Lecture 22 Highlights
Phys 402

To allow for all possible "impact parameters" we have to allow for every possible angular momentum quantum number in the solution to the angular equation (note that classically the angular momentum of the incoming particle is $L = mvb$, which means that a sum over ℓ is roughly analogous to a sum over impact parameters). This means the solution is in the form of an infinite sum:

$\psi(r,\theta) = A\left\{e^{ikz} + \sum_{\ell,m} C_{\ell,m}\, h_\ell^{(1)}(kr)\; Y_{\ell,m}(\theta,\phi)\right\}$, where the $C_{\ell,m}$ are unknown expansion coefficients. However, because we shall assume that the scattering potential is azimuthally symmetric, only the $m = 0$ terms are relevant to the expansion. Since $Y_{\ell,m}(\theta,\phi) \sim e^{im\varphi}$, it effectively reduces to just the Legendre polynomials as a function of θ: $Y_{\ell,m=0}(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$. Re-writing the expansion coefficients as $C_{\ell,0} = i^\ell\, k\,\sqrt{4\pi(2\ell+1)}\, a_\ell$ (to make it compatible with a future expression for the incoming wave), where we have now defined the unknown complex partial wave amplitudes a_ℓ. The solution to the scattering problem can now be written as $\psi(r,\theta) = A\left\{e^{ikz} + k\sum_\ell i^\ell\,(2\ell+1)\, a_\ell\, h_\ell^{(1)}(kr)\; P_\ell(\cos\theta)\right\}$. The expansion of the outgoing wave as a sum over coefficients times the Legendre polynomial takes advantage of the completeness property of the $P_\ell(\cos\theta)$ in expressing any function of angle θ.

By looking in the limit $kr \gg 1$ and using the asymptotic form for the spherical Hankel function, we find the solution reduces to the form of Eq (1) with the scattering amplitude $f(\theta) = \sum_{\ell=0}\,(2\ell+1)\, a_\ell\; P_\ell(\cos\theta)$, written in terms of the partial wave amplitudes.

$$\psi(r,\theta) = A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\}, \tag{1}$$

This allows us to write the total scattering cross section as $\sigma = \iint D(\theta)\, d\Omega = \iint |f(\theta)|^2\, d\Omega = 4\pi\sum_{\ell=0}^{\infty}(2\ell+1)\,|a_\ell|^2$. The total cross section is thus simply related to the weighted sum of the absolute squares of the partial wave amplitudes. To find these amplitudes we need to solve the full Schrodinger equation (Eq. (2) below) including the scattering potential $V(r)$ in the **Interior region** and match the boundary conditions with the intermediate and radiation zone solutions.

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right]u = Eu \tag{2}$$

A technical step is taken to re-express the e^{ikz} incoming wave with Rayleigh's formula as a sum over all angular momenta, so that the full solution becomes: $\psi(r,\theta) = A\left\{\sum_\ell i^\ell\,(2\ell+1)\left[j_\ell(kr) + i\,k\,a_\ell\, h_\ell^{(1)}(kr)\right] P_\ell(\cos\theta)\right\}$. Since angular momentum (parameterized by ℓ) is conserved upon elastic scattering from a spherically-symmetric potential, each term in this sum is independent. This is called the partial wave expansion for the scattering wavefunction.

As an example we considered the quantum version of hard-sphere scattering. This is a potential described by $V(r) = \begin{cases}\infty \text{ for } r \le a\\ 0 \text{ for } r > a\end{cases}$. The solution to the full Schrodinger equation is pretty straightforward in this case. We simply require "hard sphere boundary conditions", namely $\psi(a,\theta) = 0$. Due to the independence of each term in the sum on ℓ, each term must separately be zero, yielding $a_\ell = i\,\frac{j_\ell(ka)}{k\,h_\ell^{(1)}(ka)}$. The total scattering cross section can be written as $\sigma = 4\pi \sum_{\ell=0}^{\infty}(2\ell+1)\,|a_\ell|^2 = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\,\left|\frac{j_\ell(ka)}{h_\ell^{(1)}(ka)}\right|^2$. This expression is not particularly informative. However, consider the "small sphere" limit $ka \ll 1$, which means that the sphere is much smaller than the deBroglie wavelength of the incident particle, or alternatively the incident particle has "low energy." By examining the Bessel functions in the small argument limit, one arrives at the further rather un-helpful result: $\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}\frac{1}{2\ell+1}\left|\frac{2^\ell \ell!}{(2\ell)!}\right|^4 (ka)^{4\ell+2}$. But in the $ka \ll 1$ limit we can take just the first term in the sum since ka appears to such a high power, leading to $\sigma \approx 4\pi a^2$, which corresponds not to the cross-sectional area presented by the sphere, but rather its entire surface area! The quantum waves somehow feel their way around the entire sphere during the scattering process.

Partial Wave Phase Shifts

We continued the discussion of scattering by considering a reformulation of the scattering from a spherically-symmetric potential in terms of partial wave phase shifts. Consider scattering against a hard-wall potential in one-dimension. An incident particle from one side of the barrier will be fully reflected, hence far from barrier the amplitude of the reflected and incident waves will be identical because probability is conserved. Thus the only effect of a complicated scattering potential $V(x)$ localized near the barrier will simply be a phase shift of the reflected wave relative to the incident wave. By convention this phase shift is taken to be 2δ. One writes the total wavefunction for the scattering process as $\psi(x) = A\{e^{ikx} - e^{i(2\delta - kx)}\}$, where the first term represents an incident right-going wave and the second term is the reflected and phase shifted wave. Note that this wavefunction is written in the radiation zone far from the potential. One can find the phase shift δ by solving the Schrodinger equation in the scattering region and matching the result onto the radiation zone. Alternatively, one can measure the phase shift as a function of the energy of the incident particle. From the dependence $\delta(k)$ one could in principle deduce the potential function $V(x)$ of the scattering region.

Now take this idea to the case of 3D scattering. By writing the incident wave e^{ikz} as

$\psi_0 = \sum_\ell i^\ell\,(2\ell+1)\,j_\ell(kr)\;P_\ell(\cos\theta)$,

we can think of it in terms of partial waves of the form:

$$\psi_0^{(\ell)} = A\,i^\ell\,(2\ell+1)\,j_\ell(kr)P_\ell(\cos\theta)$$

Writing $j_\ell(kr) = \frac{1}{2}\left[h_\ell^{(1)}(kr) + h_\ell^{(2)}(kr)\right]$ in the asymptotic (radiation) regime these partial waves become:

$\psi_0^{(\ell)} = \frac{A\,(2\ell+1)}{2i}\left[\frac{e^{ikr}}{kr} - (-1)^\ell\,\frac{e^{-ikr}}{kr}\right]P_\ell(\cos\theta)$.

The first term in the bracket represents the outgoing wave while the second term represents a converging incident spherical wave. The effect of a non-zero scattering potential will be to add a phase shift $2\delta_\ell$ to the outgoing wave, unique to each partial wave. Thus, the wave measured in the radiation regime will be modified to be:

$\psi^{(\ell)} = \frac{A\,(2\ell+1)}{2i}\left[\frac{e^{i(kr+2\delta_\ell)}}{kr} - (-1)^\ell\,\frac{e^{-ikr}}{kr}\right] P_\ell(\cos\theta)$.

By comparing this to the form of the original partial wave solution: $\psi(r,\theta) = A\left\{e^{ikz} + k\,\sum_\ell i^{\ell+1}\,(2\ell+1)\,a_\ell\,h_\ell^{(1)}(kr)\;P_\ell(\cos\theta)\right\}$, substituting the asymptotic form for $\psi_0^{(\ell)}$ in place of e^{ikz}, and then equating term by term in the angular momentum sum, one finds the relationship between the partial wave amplitudes a_ℓ and the phase shifts δ_ℓ of $a_\ell = \frac{1}{2ik}\left(e^{i2\delta_\ell} - 1\right) = \frac{1}{k}e^{i\delta_\ell}\sin\delta_\ell$. Note that we have replaced the complex partial wave amplitude a_ℓ with a single real quantity, the partial wave phase shift δ_ℓ. This is possible because the scattering potential $V(r)$ is assumed to be spherically symmetric and therefore conserves angular momentum.

We can now express the scattering amplitude as $f(\theta) = \sum_{\ell=0}(2\ell+1)\,a_\ell\;P_\ell(\cos\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_\ell}\;\sin\delta_\ell\,P_\ell(\cos\theta)$. The total scattering cross section can be written as $\sigma = 4\pi\sum_{\ell=0}^{\infty}(2\ell+1)\,|a_\ell|^2 = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\;\sin^2(\delta_\ell)$.

As an example we returned to the quantum hard sphere scattering case with $V(r) = \begin{cases}\infty \text{ for } r \le a\\ 0 \text{ for } r > a\end{cases}$. We found above that the partial wave amplitudes are given by $a_\ell = i\,\frac{j_\ell(ka)}{k\,h_\ell^{(1)}(ka)}$. Equate the real and imaginary parts of this expression to $\frac{1}{k}e^{i\delta_\ell}\sin\delta_\ell = \frac{1}{k}\,(\cos\delta_\ell\sin\delta_\ell + i\;\sin^2(\delta_\ell))$ to find that $\delta_\ell = \tan^{-1}\left(\frac{j_\ell(ka)}{n_\ell(ka)}\right)$. We can evaluate this phase shift for the $\ell = 0$ partial wave to find $\delta_0 = -\tan^{-1}(\tan(ka)) = -ka$. Calculating the total scattering cross section $\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\;\sin^2(\delta_\ell)$, and assuming that the $\ell = 0$ term dominates and $ka \ll 1$, yields $\sigma \cong 4\pi a^2$, which is the same result derived by partial wave analysis in the "small sphere" limit $ka \ll 1$.