I. Time-dependent phenomena

I.1 Time-dependent perturbation theory

How to solve the time evolution of a quantum system after switching on a "small", possibly time-dependent perturbation? λ acts as formal smallness parameter which will be set to 1 later:

(1) $\hat{H} = \hat{H}_0 \rightarrow \hat{H} = \hat{H}_0 + \lambda \hat{H}_1(t) \qquad i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$

Assume that we know spectrum of $\hat{H}_0$

(2) $\hat{H}_0 |n\rangle = \varepsilon_n |n\rangle \qquad \{|n\rangle\}$ complete ONB

consider $|\psi(t=0)\rangle = |m\rangle$ what is $|\psi(t>0)\rangle$?

expand $|\psi(t)\rangle$ into basis $\{|n\rangle\}$

(3) $$|\psi(t)\rangle = \sum_n a_n(t)\, e^{-i\varepsilon_n t/\hbar} |n\rangle$$

if $\lambda = 0$: $|\psi(t)\rangle$ solution of (1) with $a_n(t) = \text{const}_t$

substitution in (1)

(4) $$\sum_n \left(i\hbar \frac{d}{dt} a_n(t) + \varepsilon_n a_n(t) \right) e^{-i\varepsilon_n t/\hbar} |n\rangle = \sum_n \left(\varepsilon_n a_n(t) + \lambda \hat{H}_1(t)\, a_n(t) \right) e^{-i\varepsilon_n t/\hbar} |n\rangle$$

$$(5) \Rightarrow \quad i\hbar \frac{d a_m(t)}{dt} = \lambda \sum_n \langle m | H_1(t) | n \rangle e^{i\omega_{mn} t} a_n(t)$$

<u>transition frequency</u> (6) $\omega_{mn} = \dfrac{(\varepsilon_m - \varepsilon_n)}{\hbar}$

Equation (5) is a <u>matrix differential equation</u> with time dependent coefficients. The dimension of the matrix

$$\lambda \langle m | H_1(t) | n \rangle e^{i\omega_{mn} t} \quad \text{is } N \times N$$

where N is the Hilbert space dimension!

Way too large $\Rightarrow$ approximation using smallness of λ

(A) Perturbation expansion

$$(7) \quad a_n(t) = a_n^{(0)}(t) + \lambda a_n^{(1)}(t) + \lambda^2 a_n^{(2)}(t) + \cdots$$

plug into (5) and sort in powers of $\lambda \Rightarrow$ <u>hierarchy</u>

$$i\hbar \frac{d a_m^{(0)}(t)}{dt} = 0 \qquad a_m^{(0)}(t) = a_m^{(0)}(0)$$

$$(8) \quad i\hbar \frac{d a_m^{(1)}(t)}{dt} = \lambda \sum_n \langle m | H_1(t) | n \rangle e^{i\omega_{mn} t} a_n^{(0)}(t)$$

...

$$i\hbar \frac{d a_m^{(\ell+1)}(t)}{dt} = \lambda \sum_n \langle m | H_1(t) | n \rangle e^{i\omega_{mn} t} a_n^{(\ell)}(t)$$

$\boxed{\lambda^1}$ first order solution:

$$(9)\quad a_m^{(1)}(t) = -\frac{i}{\hbar}\lambda \sum_n \int_0^t d\tau \, \overbrace{\langle m | H_1(\tau) | n \rangle}^{\equiv H_{1mn}(\tau)} e^{i\omega_{mn}\tau} \, a_n(0)$$

if $|\psi(0)\rangle = |n\rangle \Rightarrow \quad a_n(0) = 1 \quad a_{n'}(0) = 0 \quad n' \neq n$

$$(10)\quad a_f^{(1)}(t) = -\frac{i}{\hbar}\lambda \int_0^t d\tau \, \langle f | H_1(\tau) | i \rangle e^{i\omega_{fi}\tau}$$

$|f\rangle$: final state $\quad |i\rangle \; (= |n\rangle)$ initial state

With this we can calculate the probability that the state remains in the initial state

$$1 = \langle \psi(t) | \psi(t) \rangle = |a_i(t)|^2 + \underbrace{\sum_{n \neq i} |a_n(t)|^2}_{\mathcal{O}(\lambda^2)}$$

$$(11)\quad p_i(t) = 1 - \mathcal{O}(\lambda^2)$$

probability of initial state only modified in 2nd order of λ

transition probabilities

$$(12)\quad \boxed{c_f^{(1)}(t) = -\frac{i}{\hbar}\int_0^t d\tau \, \lambda H_{1fi}(\tau) \, e^{i\omega_{fi}\tau}}$$

(13) $$\boxed{\begin{aligned} P^{(1)}_{i\to f}(t) &= |C^{(1)}_{fi}(t)|^2 = \\ &= \frac{1}{\hbar^2}\left|\int_0^t d\tau\, \lambda H_{1fi}(\tau)\, e^{i\omega_{fi}\tau}\right|^2 \end{aligned}}$$

$\boxed{\lambda^2}$ <u>second order</u>

(14) $$C_f^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \int_0^t d\tau \int_0^\tau d\tau'\, \lambda^2 \sum_e H_{1fe}(\tau) H_{1ei}(\tau')\, e^{i\omega_{fe}\tau}\, e^{i\omega_{ni}\tau'}$$

(B) Formal time-dependent perturbation theory

<u>interaction picture</u> $\qquad H = H_0 + H_1 \qquad (\lambda = 1)$

(15) $$|\psi_I(t)\rangle \equiv U_I(t,t_0)\,|\psi(t_0)\rangle$$

here H_1 = const. for simplicity

where $U_I(t,t_0) \equiv U_0^{-1}(t,t_0)\, U(t,t_0)$

<u>time evolution operator in the interaction picture</u>

$$U_0(t,t_0) = \exp\left\{-\frac{i}{\hbar} H_0 (t-t_0)\right\}$$ unperturbed time evolution

$$U(t,t_0) = \exp\left\{-\frac{i}{\hbar} H (t-t_0)\right\}$$ total time evolution

- equation of motion in interaction picture

$$\frac{d}{dt}|\psi_I(t)\rangle = \frac{d}{dt}U_I(t,t_0)\,|\psi(t_0)\rangle$$

(16) $$= \underbrace{\left(\frac{d}{dt}U_I(t,t_0)\right)U_I^{-1}(t,t_0)}_{=\,?}\,|\psi_I(t)\rangle$$

$$\frac{dU_I}{dt} = \frac{d}{dt}\left[e^{\frac{i}{\hbar}H_0(t-t_0)}e^{-\frac{i}{\hbar}H(t-t_0)}\right] = \frac{i}{\hbar}H_0U_I - \frac{i}{\hbar}U_IH$$

(17) $$= \frac{i}{\hbar}\left(H_0 - U_IHU_I^{-1}\right)U_I$$

now

$$U_IHU_I^{-1} = e^{\frac{i}{\hbar}H_0(t-t_0)}\underbrace{e^{-\frac{i}{\hbar}H(t-t_0)}He^{\frac{i}{\hbar}H(t-t_0)}}_{=\,H\,=\,H_0+H_1}e^{-\frac{i}{\hbar}H_0(t-t_0)}$$

$$= H_0 + U_0^{-1}H_1U_0 = H_0 + H_{1I}(t)$$

where we have introduced the interaction Hamiltonian in the interaction picture

(18) $$H_{1I}(t) \equiv e^{\frac{i}{\hbar}H_0(t-t_0)}\,H_1\,e^{-\frac{i}{\hbar}H_0(t-t_0)}$$

Note that $H_{1I}(t)$ is in general time-dependent since $[H_0, H_1] \neq 0$ in general

With this we find for the time evolution operator from eq. (17)

$$\boxed{\frac{d}{dt} U_I = -\frac{i}{\hbar} H_{1I}(t)\, U_I} \tag{19}$$

If eq. (19) would be a c-number equation, the solution would simply read

$$U_I(t,t_0) = \exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau\, H_{1I}(\tau)\right\}$$

but this is wrong! since

$$[H_{1I}(t), H_{1I}(t')] \neq 0 \quad \text{in general}$$

Thus we have to be more careful with the solution of (19). For small time steps we find

$$U_I(t+\delta t, t) = \mathbb{1} - \frac{i}{\hbar} H_{1I}(t)\,\delta t \tag{20}$$

Iteration and using the group property

$$U(t_3,t_1) = U(t_3,t_2)\,U(t_2,t_1)$$

$$\Rightarrow U_I(t+2\delta t, t) = U_I(t+2\delta t, t+\delta t)\, U_I(t+\delta t, t)$$

$$= \left(1-\frac{i}{\hbar} H_{1I}(t+\delta t)\,\delta t\right)\left(1-\frac{i}{\hbar} H_{1I}(t)\,\delta t\right)$$

$$= 1 - \frac{i}{\hbar}\left(H_{1I}(t+\delta t) + H_{1I}(t)\right)\delta t$$

$$+ \left(-\frac{i}{\hbar}\right)^2 \underline{H_{1I}(t+\delta t)\, H_{1I}(t)}\, \delta t^2$$

note the order of times!

for N infinitesimal time steps

$$U_I(t+N\delta t, t) = 1 - \frac{i}{\hbar} \sum_{j=0}^{N-1} H_{1I}(t+j\delta t)\, \delta t$$

$$+ \left(-\frac{i}{\hbar}\right)^2 \sum_{j_1=0}^{N-1} \sum_{j_2=0}^{j_1} H_{1I}(t+j_1\delta t)\, H_{1I}(t+j_2\delta t)\, \delta t^2$$

$$+ \cdots$$

now take limit $N \to \infty$ and $N\delta t = T = \text{konst}$

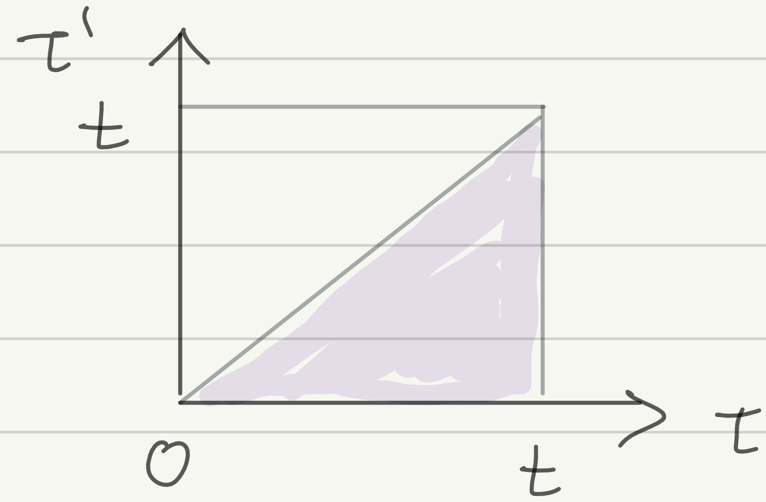
$\Rightarrow$

Dyson series

$$\boxed{\begin{aligned} U_I(t,t_0) = 1 &+ \left(-\frac{i}{\hbar}\right) \int_{t_0}^{t} d\tau\, H_{1I}(\tau) \\ &+ \left(-\frac{i}{\hbar}\right)^2 \int_0^t d\tau \int_0^{\tau} d\tau'\, H_{1I}(\tau)\, H_{1I}(\tau') \\ &+ \left(-\frac{i}{\hbar}\right)^3 \int_0^t d\tau \int_0^{\tau} d\tau' \int_0^{\tau'} d\tau''\, H_{1I}(\tau)\, H_{1I}(\tau')\, H_{1I}(\tau'') \\ &+ \cdots \end{aligned}} \qquad (21)$$

Note that the upper integration limits of the integrals reflect that operators appear in an ordered way defined by their time arguments. Also note that there are no factors $1/2!$, $1/3!$ etc.

second integral



If $[H_{1I}(\tau), H_{1I}(\tau')] = 0$ than

$$\int_{t_0}^{t} d\tau \int_{t_0}^{\tau} d\tau' \, H_{1I}(\tau) H_{1I}(\tau') = \frac{1}{2!} \int_{t_0}^{t} d\tau \int_{t_0}^{t} d\tau' \, H_{1I}(\tau) H_{1I}(\tau')$$

and the Dyson series could be summed up to an exponential function.

Using a formal trick this can be achieved, however, also for non-commuting $H_{1I}(t)$

<u>Def:</u> <u>time-ordering operator</u> T

$$(22) \qquad \boxed{T \hat{A}(t_1) \hat{B}(t_2) = \begin{cases} \hat{A}(t_1) \hat{B}(t_2) & t_1 > t_2 \\ \hat{B}(t_2) \hat{A}(t_1) & t_1 < t_2 \end{cases}}$$

(23) $$\boxed{T^{-1}\hat{A}(t_1)\hat{B}(t_2) = \begin{cases} \hat{B}(t_2)\hat{A}(t_1) & t_1 > t_2 \\ \hat{A}(t_1)\hat{B}(t_2) & t_1 < t_2 \end{cases}}$$

with this we find

(24) $$\boxed{\begin{aligned} U_I(t,t_0) &= T\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau\, H_{1I}(\tau)\right\} \\ U_I^{-1}(t,t_0) &= T^{-1}\exp\left\{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau\, H_{1I}(\tau)\right\} \end{aligned}}$$

Eq. (24) remains correct if $H_1 = H_1(t)$ is time dependent
With (24) time-dependent perturbation theory is just an expansion of the exponential in powers of H_{1I}

(25) $$|\psi_I^{(1)}(t)\rangle = \left[1 - \frac{i}{\hbar}\int_{t_0}^{t} d\tau\, H_{1I}(\tau)\right]|\psi_I(t_0)\rangle$$

(26) $$|\psi_I^{(2)}(t)\rangle = \left[1 - \frac{i}{\hbar}\int_{t_0}^{t} d\tau\, H_{1I}(\tau) + \frac{1}{2!}\left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} d\tau \int_{t_0}^{t} d\tau'\, T H_{1I}(\tau) H_{1I}(\tau')\right]|\psi_I(t_0)\rangle$$

etc.