

**POSTECH 이성익 교수의
양자 세계에 관한 강연**

- 15장 -

편집 도우미: POSTECH 학부생 임향택

Chapter 15

Time-Dependent Perturbation Theory

$$H = H_0 + V(t)$$

assumption

$$H_0 \psi_n = E_n \psi_n$$

풀어야 할 방정식

$$H\psi = i\hbar \frac{\partial \psi}{\partial t}$$

$$\begin{aligned} H(t) &= \sum_n C_n(t) \psi_n(t) \\ &= \sum_n C_n(t) \psi_n \cdot e^{-i\frac{E_n t}{\hbar}} \end{aligned}$$

위의 equation에 넣는다.

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \sum_n C_n(t) \psi_n \cdot e^{-i\frac{E_n t}{\hbar}} &= H \sum_n C_n(t) \psi_n e^{-i\frac{E_n t}{\hbar}} \\ &= [H_0 + V(t)] \sum_n C_n(t) \psi_n \cdot e^{-i\frac{E_n t}{\hbar}} \\ &= \sum_n C_n(t) \cdot \psi_n E_n e^{-i\frac{E_n t}{\hbar}} + \sum_n V(t) C_n(t) \psi_n e^{-i\frac{E_n t}{\hbar}} \end{aligned}$$

$$\text{左} = \sum_n i\hbar \frac{\partial C_n(t)}{\partial t} \psi_n e^{-i\frac{E_n t}{\hbar}} + \sum_n C_n(t) \psi_n E_n e^{-i\frac{E_n t}{\hbar}}$$

$$\int \psi_m^* \cdot dt \quad \text{ㅁ}$$

$$i\hbar \frac{\partial C_m(t)}{\partial t} e^{-i\frac{E_m t}{\hbar}} = \sum_n \langle \psi_m | V(t) | \psi_n \rangle C_n(t) e^{-i\frac{E_n t}{\hbar}}$$

$$i\hbar \frac{\partial C_m(t)}{\partial t} = \sum_n \langle \psi_m | V(t) | \psi_n \rangle C_n(t) e^{-i\left(\frac{E_n - E_m}{\hbar}\right)t}$$

$$\therefore i\hbar \frac{\partial C_m(t)}{\partial t} = \sum_n C_n(t) \cdot \langle \psi_m | V(t) | \psi_n \rangle e^{i\left(\frac{E_m - E_n}{\hbar}\right)t}$$

Initial Condition

$$C_n(0) = \delta_{nx}$$

$$\therefore i\hbar \frac{dC_m}{dt} = V_{ml}(t) e^{i\frac{(E_m - E_l)t}{\hbar}}$$

The solution of these equations,

$$C_l(t) = 1 + \frac{1}{i\hbar} \int_0^t V_{ll}(t) dt$$

$$C_n(t) = \frac{1}{i\hbar} \int_0^t V_{nl}(t) e^{i\frac{(E_n - E_l)t}{\hbar}} dt$$

Constant Perturbation

$$C_l(t) = 1 + \frac{V_{ll}}{i\hbar} t$$

$$C_n(t) = \frac{V_{nl}}{E_n - E_l} \cdot \frac{1}{i\hbar} \left(1 - e^{i\frac{(E_n - E_l)t}{\hbar}} \right) \quad (n \neq l)$$

Initial state가 어떻게 변화하나?

$$\begin{aligned} &= C_l(t) \psi_l e^{-i\frac{E_l t}{\hbar}} \\ &= \psi_l e^{-i\frac{E_l t}{\hbar}} \left(1 - \frac{i}{\hbar} V_{ll} t \right) \\ &= \psi_l e^{-i\frac{E_l t}{\hbar}} \cdot e^{-i\frac{V_{ll} t}{\hbar}} \\ &= \psi_l e^{-i\frac{(E_l + V_{ll})t}{\hbar}} \end{aligned}$$

phase만 변한다.

$$\begin{aligned}
|C_n(t)|^2 &= \frac{|V_{nl}|^2}{(E_n - E_l)^2} \left| 1 - e^{\frac{i(E_n - E_l)t}{\hbar}} \right|^2 \\
&= \frac{|V_{nl}|^2}{|E_n - E_l|^2} \left| 2 \cdot \sin \frac{E_n - E_l}{\hbar} t \right|^2
\end{aligned}$$

이 식은 $C_n(t)$ 가 매우 작을 때 성립한다.

1. 만약 V_{nl} 가 작다면 O.K.
2. 만약 $E_n \neq E_l$ 매우 다르면

$$|C_n|_{\max}^2 = \frac{4|V_{nl}|^2}{|E_n - E_l|^2} \rightarrow \text{zero}$$

Transition을 보자.

$$\begin{aligned}
\int |C_n(t)|^2 dE_n &= 4|V_{nl}|^2 \int_{-\infty}^{\infty} \sin^2 \frac{(E_n - E_l)t}{2\hbar} \cdot \frac{dE_n}{(E_n - E_l)^2} \\
&= 4|V_{nl}|^2 \int_{-\infty}^{\infty} \sin^2 x \cdot \left(\frac{t}{2\hbar x} \right)^2 \cdot dx \frac{2\hbar}{t} \quad \left[\frac{(E_n - E_l)}{2\hbar} t = x \right] \\
&= 4|V_{nl}|^2 \cdot \frac{t^2}{4\hbar^2} \frac{2\hbar}{t} \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx \\
&= \frac{2t}{\hbar} |V_{nl}|^2 \cdot \pi \quad \left(\because \int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \pi \right)
\end{aligned}$$

Hence

$$|C_n(t)|^2 = \frac{2\pi}{\hbar} |V_{nl}|^2 \cdot t \cdot \delta(E_n - E_l)$$

Total transition probability

$$\begin{aligned}
\int |C_n(t)|^2 \rho(E_n) dE_n &= \frac{2\pi t}{\hbar} \int |V_{nl}|^2 \cdot \delta(E_n - E_F) \rho(E_n) dE_n \\
&= \frac{2\pi t}{\hbar} |V_{nl}|^2 \rho(E_F)
\end{aligned}$$

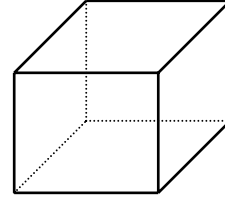
This quantity increase linearly with t

$$W_{FI} = \frac{2\pi}{\hbar} |V_{FI}|^2 \rho(E_F)$$

Box normalization

$$H_0 = \frac{p^2}{2m}$$

$$\psi_I = \frac{1}{\sqrt{L^3}} \exp(i\vec{k} \cdot \vec{r}), \quad \psi_F = \frac{1}{\sqrt{L^3}} \exp(i\vec{k}' \cdot \vec{r})$$



1. Normalization Condition이 만족된다.
2. Periodic Boundary Condition

$$KL = 2n\pi$$

$$\therefore k_x = \frac{2n_x\pi}{L}, k_y = \frac{2n_y\pi}{L}, k_z = \frac{2n_z\pi}{L}$$

$$n = (n_x^2 + n_y^2 + n_z^2)^{\frac{1}{2}}$$

$$\rho(E)dE = n^2 dn d\Omega$$

$$= \left(\frac{L}{2\pi}\right)^3 k^2 dk d\Omega$$

$$n = \frac{kL}{2\pi}$$

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

$$dE = \frac{\hbar^2}{2m} 2k dk$$

$$= \frac{V}{8\pi^3} k \cdot k dk \cdot d\Omega$$

$$= \frac{V}{8\pi^3} \cdot \frac{m dE}{\hbar^2} \cdot \sqrt{\frac{2mE}{\hbar^2}} d\Omega$$

$$\therefore \rho(E) = \frac{V}{8\pi^3} \cdot \frac{m}{\hbar^2} \sqrt{\frac{2mE}{\hbar^2}} d\Omega$$

$$= \frac{V}{8\pi^3} \cdot \frac{m}{\hbar^3} \sqrt{2mE} d\Omega$$

$$V_{FI} = (\psi_F, V\psi_I)$$

$$= \frac{1}{L^3} \int \exp(-i\vec{k}' \cdot \vec{r}) V(r) \exp(i\vec{k} \cdot \vec{r}) d\vec{r}$$

$$\begin{aligned}
W_{FI} &= \frac{2\pi}{\hbar} |V_{FI}|^2 \rho(E_F) \\
\therefore &= \frac{2\pi}{\hbar} |V_{FI}|^2 \cdot \frac{V}{8\pi^3} \cdot \frac{m}{\hbar^3} \cdot \sqrt{2mE} d\Omega \\
&= \frac{2\pi}{\hbar} \cdot \frac{1}{V} \cdot \frac{1}{8\pi^3} \cdot \frac{m}{\hbar^3} \sqrt{2mE} d\Omega \cdot \left| \int \exp(-i\vec{k}' \cdot \vec{r}) V(r) \exp(i\vec{k} \cdot \vec{r}) d\vec{r} \right|^2 \\
W_{FI} &= S_i \sigma(\vec{k}, \vec{k}') d\Omega \\
&= \frac{\hbar k}{mL^3} \sigma(\vec{k}, \vec{k}') d\Omega
\end{aligned}$$

Combine this expression

$$\sigma(\vec{k}, \vec{k}') = \left| \frac{1}{4\pi} \frac{2m}{\hbar^2} \int V(r) \exp[i(\vec{k} - \vec{k}') \cdot \vec{r}] d\vec{r} \right|^2$$

Schrödinger Equation

$$Eu(\vec{r}) = \left[-\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right] u(\vec{r})$$

$$E = \frac{\hbar^2 k^2}{2\mu}$$

$$\rightarrow \therefore \left[\nabla^2 + k^2 - V(r) \right] u(\vec{r}) = 0 \quad V(r) = \frac{2\mu}{\hbar^2} V(r)$$

Let $u(\vec{r}) = \sum_{l,m} R_l(r) Y_{lm}(\theta, \phi)$

with $R_l(r)$ satisfying

$$0 = \frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR_l}{dr} \right) + \left(k^2 - \frac{l(l+1)}{r^2} - V(r) \right) R_l$$

or $\chi_l(r) \equiv rR_l(r)$, then

$$\chi_l'' + \left[k^2 - \frac{l(l+1)}{r^2} - V(r) \right] \chi_l(r) = 0$$

만약 $r \rightarrow \infty$

$$\chi_l'' + k^2 \chi_l = 0$$

$$\therefore \chi_l = e^{\pm ikr}$$

Put $\chi_l \equiv v_l(r) e^{\pm ikr}$

$$\Rightarrow v_l'' \pm 2ikv_l' - k^2 v_l + \left(k^2 - \frac{l(l+1)}{r^2} - V(r) \right) v_l = 0$$

for smooth Potential, $|v_l''| \ll |kv_l'|$

$$\pm 2i \cdot \frac{v_l'}{v_l} = V(r) + \frac{l(l+1)}{r^2}$$

$$\therefore \pm 2i \ln v_l = \int \left[V(r) + \frac{l(l+1)}{r^2} \right] dr + \text{const}$$

If $V(r) \xrightarrow{r \rightarrow \infty} \frac{\text{const}}{r^{1+S}} \quad (S \gg 0)$

$$\begin{aligned} \pm 2i \ln v_l &\xrightarrow{r \rightarrow \infty} \text{const} \\ &\xrightarrow{\text{Coulomb potential}} \ln r \quad (S = 0) \end{aligned}$$

If $S > 0$

$$\chi_l(r) \rightarrow A \sin(kr + \delta) \text{ and } B \cos(kr + \delta)$$

Thm.

For $S > 0$, $\exists a > 0$, such that for $r > a$,

$$V_{\text{eff}} = 0$$

Exact Solution for $r > a$

$$\frac{d^2 R_l}{dr^2} + \frac{2}{r} \frac{dR_l}{dr} + \left(k^2 - \frac{l(l+1)}{r^2} \right) R_l = 0$$

$$\begin{aligned} R_l &= A_l j_l(kr) + B_l n_l(kr) \\ \rightarrow &= A_l (j_l(kr) \cos \delta_l - n_l(kr) \sin \delta_l) \end{aligned}$$

$r \rightarrow \infty$

$$R_l \rightarrow A_l \left[\frac{\cos\left(kr - \frac{l+1}{2}\pi\right)}{kr} \cos \delta_l - \frac{\sin\left(kr - \frac{l+1}{2}\pi\right)}{kr} \sin \delta_l \right]$$

$$= \frac{A_l}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$$

δ_l : phase shift

Born Approximation

Consider $(H - E)\psi(\vec{r}) = \chi(\vec{r})$

a) $H = H(r)$ Hermitian Operator

b) Assume known $(H(r) - E)\phi_E(\vec{r}) = 0$

$\{\phi_E(\vec{r})\}$ is complete set

Let $\psi(\vec{r}) = \int dE' A(E') \phi_{E'}(\vec{r})$

then

$$\begin{aligned} \chi(r) &= (H - E)\psi(\vec{r}) \\ &= (H - E) \int dE' A(E') \phi_{E'}(\vec{r}) \\ &= \int dE' A(E') (E' - E) \phi_{E'}(\vec{r}) \end{aligned}$$

Multiply $\int d^3r \phi_{E''}^*(\vec{r})$

$$\int d^3r \phi_{E''}^*(\vec{r}) = \int dE' A(E')(E' - E) \int d^3r \phi_{E'}(\vec{r}) \phi_{E''}^*(\vec{r})$$

$$= A(E'')(E'' - E) \int d^3r \phi_{E''}(\vec{r}) \phi_{E''}^*(\vec{r})$$

$\swarrow \delta(E' - E'')$

$$\therefore A(E') = \frac{1}{E' - E} \int d^3r' \phi_{E'}^*(\vec{r}') \cdot \chi(\vec{r}')$$

$$\psi(\vec{r}) = \int dE' \phi_{E'}(\vec{r}) \cdot \frac{1}{E' - E} \int d^3r' \phi_{E'}^*(\vec{r}') \chi(\vec{r}')$$

$$\therefore = \int d^3r' \left[\int dE' \frac{\phi_{E'}(\vec{r}) \phi_{E'}^*(\vec{r}')}{E' - E} \right] \chi(\vec{r}')$$

Let $G_E^{(\pm)}(\vec{r}, \vec{r}') = \lim_{\varepsilon \rightarrow 0} \int dE' \frac{\phi_{E'}(\vec{r}) \phi_{E'}^*(\vec{r}')}{E' - (E \pm i\varepsilon)}$

then $\psi(\vec{r}) = \int d^3r' G_E^{(\pm)}(\vec{r}, \vec{r}') \chi(\vec{r}')$

$$(H - E)G_E^{(\pm)}(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}')$$

$$(H - E)\phi = 0$$

$$\therefore \psi(\vec{r}) = \phi + \int d^3r' G_E^{(\pm)}(\vec{r}, \vec{r}') \chi(\vec{r}')$$

where $(H - E)\phi = 0$

$$(H - E)G_E^{(\pm)}(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}')$$

For Schrödinger equation

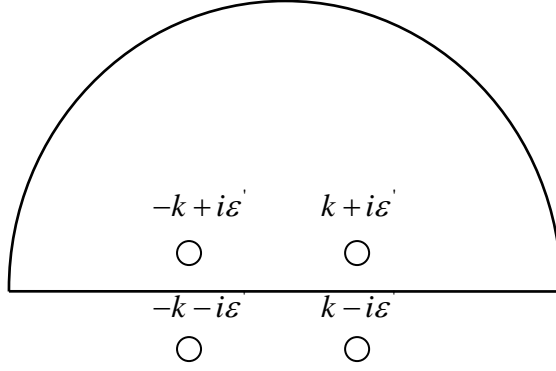
$$\left(-\frac{\hbar^2}{2\mu} \nabla^2 - E \right) \psi(\vec{r}) = -V(\vec{r})\psi(\vec{r})$$

$$\left(-\frac{\hbar^2}{2\mu} \nabla^2 - E \right) \phi(\vec{r}) = 0 \quad \therefore \phi(\vec{r}) = A e^{i\vec{k} \cdot \vec{r}} + B e^{-i\vec{k} \cdot \vec{r}}$$

$$\phi_E(\vec{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{i\vec{k} \cdot \vec{r}}$$

$$= \phi_k(\vec{r})$$

$$\begin{aligned}
G_E^{(\pm)}(\vec{r}, \vec{r}') &= \lim_{\varepsilon \rightarrow 0^+} \int dE' \frac{\phi_{E'}(\vec{r}) \phi_{E'}^*(\vec{r}')}{E' - (E \pm i\varepsilon)} \\
&= \lim_{\varepsilon \rightarrow 0^+} \int d^3k' \cdot \frac{1}{(2\pi)^3} \frac{\exp[i\vec{k}' \cdot (\vec{r} - \vec{r}')] }{\frac{\hbar^2 k'^2}{2\mu} - \left(\frac{\hbar^2 k'^2}{2\mu} \pm i\varepsilon \right)} \\
&= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{(2\pi)^3} \cdot \frac{2\mu}{\hbar^2} \cdot \int \frac{d^3k' e^{i\vec{k}' \cdot (\vec{r} - \vec{r}')}}{k'^2 - (k \pm i\varepsilon)^2} \\
&= \lim_{\varepsilon \rightarrow 0^+} \frac{1}{(2\pi)^3} \cdot \frac{2\mu}{\hbar^2} \cdot 2\pi \cdot \int_0^\infty \frac{k'^2 dk'}{k'^2 - (k \pm i\varepsilon)^2} \int_{-1}^1 d\mu e^{ik|\vec{r}-\vec{r}'|\mu} \quad (\mu = \cos \theta) \\
&= \frac{1}{(2\pi)^2} \cdot \frac{2\mu}{\hbar^2} \cdot \frac{1}{i|\vec{r} - \vec{r}'|} \lim_{\varepsilon \rightarrow 0^+} \int_0^\infty k' dk' \frac{e^{ik|\vec{r}-\vec{r}'|} - e^{-ik|\vec{r}-\vec{r}'|}}{k'^2 - (k \pm i\varepsilon)^2}
\end{aligned}$$



$$= \frac{1}{(2\pi)^2} \cdot \frac{2\mu}{\hbar^2} \cdot \frac{1}{i|\vec{r} - \vec{r}'|} \lim_{\varepsilon \rightarrow 0^+} \int_{-\infty}^{\infty} dk' \frac{k' e^{ik|\vec{r}-\vec{r}'|}}{[k' - (k \pm i\varepsilon)][k' + (k \pm i\varepsilon)]}$$

$$\oint_c = 2\pi i \times \text{Residue at } R' = R + i\varepsilon'$$

$$\begin{aligned}
&\left[\Rightarrow \frac{k + i\varepsilon'}{2(k + i\varepsilon')} e^{i(k+i\varepsilon)|\vec{r}-\vec{r}'|} \right] \\
&= \pi i e^{i(k+i\varepsilon)|\vec{r}-\vec{r}'|}
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{(2\pi)^2} \cdot \frac{2\mu}{\hbar^2} \cdot \frac{1}{i|\vec{r} - \vec{r}'|} \pi i e^{\pm ik|\vec{r}-\vec{r}'|} \\
&= \frac{1}{4\pi} \cdot \frac{2\mu}{\hbar^2} \cdot \frac{e^{\pm ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|}
\end{aligned}$$

$$\begin{aligned}
G_E(\vec{r}, \vec{r}') &= \alpha G_E^{(+)} + \beta G_E^{(-)} \\
&= \frac{1}{4\pi} \cdot \frac{2\mu}{\hbar^2} \cdot \frac{\alpha e^{ik|\vec{r}-\vec{r}'|} + \beta e^{-ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \quad (\alpha + \beta = 1) \\
&= Ae^{i\vec{k}\cdot\vec{r}} + Be^{-i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \cdot \frac{2\mu}{\hbar^2} \int \frac{\alpha e^{ik|\vec{r}-\vec{r}'|} + \beta e^{-ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi(\vec{r}') d^3r' \\
&\quad \begin{array}{c} \longrightarrow \quad \longleftarrow \\ \quad \quad \quad \begin{array}{c} \longleftarrow \uparrow \quad \longrightarrow \\ \quad \quad \quad \longleftarrow \downarrow \end{array} \end{array}
\end{aligned}$$

Boundary condition

$$B = 0, \beta = 0 \quad (\alpha = 1)$$

$$\therefore \psi(\vec{r}) = Ae^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \cdot \frac{2\mu}{\hbar^2} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi(\vec{r}') d^3r'$$

$$\frac{1}{|\vec{r}-\vec{r}'|} \rightarrow \frac{1}{r}$$

$$\begin{aligned}
|\vec{r}-\vec{r}'| &= r \left(1 - \frac{2\hat{r}\cdot\vec{r}'}{r} + \dots \right)^{\frac{1}{2}} \\
&= r - \hat{r}\cdot\vec{r}'
\end{aligned}$$

$$\therefore \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} = \frac{1}{r} e^{ikr} e^{-i\vec{k}\cdot\vec{r}'} \quad k\hat{r} = \vec{k}_r$$

$$r \rightarrow \infty \Rightarrow Ae^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \frac{2\mu}{\hbar^2} \frac{e^{ikr}}{r} \int e^{i\vec{k}_r\cdot\vec{r}'} V(\vec{r}') \psi(\vec{r}') d^3r'$$

$$f(\vec{k}, \vec{k}_r) = -\frac{1}{4\pi} \frac{2\mu}{\hbar^2} \int e^{-i\vec{k}_r\cdot\vec{r}'} V(\vec{r}') \cdot \frac{\psi(\vec{r}')}{A} d^3r'$$

So far f is exact

$$\psi(\vec{r}) = Ae^{i\vec{k}\cdot\vec{r}}$$

$$f_{\text{1st Born approx}}(\vec{k}, \vec{k}_r) = -\frac{1}{4\pi} \frac{2\mu}{\hbar^2} \int d^{i(\vec{k}-\vec{k}_r)\cdot\vec{r}'} V(\vec{r}') d^3r'$$

Summary

$$\psi(\vec{r}) = A \left[\overset{\psi_{\text{inc}}}{e^{i\vec{k}\cdot\vec{r}}} - \frac{1}{4\pi} \frac{2\mu}{\hbar^2} \int \overset{\psi_{\text{scatt}}}{\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}} V(\vec{r}') e^{i\vec{k}\cdot\vec{r}'} d^3r' \right]$$

1st Born Approx.

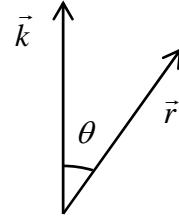
$$= A \left[e^{i\vec{k}\cdot\vec{r}} - \frac{e^{ikr}}{r} \frac{1}{4\pi} \cdot \frac{2\mu}{\hbar^2} \int e^{-i\vec{k}_r\cdot\vec{r}'} V(\vec{r}') e^{i\vec{k}\cdot\vec{r}'} d^3r' \right]$$

Validity for Born Approximation

$$|\psi_{\text{in}}(\vec{r})| \gg |\psi'_{\text{scatt}}| \quad \text{necessary condition}$$

$$\rightarrow |A|^2 \gg |A|^2 \left| -\frac{1}{4\pi} \frac{2\mu}{\hbar^2} \int \frac{e^{-i\vec{k}_r\cdot\vec{r}'}}{r'} V(\vec{r}') e^{i\vec{k}\cdot\vec{r}'} d^3r' \right|^2$$

$$\Rightarrow 1 \gg \left| -\frac{1}{4\pi} \cdot \frac{2\mu}{\hbar^2} \cdot \frac{4\pi}{K} \int_0^\infty dr' \cdot \sin Kr' \cdot V(\vec{r}') \right| \quad \vec{K} = \vec{k} - \vec{k}_r$$



Born Approximation is useful

when

- (a) Velocity of incident particle is large
- (b) weak int.