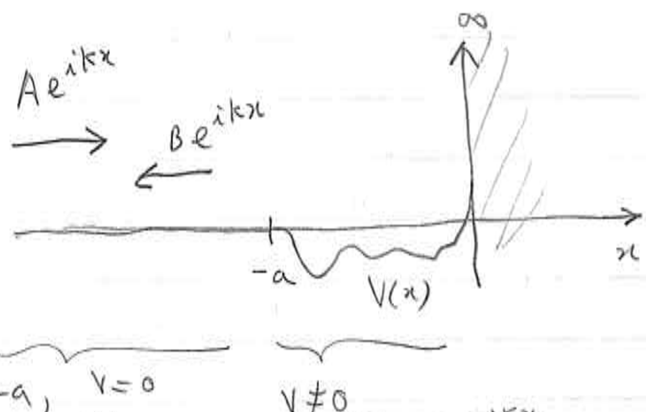
P423 – Lecture 21 : Scattering : Phase shifts and Born approximation

Phase shifts : A better way to represent scattering amplitude a_ℓ

1d example : Hard wall scattering



In the $x<-a$ region, $\psi_{x<-a}(x) = Ae^{ikx} + Be^{-ikx}$.

In this case the wave has to be fully reflected, with $|B| = |A|$ to conserve probability. If $V=0$ everywhere, we would have $\psi(x) = A(e^{ikx} - e^{-ikx})$ with $B=-A$ so that $\psi(x=0)=0$. When $V\neq 0$ we write: $\boxed{B = -Ae^{2\delta_k i}}$ where δ_k is called phase shift.

$$\Rightarrow \quad \psi_{x<-a}(x) = A\left[e^{ikx} - e^{i(2\delta_k - kx)}\right]$$

When $V\neq 0$ in the $x\in[-a,0]$ region we get $\delta_k \neq 0$. How to calculate δ_k? Find exact wave func in the scattering region $[-a,0]$ and match to the $x<-a$ solution.
The effect of $V\neq 0$ is encoded in δ_k.

Apply same idea to 3d scattering :

When $V=0$, $a_\ell = 0$ so the "scattered wave" is just

$$\psi(\vec{r}) = Ae^{ikz} = A\sum_{\ell=0}^{\infty} \underbrace{i^\ell (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta)}_{\psi^{(\ell)}(\vec{r})} \qquad \text{(Rayleigh)}$$

At large kr:

$$j_\ell(kr) \approx \frac{1}{2kr}\left[(-i)^{\ell+1} e^{ikr} + (i)^{\ell+1} e^{-ikr}\right] \qquad \begin{pmatrix} kr \gg 1 \\ V \equiv 0 \end{pmatrix}$$

So the ℓ^{th} partial wave becomes

$$\psi^{(\ell)}(\vec{r}) \approx \frac{A(2\ell+1)}{2ikr}\Big[\underbrace{e^{ikr}}_{\text{outgoing}} - \underbrace{(-1)^{\ell} e^{-ikr}}_{\text{incoming}}\Big] P_\ell(\cos\theta) \qquad \begin{pmatrix} kr \gg 1 \\ V \equiv 0 \end{pmatrix}$$

When we turn on a spherically symmetric $V(r)$, the outgoing wave "picks up a phase" $e^{2\delta_\ell i}$.
(Note ~~that~~ this is true only for spherically symmetric potentials)
Because only in this case the amplitude of the ℓ^{th} state will not be transposed to an ℓ'^{th} (conservation of angular momentum).

Thus with $V \neq 0$:

$$\psi^{(\ell)}(\vec{r}) \approx \frac{A(2\ell+1)}{2ikr}\left[e^{i(kr+2\delta_\ell)} - (-1)^{\ell} e^{-ikr}\right] P_\ell(\cos\theta) \qquad \begin{pmatrix} kr \gg 1 \\ V \neq 0 \end{pmatrix}$$

Compare this to the exact solution in the $kr \gg 1$ region (as a fnc of a_ℓ):

$$\psi^{(\ell)}(\vec{r}) \approx A\left\{\frac{(2\ell+1)}{2ikr}\left[e^{ikr} - (-1)^{\ell} e^{-ikr}\right] + \frac{(2\ell+1)}{r} a_\ell e^{ikr}\right\} P_\ell(\cos\theta)$$

$$\Rightarrow \frac{(2\ell+1)}{2ikr} e^{i(kr+2\delta_\ell)} = \frac{(2\ell+1)}{2ikr} e^{ikr} + \frac{(2\ell+1)}{r} a_\ell e^{ikr}$$

$$\Rightarrow \frac{1}{2ik}\left[e^{(2\delta_\ell)i} - 1\right] = a_\ell \Rightarrow \boxed{a_\ell = \frac{e^{i\delta_\ell}}{k}\sin(\delta_\ell)}$$

Note the advantage of working with phase shifts: Instead of working with a complex number a_ℓ, we now worry only about a single real number δ_ℓ.

Hence we have:

$$\Rightarrow \boxed{f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1) e^{i\delta_\ell}\sin(\delta_\ell) P_\ell(\cos\theta)} \quad \text{and} \quad \boxed{\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2(\delta_\ell)}$$

Born approximation

Integral form of the Schrödinger's eqn

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

where $E = \frac{\hbar^2}{2m}k^2$ can be written as

$$(\nabla^2 + k^2)\psi = \underbrace{\left(\frac{2m}{\hbar^2} V(\vec{r})\psi(\vec{r})\right)}_{\equiv\, \varphi(\vec{r})}$$

Looks like a Helmholtz eqn, but with a source that depends on $\psi(\vec{r})$ itself:

$$(\nabla^2 + k^2)\psi = \varphi$$

Suppose we find the Green's fnc associated to the Helmholtz eqn:

$$(\nabla^2 + k^2)G(\vec{r}) = \delta(\vec{r})$$

In that case our inhomogeneous solution (dependent on source) is just:

$$\psi(\vec{r}) = \int d^3r_0\, G(\vec{r}-\vec{r}_0)\,\varphi(\vec{r}_0)$$

Proof:

$$(\nabla_r^2 + k^2)\psi = \int d^3r_0\, \underbrace{(\nabla_r^2 + k^2)G(\vec{r}-\vec{r}_0)}_{=\,\delta(\vec{r}-\vec{r}_0)}\,\varphi(\vec{r}_0) = \varphi(\vec{r}) \quad //$$

(use $\nabla_r^2 = \nabla^2_{(\vec{r}-\vec{r}_0)}$)

④

This Green's func is well known; we have (see book for a formal derivation):

$$\boxed{G(\vec{r}) = -\frac{e^{ikr}}{4\pi r}}$$

Thus we get a formal solution to the Schrödinger's eqn:

$$\psi(\vec{r}) = \underbrace{\psi_0(\vec{r})}_{\substack{\text{Homogeneous solution,} \\ (\nabla^2+k^2)\psi_0(\vec{r})=0}} + \underbrace{\frac{2m}{\hbar^2}\int d^3r_0 \left(-\frac{1}{4\pi}\right)}_{\substack{\text{Inhomogeneous solution,} \\ (\nabla^2+k^2)(\cdot) = Q(\vec{r})}} \frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} V(\vec{r}_0)\psi(\vec{r}_0)$$

$$\boxed{\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{m}{2\pi\hbar^2}\int d^3r_0 \frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} V(\vec{r}_0)\psi(\vec{r}_0)}$$

Note how this "formal solution" is self consistent: The RHS has an integral that depends on the solution $\psi(\vec{r})$ itself. I.e., you can only use ~~it~~ to solve the Schrödinger eqn exactly if you already know the answer!

<u>1st Born approximation</u>

Suppose $V(\vec{r}_0)$ is localized around $\vec{r}_0 \approx 0$, and we want to compute $\psi(\vec{r})$ for $|\vec{r}| \gg |\vec{r}_0|$ (points far away).

In this case we can approximate $(\vec{r}-\vec{r}_0)$ in the integrand:

$$|\vec{r}-\vec{r}_0| = \sqrt{r^2+r_0^2 - 2\vec{r}\cdot\vec{r}_0} = r\left[1 + \underbrace{\frac{r_0^2}{r^2}}_{\text{drop}} - \frac{2\hat{r}\cdot\vec{r}_0}{r}\right]^{1/2}$$

$$\approx r\left[1 - \frac{\hat{r}\cdot\vec{r}_0}{r}\right] \approx r - \hat{r}\cdot\vec{r}_0$$

Define "scattered wave vector" as $\vec{k} = k\hat{r}$ (points along detector), so

$$\frac{e^{ik|\vec{r}-\vec{r}_0|}}{|\vec{r}-\vec{r}_0|} \approx \frac{e^{i\vec{k}\cdot[\vec{r}-\vec{r}_0]}}{r-\hat{r}\cdot\vec{r}_0} \approx \frac{e^{ikr}e^{-i\vec{k}\cdot\vec{r}_0}}{r}\left[1+\underbrace{\frac{\hat{r}\cdot\vec{r}_0}{r}}_{\text{drop}}\right]$$

And choose as the homogeneous solution the incident plane wave:

$$\psi_0(\vec{r}) = Ae^{ikz}$$

Thus, for large r:

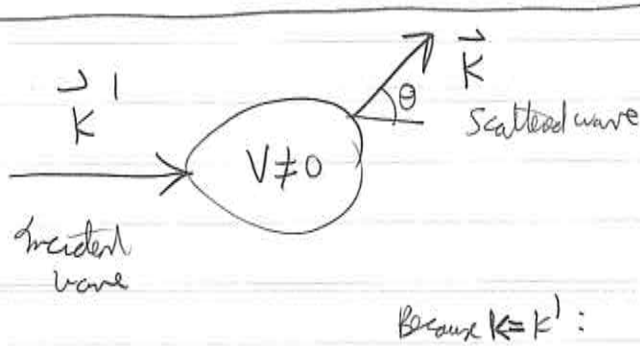
$$\psi(\vec{r}) \approx Ae^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3r_0\, e^{-i\vec{k}\cdot\vec{r}_0}\, V(\vec{r}_0)\psi(\vec{r}_0)$$

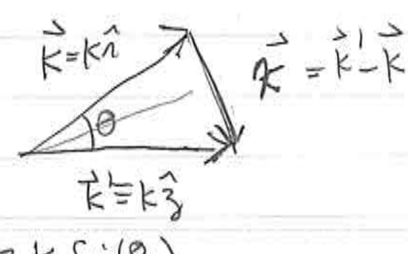
Leading to an expression for the scattered amplitude:

$$\boxed{f(\theta,\phi) = -\frac{m}{2\pi\hbar^2 A}\int d^3r_0\, e^{-i\vec{k}\cdot\vec{r}_0}\, V(\vec{r}_0)\psi(\vec{r}_0)} \quad \text{(exact!)}$$

Suppose the scattering potential is "weak", so that the scattered wave is much smaller than Ae^{ikz}.
The 1st Born approx. consists in plugging $\psi(\vec{r}_0) \approx Ae^{i\vec{k}'\cdot\vec{r}}$, $\boxed{\vec{k}' = k\hat{z}}$, in the integrand:

$$\boxed{f_{1^{st}\,Born}(\theta,\phi) \approx -\frac{m}{2\pi\hbar^2}\int d^3r_0\, e^{i(\vec{k}'-\vec{k})\cdot\vec{r}_0}\, V(\vec{r}_0)}$$





Because $k = k'$: $|\kappa| = 2k\sin\left(\frac{\theta}{2}\right)$

When $|\vec{k}| = |\vec{k}'| << \frac{1}{a}$ (range of potential) we can approximate the exponential to ≈ 1:

$$\boxed{f_{1^{st}\,\text{Born}}(\theta, \phi) \approx -\frac{m}{2\pi\hbar^2} \int d^3r_0 \, V(\vec{r}_0)} \quad \left(\text{low energy } |k| << \frac{1}{a}\right)$$

<u>Example</u>: Soft sphere scattering:

$$V(\vec{r}) = \begin{cases} V_0 & \text{for } r \leq a \\ 0 & \text{for } r > a \end{cases}$$

we get at $ka << 1$: (low energy)

$$f(\theta, \phi) \approx -\frac{m}{2\pi\hbar^2} V_0 \left(\frac{4}{3}\pi a^3\right) = -\frac{2}{3}\frac{mV_0a^3}{\hbar^2}$$

$$\Rightarrow \quad \frac{d\sigma}{d\Omega} = |f|^2 = \left(\frac{2mV_0a^3}{3\hbar^2}\right)^2$$

$$\sigma \approx 4\pi\left(\frac{2mV_0a^3}{3\hbar^2}\right)^2$$

This is only valid when $|f| << a$ i.e. $\frac{mV_0a^3}{\hbar^2} << a$. Otherwise our 1^{st} order approx. breaks down!

$$\Rightarrow \quad \boxed{V_0 << \frac{\hbar^2}{ma^2}}$$

Note how hard sphere case ($V_0 \to \infty$), exactly solvable with partial waves, can not be solved this way.

Higher orders: Born series

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int d^3 r_0 \; g(\vec{r}-\vec{r}_0)\, V(\vec{r}_0)\, \psi(\vec{r}_0),$$

where $g(\vec{r}) \equiv -\frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}$, or

$$\psi = \psi_0 + \int g V \psi$$

Plug the RHS in the integrand:

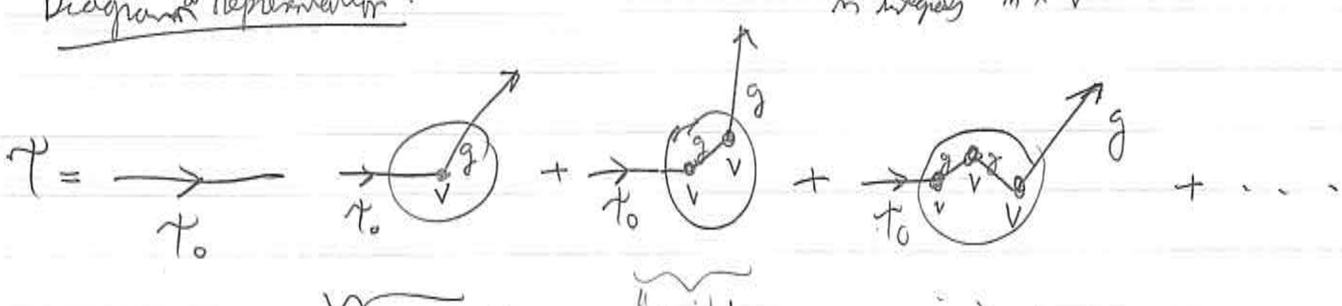
$$\psi = \psi_0 + \int g V \psi_0 + \int\int g V g V \psi$$

Do it several times:

$$\psi = \psi_0 + \int g V \psi_0 + \int\int g V g V \psi_0 + \int\int\int g V g V g V \psi_0 + \dots +$$

$$+ \underbrace{\int \dots \int}_{n \text{ integrals}} \underbrace{g V g V g V \dots g V}_{n \times V} \psi_0 + \dots$$

Diagrammatic representation:



1st order: "kicked once by the potential"

"kicked twice"