# 7. Response fn's

Schrödinger, Heisenberg & interaction

Quick rehash:

S: $i\hbar \partial_t |\psi^S(t)\rangle = H|\psi^S(t)\rangle$ $\qquad \boxed{|\psi^S(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\psi^S(t=0)\rangle}$

$\langle \psi_1^S(t)|O^S|\psi_2^S(t)\rangle$ = matrix element $O_{12}(t)$

H: here, states are t-indep, but operators depend on t

$$\langle \psi_1^S(t)|O^S|\psi_2^S(t)\rangle = \langle \psi_1^S(t=0)|\underbrace{e^{\frac{i}{\hbar}Ht}O^S e^{-\frac{i}{\hbar}Ht}}_{O^H(t)}\underbrace{|\psi_2^S(t=0)\rangle}_{|\psi_2^H\rangle}$$

so $|\psi^H\rangle \equiv |\psi^S(t=0)\rangle$

& $O^H(t)$ obeys $\frac{d}{dt}O^H(t) = \frac{i}{\hbar}[H, O^H(t)] + [\partial_t O]^H$

$+ \; e^{\frac{i}{\hbar}Ht}\partial_t O^S e^{-\frac{i}{\hbar}Ht}$

Interaction picture.

Generic $H(t) = H_0 + V^S(t)$

Let $\{|\alpha^0\rangle\}$ be a complete set of eigenstates of $H_0$

$$H_0|\alpha^0\rangle = E_{\alpha^0}|\alpha^0\rangle$$

Idea: "Heisenberging" the $H_0$ part only.

Namely: $\mathcal{O}^I(t) = e^{\frac{i}{\hbar}H_0 t}\,\mathcal{O}^S\,e^{-\frac{i}{\hbar}H_0 t}$

$$\partial_t\left\{e^{\frac{i}{\hbar}H_0 t}|\psi^S(t)\rangle\right\} = \left[\frac{i}{\hbar}H_0 + \frac{1}{i\hbar}H(t)\right]e^{\frac{i}{\hbar}H_0 t}|\psi^S(t)\rangle$$

$$\rightarrow \quad |\psi^I(t)\rangle \equiv e^{\frac{i}{\hbar}H_0 t}\,\underline{|\psi^S(t)\rangle}$$

Look at $i\hbar\partial_t|\psi^I(t)\rangle = \left[-H_0 + H(t)\right]e^{\frac{i}{\hbar}H_0 t}|\psi^S(t)\rangle = e^{\frac{i}{\hbar}H_0 t}V^S(t)|\psi^S(t)\rangle$

$$\rightarrow \quad i\hbar\partial_t|\psi^I(t)\rangle = V^I(t)|\psi^I(t)\rangle$$

$$\uparrow \; e^{\frac{i}{\hbar}H_0 t}V^S(t)e^{-\frac{i}{\hbar}H_0 t}$$

$\cdot \quad i\hbar\,\partial_t |\psi^I(t)\rangle = V^I(t)|\psi^I(t)\rangle$

Formal sol$^{\underline{n}}$ $\cdot \; |\psi^I(t)\rangle = U^I(t,t_0)|\psi^I(t_0)\rangle$

Special case of $V^S(t)$ being time-indep $V^S(t) = V^S$

Then $\quad U^I(t,t_0) = e^{\frac{i}{\hbar}H_0 t}\, e^{-\frac{i}{\hbar}H(t-t_0)}\, e^{-\frac{i}{\hbar}H_0 t_0}$

In general

$$i\hbar\,\partial_t U^I(t,t_0)|\psi^I(t_0)\rangle = V^I(t)\,U^I(t,t_0)|\psi^I(t_0)\rangle$$

is satisfied if $\quad i\hbar\,\partial_t U^I(t,t_0) = V^I(t)\,U^I(t,t_0) \quad *$

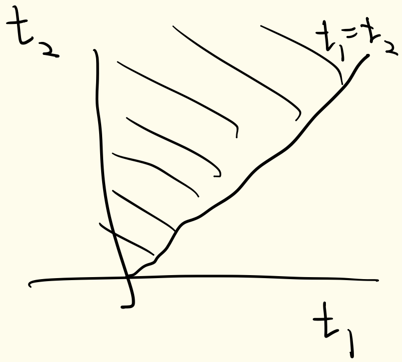
Boundary cond$^{\underline{n}}$ $\quad U^I(t_0,t_0) = \mathbb{1}$

Integrate $*$ from $t_0$ to $t$ : $\quad U^I(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\, V^I(t_1)\,U^I(t_1,t_0)$

Series $\quad U^I(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\, V^I(t_1)\left\{\mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t_1} dt_2\, V^I(t_2)\left\{\mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t_2} dt_3\, V^I(t_3)\left\{\mathbb{1} \cdots\right.\right.\right.$

Series sol$^{\underline{n}}$:

$$U^I(t,t_0) = \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n\, V^I(t_1)\cdots V^I(t_n)$$




$$= \sum_{n=0}^{\infty} \frac{(-i/\hbar)^n}{n!} \int_{t_0}^{t} dt_1 \ldots dt_n\, T_t\left[V^I(t_1)\ldots V^I(t_n)\right]$$

$$= T_t \sum_{n=0}^{\infty} \frac{(-i/\hbar)^n}{n!} \ldots$$

"time ordering" operator

$$T_t\left[A(t_1)B(t_2)\right] = \begin{cases} A(t_1)B(t_2) & t_1 > t_2 \\ B(t_2)A(t_1) & t_1 < t_2 \end{cases}$$

so the sol$^{\underline{n}}$ is

$$\boxed{U^I(t,t_0) = T_t\left\{e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, V^I(t')}\right\}}$$

Reminder: Fermi's Golden Rule

Start at $t = -\infty$ in the "free" system

Apply a pert$^n$ $V(t) = V e^{-i\omega t + \eta t}$ $\quad \eta \to 0^+$

Assume initial state at $t_0$ $\quad |\psi^S(t=t_0)\rangle = |\alpha_i^0\rangle$

Q: what is the proba of finding the system in state $|\alpha_f^0\rangle$ at time $t$?

A: $P_{f \leftarrow i}(t) = |\langle \alpha_f^0 | \psi(t)\rangle|^2$ $\quad$ (assume $f \neq i$)

Calculate: $\langle \alpha_f^0 | \psi^S(t)\rangle = \langle \alpha_f^0$

Step by step: $|\psi^I(t)\rangle = U^I(t, t_0)|\psi^I(t_0)\rangle$,

But $|\psi^I(t_0)\rangle = e^{\frac{i}{\hbar} H_0 t_0} |\psi^S(t_0)\rangle$

Here, $|\psi^I(t_0)\rangle = e^{\frac{i}{\hbar} E_{\alpha_i^0}} |\alpha_i^0\rangle$

So:
$$\langle \alpha_f^0 | \psi^S(t) \rangle = \langle \alpha_f^0 | e^{-\frac{i}{\hbar}H_0 t_0} U^I(t,t_0) e^{\frac{i}{\hbar}H_0 t_0} | \alpha_i^0 \rangle = e^{-\frac{i}{\hbar}\left(E_{\alpha_f^0} - E_{\alpha_i^0}\right)t_0} \langle \alpha_f^0 | U^I(t,t_0) | \alpha_i^0 \rangle$$

Use series exp$^{\underline{n}}$ for $U^I$:
$$\langle \alpha_f^0 | U^I(t,t_0) | \alpha_i^0 \rangle = \underbrace{\langle \alpha_f^0 | \alpha_i^0 \rangle}_{0 \text{ by assumption } f \neq i} - \frac{i}{\hbar}\int_{t_0}^{t} dt' \langle \alpha_f^0 | V^I(t') | \alpha_i^0 \rangle + \underbrace{O(V^2)}_{\text{drop}}$$

$$= -\frac{i}{\hbar}\int_{t_0}^{t} dt' \langle \alpha_f^0 | e^{\frac{i}{\hbar}H_0 t'} \underbrace{V(t')}_{Ve^{-i\omega t' + \eta t'}} e^{-\frac{i}{\hbar}H_0 t'} | \alpha_i^0 \rangle = -\frac{i}{\hbar}\int_{t_0}^{t} dt' \, e^{\frac{i}{\hbar}\left[E_{\alpha_f^0} - E_{\alpha_i^0} - \hbar\omega - i\hbar\eta\right]t'} \times \langle \alpha_f^0 | V | \alpha_i^0 \rangle$$

$$= -\frac{\langle \alpha_f^0 | V | \alpha_i^0 \rangle}{E_{\alpha_f^0} - E_{\alpha_i^0} - \hbar\omega - i\hbar\eta} \, e^{\frac{i}{\hbar}[\;]t'} \Big|_{t_0}^{t} \xrightarrow[t_0 \to -\infty]{} - \frac{\langle \alpha_f^0 | V | \alpha_i^0 \rangle \, e^{\frac{i}{\hbar}[\;]t}}{\left[E_{\alpha_f^0} - E_{\alpha_i^0} - \hbar\omega - i\hbar\eta\right]}$$

So $\langle \alpha_f^0 | \psi^S(t) \rangle = \dfrac{\langle \alpha_f^0 | V | \alpha_i^0 \rangle}{\hbar\omega - (E_{\alpha_f^0} - E_{\alpha_i^0}) + i\hbar\eta} e^{-\frac{i}{\hbar} E_{\alpha_i^0}(t-t_0)} e^{-i\omega t + \eta t} + O(V^2)$

Thus: $P_{f\leftarrow i}(t) = | \text{"} |^2 = \dfrac{|\langle \alpha_f^0 | V | \alpha_i^0 \rangle|^2 e^{2\eta t}}{[\hbar\omega - (E_{\alpha_f^0} - E_{\alpha_i^0})]^2 + \hbar^2\eta^2}$ $\qquad \Delta E = E_f - E_i$

<u>Rate</u> of transition:

$$\frac{d}{dt} P_{f\leftarrow i}(t) = |\langle \alpha_f^0 | V | \alpha_i^0 \rangle|^2 \lim_{\eta\to 0^+} \frac{2\eta}{(\hbar\omega - \Delta E_{fi})^2 + \hbar^2\eta^2}$$

Use $\delta(x) = \lim_{\eta\to 0} \frac{1}{\pi} \frac{\eta}{x^2+\eta^2}$

FGR

$$\longrightarrow \boxed{\frac{d}{dt} P_{f\leftarrow i}(t) = \frac{2\pi}{\hbar} |\langle \alpha_f^0 | V | \alpha_i^0 \rangle|^2 \delta\left(\hbar\omega - (E_{\alpha_f^0} - E_{\alpha_i^0})\right)}$$

# Linear response theory

$$\hat{H}(t) = \hat{H}_0 + F(t)\hat{P}$$

Q: How does P affect expectation values

$$\bar{O}(t) = \langle\psi(t)|\hat{O}|\psi(t)\rangle$$

$$\bar{O}(t) = \langle\psi^I(t)|\hat{O}^I(t)|\psi^I(t)\rangle \qquad U^I(t,t_0) = T_t\, e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, F(t')\hat{P}^I(t')}$$

$$U^I(t,t_0)|\psi^I(t_0)\rangle \qquad = \mathbb{1} - \frac{i}{\hbar}\int \dots + \mathcal{O}(F^2)$$

$$= \langle\psi^I(t_0)|\left[U^I(t,t_0)\right]^\dagger O^I(t)\, U^I(t,t_0)|\psi^I(t_0)\rangle \qquad \text{Let } |\psi^I(t_0)\rangle = |\psi_0\rangle$$

Let $t_0 \to -\infty$

$$= \underbrace{\langle\psi_0|O|\psi_0\rangle}_{\bar{O}_{\psi_0}} - \frac{i}{\hbar}\int_{-\infty}^{t} dt' \langle\psi_0|\left[O^I(t), P^I(t')\right]|\psi_0\rangle F(t') + \mathcal{O}(2)$$

Nomenclature: <u>retarded</u> correl$^n$ f$^{n}$ $\quad C^{\hat{O},\hat{P}}_{ret,\psi}(t-t') = -i\Theta(t-t')\langle\psi|\left[\hat{O}^I(t), P^I(t')\right]|\psi\rangle$

Conclusion: to linear order in the pert$^n$, the observable is

$$\boxed{\bar{O}(t) = \bar{O}_{\psi_0} + \int_{-\infty}^{\infty} dt' \; C^{O,P}_{ret,\psi_0}(t-t')F(t') + O(F^2)}$$

This is known as the Kubo formula.

To an accuracy of 1 in a million, __every__ exp $\leftrightarrow$ th correspondence is made through Kubo.

# Frequency-dependent correl$^{\text{n}}$ f$^{\text{ns}}$

$$C^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(t) = -i\Theta(t)\langle\psi_\alpha|\underbrace{[O^I(t),P^I(0)]}_{e^{iH_0t}O e^{-iH_0t}P - Pe^{iH_0t}Oe^{-iH_0t}}|\psi_\alpha\rangle$$

Introduce $\mathbb{1} = \sum_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ & matrices ~~elements~~ $\langle\psi_\alpha|A|\psi_{\alpha'}\rangle = A_{\alpha\alpha'}$

eigenstates of $H_0$

$$\Rightarrow C^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(t) = -i\Theta(t)\sum_{\alpha'}\left\{O_{\alpha\alpha'}P_{\alpha'\alpha}\,e^{i(E_\alpha-E_{\alpha'})t} - P_{\alpha\alpha'}O_{\alpha'\alpha}\,e^{-i(E_\alpha-E_{\alpha'})t}\right\}$$

Recap:

$$\langle\psi_\alpha|e^{iH_0t}O\,\underset{\mathbb{1}}{}\,e^{-iH_0t}P|\psi_\alpha\rangle = \sum_{\alpha'}\langle\psi_\alpha|e^{iE_\alpha t}O e^{-iE_{\alpha'}t}|\psi_{\alpha'}\rangle\langle\psi_{\alpha'}|P|\psi_\alpha\rangle$$

$\mathbb{1} = \sum_{\alpha'}|\psi_{\alpha'}\rangle\langle\psi_{\alpha'}|$

$$= \sum_{\alpha'} e^{i(E_\alpha-E_{\alpha'})t}\underbrace{\langle\psi_\alpha|O|\psi_{\alpha'}\rangle}_{O_{\alpha\alpha'}}\underbrace{\langle\psi_{\alpha'}|P|\psi_\alpha\rangle}_{P_{\alpha'\alpha}}$$

Introduce FT in time:

$$C^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(\omega) \equiv \int_{-\infty}^{\infty}dt\; C^{\hat{O},\hat{P}}_{ret,\psi_\alpha}(t)\,e^{i\omega t-\eta|t|}$$

$$\mathcal{C}^{O,P}_{ret,\psi_\alpha}(\omega) = \int_{-\infty}^{\infty} dt \left[-i\Theta(t)\right] \sum_{\alpha'} O_{\alpha\alpha'} P_{\alpha'\alpha}\, e^{i\left[E_\alpha - E_{\alpha'} + \omega\right]t - \eta|t|} + 2^{nd} \text{ term}$$

$$= -i \int_{0}^{\infty} dt \sum_{\alpha'} O_{\alpha\alpha'} P_{\alpha'\alpha}\, e^{i\left[E_\alpha - E_{\alpha'} + \omega + i\eta\right]t} + 2^{nd} \text{ term}$$

$$= \sum_{\alpha'} \left\{ \frac{O_{\alpha\alpha'} P_{\alpha'\alpha}}{\omega + E_\alpha - E_{\alpha'} + i\eta} - \frac{P_{\alpha\alpha'} O_{\alpha'\alpha}}{\omega - (E_\alpha - E_{\alpha'}) + i\eta} \right\}$$

Such a repres$^{n}$ for a correl$^{n}$ f$^{n}$ is called a

<u>Lehmann representation</u>

Other types of correl$^{\underline{ns}}$s:

<u>Advanced</u> $f^{\underline{n}}$ $\quad \mathcal{C}^{\hat{O},\hat{P}}_{adv,\psi}(t-t') \equiv i\,\Theta(t'-t)\langle\psi|[\hat{O}^I(t),\hat{P}(t')]|\psi\rangle$

(see notes for its Lehmann repres$^{\underline{n}}$)

<u>Real-time</u> $f^{\underline{n}}$: $\quad \mathcal{C}^{\hat{O},\hat{P}}_{\psi}(t-t') \equiv -i\langle\psi|T_t\{O^I(t)P^I(t')\}|\psi\rangle$