First we write down the series for $\psi_{sc}(\vec{r}) = \psi(\vec{r}) - \psi_{inc}(\vec{r})$,

$$\psi_{sc}(\vec{r}) = 4\pi \sum_{lm} i^l \left[A_{lm} R_l(r) - Y^*_{lm}(\hat{k}) \, j_l(kr) \right] Y_{lm}(\hat{r}),$$

and then take the large r limit of the expression $[\ ]$, which contains the radial dependence of the partial wave lm. This gives

$$[\ ] \xrightarrow[r\to\infty]{} \frac{1}{kr}\left[A_{lm} \sin(kr - l\pi/2 + \delta_l) - Y^*_{lm}(\hat{k}) \sin(kr - l\pi/2) \right].$$

2/14/08

On physical grounds we require this to consist purely of an outgoing wave, since any incoming wave would represent particles streaming in toward the scatterer from all directions. The incoming part is

$$(\text{factors}) \left[A_{\ell m}\, e^{-i(kr - \ell\pi/2 + \delta_\ell)} - Y^*_{\ell m}(\hat{k})\, e^{-i(kr - \ell\pi/2)} \right]$$

$$= (\text{factors})\, e^{-i(kr-\ell\pi/2)} \left[A_{\ell m}\, e^{-i\delta_\ell} - Y^*_{\ell m}(\hat{k}) \right] = 0 \quad (\text{demand}),$$

so we obtain

$$A_{\ell m} = e^{i\delta_\ell}\, Y^*_{\ell m}(\hat{k}).$$

Plugging this back into the expansion of $\psi_{sc}(\vec{r})$, which now contains only outgoing waves, we obtain

$$\psi_{sc}(\vec{r}) = 4\pi \sum_{\ell m} i^\ell \left[e^{i\delta_\ell} R_\ell(r) - j_\ell(kr) \right] Y^*_{\ell m}(\hat{k})\, Y_{\ell m}(\hat{r})$$

$$\underset{r\to\infty}{\sim} 4\pi \sum_{\ell m} i^\ell \left(\frac{1}{2i}\right) \left(\frac{1}{kr}\right) \left[e^{i\delta_\ell} e^{i(kr-\ell\pi/2+\delta_\ell)} - e^{i(kr-\ell\pi/2)} \right] Y^*_{\ell m}(\hat{k})\, Y_{\ell m}(\hat{r})$$

$$= \frac{e^{ikr}}{r} f(\theta,\phi),$$

where

$$f(\theta,\phi) = \frac{4\pi}{k} \sum_{\ell m} \underbrace{\left(\frac{e^{2i\delta_\ell} - 1}{2i} \right)}_{= e^{i\delta_\ell} \sin\delta_\ell} Y^*_{\ell m}(\hat{k})\, Y_{\ell m}(\hat{r})$$

We see that the scattered wave does have the asymptotic form

2/14/08

we argued for previously on somewhat intuitive grounds, and we get an explicit formula for the scattering amplitude in terms of the phase shifts δ_ℓ. That formula can be simplified by using the addition thm. for spherical harmonics,

$$f(\theta) = \frac{1}{k}\sum_\ell (2\ell+1)\left(e^{i\delta_\ell}\sin\delta_\ell\right) P_\ell(\hat{k}\cdot\hat{r})$$

Notice that if we put $\hat{k}=\hat{z}$, then $\hat{k}\cdot\hat{r}=\cos\theta$ and the scattering amplitude is independent of ϕ, as is clear it must be because of the azimuthal symmetry of the potential and the boundary conditions,

From $f(\theta)$ we can compute the differential cross section. We'll use the $Y_{\ell m}$-form for this:

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{(4\pi)^2}{k^2}\sum_{\substack{\ell m\\ \ell' m'}} e^{i\delta_\ell}\sin\delta_\ell\, Y^*_{\ell m}(\hat{k})\,Y_{\ell m}(\hat{r})\, e^{-i\delta_{\ell'}}\sin\delta_{\ell'}\, Y_{\ell' m'}(\hat{k})\,Y^*_{\ell' m'}(\hat{r})$$

It has a lot of cross terms that tend to make oscillations (interference patterns) in $\frac{d\sigma}{d\Omega}$, as observed experimentally. But when we integrate over solid angles to get the total cross section, the interference terms disappear,

$$\int d\Omega \, Y_{\ell m}(\hat{r}) \, Y^*_{\ell' m'}(\hat{r}) = \delta_{\ell\ell'} \delta_{mm'}$$

so

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \frac{(4\pi)^2}{k^2} \sum_{\ell m} \sin^2\delta_\ell \, |Y_{\ell m}(\hat{k})|^2$$

or

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

where we use the addition thm. again.

To determine f, $\frac{d\sigma}{d\Omega}$, and σ, for central force problems, we need the phase shifts δ_ℓ. Sakurai discusses hard sphere scattering (also discussed in class.)