Time-dependent perturbation theory

- Heisenberg, Schrödinger and interaction pictures
- 1st order time-dependent perturbation theory

Schrödinger picture:

state vector

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle$$

Hamiltonian (operator) $H = \hat{H}$

Funny: $i\hbar \frac{\partial}{\partial |t\rangle} |t\rangle = H(t) |\Psi(t)\rangle$??

Lets add "S" to denote the picture $\Rightarrow i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle_S = H_S(t) |\Psi(t)\rangle_S$

Note: a) this is true for many body systems as well. H and $|\Psi\rangle$ just become more complicated then.

b) H can have time-dependence.

Solve $\Rightarrow |\Psi(t)\rangle_S = U(t) |\Psi(0)\rangle_S$

time-evolution operator

example from eigenstates?

If H is time-independent: $U(t) = e^{-\frac{i}{\hbar}\hat{H}t}$

Schrödinger eq $\Leftrightarrow$ $|\Psi(t)\rangle_S = |\Psi(0)\rangle_S - \frac{i}{\hbar}\int_0^t dt' \, H_S(t') |\Psi(t')\rangle_S$

... iterate

$$\Rightarrow |\Psi(t)\rangle_S = \left[1 - \frac{i}{\hbar}\int_0^t dt' H_S(t') + \frac{i^2}{\hbar^2}\int_0^t dt' \int_0^{t'} dt'' \, H_S(t') H_S(t'') \dots \right] |\Psi(0)\rangle_S$$

$$\Rightarrow U(t) = T e^{-\frac{i}{\hbar}\int_0^t d\tau \, H_S(\tau)}$$

T = time-ordering operator = operators so that earlier on the right

$T[A(t_1)A(t_2)A(t_3)] = A(t_3)A(t_1)A(t_2)$

if $t_3 > t_1 > t_2$ exercises ↑!

Why do we need time-ordering? Commutation not obvious if $H_S(t)$.

$$U(t,t_0) = T\, e^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau\, H(\tau)} \Rightarrow |\Psi(t)\rangle_S = U(t,t_0)|\Psi(t_0)\rangle_S$$

Observable $A_S(t) \rightarrow \langle A_S(t)\rangle = {}_S\langle\Psi(t)|A_S(t)|\Psi(t)\rangle_S$

How does this expectation vary in time?

$$i\hbar \frac{d}{dt}\langle A_S(t)\rangle = i\hbar\Big[\Big(\frac{d}{dt}\,{}_S\langle\Psi(t)|\Big)A_S|\Psi(t)\rangle_S + {}_S\langle\Psi(t)|A_S\Big(\frac{d}{dt}|\Psi(t)\rangle_S\Big)$$
$$+\ {}_S\langle\Psi(t)|\Big(\frac{dA_S}{dt}\Big)|\Psi(t)\rangle_S\Big]$$

↖ often vanishes

Schrödinger picture: state evolves in time, but operators for observables (typically) time-independent.

Heisenberg picture: constant states, but operators have time-dependence.

You can change basis by unitary transformation ... especially

$|\psi\rangle_S \rightarrow U^{-1}|\psi\rangle_S$ removes time-dependence of

↖ inverse of U

Schrödinger picture states.

$$|\Psi(t)\rangle_H = U(t)^{-1}|\Psi(t)\rangle_S$$

$$\Rightarrow |\Psi(t)\rangle_H = U^{-1}U|\Psi(0)\rangle_S = |\Psi(0)\rangle_S = |\Psi\rangle_H$$

Expectation values? $\Rightarrow$ need to transform the operators also

$$A_H(t) = U(t)^{-1}A_S U(t)$$

Hamiltonian in particular: $H_H(t) = U(t)^{-1}H_S U(t)$

For time-independent H_S, we have $H_S = H_H$ why?

$${}_H\langle\Psi|A_H(t)|\Psi\rangle_H = {}_S\langle\Psi(t)|A_S|\Psi(t)\rangle_S \quad \text{why?}$$

$\Rightarrow$ expectations are the same!

$$i\hbar\frac{d}{dt}A_H(t) = i\hbar\left(\frac{d}{dt}U^{-1}\right)A_S U + U^{-1}A_S\, i\hbar\frac{d}{dt}U$$

Ex 1 $\Rightarrow$ $i\hbar\frac{d}{dt}A_H(t) = -H_H(t)A_H(t) + A_H(t)H_H(t) = [A_H, H_H]$

Heisenberg's equation of motion

Interaction picture:

Say we have Hamiltonian H_0 we can actually solve exactly (meaning?) and something tricky $V(t)$

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

often H_0 = BIG, $V(t)$ = small

Such a picture where state evolution from H_0 removed a'la Heisenberg, but state evolution from $V(t)$ kept!

define $U_0(t) = T e^{-\frac{i}{\hbar}\int_0^t d\tau\, H_0(\tau)}$

assume $H_0(t) = H_0 \Rightarrow$ Integral just $H_0 t$, no need for T

$$|\psi(t)\rangle_I = e^{iH_0t/\hbar}|\psi(t)\rangle_S = e^{iH_0t/\hbar}\, T e^{-\frac{i}{\hbar}\int_0^t d\tau\, H(\tau)}|\psi(0)\rangle_S$$

$$= e^{iH_0t/\hbar}\, T e^{-\frac{i}{\hbar}\int_0^t d\tau\, H(\tau)}|\psi(0)\rangle_I$$

$$i\hbar\frac{d}{dt}|\psi(t)\rangle_I = -H_0 e^{iH_0t/\hbar}\, T e^{-\frac{i}{\hbar}\int_0^t d\tau\, H(\tau)}|\psi(0)\rangle_I + e^{iH_0t/\hbar} H(t)\, T e^{-\frac{i}{\hbar}\int_0^t d\tau\, H(\tau)} \cdot|\psi(0)\rangle_I$$

$$= -H_0|\psi(t)\rangle_I + H_I(t)|\psi(t)\rangle_I$$

$$= V_I(t)|\psi(t)\rangle_I$$ Kind of like Schrödinger, but why?

$$V_I(t) = e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar}$$

More generally $O_I = e^{iH_0t/\hbar}\, O\, e^{-iH_0t/\hbar}$

$\Rightarrow |\psi(t)\rangle_I = U_I(t)|\psi(0)\rangle_I$, $U_I(t) = T e^{-\frac{i}{\hbar}\int_0^t d\tau\, V_I(\tau)}$

... if V = small $\Rightarrow$ perturbation expansion!

$V = \lambda H'$ to assist seeing the order.

Exercise 1

$$\Rightarrow U_I(t) = 1 + \sum_{n=1}^{\infty}\left(-\frac{i\lambda}{\hbar}\right)^n \int_0^t d\tau_n \int_0^{\tau_n} d\tau_{n-1} \cdots \int_0^{\tau_2} d\tau_1 \Big\{ U_0(0,\tau_n)H_S'(\tau_n)U_0(\tau_n,\tau_{n-1})H_S'(\tau_{n-1})\ldots U_0(\tau_2,\tau_1)H_S'(\tau_1)U_0(\tau_1,0)\Big\}$$

Hopefully first terms are enough!

Perturbation theory:

Reminder time-independent perturbation theory:

- get approximate eigenstates and eigenvalues.

Time-dependent perturbation theory:

$H = H_0 + V(t) \Rightarrow |\Psi(t)\rangle_I = U_I(t,t_0)\,|\Psi(t_0)\rangle_I$

(assume $V(t)=0$ for $t<t_0$)

$$U_I(t,t_0) = 1 + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, V_I(t') + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^{t} dt'\, V_I(t') \int_{t_0}^{t'} dt''\, V_I(t'') + \dots$$

$$V_I(t') = e^{iH_0(t'-t_0)/\hbar}\, V(t')\, e^{-iH_0(t'-t_0)/\hbar}$$

$$U_I(t,t_0) = T e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt'\, V_I(t')} \quad \text{also}$$

1st order time-dependent perturbation obtained from:

$$U_I(t,t_0) \approx 1 + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, V_I(t')$$

Usually not worth it to go beyond 2nd order!

$$\Rightarrow |\psi(t)\rangle_I \approx \left[1 + \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, V_I(t') + \mathcal{O}(V_I^2)\right]|\psi(t_0)\rangle_I$$

we are interested in transition amplitudes between different eigenstates of H_0.

$$|\psi(t_0)\rangle_I = |l\rangle \leftarrow H_0|l\rangle = E_l|l\rangle$$

$$\Rightarrow \langle k|\psi(t)\rangle_I \approx \langle k|l\rangle + \frac{1}{i\hbar}\int_{t_0}^{t} dt' \langle k|V_I(t')|l\rangle + \mathcal{O}(V_I^2)$$

$H_0|k\rangle = E_k|k\rangle$

operator stuff

Assume $V(t) = \underbrace{\lambda f(t)}_{\text{just a function}} H'$

$$\Rightarrow V_I(t') = e^{iH_0(t'-t_0)/\hbar}\lambda H' f(t') e^{-iH_0(t'-t_0)/\hbar}$$

when $k \neq l$ $\langle k|l\rangle = 0$ why?

$$\langle k|\psi(t)\rangle_I = \frac{\lambda\langle k|H'|l\rangle}{i\hbar}\int_{t_0}^{t} dt'\, e^{i(E_k-E_l)t/\hbar} f(t') + \mathcal{O}(V_I^2) \quad \text{why?}$$

$$\Rightarrow \text{probability: } |\langle k|\psi(t)\rangle_I|^2 \approx \frac{\lambda^2|\langle k|H'|l\rangle|^2}{\hbar^2}\left|\int_0^t dt'\, e^{i(E_k-E_l)t'/\hbar} f(t')\right|^2$$

(choose $t_0 = 0$)

if $\langle k|l\rangle \neq 0$ need also the 2nd order term.

Example: harmonic perturbation

$f(t) = 2\cos\omega t$

$$\Rightarrow \langle k|\psi(t)\rangle_I \approx \frac{\lambda\langle k|H'|l\rangle}{i\hbar}\int_0^t dt\, e^{i(E_k-E_l)t'/\hbar}\left(e^{i\omega t'} + e^{-i\omega t'}\right)$$

$$\Rightarrow \langle k|\psi\rangle_I = -2i\lambda \underbrace{H'_{kl}}_{\langle k|H'|l\rangle} \left[\frac{e^{i(E_k - E_l - \hbar\omega)t/2\hbar}}{E_k - E_l - \hbar\omega} \sin\frac{(E_k - E_l - \hbar\omega)t}{2\hbar} + \frac{e^{i(E_k - E_l + \hbar\omega)t/2\hbar} \sin\frac{(E_k - E_l + \hbar\omega)t}{2\hbar}}{E_k - E_l + \hbar\omega} \right]$$

1st term: absorption of a "photon"

2nd term: emission of a "photon"

why?

Semiclassical since we didn't treat the field quantum mechanically here.

Adiabatic perturbation:

Integrate by parts ($t_0 = 0$)

$$\Rightarrow \langle k|\psi\rangle_I \simeq \frac{\lambda \langle k|H'|l\rangle}{i\hbar (E_k - E_l) i/\hbar} \left[f(t) e^{i(E_k - E_l)(t - t_0)/\hbar} \underbrace{- \int_{t_0}^{t} dt' \, e^{i(E_k - E_l)t'/\hbar} \frac{d}{dt'} f(t') \Big]}_{\text{small if the perturbation slowly varying}}$$

Exercise 2 for bit more...

Example on Heisenberg formalism: harmonic oscillator (mainly for curiosity)

Hamiltonian: $H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$ (x, p are operators)

Heisenberg's equations of motion for x and p..

$$i\hbar \frac{dx}{dt} = [x, H] = [x, \frac{p^2}{2m}] = \frac{1}{2m}(xp^2 - p^2 x)$$

$xp - px = i\hbar$
$\Rightarrow px = xp - i\hbar$

$$= \frac{1}{2m}(xp^2 - p(xp - i\hbar))$$

$$= \frac{1}{2m}(xp^2 - pxp + i\hbar p) = \frac{1}{2m}(xp^2 - xp^2 + 2i\hbar p)$$

$$= \frac{i\hbar}{m} p \Rightarrow \frac{dx}{dt} = \frac{p}{m}$$ (of course)

Same way: $\frac{dp}{dt} = -m\omega^2 x$ (of course)

$$\frac{d^2x}{dt^2} = \frac{1}{m}\frac{dp}{dt} = -\omega^2 x \Rightarrow x(t) = A\cos\omega t + B\sin\omega t$$

$$p(t) = -mA\omega \sin\omega t + mB\omega\cos\omega t$$

$x(t=0) = x_0 \Rightarrow A = x_0$ (initial conditions)
$p(t=0) = p_0 \Rightarrow B = p_0/m\omega$

$x(t) = x_0 \cos\omega t + p_0/m\omega \sin\omega t$ (*)
$p(t) = p_0 \cos\omega t$

Eigenstates ???
Say we have eigenstates $|n\rangle$ and $|n'\rangle$ with energies E_n and $E_{n'}$
Matrix elements for $x(t)$: $\langle n'|x(t)|n\rangle = \langle n'|e^{iHt/\hbar} x_0 e^{-iHt/\hbar}|n\rangle$

$$= e^{it/\hbar (E_{n'} - E_n)} \langle n'|x_0|n\rangle$$

we can also use (*)

$$\Rightarrow \langle n'| x_0 \cos\omega t + \frac{p_0}{m\omega} \sin\omega t |n'\rangle = \langle n'| \frac{x_0}{2}(e^{i\omega t} + e^{-i\omega t})$$

$$+ \frac{p_0}{2im\omega}(e^{i\omega t} - e^{-i\omega t}) |n\rangle$$

$$= \frac{e^{i\omega t}}{2} \langle n'|(x_0 - i\frac{p_0}{m\omega})|n\rangle + \frac{e^{-i\omega t}}{2} \langle n'| x_0 + \frac{p_0}{m\omega} |n\rangle$$

assume $E_{n'} > E_n$, note also that $\omega > 0$
Since expressions must be the same ... $e^{-i\omega t}$ - term must vanish

$$\Rightarrow \langle n'| x_0 + \frac{ip_0}{m\omega} |n\rangle = 0 \qquad (**)$$

ALSO: $e^{\frac{it}{\hbar}(E_{n'} - E_n)} = e^{i\omega t} \Rightarrow \boxed{E_{n'} = E_n + \hbar\omega}$

We can apply the same to n'' $E_{n''} > E_{n'}$

$$\Rightarrow E_{n''} = E_{n'} + \hbar\omega$$

$\Rightarrow E_n, E_n + \hbar\omega, E_n + 2\hbar\omega, \ldots$

H is a sum of two positive terms, so there must be a lowest state E_0.

If we assume $E_{n'} < E_n$ same logic gives

$$E_{n'} = E_n - \hbar\omega \text{ etc.}$$

$E_n = E_0 + n\hbar\omega$

Apply specifically to $n' = 1$, $n = 0$

(**) $\Rightarrow \langle 1| x_0 + \frac{ip_0}{m\omega} |0\rangle = 0$

In fact all $\langle n|x_0|0\rangle$ and $\langle n|p_0|0\rangle$ must vanish since they are associated with $e^{in\omega t}$ phase-factors that cannot be there.

$(x_0 + \frac{ip_0}{m\omega})|0\rangle$ doesn't have matrix element with $|1\rangle$ or any other $|n\rangle$

$$\Rightarrow \left(x_0 + \frac{ip_0}{m\omega}\right)|0\rangle = 0$$

$$\Rightarrow \left(x_0 - \frac{ip_0}{m\omega}\right)\left(x_0 + \frac{ip_0}{m\omega}\right)|0\rangle = 0$$

$$\left(x_0^2 + \frac{i}{m\omega}\underbrace{(x_0 p_0 - p_0 x)}_{i\hbar} + \frac{p_0^2}{m^2\omega^2}\right)|0\rangle = 0$$

$$\Rightarrow \left(x_0^2 + \frac{p_0^2}{m^2\omega^2} - \frac{\hbar}{m\omega}\right)|0\rangle = 0 \quad \Big|\Big| \cdot \frac{m\omega^2}{2}$$

$$\Rightarrow \left(\frac{m\omega^2}{2}x_0^2 + \frac{p_0^2}{2m} - \frac{\hbar\omega}{2}\right)|0\rangle = 0$$

$$\Rightarrow \left(E_0 - \frac{\hbar\omega}{2}\right)|0\rangle = 0 \Rightarrow E_0 = \hbar\omega/2$$

So we could figure out eigenenergies and quite a bit about matrix element starting from Heisenberg's equations of motion.