Examples:

(1) $H_0 = \frac{p^2}{2m} + \frac{1}{2} m w_0^2 x^2$.

$V = \frac{1}{2} \varepsilon m w_0^2 x^2$. $\varepsilon \to 0$.

$H = H_0 + V = \frac{p^2}{2m} + \frac{1}{2} m (\sqrt{1+\varepsilon}\, w)^2 x^2$.

$w_{new} = \sqrt{1+\varepsilon}\, w$.

$E_0 = \frac{1}{2}\hbar\sqrt{1+\varepsilon}\, w$.

$E_0^{(0)} = \frac{1}{2}\hbar w$.

$E_0^{(1)} = \langle \varphi_n^{(0)} | V | \varphi_n^{(0)} \rangle = \langle 0 | \frac{1}{2}\varepsilon m w^2 x^2 | 0 \rangle$

$x = \frac{1}{\sqrt{2}}(a^+ + a)\sqrt{\frac{\hbar}{mw}}$. 谐振子模型.

$\therefore E_0^{(1)} = \langle 0 | x^2 | 0 \rangle = \frac{\hbar}{2mw} \langle 0 | (a^+ + a)^2 | 0 \rangle$

$(\frac{1}{2} m \varepsilon w^2)$

$= \frac{\hbar}{2mw} \langle 0 | (a^+)^2 + a^+ a + a a^+ + a^2 | 0 \rangle$

$\langle 0 | (a^+)^2 | 0 \rangle = 0$. $\langle 0 | a^+ a | 0 \rangle = 0$

$\langle 0 | a^2 | 0 \rangle = 0$. $\langle 0 | a a^+ | 0 \rangle = 1$

$E_0^{(1)} = \frac{1}{2} m \varepsilon w^2 \cdot \frac{\hbar}{2mw} \times 1 = \frac{\varepsilon \hbar w}{4}$

$E_0^{(2)} = \sum_{n \neq 0} \frac{|\langle n | V | 0 \rangle|^2}{-E_n^{(0)} + E_0^{(0)}}$

$\langle n | (a^+ + a)^2 | 0 \rangle = \langle n | (a^+)^2 + a^2 + a^+ a + a a^+ | 0 \rangle$

$= \langle n | (a^+)^2 + a a^+ | 0 \rangle$

$\langle n | a a^+ | 0 \rangle = 0$ for $n \neq 0$.

$\langle n | (a^+)^2 | 0 \rangle = \langle n | a^+ | 1 \rangle = \sqrt{2} \langle n | 2 \rangle$. $a^+ | n \rangle = \sqrt{n+1}\, | n+1 \rangle$.

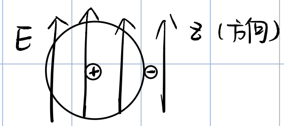
$\therefore E_0^{(2)} = \sum_{n \neq 0} \frac{|\langle n | V | 0 \rangle|^2}{E_0^{(0)} - E_n^{(0)}} = \frac{|\langle 2 | V | 0 \rangle|^2}{E_0^{(0)} - E_2^{(0)}} = \frac{|\frac{1}{2}\varepsilon m w^2 \cdot \frac{\hbar}{2mw} \cdot \sqrt{2}|^2}{[\frac{1}{2} - (2 + \frac{1}{2})]\hbar w} = -\frac{\varepsilon^2 \hbar w}{16}$.

$E_0 = \frac{1}{2}\hbar w + \frac{\varepsilon \hbar w}{4} - \frac{\varepsilon^2}{16}\hbar w = \frac{1}{2}\hbar w (1 + \frac{1}{2}\varepsilon - \frac{1}{8}\varepsilon^2 + \cdots)$

$E_0 = \frac{1}{2}\hbar\sqrt{1+\varepsilon}\, w = \frac{1}{2}\hbar w (1 + \frac{1}{2}\varepsilon - \frac{1}{8}\varepsilon^2 + \cdots)$ 泰勒展开.

(2) Linear Stark Effect.

$V = -ez|E|$.



1s, 2s, 2p, 3s, 3p, 3d.

$E_n = -\frac{E_0}{n^2}$.

2s: $n=2$. $l=0$. $m=0$

2p: $n=2$. $l=1$. $m=-1.0.1$.

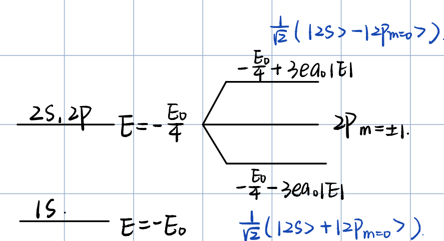
$$V = \begin{array}{c} \begin{array}{cccc} 2s & 2p_{m=0} & 2p_{m=1} & 2p_{m=-1} \end{array} \\ \left(\begin{array}{cccc} \; & \; & \; & \; \\ \; & \; & \; & \; \end{array} \right) \end{array}$$

$\langle 2s|V|2s\rangle = 0$. V是沿z方向的. 2s轨道是球. 平均值是0.

$\langle 2s|V|2p_{m=0}\rangle = 3ea_0|E|$

$\langle 2s|V|2p_{m=\pm1}\rangle = 0$ 　　对径.

$$V = \begin{array}{c} \begin{array}{cccc} |200\rangle & |210\rangle & |211\rangle & |21-1\rangle \end{array} \\ \left(\begin{array}{cc|cc} 0 & 3ea_0|E| & & \\ 3ea_0|E| & 0 & & \\ \hline & & 0 & \\ & & & 0 \end{array} \right) \end{array}$$



$\Delta_\pm = \pm 3ea_0|E|$.

$\langle n'l'm'|z|nlm\rangle = 0$ $\begin{cases} l' = l \pm 1 \\ m' = m. \end{cases}$

selection rule.

Density Operator

$\hat{\rho} = |\varphi\rangle\langle\varphi|$

$\langle A\rangle = \langle\varphi|\hat{A}|\varphi\rangle = tr(|\varphi\rangle\langle\varphi|\hat{A}) = tr(\hat{\rho}\hat{A})$ 　　trace 迹，对角线求和.

$tr(\hat{\rho}) = tr(\hat{\rho}\cdot\hat{I}) = tr(|\varphi\rangle\langle\varphi|\hat{I}) = \langle\varphi|I|\varphi\rangle = 1$.

$\begin{cases} \hat{A} = \sum_{nm} A_{mn}|m\rangle\langle n|. \\ tr\hat{A} = \sum_n A_{nn} \end{cases}$

$tr\hat{A} = \sum_k \langle k|\hat{A}|k\rangle = tr(A\sum_k |k\rangle\langle k|) = tr(A\cdot I) = \sum_k \langle k|\sum_{mn} A_{mn}|m\rangle\langle n|k\rangle$

$= \sum_{kmn} A_{mn} \delta_{km} \delta_{kn}$

$= \sum_k A_{kk}$.

$\rho^2 = |\psi\rangle\underbrace{\langle\psi|\psi\rangle}_{\mathrm{I}}\langle\psi| = |\psi\rangle\langle\psi| = \rho$

$\rho^2 = \rho$. ρ is in a pave state

$\rho = \sum_{mn} \rho_{mn} |\varphi_n\rangle\langle\varphi_m|$

$\rho^2 = \sum_{mn} \rho_{mn} |\varphi_n\rangle\langle\varphi_m| \sum_{kl} \rho_{kl} |\varphi_l\rangle\langle\varphi_k|$

$= \sum_{mnk} \rho_{mn} \rho_{mk} |\varphi_n\rangle\langle\varphi_k| \neq \rho$ mixed state

$\rho = \sum_i w_i |\varphi_i\rangle\langle\varphi_i|$

$\mathrm{tr}\,\rho = 1 \Rightarrow \sum_i w_i = 1$.

$\langle A\rangle = \mathrm{tr}(\rho A) = \sum_i w_i \langle\varphi_i|A|\varphi_i\rangle$

ensemble average 统计平均值.

Time Evolution of ρ.

$$\frac{\partial\rho}{\partial t} = \sum_i w_i \frac{\partial}{\partial t}|\varphi_i\rangle\langle\varphi_i| + \sum_i w_i |\varphi_i\rangle\frac{\partial}{\partial t}\langle\varphi_i|$$

$$= \sum_i w_i \left(\frac{H}{i\hbar}|\varphi_i\rangle\langle\varphi_i| + |\varphi_i\rangle\langle\varphi_i| \cdot \frac{-H}{i\hbar} \right)$$

$$= -\frac{i}{\hbar}(H\rho - \rho H)$$

$$= -\frac{i}{\hbar}[H, \rho]$$

$$\boxed{\begin{array}{l} i\hbar\frac{\partial}{\partial t}|\varphi_i\rangle = H|\varphi_i\rangle \\ -i\hbar\frac{\partial}{\partial t}\langle\varphi_i| = \langle\varphi_i|H. \end{array}}$$

Schrödinger Picture

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

$\frac{\partial\rho_s}{\partial t} = -\frac{i}{\hbar}[H, \rho_s]$

Heisenberg Picture

$|\psi\rangle_H = e^{\frac{iH}{\hbar}t}|\psi\rangle_s$.

$\Downarrow$

$\frac{\partial}{\partial t}|\psi\rangle_H = 0$

$\frac{\partial}{\partial t}\rho_H = 0.$

$$\frac{\partial}{\partial t}|\psi\rangle_H = \frac{iH}{\hbar}|\psi\rangle_H + \underbrace{e^{\frac{iH}{\hbar}}\left(-\frac{iH}{\hbar}\right)|\psi\rangle_s}_{-\frac{iH}{\hbar}|\psi\rangle_H} = 0.$$

$$\rho_H = e^{\frac{iHt}{\hbar}}\rho_s e^{-\frac{iHt}{\hbar}}$$

$$\frac{\partial \rho_H}{\partial t} = e^{\frac{iHt}{\hbar}} \cdot \frac{iH}{\hbar}\rho_s e^{\frac{iHt}{\hbar}} + e^{\frac{iHt}{\hbar}}\rho_s \cdot \left(-\frac{iH}{\hbar}\right) e^{-\frac{iHt}{\hbar}}$$

$$+ e^{\frac{iHt}{\hbar}}\left(-\frac{i}{\hbar}\right)[H, \rho_s] e^{-\frac{iHt}{\hbar}} = 0.$$

$\hat{A}$

Heisenberg

$\hat{A}_H = e^{\frac{iHt}{\hbar}} A_s e^{-\frac{iHt}{\hbar}}$

propogate

$$\langle A\rangle = tr(\rho_H A_H) = tr\left(e^{\frac{iHt}{\hbar}}\rho_s \underbrace{e^{-\frac{iHt}{\hbar}} e^{\frac{iHt}{\hbar}}}_{=1} A_s e^{-\frac{iHt}{\hbar}}\right)$$

$$= tr\left(e^{\frac{iHt}{\hbar}}\rho_s A_s e^{-\frac{iHt}{\hbar}}\right) \qquad tr(AB) = tr(BA)$$

$$= tr\left(\rho_s A_s e^{-\frac{iHt}{\hbar}} e^{\frac{iHt}{\hbar}}\right)$$

$$= tr(\rho_s A_s).$$

Interaction Picture

$H = H_0 + V(t)$

$|\psi\rangle_I = e^{\frac{iH_0t}{\hbar}}|\psi\rangle_s$

$\rho_I = e^{\frac{iH_0t}{\hbar}}\rho_s e^{-\frac{iH_0t}{\hbar}}$

$O_I = e^{\frac{iH_0t}{\hbar}} O_s e^{-\frac{iH_0t}{\hbar}}$

$tr(O_I\rho_I) = tr(\rho_s O_s) = tr(\rho_H O_H)$

$$\frac{\partial}{\partial t}\psi_I = \underbrace{e^{\frac{iH_0t}{\hbar}} \cdot \left(\frac{iH_0}{\hbar}\right)}_{[A, e^A] = 0.}|\psi\rangle_s + e^{\frac{iH_0t}{\hbar}}\left(+\frac{H}{i\hbar}\right)|\psi_s\rangle$$

$$= e^{\frac{iH_0t}{\hbar}}\left(\frac{iH_0}{\hbar} - \frac{iH}{\hbar}\right)|\psi_s\rangle$$

$$= -\frac{i}{\hbar} e^{\frac{iH_0t}{\hbar}} V e^{-\frac{iH_0t}{\hbar}} e^{\frac{iH_0t}{\hbar}}|\psi_s\rangle$$

$$= -\frac{i}{\hbar} V_I |\psi_I\rangle$$

证明：$\frac{\partial}{\partial t}\rho_I = -i[V_I, \rho_I]$

$\frac{\partial}{\partial t}O_I = i[H_0, O_I]$

$\hat{H}\lvert\psi(t)\rangle$ Schrödinger	$\hat{H}(t)\lvert\psi\rangle$ Heisenberg	$\hat{H}(t)\lvert\psi(t)\rangle$ Interaction
$i\hbar\frac{\partial}{\partial t}\lvert\psi\rangle_S = H\lvert\psi\rangle_S$	$i\hbar\frac{\partial}{\partial t}\lvert\psi\rangle_H = 0.$	$i\hbar\frac{\partial}{\partial t}\lvert\psi\rangle_I = V_I\lvert\psi\rangle_I.$
$i\hbar\frac{\partial}{\partial t}\rho_S = [H,\rho_S]$	$i\hbar\frac{\partial}{\partial t}\rho_H = 0$	$i\hbar\frac{\partial}{\partial t}\rho_I = [V_I,\rho_I]$
$\frac{\partial O_S}{\partial t} = 0.$	$i\hbar\frac{\partial}{\partial t}\hat{O}_H = [H,\hat{O}_H]$	$i\hbar\frac{\partial}{\partial t}O_I = -[H_0, O_I]$

$$\lvert\psi\rangle_I = \sum_n C_n(t)\lvert n\rangle.$$

$$\langle n\rvert\, i\hbar\frac{\partial}{\partial t}\lvert\psi\rangle_I \overset{\langle n\rvert}{=} V_I\lvert\psi\rangle_I$$

$\langle n$ 插入了 $\sum_m V_I\lvert m\rangle\langle m\rvert V_I\rangle$

$$i\hbar\frac{\partial}{\partial t}C_n(t) = \sum_m \langle n\rvert V_I\lvert m\rangle C_m$$

$$\langle n\rvert V_I\lvert m\rangle = \langle n\rvert e^{\frac{iHt}{\hbar}} V e^{-\frac{iHt}{\hbar}}\lvert m\rangle$$

$$= e^{\frac{iE_nt}{\hbar}}\langle n\rvert V\lvert m\rangle e^{\frac{-iE_mt}{\hbar}}$$

$$i\hbar\frac{\partial}{\partial t}C_n = \sum_m \lambda V_{nm} e^{i\omega_{nm}t} C_m. \qquad \omega_{nm} = \frac{E_n-E_m}{\hbar}$$

$$H = H_0 + \lambda V.$$

$$C_n = C_n^{(0)} + \lambda C_n^{(1)} + \lambda^2 C_n^{(2)} + \cdots$$

initial condition

$$\lambda^0:\quad i\hbar\frac{\partial}{\partial t}C_n^{(0)} = 0. \quad\Rightarrow\quad \boxed{C_n^{(0)} = \text{Const} \qquad C_n^{(0)} = \delta_{ni}}$$

$$\lvert\psi(0)\rangle = \lvert i\rangle$$

$$\lambda^1:\quad i\hbar\frac{\partial}{\partial t}C_n^{(1)} = \sum_m V_{nm} e^{i\omega_{nm}t} C_m^{(0)}$$

$$= \sum_m V_{nm} e^{i\omega_{nm}t}\delta_{mi}$$

$$= V_{ni} e^{i\omega_{ni}t}.$$

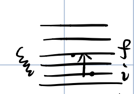
$$C_n^{(1)} = \frac{1}{i\hbar}\int_0^t e^{i\omega_{ni}t'} V'_{ni}(t)\,dt'.$$

$$C_f = C_f^{(0)} + C_f^{(1)} + C_f^{(2)} + \cdots\cdots \qquad (i\neq f).$$

$$\approx C_f^{(1)}$$

$$= \frac{1}{i\hbar}\int_0^t e^{i\omega_{fi}t'} V_{fi}(t')\,dt'.$$

$$P_{i\to f} = \lvert C_f\rvert^2 = \frac{1}{\hbar^2}\left\lvert\int_0^t e^{i\omega_{fi}t'} V_{fi}(t')\,dt'\right\rvert^2.$$



$\langle f\rvert V\lvert i\rangle$

跃迁的可能性.

$$= \Gamma_{i\to f}\cdot t$$

$\hat{V}(t) = V_{st}\cos(wt)$.

$$C_f^{(1)} = \frac{1}{i\hbar}\int_0^t e^{iw_{fi}t}\,\frac{1}{2}\left(e^{iwt}+e^{-iwt}\right)\langle f|V_{st}|i\rangle\, dt'$$

$$C_f^{(1)} = \frac{V_{fi}}{2i\hbar}\int_0^t e^{i(w_{fi}-w)t'} + e^{i(w_{fi}+w)t'}\, dt'$$

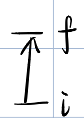
$$= \frac{V_{fi}}{2\hbar}\left[\frac{1-e^{i(w_{fi}-w)t}}{w_{fi}-w} + \frac{1-e^{i(w_{fi}+w)t}}{w_{fi}+w}\right]$$

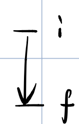
$w \approx w_{fi} = w_f - w_i$ $\qquad$ $x = \frac{w_{fi}-w}{2}$

$$P_{fi} = |C_f^{(1)}|^2 = \frac{|V_{fi}|^2}{4\hbar^2}\left(\frac{\sin(w_{fi}-w)\cdot\frac{t}{2}}{(w_{fi}-w)/2}\right)^2 \qquad \lim_{x\to 0}\frac{\sin xt}{x} = t.$$

$$= \frac{|V_{fi}|^2}{4\hbar^2}t^2.$$

$\underset{\sim}{w}$





$\underset{\sim}{w = w_{if}}$

$w = -w_{fi} = w_i - w_f$.

Const perturbation

$\hat{V}(t) = V_{st}\cos(wt)$.

$w=0$. $\hat{V}(t) = V_{st}$

$$P_{fi} = \frac{|V_{fi}|^2}{\hbar^2}\left(\frac{\sin w_{fi}\cdot\frac{t}{2}}{w_{fi}/2}\right)^2 \qquad \lim_{\alpha\to\infty}\frac{1}{\pi}\cdot\frac{\sin^2\alpha x}{\alpha x^2} = \delta(x).$$

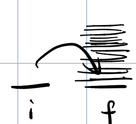
$$\lim_{t\to\infty}\left[\frac{\sin(w_{fi}\cdot\frac{t}{2})}{w_{fi}/2}\right]^2 = 2\pi t\,\delta(w_{fi})$$

$$= \frac{2\pi|V_{fi}|^2}{\hbar^2}\delta(w_{fi})\,t$$

$$= T_{fi}\cdot t$$

$$\underset{\sim}{T_{fi}} = \frac{2\pi|V_{fi}|^2}{\hbar^2}\delta(w_f-w_i).$$

跃迁概率



$$\sum_f T_{fi} = \frac{2\pi}{\hbar}|V_{fi}|^2\delta(w_f-w_i)$$ $\qquad$ Fermi's Gorden Rule

$$= \frac{2\pi}{\hbar}|V_{fi}|^2\rho(E_f)|_{E_f=E_i}$$

$V\cos(wt)$

$$k_{fi} = \frac{2\pi}{\hbar}|V_{fi}|^2 \rho(E_f)\Big|_{E_f = E_i = \hbar w}$$

$$k_{fi} = \frac{2\pi}{\hbar}|V_{fi}|^2 \rho(E_f)\Big|_{E_f = E_i = -\hbar w.}$$