20190528 Ch5 approximation methods

Monday, May 27, 2019 2:40 PM

HW. with $H = \hbar\omega a^\dagger a + \hbar\eta(a + a^\dagger)$, with $\eta \ll \omega$, use perturbation theory to calculate the energy shift to the second order $E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)}$, and the perturbed eigenstate to first order $|n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle$.

recap

6月11日下午考试教室改到了5503教室，final exam will be at room 5503, June 11.

$H = H_0 + H'$, $\quad H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$,

use perturbation theory,

first order $E_n = E_n^{(0)} + E_n^{(1)}$, $\quad |n\rangle = |n^{(0)}\rangle + |n^{(1)}\rangle$

$$E_n^{(1)} = \langle n^{(0)}|H'|n^{(0)}\rangle, \qquad |n^{(1)}\rangle = \sum_{k\neq n} \frac{\langle k^{(0)}|H'|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} \cdot |k^{(0)}\rangle.$$

- second order perturbation

$H = H_0 + H'$, let $H' = \lambda V$, $\lambda \ll 1$

$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$, $\quad \begin{cases} E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \\ |n\rangle = |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle \end{cases}$

↑

"e-n-not"

$H|n\rangle = E_n|n\rangle$

$$\Rightarrow (H_0 + \lambda V)\cdot(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots)$$
$$= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots)\cdot(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots)$$

terms proportional to λ^2.

$$H_0|n^{(2)}\rangle + V|n^{(1)}\rangle = E_n^{(0)}|n^{(2)}\rangle + E_n^{(1)}|n^{(1)}\rangle + E_n^{(2)}|n^{(0)}\rangle.$$

we are interested in $E_n^{(2)}$

apply $\langle n^{(0)}|$ on the left.

with $\langle n^{(0)}| H_0 | n^{(2)}\rangle = E_n^{(0)} \langle n^{(0)} | n^{(2)}\rangle$

and $\langle n^{(0)} | n^{(1)}\rangle = 0$

$\langle n^{(0)} | n^{(0)}\rangle = 1$

$\Rightarrow \quad E_n^{(2)} = \langle n^{(0)} | V | n^{(1)}\rangle$

$$|n^{(1)}\rangle = \sum_{k\neq n} \frac{\langle k^{(0)} | V | n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle$$

$$\Rightarrow \quad E_n^{(2)} = \sum_{k\neq n} \frac{\langle k^{(0)} | V | n^{(0)}\rangle \cdot \langle n^{(0)} | V | k^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}}$$

short hand $\quad V_{kn} = \langle k^{(0)} | V | n^{(0)}\rangle$

$$E_n^{(2)} = \sum_{k\neq n} \frac{|V_{kn}|^2}{E_n^{(0)} - E_k^{(0)}}$$

up to 2nd order

$$\Rightarrow \quad E_n = E_n^{(0)} + \lambda \langle n^{(0)} | V | n^{(0)}\rangle + \lambda^2 \sum_{k\neq n}$$

$$\boxed{E_n = E_n^{(0)} + \langle n^{(0)} | H' | n^{(0)}\rangle + \sum_{k\neq n} \frac{|H'_{kn}|^2}{E_n^{(0)} - E_k^{(0)}}}$$

discussion:

① second order perturbation for ground is always making energy going lower.

② if there are degeneracies, then the above theory would not work.
and it would starts to fail even when the energies are very close.

example:

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + \frac{1}{2}\epsilon m\omega^2 x^2, \quad \epsilon \ll 1$$

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$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega'^2 x^2, \qquad \omega' = \underline{\sqrt{1+\epsilon}}\,\omega.$$

$$E_n = \hbar\omega'(n+\tfrac{1}{2}) = \hbar\omega(n+\tfrac{1}{2})\cdot(1 + \tfrac{1}{2}\epsilon - \tfrac{1}{8}\epsilon^2 + \cdots)$$

next apply perturbation theory to check this correct.

① identify $H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$, $H' = \frac{1}{2}\epsilon m\omega^2 x^2$.

$$H_0 = \hbar\omega(a^\dagger a + \tfrac{1}{2}), \quad x = \sqrt{\frac{\hbar}{2m\omega}}\,(a+a^\dagger)$$

$$\Rightarrow H' = \frac{1}{2}\epsilon m\omega^2 \cdot \frac{\hbar}{2m\omega}(a+a^\dagger)^2$$

$$= \frac{1}{4}\epsilon\hbar\omega\,(a^2 + a^{\dagger 2} + aa^\dagger + a^\dagger a).$$

$|n^{(0)}\rangle$ = the "Fock" state

$$\begin{cases} a|n^{(0)}\rangle = \sqrt{n}\,|(n-1)^{(0)}\rangle \\ a^\dagger|n^{(0)}\rangle = \sqrt{n+1}\,|(n+1)^{(0)}\rangle \end{cases}$$

$$E_n^{(0)} = \hbar\omega(n+\tfrac{1}{2})$$

$$E_n^{(1)} = \langle n^{(0)}|H'|n^{(0)}\rangle = \frac{1}{4}\epsilon\hbar\omega\Big(\cancel{\langle a^2\rangle}^{\,0} + \cancel{\langle a^{\dagger 2}\rangle}^{\,0} + \langle aa^\dagger\rangle + \langle a^\dagger a\rangle\Big)$$

$$\langle aa^\dagger\rangle = n+1$$
$$\langle a^\dagger a\rangle = n$$

$$\Rightarrow E_n^{(1)} = \frac{1}{2}\hbar\omega\,\epsilon\,(n+\tfrac{1}{2}).$$

$$E_n^{(2)} = \sum_{k\neq n}\frac{|H'_{kn}|^2}{E_n^{(0)} - E_k^{(0)}}$$

$$H'_{kn} = \langle k^{(0)}|H'|n^{(0)}\rangle$$

$\rightarrow \delta_{\xi,\eta} = 1$ if $\xi = \eta$.

$H'_{kn} = \langle k^{(0)} | H' | n^{(0)} \rangle$ $\rightarrow$ $\delta_{\xi,\eta} = 1$ if $\xi = \eta$.

$\langle k^{(0)} | a^2 | n^{(0)} \rangle = \sqrt{n(n-1)}\ \delta_{k-2,n}$

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

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

$$\Rightarrow \quad E_n^{(2)} = \frac{(\frac{1}{4}\hbar\omega\epsilon)^2}{\hbar\omega}\left(\frac{n(n-1)}{+2} + \frac{(n+1)(n+2)}{-2} \right)$$

$$= -\frac{1}{8}\hbar\omega\epsilon^2(n+\tfrac{1}{2})$$

up to 2nd order.

$\Rightarrow$ $E_n = \hbar\omega(n+\frac{1}{2})(1+\frac{1}{2}\epsilon - \frac{1}{8}\epsilon^2)$ matching with the exact solution.

o skip degenerate time-independent perturbation. see Sakurai if interested.

* §2. time-dependent perturbation (not in exam).

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

Schrödinger's equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = (H_0 + \lambda V(t))|\psi(t)\rangle.$$

$$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$$

$$|\psi(t)\rangle = \sum_n a_n(t)\, e^{-i\frac{E_n^{(0)}t}{\hbar}}|n^{(0)}\rangle.$$

if $\lambda = 0$, $a_n(t) = a_n$. time-independent.

next we can apply perturbation to $a_n(t)$.

$$a_n(t) = a_n + \lambda a_n^{(1)}(t) + \lambda^2 a_n^{(2)}(t) + \cdots$$

plug $|\psi(t)\rangle$ back to Schrödinger's equation.

$$\Rightarrow \quad i\hbar \sum_n \left(\frac{d a_n(t)}{dt} e^{-i\frac{E_n^{(0)} t}{\hbar}} \right) = \sum_{n'} \lambda V(t)\, a_{n'}(t)\, e^{-i\frac{E_{n'}^{(0)} t}{\hbar}} |n'^{(0)}\rangle$$

in the following $n' = m$

$$i\hbar \frac{d a_n(t)}{dt} = \lambda \sum_m a_m(t) \langle n | V(t) | m \rangle e^{i\frac{(E_n^{(0)} - E_m^{(0)})t}{\hbar}}$$

denote $\omega_{nm} = \dfrac{E_n^{(0)} - E_m^{(0)}}{\hbar}$ ← energy difference

$$\boxed{i\hbar\, \dot{a}_n(t) = \lambda \sum_m a_m V_{nm} e^{i\omega_{nm} t}} \qquad \dot{x} = \frac{dx}{dt}$$

time-dependent perturbation.

apply expansion

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

$$\lambda^0: \quad i\hbar \frac{d a_n^{(0)}}{dt} = 0 \quad ✓$$

$$\lambda^1: \quad i\hbar\, \dot{a}_n^{(1)}(t) = \underbrace{\sum_m a_m^{(0)} V_{nm}(t) e^{i\omega_{nm} t}}_{\text{known.}}$$

$$a_n^{(1)}(t) = \frac{1}{i\hbar} \int_0^t dt'\, a_m^{(0)} V_{nm}(t') e^{i\omega_{nm} t'}.$$

for $t \gg \dfrac{2\pi}{\omega_{nm}}$ $\quad \int_0^t dt'\, e^{i\omega_{nm} t'} \xrightarrow{\text{compart to } t} 0.$

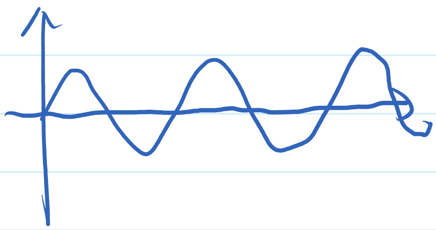
$e^{-i\omega_{nm} t'}$

ω_{nm} $\gg 0$

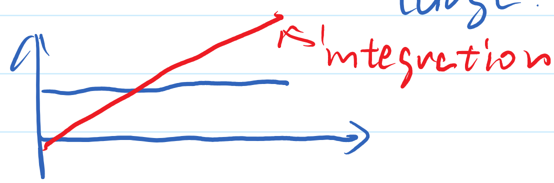
So the interesting case is $V_{nm}(t') \sim e^{-i\omega_{nm}t'}$ which cancels the fast oscillation.

$$\int_0^t dt' \, a_m^{(0)} V_{nm}(t') e^{i\omega_{nm}t'} \propto t' a_m^{(0)}$$

large.



not accumulating.

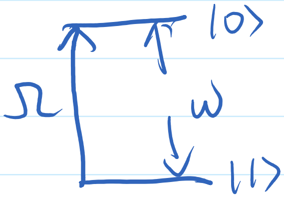


accumulating.

$V_{nm}(t') \sim e^{-i\omega_{nm}t'} \longrightarrow$ a resonance.

Example.

$$H = \hbar \frac{\omega}{2} \sigma_z + \hbar \Omega \sigma_x \cos \omega t.$$



drive 驱动

on resonance 共振

exact solution: applying transformation $|\psi\rangle = e^{-i\frac{H_0 t}{\hbar}} |\phi\rangle$

$H_0 = \hbar \frac{\omega}{2} \sigma_z$.

apply rotating wave approximation $\rightarrow H_{int} = \frac{\hbar\Omega}{2} \sigma_x$

with $|\psi(t=0)\rangle = |0\rangle \rightarrow |\psi(t)\rangle = \cos\frac{\Omega t}{2}|0\rangle - i \sin\frac{\Omega t}{2}|1\rangle$

$$\xrightarrow{\Omega \ll \frac{2\pi}{t}} |\phi(t)\rangle \simeq |0\rangle - i\frac{\Omega t}{2}|1\rangle.$$

the following we are going to compare this with time-dependent perturbation.

$$|\phi(t)\rangle = a_0(t)|0\rangle + a_1(t)|1\rangle.$$

$$\begin{cases} a_0^{(0)}(t) = 1, \quad a_1^{(0)}(t) = 0. \qquad \omega_{01} = \omega, \ \omega_{10} = -\omega \\ |\psi(t=0)\rangle = |0\rangle. \end{cases}$$

$$a_0^{(1)}(t) = \frac{1}{i\hbar}\int_0^t \sum_{j=0,1} a_j^{(0)}(t') H'_{0j}(t') e^{i\omega_{0j}t'} dt'$$

$$H'_{00}(t') = \hbar\Omega\cos\omega t' \quad \langle 0|\sigma_x|0\rangle = 0.$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$H'_{11}(t') = 0.$$

$$H'_{01}(t') = \hbar\Omega\cos\omega t' \underbrace{\langle 0|\sigma_x|1\rangle}_{1} = \hbar\Omega\cos\omega t'$$

$$H'_{10}(t') = \hbar\Omega\cos\omega t'$$

$$\Rightarrow \quad a_0^{(1)}(t) = \frac{1}{i\hbar}\int_0^t \underbrace{a_1^{(0)}(t')}_{0} H'_{01}(t') e^{i\omega_{01}t'} dt'$$

$$= 0$$

$$a_1^{(1)}(t) = \frac{1}{i\hbar}\int_0^t \underbrace{a_0^{(0)}(t')}_{1} H'_{10}(t') e^{i\omega_{10}t'} dt'$$

$$= \frac{1}{i\hbar}\int_0^t \hbar\Omega \underbrace{\cos\omega t'}_{\frac{1}{2}(e^{i\omega t'} + e^{-i\omega t'})} e^{-i\omega t'} dt'$$

$$= \frac{\Omega}{2i}\int_0^t 1 + e^{-2i\omega t'} dt'$$

$$= \frac{\Omega}{2i} t + \frac{\Omega}{2i} \frac{e^{-2i\omega t} - 1}{-2i\omega}$$

$$= \frac{\Omega}{2i} t + \frac{\Omega}{2i} \frac{e^{\quad} - 1}{-2iw}$$

$$\Rightarrow a_1^{(1)}(t) = -i\frac{\Omega t}{2} + \frac{\Omega}{4w}\left(e^{-2iwt} - 1\right).$$

for $t \ll \frac{2\pi}{\Omega}$, but $t \gg \frac{2\pi}{w}$, w is large, Ω is small

$$\Omega t \gg \frac{\Omega}{w}$$

$$\Rightarrow a_1^{(1)}(t) = -i\frac{\Omega t}{2}, \quad a_0^{(1)}(t) = 0.$$

$$\Rightarrow |\psi(t)\rangle \xrightarrow{1^{st}\text{ order}} |0\rangle - i\frac{\Omega t}{2}|1\rangle$$

matches with basis transformation and Rotating wave approximation.