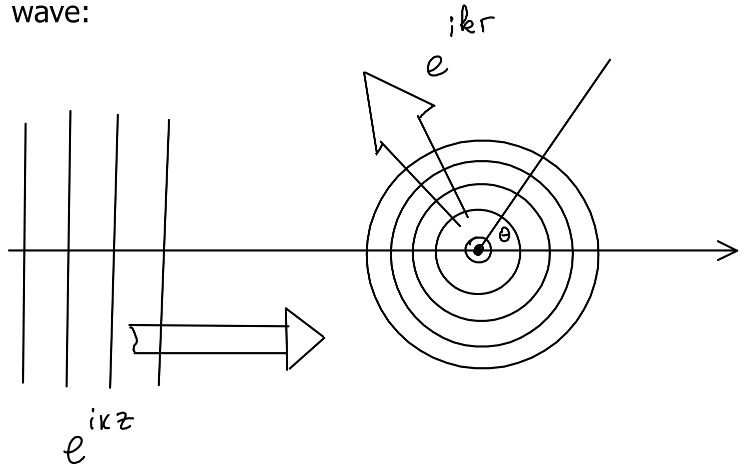
Lecture 19

Quantum scattering theory

Our problem: incident plane wave

$$\psi(z) = A e^{ikz}$$

traveling in Z direction encounters a scattering potential that produces outgoing spherical wave:



Therefore, the solutions of the Schrödinger equation have the general form:

$$\psi(r,\theta) \approx A\left\{ \underbrace{e^{ikz}}_{\text{plane wave}} + \underbrace{f(\theta)\frac{e^{ikr}}{r}}_{\text{spherical wave}} \right\} \quad \text{for large } r$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

E ← energy of the incident particle

The quantity $f(\theta)$ called scattering amplitude is the probability of scattering in a given direction.

The differential cross-section is given by

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

Therefore, to solve the scattering problem, we need to calculate the scattering amplitude $f(\theta)$.

Partial wave analysis

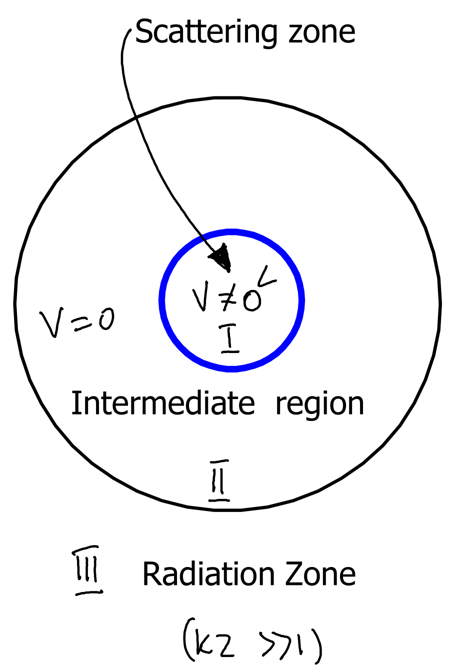
Our potential is spherically symmetric $\Longrightarrow$

The solutions of the Schrödinger equation are $\psi(r,\theta,\phi) = \underbrace{\frac{1}{r}u(r)}_{R_{n\ell}(r)} Y_\ell^m(\theta,\phi)$

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

"centrifugal contribution"

Our goal is to develop method that would allow us to find the scattering amplitude.
We separate our space into three zones:



Both V=0 and centrifugal term may be taken to be zero.

In **Zone III** the radial Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} \approx Eu$$

$$\frac{d^2u}{dr^2} \approx -k^2u$$

$$u = Ce^{ikr}$$

$$\boxed{R(r) = C\frac{e^{ikr}}{r}}$$

(outgoing spherical wave as we assumed earlier)

In **Zone II** we can neglect the potential term, but not the centrifugal term:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}u = Eu$$

$$\frac{d^2u}{dr^2} - \frac{\ell(\ell+1)}{r^2}u = -k^2u$$

The solutions of this equation are spherical Bessel functions:

$$u(r) = A r\, j_\ell(kr) + B r\, n_\ell(kr)$$

The problem is that neither $j_\ell(kr)$ nor $n_\ell(kr)$ represents an outgoing or incoming wave.

However, the spherical Hankel functions

$$h_\ell^{(1)}(x) \equiv j_\ell(x) + i n_\ell(x)$$

$$h_\ell^{(2)}(x) \equiv j_\ell(x) - i n_\ell(x)$$

have asymptotic behavior that we need (x » 1):

$$h_\ell^{(1)} \to \frac{1}{x}(-i)^{\ell+1} e^{ix} \quad \left(\text{like } \frac{e^{ikr}}{r}, \text{ represents outgoing wave}\right)$$

$$h_\ell^{(2)} \to \frac{1}{x}(i)^{\ell+1} e^{-ix} \quad \left(\text{like } \frac{e^{-ikr}}{r}, \text{ represents incoming wave}\right)$$

We need outgoing wave so we pick Hankel function of the first kind $h_\ell^{(1)}$:

$$u(r) = A r h_\ell^{(1)} \Rightarrow R(r) = \frac{u}{r} \sim h_\ell^{(1)}$$

Summary: outside of the scattering region the exact wave function is

$$\psi(r,\theta,\phi) = A\left\{ \underbrace{e^{ikz}}_{\text{incident plane wave}} + \sum_{\ell,m} C_{\ell,m} \underbrace{h_\ell^{(1)}(kr)}_{\text{scattered wave}} Y_\ell^m(\theta,\phi)\right\}$$

Since the potential is spherically symmetric, the wave function can not depend on $\phi \Rightarrow$ $m=0$ since $Y_\ell^m \sim e^{im\phi}$ and only terms

$$Y_\ell^0(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}}\, \underbrace{P_\ell(\cos\theta)}_{\ell^{th} \text{ Legendre polynomial}}$$

contribute to the wave function above.

For convenience, we rename the coefficients C as

$$C_{\ell,0} = i^{\ell+1} k \sqrt{4\pi(2\ell+1)} \, a_\ell .$$

Plugging in the expressions for $C_{\ell,0}$ and Y_ℓ^0 we get

$$\psi(r,\theta) = A \left\{ e^{ikz} + k \sum_{\ell=0}^{\infty} i^{\ell+1} (2\ell+1) a_\ell h_\ell^{(1)}(kr) P_\ell(\cos\theta) \right\}$$

for large r, the Hankel function behaves as $(-i)^{\ell+1} \dfrac{e^{ikr}}{kr}$

and the wave function becomes

$$\psi(r,\theta) = A \left\{ e^{ikz} + \underbrace{\sum_{\ell=0}^{\infty} (2\ell+1) a_\ell P_\ell(\cos\theta)} \frac{e^{ikr}}{r} \right\} .$$

Comparing this formula with

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

gives the scattering amplitude

$$\boxed{f(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1) a_\ell P_\ell(\cos\theta)}$$

a_ℓ is called partial wave amplitude (since waves with different values of orbital angular momentum ℓ are referred to as partial waves). This is why this method is called **partial wave analysis**.

The differential cross-section is the given by

$$\boxed{D(\theta) = |f(\theta)|^2 = \sum_\ell \sum_{\ell'} (2\ell+1)(2\ell'+1) a_\ell^* a_{\ell'} P_\ell(\cos\theta) P_{\ell'}(\cos\theta)}$$

The total cross section is

$$\sigma = \int D \, d\Omega = 4\pi \int_0^\pi \sum_\ell \sum_{\ell'} (2\ell+1)(2\ell'+1) a_\ell^* a_{\ell'} P_\ell(\cos\theta) P_{\ell'}(\cos\theta) \sin\theta \, d\theta$$

$$\boxed{\sigma = 4\pi \sum_{\ell=0}^{\infty} (2\ell+1)\,|a_\ell|^2},$$

were we used orthogonality condition for Legendre polynomials

$$\int_{-1}^{1} P_\ell(x)\, P_{\ell'}(x)\, dx = \frac{2}{2\ell+1}\,\delta_{\ell\ell'}.$$

Strategy how to solve scattering problems using the partial wave analysis:

Solve Schrödinger equation in the interior region (where V≠0) and match this solution to the exterior solution that we have derived using the boundary conditions. This procedure will give the partial wave amplitude a_ℓ . Then, plug in the partial wave amplitude into the formulas for the differential and/or total scattering cross-sections.

However, before considering an example we note that our expression for the exterior wave function is in mixed coordinates: the incoming wave is in cartesian coordinates while the outgoing wave is in spherical coordinates. We can re-write the expression for the incoming wave in spherical coordinates by using the expansion for the exponential

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta).$$

Then, the exterior solution may be written in spherical coordinates as

$$\psi(r,\theta) = A \sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\left[j_\ell(kr) + ik\, a_\ell\, h_\ell^{(1)}(kr)\right] P_\ell(\cos\theta).$$

We note that amplitude of the incoming wave has to be equal to the amplitude of the outgoing wave (by conservation of probability), so we can reformulate our scattering problem in terms of calculating the **phase shifts** rather than partial wave amplitudes defined as:

$$a_\ell = \frac{1}{2ik}\left(e^{2i\delta_\ell} - 1\right) = \frac{1}{k}\, e^{i\delta_\ell} \sin(\delta_\ell).$$

Then, the scattering amplitude is given by

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

and total cross-section is given by

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

Example

Quantum hard-sphere scattering

The potential is $V(r) = \begin{cases} \infty, & \text{for} \quad r \leq a \\ 0, & \text{for} \quad r > a \end{cases}$

The boundary condition is $\psi(a, \theta) = 0$.
Matching it with the exterior solution gives

$$\sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1)\left[j_\ell(ka) + ika_\ell h_\ell^{(1)}(ka)\right] P_\ell(\cos\theta) = 0$$

In homework #8 your will prove that then

$$a_\ell = -i \frac{j_\ell(ka)}{k h_\ell^{(1)}(ka)}.$$

The total cross-section is

$$\sigma = 4\pi \sum_{\ell=0}^{\infty} (2\ell+1)|a_\ell|^2 = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell+1) \left|\frac{j_\ell(ka)}{h_\ell^{(1)}(ka)}\right|$$

It is possible to show that for low-energy scattering $(ka \ll 1)$

$$\sigma \approx 4\pi a^2.$$

This is 4 times larger than the classical result for hard-sphere scattering πa^2 !
In the classical case, the result that we got was the geometrical cross-section of the sphere. In the quantum case, the scattering cross-section is the total surface area of the sphere. This is characteristic of the long-wavelength scattering.