Lect 28 Formal theory of Scattering

§ Time-dependent method

$$i\hbar \frac{\partial}{\partial t} \Psi(t) = (H_0 + V)\Psi(t), \quad \text{where } H_0 = -\frac{i\hbar \nabla^2}{2m}, \quad V : \text{short ranged}$$

at $t \to -\infty$, $\Psi(t)$ should be a wave packet with well-defined momentum as

$$\phi_0(r,t) = \int C(p; P_0 \Delta P_0) \frac{1}{(2\pi\hbar)^{3/2}} e^{i(pr - E(p)t)/\hbar} d^3\vec{p}$$

$C(p; P_0 \Delta P_0)$ is a sharp distribution around P_0 with the width ΔP_0.

If $\Delta P_0 \to 0$, then $C(p; P_0 \Delta P_0) \longrightarrow \delta(\vec{p} - \vec{P}_0)$. $\phi_0(r,t)$ satisfies

$$i\hbar \frac{\partial}{\partial t} \phi_0(r,t) = H_0 \phi(r,t).$$

Let us suppose at $t \leq T$, (T is a certain negative time in the distant past).

$$\boxed{\Psi(t) = \phi_0(t), \text{ at } t \leq T.}$$

Now take T as the initial time, and $\Psi(T) = \phi_0(T)$ as the initial condition

$$\Psi(t) = e^{-iH(t-T)/\hbar} \phi_0(T) = e^{-iHt} \underbrace{e^{iHT/\hbar} \phi_0(T)} = e^{-iHt} \Psi(0)$$

define

$$\Psi(0) = \lim_{T \to -\infty} e^{iHT/\hbar} \phi_0(T)$$

$$= \lim_{T \to -\infty} e^{iHT/\hbar} e^{-iH_0T/\hbar} \underbrace{e^{iH_0T/\hbar} \phi_0(T)}_{\phi_0(0)}$$

$$= \lim_{T \to \infty} \mathcal{U}(0, T)\, \phi_0(0)$$

$t = 0$ is the instant that particle moves to the centeral region of $V(r)$

$$\mathcal{U}(0,T) = e^{iHT/\hbar}\, e^{-iH_0T/\hbar}$$, thus $\psi(0)$ is different from the free state.

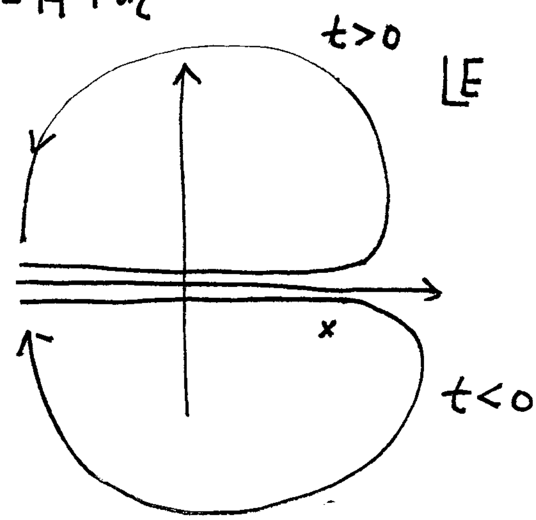
$$\frac{\partial}{\partial T}\mathcal{U}(0,T) = \frac{i}{\hbar} e^{iHT/\hbar}(H-H_0)\, e^{-iH_0T/\hbar} = \frac{i}{\hbar} e^{iHT/\hbar}\, V\, e^{-iH_0T/\hbar}$$

$$\mathcal{U}(0,T) = 1 + \frac{1}{i\hbar}\int_T^0 dt\; e^{iHt/\hbar}\, V\, e^{-iH_0t/\hbar}$$

$$T \to -\infty \Rightarrow \mathcal{U}(0,-\infty) = 1 + \frac{1}{i\hbar}\int_{-\infty}^0 dt\; e^{iHt/\hbar}\, V\, e^{-iH_0t/\hbar}$$

use the identity

$$\Theta(-t)\, e^{iHt/\hbar} = \frac{i}{2\pi}\lim_{\eta\to 0^+}\int_{-\infty}^{+\infty} dE\; \frac{e^{iEt/\hbar}}{E-H+i\eta}$$



$$\Rightarrow \mathcal{U}(0,-\infty) = 1 + \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dE \int_{-\infty}^{+\infty} dt\; \frac{i}{2\pi}\, \frac{e^{iEt/\hbar}}{E-H+i\eta} \cdot V\, e^{-iH_0t/\hbar}$$

perform the integral of $\int_{-\infty}^{+\infty} dt\; e^{iEt/\hbar}\, e^{-iH_0t/\hbar}$

$$= 2\pi\,\delta\!\left(\frac{E-H_0}{\hbar}\right) = 2\pi\hbar\,\delta(E-H_0)$$

$$\boxed{\mathcal{U}(0,-\infty) = 1 + \int_{-\infty}^{+\infty} dE\; \frac{1}{E-H+i\eta}\, V\, \delta(E-H_0)}$$

define $\Omega_+(E) = 1 + \frac{1}{E-H+i\eta} V$, we have

$$\psi(0) = \mathcal{U}(0,-\infty)\,\phi(0) = \int dp\; C(p;p_0\Delta p)\; \mathcal{U}(0,-\infty)\,|p\rangle$$ ← plane wave

define $\psi_p^+ = \mathcal{U}(0,-\infty)|p\rangle$, then $\psi(0) = \int dp\; C(p;p_0\Delta p)\,\psi_p^+$

$$\boxed{\begin{aligned}\psi_p^{+} &= \left(1+\int_{-\infty}^{+\infty} dE \; \frac{1}{E-H+i\eta}\, V\, \delta(E-H_0)\right)|p\rangle \\ &= \left(1 + \frac{1}{E(p)-H+i\eta} V\right)|p\rangle = \Omega_{+}(E(p))\,|p\rangle\end{aligned}}$$

$$E(p) = \hbar^2 p^2/2m$$

Comments: ① ψ_p^{+} is the eigenstate of H

Proof:
$$H\psi_p^{+} = \left[H + \frac{1}{E-H+i\eta} H V\right]|p\rangle$$

$$= \left(H_0 + \cancel{V} + \frac{1}{E-H+i\eta}(\cancel{-E+H})V + \frac{1}{E-H+i\eta} V E\right)|p\rangle$$

$$= H_0 + \frac{1}{E-H+i\eta} V H_0 |p\rangle = \Omega_{+}(E)\, H_0 |p\rangle = E_p\, \psi_p^{+} .$$

later, we will show

$$\langle r|\psi_p^{+}\rangle \xrightarrow{r\to\infty} \frac{1}{(2\pi\hbar)^{3/2}}\left(e^{i\vec{p}\cdot\vec{r}/\hbar} + \frac{e^{ikr}}{r} f(\theta,\varphi)\right)_{k=p/\hbar}$$

outgoing eigenstate, which is just the boundary condition that is used for time-independent method.

② Similarly we can formally definite the state $\psi'(0)$ from the future by setting $T\to+\infty$. Then

$$\psi'(0) = \lim_{T\to\infty} \mathcal{U}(0,T)\;\phi_0(0)$$

$$\mathcal{U}(0,+\infty) = 1 + \frac{1}{i\hbar}\int_0^{\infty} dt\; e^{iHt/\hbar}\, V e^{-iH_0 t/\hbar} \quad \text{(exercise).}$$

$$= 1 + \int_{-\infty}^{+\infty} dE\; \frac{1}{E-H-i\eta}\, V\, \delta(E-H_0)$$

$$\int dp\, |\psi_p^+\rangle\langle\psi_p^+| = \int dp\, |\psi_p^-\rangle\langle\psi_p^-| \neq 1$$

$$|\psi_p^+\rangle = U(0,-\infty)|p\rangle, \quad |\psi_p^-\rangle = U(0,+\infty)|p\rangle$$

$$\Rightarrow U(0,-\infty)\int dp\,|p\rangle\langle p|\, U(-\infty,0) = U(0,+\infty)\int dp\, |p\rangle\langle p|\, U(+\infty,0)$$

$$\Rightarrow \boxed{U(0,-\infty)\,U(-\infty,0) = U(0,+\infty)\,U(+\infty,0) \neq 1.}$$

Derive Lipman-Schwinger Eq

$$\Omega_+ = 1 + \frac{1}{E-H+i\eta} V$$

$$\frac{1}{E-H+i\eta} = \frac{1}{E-H_0+i\eta} + \frac{1}{E-H_0+i\eta} V \frac{1}{E-H_0+i\eta} + \cdots$$

$$= \frac{1}{E-H_0+i\eta} + \frac{1}{E-H_0+i\eta} V \frac{1}{E-H+i\eta}$$

$$\Omega_+ = 1 + \frac{1}{E-H_0+i\eta} V\left[1 + \frac{1}{E-H+i\eta} V\right] = \boxed{\Omega_+ = 1 + \frac{1}{E-H_0+i\eta} V\Omega_+}$$

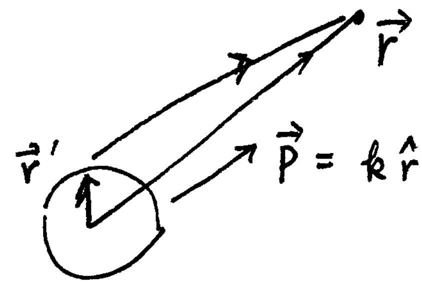
$$\boxed{|\psi_{p_0}^+\rangle = |p_0\rangle + \frac{1}{E-H_0+i\eta} V\, |\psi_{p_0}^+\rangle} \xrightarrow{\text{coordinate Rep}}$$

$$\psi_{p_0}^+(r) = \frac{1}{(2\pi\hbar)^{3/2}} e^{ip_0 r/\hbar} + \int \langle r| \frac{1}{E-H_0+i\eta} |r'\rangle\, V(r')\, \psi_{p_0}^+(r')\, dr'$$

$$= \frac{1}{(2\pi\hbar)^{3/2}} e^{ip_0 r/\hbar} - \frac{m}{2\pi\hbar^2}\int \frac{e^{ik_0|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(r')\, \psi_{p_0}^+(r')\, dr'$$

$$|\vec{r}-\vec{r}'| = r - \vec{r}'\cdot\hat{r}$$

$$e^{ik_0|\vec r-\vec r'|} = e^{ik_0 r}\, e^{ik\hat r\cdot\vec r'}$$



$$\Rightarrow \psi^+_{p_0}(\vec r) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec p_0\cdot\vec r/\hbar} - \frac{m}{2\pi\hbar^2}\frac{e^{ik_0 r}}{r}$$

$$(2\pi\hbar)^{3/2}\int \frac{e^{i\vec p\cdot\vec r'}}{(2\pi\hbar)^{3/2}} V(r')\,\psi^+_{p_0}(r')\,d\vec r'$$

$$= \frac{1}{(2\pi\hbar)^{3/2}}\left[e^{i\vec p_0\cdot\vec r/\hbar} - \frac{m}{2\pi\hbar^2}\cdot 8\pi^3\hbar^3\,\frac{e^{ik_0 r}}{r}\,\langle p|V|\psi^+_{p_0}(r)\rangle\right]$$

$$\Rightarrow \boxed{f(\theta,\varphi) = -4\pi^2\hbar m\,\langle p|V|\psi^+_{p_0}\rangle}$$

, where $\vec p$ along the direction of $\vec r$.

$$\langle p|V|\psi^+_{p_0}\rangle = \langle p|V\ \cancel{+V}\frac{1}{E-H+i\eta}\,V\,|p_0\rangle$$

$$= \langle p|\left(1+V\frac{1}{E-H+i\eta}\right)V|p_0\rangle$$

$$= \left\langle \left(1+\frac{1}{E-H-i\eta}V\right)p\right|V|p_0\rangle = \langle\psi^-_p|V|p_0\rangle$$

$$\boxed{f(\theta,\varphi) = -4\pi^2\hbar m\,\langle\psi^{(-)}_p|V|p_0\rangle}$$

check unit

$|p\rangle$ normalized to $\delta^{(3)}(p-p)$

$\langle\psi_p|V|p_0\rangle \to p^{-3}\frac{p^2}{2m} = \frac{1}{mp}$

$[f] = \hbar/p = [1/k] =$ length

§ Cross-section & optical theorem

we write $\psi(t) = \phi_0(t) + W(t)$; $\phi_0(t)$ is the incident wavepacket and $W(t)$ is the scattering wave. $\phi_0(t) \longrightarrow e^{-iE_0 t/\hbar} |\vec{p}_0\rangle$.

The scattering rate to the state $|\vec{p}\rangle$

$$\omega_p \, d^3\vec{p} = \frac{\partial}{\partial t} |\langle p | W(t)\rangle|^2 \, d^3\vec{p} ,$$

$$\begin{cases} \sigma(\theta, \varphi)\, d\Omega = \dfrac{(2\pi\hbar)^3}{v_0} d\Omega \displaystyle\int_0^{+\infty} \omega_p \, p^2 dp \\ v_0 = \dfrac{p_0}{m} \end{cases}$$

$|p\rangle$ normalization according to $\delta^{(3)}(p-p')$

check dimension

ω_p - dimension $[p]^{-6}[T]^{-1}$

$$\rightarrow [\sigma] = \frac{[\hbar]^3 [p]^{-3} [T]^{-1}}{[L][T]^{-1}} = [L]^2$$

$$\frac{\partial}{\partial t} |\langle p | W(t)\rangle|^2 = \langle W(t)|p\rangle\langle p|\dot{W}(t)\rangle + c.c.$$

$$\frac{d}{dt} W(t) = \frac{1}{i\hbar}\left[H\psi(t) - H_0 \phi_0(t)\right]$$

$$= \frac{1}{i\hbar}\left[H_0\psi(t) + V\psi(t) - H_0\phi_0(t)\right]$$

$$= \frac{1}{i\hbar}\left[V\psi(t) + H_0 W(t)\right]$$

$$\frac{\partial}{\partial t} |\langle p | W(t)\rangle|^2 = \frac{1}{i\hbar}\left\{\langle W(t)|p\rangle\langle p|V|\psi(t)\rangle + E_p \langle W(t)|p\rangle\langle p|W(t)\rangle\right\} + c.c.$$

$$= \frac{1}{i\hbar} \langle W(t)|p\rangle\langle p|V|\psi(t)\rangle + c.c.$$

$$\sigma_T = \int \sigma(\theta,\varphi)\,d\Omega = \frac{\partial}{\partial t}\int d^3p \,\langle w(t)|p\rangle\langle p|w(t)\rangle \frac{(2\pi\hbar)^3}{v_0}$$

$$= \left[\frac{1}{i\hbar}\int d^3p \,\langle W(t)|p\rangle\langle p|V|\psi(t)\rangle + c.c\right]\frac{(2\pi\hbar)^3}{v_0}$$

$$= \left[\frac{1}{i\hbar}\langle W(t)|V|\psi(t)\rangle + c.c\right]\frac{(2\pi\hbar)^3}{v_0}$$

$$|W(t)\rangle = |\psi(t)\rangle - |\phi_0(t)\rangle$$

$$\Rightarrow \sigma_T = \left\{\frac{-1}{i\hbar}\langle\phi_0(t)|V|\psi(t)\rangle + c.c.\right\}(2\pi\hbar)^3/v_0$$

set $\Delta p \to 0$

$$\sigma_T = -\frac{2}{\hbar}\,\mathrm{Im}\langle\vec{p}_0|V|\psi^+_{p_0}\rangle\frac{(2\pi\hbar)^3}{v_0} \leftarrow v_0 = \frac{\hbar k_0}{m}$$

$$\boxed{\sigma_T = \frac{4\pi}{k_0}\,\mathrm{Im}\,f(p_0,p_0)}$$

§. Scattering matrix

$$S = \mathcal{U}(+\infty, -\infty)$$

§ interaction picture

$$H = H_0 + V,$$

state vector $|\psi_I(t)\rangle = e^{iH_0t}\,|\psi_S(t)\rangle$

operator $O_I(t) = e^{iH_0t}\, O_S\, e^{-iH_0t}$

time evolution operator

$$|\psi_I(t)\rangle = e^{iH_0t}\,|\psi_S(t)\rangle = e^{iH_0t}\, e^{-iH(t-t_0)}\,|\psi_S(t_0)\rangle$$

$$= e^{iH_0t}\, e^{-iH(t-t_0)}\, e^{-iH_0t_0}\,|\psi_I(t_0)\rangle$$

$$\Rightarrow \boxed{\begin{array}{l} \mathcal{U}_I(t,t_0) = e^{iH_0t}\, e^{-iH(t-t_0)}\, e^{-iH_0t} \\ \mathcal{U}(t,t) = 1; \quad \mathcal{U}(t,t_1)\,\mathcal{U}(t_1,t_0) = \mathcal{U}(t,t_0); \quad \mathcal{U}^\dagger(t,t_0) = \mathcal{U}(t_0,t) = \mathcal{U}^{-1}(t,t_0) \\ i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0) = V_I(t)\,\mathcal{U}(t,t_0); \quad -i\hbar\frac{\partial}{\partial t_0}\mathcal{U}(t,t_0) = \mathcal{U}(t,t_0)\,V_I(t_0) \end{array}}$$

§ Scattering matrix

$$S = \mathcal{U}(\infty,-\infty) = \lim_{t\to+\infty}\lim_{t_0\to-\infty}\mathcal{U}(t,t_0)$$

$$= \mathcal{U}(\infty,0)\;\mathcal{U}(0,-\infty)$$

← wave operator defined in last lecture

$$\Psi_S(t=0) = \mathcal{U}(0,-\infty)\,\phi_0(0) = \lim_{T\to-\infty} e^{iHT}\,\phi_0(T) = \lim_{T\to-\infty} e^{iHT}\, e^{-iH_0T}\,\phi_0(0)$$

$\boxed{\text{In the interaction picture}}$

$$\Psi_I(t) = \mathcal{U}_I(t, 0) \Psi_I(0)$$

$$= \mathcal{U}_I(t, 0) \Psi_s(0) = \mathcal{U}_I(t, 0)\, \mathcal{U}(0, -\infty) \quad \phi_0(0) = \mathcal{U}_I(t, 0)\, \mathcal{U}_I(0, -\infty) \phi_0(0)$$

$$= \mathcal{U}_I(t, -\infty)\, \phi_0(0)$$

$$\boxed{\Psi_I(+\infty) = \mathcal{U}(+\infty, -\infty)\ \phi_0(0)}$$

$\mathcal{U}(+\infty, -\infty)$ Contains all the information of the Scattering problem.

$\mathcal{U}(+\infty, -\infty) = S$ satisfies

$t \to -t$

① $\boxed{\text{time reversal}}$ $$T\, S = T\, \mathcal{U}(+\infty, 0)\, \mathcal{U}(0, -\infty) = \mathcal{U}(-\infty, 0)\, \mathcal{U}(0, +\infty)\, T$$

$$\Rightarrow \boxed{T\, S\, T^{-1} = S^\dagger}$$

② $$H_0 S = H_0\, \mathcal{U}(+\infty, 0)\, \mathcal{U}(0, -\infty) = \mathcal{U}(+\infty, 0)\, H\, \mathcal{U}(0, -\infty)$$

$$= \mathcal{U}(+\infty, 0)\mathcal{U}(0, -\infty)\, H_0 = S\, H_0$$

③ Unitarity

Completeness for the scattering states

$$S^\dagger S = \mathcal{U}(-\infty, 0)\, \underline{\mathcal{U}(0\ \infty), \mathcal{U}(\infty, 0)}\ \mathcal{U}(0, -\infty)$$

$$= \mathcal{U}(-\infty, 0)\ \underline{\mathcal{U}(0, -\infty)\, \mathcal{U}(\infty, 0)}\ \mathcal{U}(0, -\infty)$$

$$= I \cdot I = I$$

Similarly $S S^\dagger = I$

③ S-matrix and scattering amplitude.

$$\langle p'|\, S \,|p\rangle = \langle p'|\, \mathcal{U}(+\infty,0)\, \mathcal{U}(0,-\infty)|p\rangle = \langle \psi^{-}_{p'}|\psi^{+}_{p}\rangle$$

$$|\psi^{+}_{p}\rangle - |\psi^{-}_{p}\rangle = \lim_{\eta\to 0^{+}} \left(\frac{1}{E(p)-H+i\eta} - \frac{1}{E(p)-H-i\eta} \right) V\, |p\rangle$$

$$= -2\pi i\, \delta(E(p)-H)\, V\, |p\rangle$$

$$\Rightarrow \langle p'|S|p\rangle = \langle \psi^{+}_{p'}|\psi^{+}_{p}\rangle - 2\pi i \,\langle p'|\, V\, \delta(E(p')-H)\, |\psi^{+}_{p}\rangle$$

$$= \delta(p'-p) - 2\pi i \langle p'|V|\psi^{+}_{p}\rangle\, \delta(E(p')-E(p))$$

$$= \delta(p'-p) - 2\pi i \langle \psi^{(-)}_{p'}|V|p\rangle\, \delta(E(p)-E(p'))$$

or $$\langle p'|\, S-1\, |p\rangle = -2\pi i \langle p'|\, V|\, \psi^{(+)}_{p}\rangle\, \delta(E(p')-E(p))$$

$$= -2\pi i \langle \psi^{(-)}_{p}|V|p\rangle\, \delta(E(p)-E(p'))$$

$$\Rightarrow \boxed{\begin{aligned} &\langle p|(S-1)|p_0\rangle = \frac{i}{2\pi\hbar m}\, f(p,p_0)\; \delta(E(p)-E(p_0)) \\ &\text{where } f(p,p_0) = -4\pi^2\hbar m \langle p|\, V\,|\psi^{(+)}_{p_0}\rangle \end{aligned}}$$

check unit $[\text{left}] = \delta^3(p-p_0) \sim [p]^{-3}$

$[\text{right}] = \frac{1}{\hbar m}\frac{1}{k}\cdot\frac{1}{E} = \frac{1}{pm}\frac{m}{p^2} = [p]$

④ ~~Reciprocal relation~~

$$\cancel{\langle p'|S|p\rangle} = \cancel{\langle p'|\, T^{-1} S^{\dagger}\, T\, |p\rangle} = \cancel{\langle Tp'|\, S^{\dagger}\, |Tp\rangle}$$

$$\cancel{= \langle Tp'|\, S^{\dagger}\, |Tp\rangle}$$

$$\cancel{\langle A|\, O\, |B\rangle}$$

$$\cancel{= \langle A|\, T T^{-1} O\, |B\rangle}$$

$$\cancel{= \langle}$$

★ Reciprocal relation :

T: time reversal

$$\langle A|B\rangle = \langle TA|TB\rangle^* = \langle TB|TA\rangle$$

$$\langle A|\hat{O}|B\rangle = \langle TOB|TA\rangle = \langle (TOT^{-1})TB|TA\rangle$$

$$= \langle TB|(TOT^{-1})^\dagger|TA\rangle$$

$$\Rightarrow \boxed{\langle p'|S|p\rangle} = \langle Tp|(TST^{-1})^\dagger|Tp'\rangle = \langle Tp|(S^\dagger)^\dagger|Tp'\rangle$$

$$\boxed{= \langle Tp|S|Tp'\rangle}$$

← Scattering amplitudes are the same for two processes related by TR.

i.e $f(\vec{p}\,';\vec{p}) = f(T\vec{p};T\vec{p}\,')$