plug in

$$E_{fs}^{(1)} = \frac{E_n^2}{2mc^2}\left[3 - \frac{4n}{j+\frac{1}{2}}\right] \qquad l = j - \frac{1}{2}$$

$$= \frac{E_n^2}{2mc^2}\left[3 - \frac{4n}{j+2}\right] \qquad l = j + \frac{1}{2}$$

Same result!!

$$E_{fs}' = \frac{E_n^2}{2mc^2}\left[3 - \frac{4n}{j+\frac{1}{2}}\right]$$

fs depends on j but not l!

two states with same j but different l degenerate at this order

— split by QED Lamb shift

— idea of Zeeman effect.
Put atom in external mag field
Do pert. theory.

Time-dependent Perturbation Theory

Schrödinger Equation,

$$H \Psi = i\hbar \frac{\partial}{\partial t} \Psi$$

explicitly $H(\vec{r},t)\Psi(\vec{r},t) = i\hbar \frac{\partial}{\partial t}\Psi(\vec{r},t)$

If the potential is independent of time,

$$V(\vec{r},t) \equiv V(\vec{r})$$

the time-dependent part of the wave function can be separated out

$$\Psi(\vec{r},t) = \psi(\vec{r})\, e^{-iEt/\hbar}$$

$\Rightarrow$ time-independent Schrödinger eq.

$$H(\vec{r})\psi(\vec{r}) = E\,\psi(\vec{r})$$

Remarks: ① time-dependence is trivial

② not contribute to the probability $|\Psi|^2$

③ linear combinations of these stationary states may have some time-dependence, but not Energy.

Time-dependent Potential can lead to <u>transitions</u> between different states (energy).

$\Longleftrightarrow$ Quantum dynamics.

Of course, if we can solve the time-dependent Schrödinger equation, we got the answers, and know How the transition between States happens...

However, in most cases, the time-dependent Schrödinger equation is very difficult to solve. We need to use perturbation method to get the approximate results, assuming the time-dependent part of the Hamiltonian is small, Just like the time-independent perturbation theory we have done before:

Example — Two - Level System

Suppose
$$H(t) = H_0 + H'(t)$$

and two states

$$H_0 |\psi_a\rangle = E_a |\psi_a\rangle \qquad H_0 |\psi_b\rangle = E_b |\psi_b\rangle$$
$$\equiv E_a |a\rangle \qquad \equiv E_b |b\rangle$$

with $\langle a | b \rangle = \delta_{ab}$ (orthonormal)

Any state can be expressed as a linear combination of these two states,

$$\Psi = c_a |a\rangle + c_b |b\rangle$$

where $|c_a|^2$ Represents the probability that particle is in state $|a\rangle$,

$$|c_a|^2 + |c_b|^2 = 1 \qquad \text{Normalization.}$$

Extending to time-dependent

$$\Psi(t) = c_a(t) |a\rangle + c_b(t) |b\rangle$$

The time-dependence of the wave function is represented by the time-dependence of the coefficient functions $C_a(t)$ and $C_b(t)$.

More explicitly, we write

$$\boxed{\Psi(t) = C_a(t)\, e^{-iE_a t/\hbar} |a\rangle + C_b(t) e^{-iE_b t/\hbar} |b\rangle}$$

Now, the goal is to solve ~~the~~ functions $C_a(t)$, $C_b(t)$.

Schrödinger equation

$$\hat{H}\Psi(t) = i\hbar\frac{\partial}{\partial t}\Psi(t) \qquad H = H_0 + H'(t)$$

L.H.

$$\Rightarrow \hat{H}\Psi(t) = \left(\hat{H}_0 + \hat{H}'(t)\right)\left[C_a(t) e^{-iE_a t/\hbar}|a\rangle + C_b(t) e^{-iE_b t/\hbar}|b\rangle\right]$$

$$\overset{4\text{ terms}}{=} E_a C_a(t) e^{-iE_a t/\hbar}|a\rangle + E_b C_b(t) e^{-iE_b t/\hbar}|b\rangle$$

$$+ C_a(t) e^{-iE_a t/\hbar}\hat{H}'(t)|a\rangle + C_b(t) e^{-iE_b t/\hbar}\hat{H}'(t)|b\rangle$$

R.H.

$$i\hbar\frac{\partial}{\partial t}\Psi(t) = i\hbar\frac{\partial}{\partial t}\left[C_a(t) e^{-iE_a t/\hbar}|a\rangle + C_b(t) e^{-iE_b t/\hbar}|b\rangle\right]$$

$$\overset{4\text{ terms}}{=} i\hbar\Big[-iE_a/\hbar\; C_a(t) e^{-iE_a t/\hbar}|a\rangle + (-iE_b/\hbar) C_b(t) e^{-iE_b t/\hbar}|b\rangle$$

$$\dot{C}_a(t)\, e^{-iE_a t/\hbar}|a\rangle + \dot{C}_b(t)\, e^{-iE_b t/\hbar}|b\rangle\Big]$$

$$\Rightarrow \dot{C}_a(t) e^{-iE_a t/\hbar} |a\rangle + \dot{C}_b(t) e^{-iE_b t/\hbar} |b\rangle$$

$$= \frac{-i}{\hbar}\left(C_a(t) e^{-iE_a t/\hbar} \hat{H}'(t)|a\rangle + C_b(t) e^{-iE_b t/\hbar} \hat{H}'(t)|b\rangle \right)$$

left product with $|a\rangle$

$$\dot{C}_a(t) = \frac{-i}{\hbar}\left[C_a(t) \langle a|H'(t)|a\rangle + C_b(t) \langle a|\hat{H}'(t)|b\rangle e^{-i(E_b - E_a)t/\hbar} \right]$$

$$= \frac{-i}{\hbar}\left[H'_{aa}(t)\, C_a(t) + H'_{ab}(t)\, e^{-i(E_b - E_a)t/\hbar}\, C_b(t) \right]$$

Similarly.

$$\dot{C}_b(t) = \frac{-i}{\hbar}\left[H'_{ab}(t)\, C_b(t) + H'_{ba}(t)\, e^{-i(E_a - E_b)t/\hbar}\, C_a(t) \right]$$

Comments on the Matrix $H'_{ab}(t)$

① It's time-dependent.

② Hermiticity. $H'_{ab} = (H'_{ba})^*$

③ It Mixes states.

④ $|C_a(t)|^2 + |C_b(t)|^2 = 1$ for any t.

Example:

An electron in a time-dependent Magnetic Field:

$$H(t) = -\gamma \vec{B}(t) \cdot \vec{S}$$

$\vec{S}$ is the spin for the electron

$$\left\{\begin{array}{l} S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \end{array}\right.$$

Suppose the dominant Magnetic field is in z direction,

$H_0 = -\gamma B_0 S_z$ is time-independent.

Eigenstates of H_0 : $|a\rangle = |\uparrow\rangle$, $|b\rangle = |\downarrow\rangle$

$$H_0 |\uparrow\rangle_z = -\frac{\gamma B_0 \hbar}{2} |\uparrow\rangle_z$$

$$H_0 |\downarrow\rangle_z = \frac{\gamma B_0 \hbar}{2} |\downarrow\rangle_z$$

$$E_a = -\frac{\gamma B_0 \hbar}{2} \qquad E_b = \frac{\gamma B_0 \hbar}{2}$$

$$\omega_0 = (E_b - E_a)/\hbar = \gamma B_0$$

Now, we add some perturbation, varying the magnetic field.

A) $B(t)$ in z direction

B) $B(t)$ in x direction

A). $\hat{H}'(t) = -\gamma B_z(t)\,\hat{S}_z$ — self-Mixing.

$$H'_{ab}(t) = 0 = \langle a|\hat{H}'(t)|b\rangle$$
$$= \langle\uparrow|\hat{H}'(t)|\downarrow\rangle = \langle\uparrow|\hat{S}_z|\downarrow\rangle = 0$$

$$H'_{aa} = \langle a|\hat{H}'(t)|a\rangle = \langle\uparrow|\hat{H}'(t)|\uparrow\rangle$$
$$= -\frac{\gamma}{2}B_z(t)\hbar$$

$$H'_{bb} = \frac{\gamma}{2}B_z(t)\hbar$$

$$\dot{C}_a(t) = \frac{-i}{\hbar}H'_{aa}\,C_a(t)$$
$$= \frac{i}{2}\gamma B_z(t)\,C_a(t)$$

$$\Rightarrow \begin{cases} C_a(t) = C_a(0)\,e^{\frac{i}{2}\gamma B_z(t)t/\hbar} \\ C_b(t) = C_b(0)\,e^{-\frac{i}{2}\gamma B_z(t)t/\hbar} \end{cases}$$

$$\Psi(t) = C_a(0)\,e^{\frac{i}{2}\gamma B_z(t)t/\hbar}\,e^{-iE_a t/\hbar}|\uparrow\rangle$$
$$+ C_b(0)\,e^{-\frac{i}{2}\gamma B_z(t)t/\hbar}\,e^{-iE_b t/\hbar}|\downarrow\rangle$$
$$= C_a(0)\,e^{\frac{i}{2}\gamma(B_0+B_z(t))t/\hbar}|\uparrow\rangle + C_b(0)\,e^{-i\frac{\gamma}{2}(B_0+B_z(t))t/\hbar}|\downarrow\rangle$$

i) Check $|C_a(t)|^2 + |C_b(t)|^2 = 1$

ii) if $C_a(0) = 1$ $C_b(0) = 0$

$|C_a(t)| = 1$ $C_b(0) = 0$.

No transition.

iii) $\langle S_z \rangle = \langle \psi(t) | \hat{S}_z | \psi(t) \rangle$

$$= |C_a(t)|^2 \langle a | \hat{S}_z | a \rangle - |C_b(t)|^2 \langle b | \hat{S}_z | b \rangle$$
$$= \left(|C_a(0)|^2 - |C_b(0)|^2\right) \frac{\hbar}{2}$$

is independent of time.

iv) Energy $\langle E \rangle = \langle \psi(t) | \hat{H} | \psi(t) \rangle$

$$= |C_a(t)|^2 \langle a | \hat{H} | a \rangle + |C_b(t)|^2 \langle b | \hat{H} | b \rangle$$
$$= |C_a(0)|^2 \left(-\frac{\gamma}{2}(B_0 + B_z(t))\hbar\right) + |C_b(0)|^2 \left(\frac{\gamma}{2}(B_0 + B_z(t))\hbar\right)$$
$$= \left(|C_b(0)|^2 - |C_a(0)|^2\right)\left(\frac{\gamma}{2} B_0 \hbar + \frac{\gamma}{2} B_z(t)\hbar\right)$$

depends on time, but the dependence is trivial.

2) $H'(t) = -\gamma B_x(t)\,\hat{S}_x$

$$H'_{aa} = -\gamma B_x(t)\,\langle a|\hat{S}_x|a\rangle = -\gamma B_x(t)\langle\uparrow|\hat{S}_x|\uparrow\rangle = 0$$

$$H'_{bb} = 0$$

$$H'_{ab} = -\gamma B_x(t)\,\langle\uparrow|\hat{S}_x|\downarrow\rangle = -\frac{\gamma\hbar}{2}B_x(t) = H'_{ba}(t)$$

$$\dot{C}_a(t) = \frac{-i}{\hbar}\,H'_{ab}(t)\,e^{i(E_b-E_a)t/\hbar}\,C_b(t)$$

$$= \frac{i}{2}\gamma B_x(t)\,e^{-i(E_b-E_a)t/\hbar}\,C_b(t)$$

$$\begin{cases} \dot{C}_a(t) = \frac{i}{2}\gamma B_x(t)\,e^{-i\gamma B_0 t}\,C_b(t) \\ \dot{C}_b(t) = \frac{i}{2}\gamma B_x(t)\,e^{i\gamma B_0 t}\,C_a(t) \end{cases}$$

This is a more general case, ~~that the~~ and it is difficult to solve exactly.

We need to do perturbation.

Time-dependent perturbation theory

We have the case, $H'_{aa} = 0 = H'_{bb}$ but $H'_{ab} \neq 0$.

$$\begin{cases} \dot{C}_a(t) = -\frac{i}{\hbar} H'_{ab}(t) e^{-i(E_b - E_a)t/\hbar} C_b(t) \\ \dot{C}_b(t) = -\frac{i}{\hbar} H'_{ba}(t) e^{-i(E_a - E_b)t/\hbar} C_a(t) \end{cases}$$

define $\omega_0 = E_b - E_a$.

Suppose at $t=0$, $C_a(0) = 1$, $C_b(0) = 0$.

0) Zeroth order

$H' = 0$, $H'_{ab} = 0$,

$C_a(t) = 1$ $C_b(t) = 0$ for any t.

1) First Order,

Substitute zeroth order result to the right hand sides of the equations,

$$\begin{cases} \dot{C}_a(t) = 0 \Rightarrow C_a(t) = 1 \\ \dot{C}_b(t) = -\frac{i}{\hbar} H'_{ba}(t) e^{+i\omega_0 t} \end{cases}$$

$$\boxed{C_b(t) = -\frac{i}{\hbar}\int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt'}$$

2) Second order:

Substitute the first order results to the right hand sides of the equations

$$\begin{cases} \dot{C}_a(t) = -\frac{i}{\hbar} H'_{ab}(t) e^{-i\omega_0 t} \left[-\frac{i}{\hbar} \int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt' \right] \\ \dot{C}_b(t) = -\frac{i}{\hbar} H'_{ba}(t) e^{i\omega_0 t} \end{cases}$$

is the same as the first order.

$$\Rightarrow \begin{cases} C_a(t) = 1 - \frac{1}{\hbar^2} \int_0^t H'_{ab}(t') e^{-i\omega_0 t'} \left[\int_0^{t'} H'_{ba}(t'') e^{i\omega_0 t''} dt'' \right] dt' \\ C_b(t) = C_b(t) \text{ at first order} \end{cases}$$

⋮

N). Nth order.

Substitute the (N-1)th order results to the right hand sides of the equations.

⇒ get the Nth order results are integrals of (N-1)th results

Remarks: ① order by order

② Ca is modified by even order
Cb is modified by odd order

(3) Although for every order

$$|C_a(t)|^2 + |C_b(t)|^2 \neq 1$$

For every power of H', $|C_a(t)|^2 + |C_b(t)|^2 = 1$

e.g. Zero power of H'

$C_a(t) = 1$ $\qquad C_b(t) = 0$ $\qquad$ correct.

~~one~~ power of H',

none.

two power of H',

$$|C_a(t)|^2 + |C_b(t)|^2$$

$$= 1 - \frac{2}{\hbar^2}\int_0^t H_{ab}(t')e^{-i\omega_0 t'}\left[\int_0^{t'} H'_{ba}(t'')e^{i\omega_0 t''}dt''\right]dt'$$

$$+ \frac{1}{\hbar^2}\left(\int_0^t H'_{ba}(t')e^{-i\omega_0 t'}dt'\right)^2$$

$$+ \frac{1}{\hbar^2}\int_0^t H'_{ba}(t')e^{-i\omega_0 t'}dt' \int_0^t H'_{ab}(t')e^{i\omega_0 t'}dt'$$

$= 1$ $\qquad$ correct.

Back to our example.

$$\begin{cases} \dot{C}_a(t) = \frac{i}{2}\gamma B_x(t)\, e^{-i\gamma B_0 t}\, C_b(t) \\ \dot{C}_b(t) = \frac{i}{2}\gamma B_x(t)\, e^{i\gamma B_0 t}\, C_a(t) \end{cases}$$

initial state is spin up. $|+\rangle$, like ground state

$C_a(0) = 1$ $\quad C_b(0) = 0$

Zeroth order: $C_a(t) = 1$ $\quad C_b(t) = 0$

First order: $C_a(t) = 1$

$$C_b(t) = \frac{i}{2}\gamma \int_0^t B_x(t')\, e^{i\gamma B_0 t'}\, dt' \neq 0$$

(transition ~~from~~ spin up state to spin down state)

Second order

$$C_a(t) = 1 - \frac{\gamma^2}{4}\int_0^t B_x(t')\, e^{-i\gamma B_0 t'}\, dt' \left[\int_0^{t'} B_x(t'')\, e^{i\gamma B_0 t''}\, dt''\right] dt'$$

$$C_b(t) = \frac{i}{2}\gamma \int_0^t B_x(t')\, e^{i\gamma B_0 t'}\, dt'$$

Simple case, if $B_x(t) = \alpha\, \delta(t - t_0)$

to the first order $C_a(t) = 1$.

$$C_b(t) = \begin{cases} 0 & t < t_0 \\ \frac{i}{4}\gamma\alpha\, e^{i\gamma B_0 t_0} & t = t_0 \text{ (?) Step function} \\ \frac{i}{2}\gamma\alpha\, e^{i\gamma B_0 t_0}, & t > t_0 \end{cases}$$

Now, if we mesure the spin of the electron along the $\hat{z}$ direction, it has $\frac{1}{4}\alpha^2\gamma^2$ chance with $S_z = -\frac{1}{2}\hbar$.

for $t > t_0$

$$\langle S_z \rangle = \left(|C_a(t)|^2 - |C_b(t)|^2 \right) \frac{\hbar}{2}$$

$$= \left(1 - \frac{1}{4}\gamma^2\alpha^2\right)\hbar/2 \quad (?)$$

$$= \left(|C_a(t)|^2 + |C_b(t)|^2 - 2|C_b(t)|^2 \right) \frac{\hbar}{2}$$

$$= \left(1 - \frac{1}{2}\gamma^2\alpha^2 \right) \frac{\hbar}{2} + o(\alpha^2)$$

and the energy.

$$\langle E \rangle = \langle H \rangle = \langle H_0 + H' \rangle$$

$$= \langle -\gamma B_0 \hat{S}_z - \gamma\alpha\,\cancel{\delta(t-t_0)\hat{S}_x} \rangle$$

$$= -\gamma B_0 \langle S_z \rangle = -\frac{\gamma B_0}{2}\hbar \left(1 - \frac{1}{2}\gamma^2\alpha^2\right) + o(\alpha^2)$$

Sinusoidal Perturbation

This is the most interesting case.

Suppose the perturbation has sinusoidal time dependence

$$H'(r,t) = V(r)\cos(\omega t)$$

$$\Rightarrow \quad H'_{ab}(t) = V_{ab}\cos(\omega t)$$

$$V_{ab} = \langle a | V | b \rangle$$

To the first order accuracy,

$$C_a(t) = 1$$

$$C_b(t) = -\frac{i}{\hbar}\int_0^t H'_{ab}(t)\, e^{i\omega_0 t'}\, dt'$$

$$= -\frac{i}{\hbar} V_{ab}\int_0^t \cos\omega t\ e^{i\omega_0 t'}\, dt'$$

$$= -\frac{i}{2\hbar} V_{ab}\int_0^t \left[e^{i(\omega_0+\omega)t'} + e^{+i(\omega_0-\omega)t'}\right] dt'$$

$$= \frac{V_{ab}}{2\hbar}\left[\cancel{\frac{1-e^{i(\omega_0+\omega)t}}{\omega_0+\omega}} + \frac{1-e^{+i(\omega_0-\omega)t}}{\omega_0-\omega}\right]$$

if ω is close to ω_0, drop the first term

$$= \frac{V_{ab}}{2\hbar}\ \frac{e^{-i(\omega_0-\omega)t/2} - e^{i(\omega_0-\omega)t/2}}{\omega_0-\omega}\ e^{i(\omega_0-\omega)t/2}$$

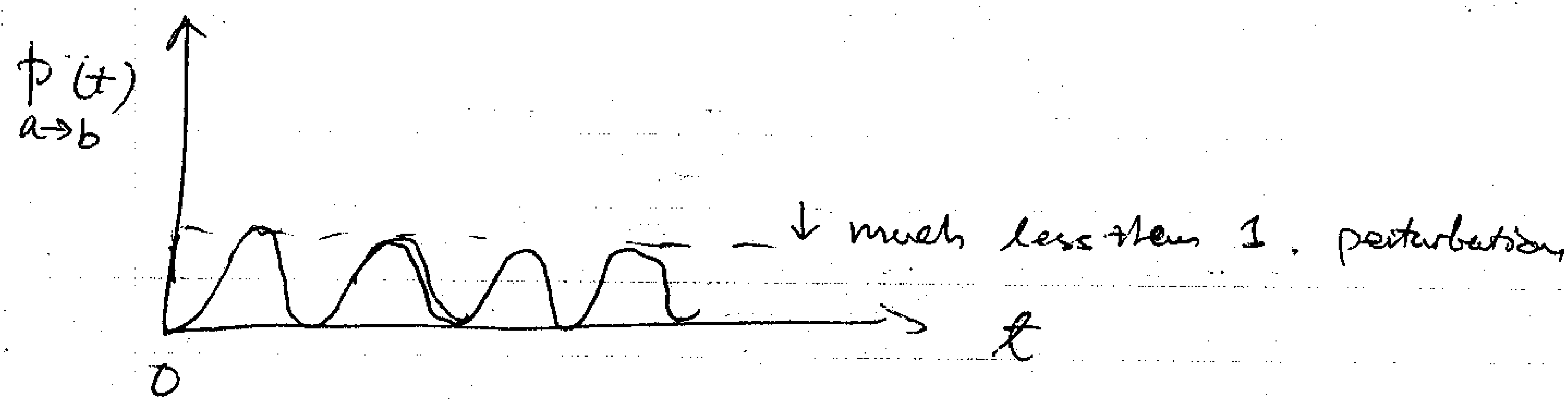
$$c_b(t) = -\frac{V_{ab}}{\hbar}\, i\, \frac{2i \sin(\omega_0-\omega)t/2}{\omega_0-\omega}\, e^{i(\omega_0-\omega)t/2}$$

which is a sinusoidal function.

The probability of the transition from $|a\rangle$ to $|b\rangle$

$$\boxed{P_{a\to b}(t) = \left(\frac{V_{ab}}{\hbar}\right)^2 \frac{\sin^2(\omega_0-\omega)t/2}{(\omega_0-\omega)^2}}$$

It oscillates sinusoidally as a function of time



Remarks:

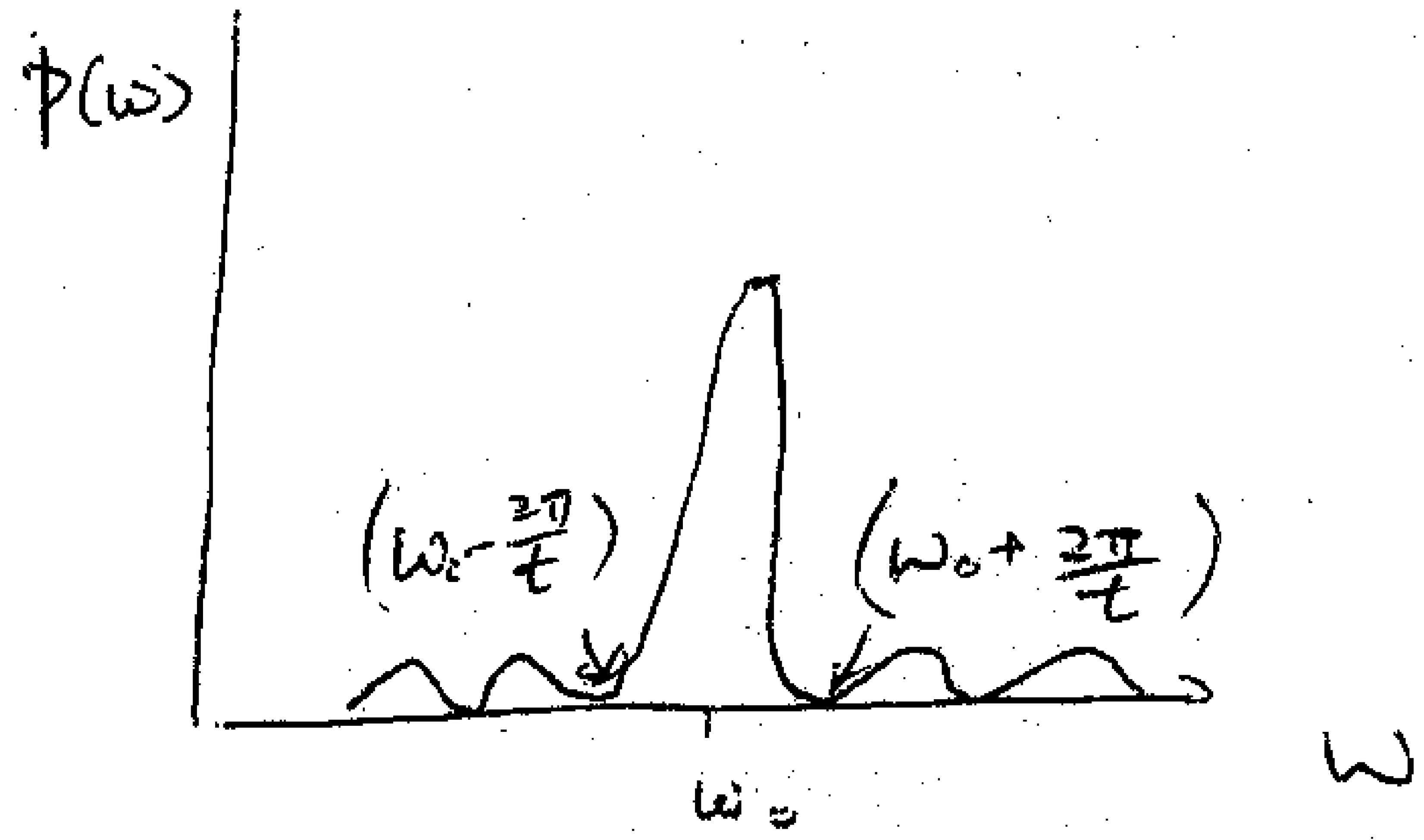
① $P_{a\to b}$ must be much less than 1

② $t_n = \frac{2n\pi}{|\omega_0-\omega|}$, $P_{a\to b} = 0$

③ $P_{a\to b}(t)$ as a function of ω

Peaks at $\omega = \omega_0$ with $\left(\frac{V_{ab}}{2\hbar} t\right)^2$ height

width $4\pi/t$.



Since perturbation works only for $P_{a\to b} < 1$, t must be small.

Back to our example, electron in a time-dependent magnetic field

$$H = -\gamma B_0 \hat{S}_z - \gamma B_x(t)\hat{S}_x$$

assume $B_x(t) = \alpha \cos\omega t$, α is a small parameter

at $t=0$, $C_a(0) = 1$, $C_b(0) = 0$

$$\psi(t=0) = |\psi_a\rangle = |\uparrow\rangle_z$$

First order perturbation.

$$C_a(t) = 1$$

$$C_b(t) = \frac{-i}{\hbar}\int_0^t H'_{ab}(t')\, e^{i\omega_0 t'}\, dt'$$

$$H'(t) = -\gamma B_x(t)\hat{S}_x = -\gamma \hat{S}_x \, \alpha \cos\omega t .$$

$$H'_{aa} = 0 = H'_{bb}$$

$$H'_{ab} = -\frac{\hbar\gamma\alpha}{2}\cos\omega t = V_{ab}\cos\omega t$$

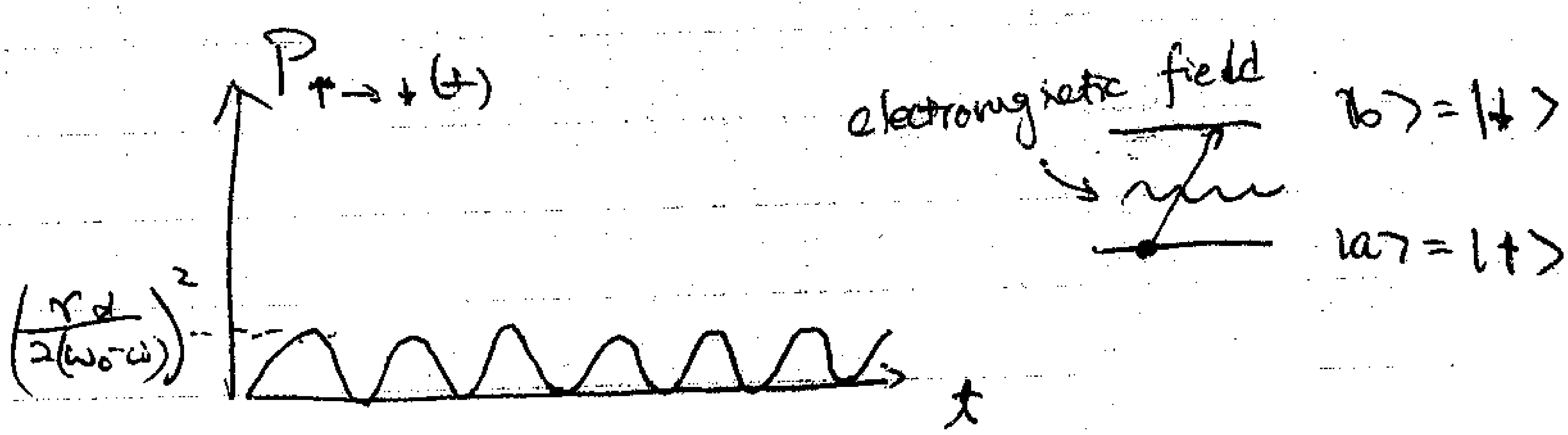
$$\Rightarrow \quad C_b(t) = -i\,\frac{V_{ab}}{\hbar}\,\frac{\sin(\omega_0-\omega)t/2}{\omega_0-\omega}\,e^{i(\omega_0-\omega)t/2}$$

$$= i\,\frac{\gamma\alpha}{2}\,\frac{\sin(\omega_0-\omega)t/2}{\omega_0-\omega}\,e^{i(\omega_0-\omega)t/2}$$

$$\omega_0 = \gamma B_0$$

$$P_{a\to b}(t) = |C_b(t)|^2$$

$$= \left(\frac{\gamma\alpha \sin(\omega_0-\omega)t/2}{2(\omega_0-\omega)}\right)^2$$



Underlying Physics : Absorbing radiation.

Limitation of treatment in book

- two levels
- $\langle a|H'|a\rangle = \langle b|H'|b\rangle = 0$

o.k. for probabilities at 1st order

more general treatment better done formally

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

now in general

$$|\Psi(t)\rangle = \hat{u}(t)\,|\Psi(0)\rangle$$

unitary (time evolution op)

why?

so

$$\hat{H}\,\hat{u}(t)\,|\Psi(0)\rangle = i\hbar\frac{\partial}{\partial t}u(t)\,|\Psi(0)\rangle$$

true for all $|\Psi(0)\rangle$ so as

operator $\hat{H}\,\hat{u}(t) = i\hbar\frac{\partial}{\partial t}\hat{u}(t)$

cute factoid — all of Q.M. is expressed in terms of matrix elements all else is unphysical (eg. wavefunction)

consider $|\Psi(t)\rangle = \hat{U}(t)\,|\Psi(0)\rangle$
$|\phi(t)\rangle = \hat{U}(t)\,|\phi(0)\rangle$

what is

$$\langle\Psi(t)|\,\hat{A}\,|\phi(t)\rangle$$

~~[illegible]~~ now I can think of this in two ways

Schrödinger picture is as written
$\hat{A}$ is time-independent
states are time-dependent

but

$$\langle\Psi(t)|\hat{A}\,|\phi(t)\rangle = \langle\Psi(0)|\,\hat{U}^{\dagger}(t)\,\hat{A}\;U(t)\,|\phi(0)\rangle$$

define $\hat{A}_H$ (Heisenberg rep) as

$$\hat{A}_H = \hat{U}^{\dagger}(t)\,\hat{A}\;U(t)$$

Now we have

$$\langle \psi(t) | \hat{A} | \phi(t) \rangle = \langle \psi(0) | \hat{A}_H(t) | \phi(0) \rangle$$

Heisenberg picture
- wave functions time independent
- all time evolution is in operators

simple case: $\hat{H}$ is time independent

$$\hat{H} \hat{u}(t) = i\hbar \frac{\partial}{\partial t} \hat{u}(t)$$

formal solution $\hat{u} = e^{-i\hat{H}t/\hbar}$ what does this mean

proof plug & chug.

Now this is very simple in eigenbasis of $\hat{H}$.

$$\hat{H}|\psi_i\rangle = E_i |\psi_i\rangle$$

$$\langle \psi_j | \hat{u} | \psi_i \rangle = \delta_{ji} \, e^{-iE_i t/\hbar}$$

$$\begin{pmatrix} e^{-iE_1 t/\hbar} & & \\ & e^{-iE_2 t/\hbar} & \\ & & \ddots \end{pmatrix}$$

Note this does not work if $\hat{H}$ is time-independent why?

Heisenberg picture is like using a time-dependent basis

Schrödinger

$\langle \Psi(t) | \hat{A} | \phi(t) \rangle =$

$\langle \Psi(t) | U U^{+} \hat{A} U U^{+} | \phi(t) \rangle =$

$(\langle \Psi(t) | U)(U^{+} \hat{A} U)(U^{+} | \phi(t) \rangle)$ note $U^{+} | \phi(t) \rangle = | \phi(0) \rangle = | \phi \rangle_H$

${}_H\langle \phi | \hat{A}_H | \phi \rangle_H$

Now suppose $\hat{H} = \hat{H}_0 + \hat{H}'$ with H_0 time independent

let us define $\hat{U}_0 = e^{-i\hat{H}_0 t/\hbar}$

any matrix element may be written as

$\langle \Psi(t) | \hat{A} | \phi(t) \rangle = \langle \Psi(t) | U_0 U_0^{+} \hat{A} U_0 U_0^{+} | \phi(t) \rangle$

$= {}_I\langle \Psi | \hat{A}_I(t) | \phi \rangle_I$ interaction picture suitable for td pert theory

with $\hat{A}_I = U_0^{+}(t) \hat{A} U_0(t)$

and $|\phi\rangle_I = U_0^{+}(t) | \phi \rangle$

Removes the time-dependence due to H_0 for $|\Psi\rangle$ but leaves time-dependence due to $\hat{H}'$

Now let us find time evolution of $|\Psi\rangle_I$ ie. $|\Psi\rangle$ in interaction rep

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle_I = i\hbar \frac{\partial}{\partial t} U_0^+(t) |\Psi\rangle$$

$$= i\hbar \left(\frac{d\hat{U}_0^+}{dt}\right) |\Psi\rangle + i\hbar\, U_0^+ \frac{\partial |\Psi\rangle}{dt}$$

but $i\hbar \frac{d\hat{U}_0}{\partial t} = \hat{H}_0 U_0$

so

$$-i\hbar \frac{d\hat{U}_0^+}{dt} = U_0^+ \hat{H}_0$$

and $i\hbar \frac{\partial |\Psi\rangle}{dt} = \hat{H} = \hat{H}_0 + \hat{H}'$

so

$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle_I = - U_0^+ \hat{H}_0 |\Psi\rangle + \hat{U}_0^+ (H_0 + H') |\Psi\rangle$$

$$= U_0^+ H' |\Psi\rangle$$

$$= U_0^+ H' U_0 \quad U^+ |\Psi\rangle$$

$$= H_I' |\Psi\rangle_I$$

so form of Schrödinger in interaction picture is same as usual with H_I' playing role Hamiltonian

so

$$|\Psi(t)\rangle_I = U_I(t)\,|\Psi(0)\rangle_I = U_I(t)\,|\Psi(0)\rangle$$

Now solving for $U_I(t)$ gives the <u>full</u> time evolution since

$$U_0^\dagger(t)\,|\Psi(t)\rangle = |\Psi(t)\rangle_I$$

or

$$|\Psi(t)\rangle = U_0(t)\,|\Psi(t)\rangle_I$$

$$= U_0(t)\,U_I(t)\,|\Psi(0)\rangle$$

Now let us solve for $U_I(t)$ perturbatively

so

$$i\hbar \frac{\partial}{\partial t} U_I(t)\,|\Psi(0)\rangle_I = H_I'\;U_I(t)\,|\Psi(0)\rangle_I$$

true for all $|\Psi(0)\rangle_I$ so

$$\boxed{i\hbar \frac{\partial}{\partial t} U_I = H_I'\,U_I}$$

Now we can solve for $\mathcal{U}_I$ perturbatively quite easily.

say that $H_I' \to \lambda H_I'$ and count powers of λ

$$\hat{\mathcal{U}}_I = \mathbb{1} + \lambda \hat{\mathcal{U}}_I^{(1)} + \lambda^2 \hat{\mathcal{U}}_I^{(2)} + \lambda^3 \mathcal{U}_I^{(3)} + \cdots$$

$\uparrow$ if $H_I = 0$ $\quad \mathcal{U}_I = \mathbb{1}$

$$\lambda \hat{H}_I' \left(\mathbb{1} + \lambda \hat{\mathcal{U}}_I^{(1)} + \lambda^2 \hat{\mathcal{U}}_I^{(2)} + \cdots\right) = i\hbar \frac{\partial}{\partial t}\left(\mathbb{1} + \lambda \hat{\mathcal{U}}_I^{(1)} + \lambda^2 \hat{\mathcal{U}}_I^{(2)} + \cdots\right)$$

so

$$\lambda^1 : \quad \hat{H}_I = i\hbar \frac{\partial \hat{\mathcal{U}}_I^{(1)}}{\partial t}$$

$$\hat{H}_I \hat{\mathcal{U}}_I^{(1)} = i\hbar \frac{\partial \hat{\mathcal{U}}_I^{(2)}}{\partial t}$$

$$\vdots$$

$$\hat{H}_I \hat{\mathcal{U}}_I^{(n)} = i\hbar \frac{\partial \hat{\mathcal{U}}_I^{(n+1)}}{\partial t}$$

so $\mathcal{U}_I^{(1)} = \frac{-i}{\hbar}\int_0^t dt' \, \hat{H}_I(t')$ integrate 1st term

$$\mathcal{U}_I^{(2)} = \frac{-i}{\hbar}\int_0^t dt'' \, H_I(t'') \, \mathcal{U}_I^{(1)}(t'') = \left(\frac{-i}{\hbar}\right)^2 \int_0^t dt'' \, \hat{H}_I(t'') \int_0^{t''} dt' \, \hat{H}_I(t')$$

$$\mathcal{U}_I^{(n)} = \frac{-i}{\hbar}\int_0^t dt''' \, H_I(t''') \, \mathcal{U}_I^{(2)}(t''') = \left(\frac{-i}{\hbar}\right)^3 \int_0^t dt''' \, H_I(t''') \int_0^{t'''} dt'' \, H_I(t'') \int_0^{t''} dt' \, H_I(t')$$

Two level system

$\langle a|H'|a\rangle = \langle b|H'|b\rangle = 0$

$H' = V \cos(\omega t)$

$$P_{a\to b} = \frac{|V_{ab}|^2}{\hbar^2} \frac{\sin^2[(\omega_0 - \omega)t/2]}{(\omega-\omega_0)^2} \qquad \text{(1st order)}$$

derived previously

answer is time-dependent.
sensible to look at time average

$$\overline{P}_{a\to b} = \frac{1}{2\hbar^2} \frac{|V_{ab}|^2}{(\omega-\omega_0)^2}$$

- gives a way to measure mag. of V_{ab}

- big for $\omega \approx \omega_0$ why?
relation to photon

what if $w = w_0$: blows up!
clearly this is wrong
why - 1^{st} order pert ~~started~~ theory
breaks down then even for small V_{ab}

when is 1^{st} order o.k.

for $\overline{P_{a\to b}} << 1$

when $w = w_0$ does 1^{st} order pert always fail?

yes for $\overline{P_{a\to b}}$

but $P_{a\to b}(t)$ is o.k. for small time

$$P_{a\to b}(t) = \frac{|V_{ab}|^2}{\hbar^2} \frac{\sin^2\left((w_0 - w)t/2\right)}{(w - w_0)^2}$$

suppose $(w-w_0)\frac{t}{2} << $
$\sin\left((w-w_0)\frac{t}{2}\right) \approx (w-w_0)\frac{t}{2}$

$$\approx \frac{|V_{ab}|^2}{\hbar^2} \frac{(w-w_0)^2 \frac{t^2}{4}}{(w-w_0)^2}$$

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

this is o.k for $P_{a\to b}(t) \ll 1$

i.e for $t \ll \frac{4\hbar^2}{|V_{ab}|^2}$

actually even when ω different from ω_0
$P_{ab}(t)$ eventually becomes bad
but $\overline{P}_{ab}$ is still O.k. why.

Key issue is time scale

Now this suggests another type of approximation method instead of looking at size of perturbation look at its speed — how fast H' changes

~~[illegible]~~

Fast or slow compared to what?

τ is time scale over which H' changes ~ eg $e^{-t/\tau}$ $\sin\left(\frac{2\pi t}{\tau}\right)$ etc.

issue is $(E_a - E_b)/\hbar \gg \tau^{-1}$
or $(E_a - E_b)/\hbar \ll \tau^{-1}$

for all a, b

first case : $(E_a - E_b)/\hbar >> T^{-1}$ is the ~~non adiabatic~~ addiabatic regime

$(E_a - E_b)/\hbar << T^{-1}$ is the ~~nonadiabatic~~ sudden regime

typical problem $\hat{H}(t)$ starts at $\hat{H}_i$ and ends at $\hat{H}_f$

$\hat{H}(t=-\infty) = \hat{H}_i$
$\hat{H}(t=+\infty) = \hat{H}_f$

with $\hat{H}_i \neq \hat{H}_f$

Now in this case it is not always clear what basis to work in the eigen basis of $\hat{H}_i$ or $\hat{H}_f$ or what

e.g. we have an atom in its ground state and turn on a mag field sudden approx is simple:

if $\hat{H}$ changes from $\hat{H}_i$ to $\hat{H}_f$ more rapidly the all time scales it the problem $\left(\frac{\hbar}{E_i - E_k} \gg T'\right)$ then wave function has no time to change during switch from $\hat{H}_i$ to $\hat{H}_f$

call the time of switch, $t_0 > 0$)

equation of motion

$$\hat{H}_i |\Psi\rangle = i\hbar \frac{\partial}{\partial t} |\Psi\rangle \quad \text{for} \quad t < t_0$$

$$\hat{H}_f |\Psi\rangle = i\hbar \frac{\partial}{\partial t} |\Psi\rangle \quad \text{for} \quad t > t_0$$

solution

$$|\Psi(t)\rangle = e^{-i\hat{H}_i t/\hbar} |\Psi(0)\rangle \quad \text{for} \quad t < t_0$$

$$|\Psi(t)\rangle = e^{-i\hat{H}_f (t-t_0)} e^{-i\hat{H}_i t_0} |\Psi(0)\rangle \quad \text{for} \quad t > t_0$$

Note $e^{-i\hat{H}_f(t-t_0)} e^{-i\hat{H}_i t_0} \neq e^{-i(\hat{H}_f(t-t_0) + \hat{H}_i t_0)/\hbar}$

unless $[\hat{H}_f, \hat{H}] = 0$

in practice the way to do this is to work in $\hat{H}_i$ basis's for $t < t_0$ and $\hat{H}_f$ basis's for $t > t_0$

eg β decay problem on exam

Now this is intellectually easy to understa. what about the opposite limit the slow or addiabatic limit

$$\tau >> \frac{\hbar}{|E_a - E_b|} \quad \text{for all } a, b$$

basic idea is quite simple

adibatic limit is opposite

Claim: in adiabatic limit state remains in an eigenstate of time local H if it began in one and phase evolves according to time dependent $\hat{H}$

$$|\Psi(t)\rangle = e^{i\phi(t)} |\Psi_i(t)\rangle \quad \text{where} \quad \hat{H}(t)|\Psi_i\rangle = E_i(t)|\Psi_i(t)\rangle$$

$$\phi(t) = -\int_0^t dt' \frac{E_i(t')}{\hbar}$$

intuitive argument:

to make a transition need Fourier components $\sim \frac{\Delta E}{\hbar}$

but as $f(t) \to f(t/\lambda)$ stretches out as $\lambda \to \infty$

$$\tilde{f}(\omega) \to \tilde{f}(\lambda\omega)$$ Fourier spectrum gets squeezed

as $\lambda \to \infty$ no Fourier compents of an size comprable to ΔE

system must stay in "same" state with level itself slowly evolving

Example

$$H(t) = -\frac{\hbar\omega_1}{2}\begin{pmatrix} 0 & e^{-i\omega t} \\ e^{+i\omega t} & 0 \end{pmatrix} \qquad \text{mag. field rotating}$$

B field with $\omega_1 = \gamma |B|$

and $\vec{B} = |B|\left(\hat{x}\cos(\omega t) + \hat{y}\sin(\omega t)\right)$

Exact Solution

$$H\chi = i\hbar\dot{\chi}$$

Claim
$$\chi(t) = \begin{pmatrix} \frac{1}{\sqrt{2}}e^{-i\omega t/2}\left(\cos(\lambda t/2) + i\frac{(\omega_1+\omega)}{\lambda}\sin(\lambda t/2)\right) \\ \frac{1}{\sqrt{2}}e^{i\omega t/2}\left(\cos(\lambda t/2) + i\frac{(\omega_1-\omega)}{\lambda}\sin(\lambda t/2)\right) \end{pmatrix}$$

$$\lambda = \sqrt{\omega^2 + \omega_1^2}$$

check: plug & chug

at $t=0$ $\quad \chi(0) = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \chi_+^x$

jets look at

$$H(0) = -\hbar\omega_1 S_x$$

$$H\left(t=\frac{\pi}{\omega}\right) = +\hbar\omega_1 S_x$$

let us look at

$$\chi\left(t=\frac{\pi}{\omega}\right) = \begin{pmatrix} \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{2}} & \cos\left(\frac{\lambda}{\omega}\frac{\pi}{2}\right) + \frac{i(\omega_1+\omega)}{\lambda}\sin\left(\frac{\lambda}{\omega}\frac{\pi}{2}\right) \\ \frac{1}{\sqrt{2}} e^{+i\pi/2} & \left(\cos\left(\frac{\lambda}{\omega}\frac{\pi}{2}\right) + \frac{i(\omega_1-\omega)}{\lambda}\sin\left(\frac{\lambda}{\omega}\frac{\pi}{2}\right)\right) \end{pmatrix}$$

first look in sudden limit

$\omega \gg \omega_1$ (why is this sudden)

$$\lambda = \sqrt{\omega^2+\omega_1^2} \approx \omega$$

$$\frac{\omega_1 \pm \omega}{\lambda} \approx \pm 1$$

$$\frac{\lambda}{\omega}\frac{\pi}{2} \approx \frac{\pi}{2}$$

so

$$\chi\left(t=\frac{\pi}{\omega}\right) \approx \begin{pmatrix} \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{2}} \left(\cos\left(\frac{\pi}{2}\right) + i\sin\left(\frac{\pi}{2}\right)\right) \\ \frac{1}{\sqrt{2}} e^{+i\pi/2} \left(\cos\left(\frac{\pi}{2}\right) - i\sin\left(\frac{\pi}{2}\right)\right) \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} e^{-i\pi/2} e^{+i\pi/2} \\ \frac{1}{\sqrt{2}} e^{-i\frac{\pi}{2}} e^{+i\frac{\pi}{2}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \chi(t=0) \quad \text{as it should}$$

Next look in addibatic limit

$\omega_1 >> \omega$

$\lambda = \sqrt{\omega^2 + \omega_1^2} \approx \omega_1$

$$\frac{\omega_1 \pm \omega}{\lambda} \approx 1$$

so

$$\chi\left(t = \frac{\pi}{\omega}\right) \approx \begin{pmatrix} \frac{i}{\sqrt{2}} e^{-i\frac{\pi}{2}} \left(\cos\left(\frac{\omega_1}{\omega}\frac{\pi}{2}\right) + i\sin\left(\frac{\omega_1}{\omega}\frac{\pi}{2}\right)\right) \\ \frac{i}{\sqrt{2}} e^{+i\frac{\pi}{2}} \left(\cos\left(\frac{\omega_1}{\omega}\frac{\pi}{2}\right) + i\sin\left(\frac{\omega_1}{\omega}\frac{\pi}{2}\right)\right) \end{pmatrix}$$

$$= \begin{pmatrix} -\frac{i}{\sqrt{2}} & e^{i\frac{\omega_1}{\omega}\frac{\pi}{2}} \\ \frac{i}{\sqrt{2}} & e^{i\frac{\omega_1}{\omega}\frac{\pi}{2}} \end{pmatrix}$$

$$= e^{i\left(\frac{\omega_1}{\omega} - 1\right)\frac{\pi}{2}} \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = \chi_{-x}$$

Phase

probability that it is down in x direction is 1 but at t=0 it was 0; with unit probability is switched

Now $H\left(t = \frac{\pi}{\omega}\right)$ has its ground state as down

"Proof" of adiabatic theorem:

$H = H(t)$

$H(t = -\infty) = H_i$

$H(t = +\infty) = H_f$

Now break this path into N section

$H_i \to H_2 \to H_3 \to H_4 \to H_5 \to H_6 \to \cdots H_f$

$\quad t_2 \quad t_3 \quad t_4$

Now suppose enouh pieces so that

$H_j \to H_{j+1}$ is a small perturbation

$H_{j+1} = H_j + H'$ with H' small

$H(t) \approx H_j + \frac{t - t_j}{\Delta t} H'$ higher derivatives neglible

Now time evolution is via pert theory in going from $t_j \to t_{j+1}$

in pert theory suppose at t_j the system is in a given eigenstate of H_j call it the α^{th} state

Now for each segment ordinary pert theory is legit.

for each segment compute

$\Delta\Psi$ via 1st order td pert
and $\delta\Psi_j$ via 1st order time ind pert.

Compare and see that ad. theorem works for each segment. then add up.

Variation Principle

Often we can not solve Schr. eq. exactly and we are interested in finding g.s. of system

Obvious point

$$E_g \leq \langle\Psi|\hat{H}|\Psi\rangle \quad \text{for any } |\Psi\rangle$$

proof $\quad |\Psi\rangle = \sum_i c_i |i\rangle$

$$\langle\Psi|\hat{H}|\Psi\rangle = \sum_i |c_i|^2 E_i \qquad \text{all } E_i \geq E_g$$

$$\text{so } \sum_i |c_i|^2 E_i \geq \sum_i |c_i|^2 E_g \geq E_g$$

to look for E_g try to find $|\Psi\rangle$ for which

$\langle\Psi|\hat{H}|\Psi\rangle$ is smallest duh!

thus $\delta\langle\Psi|\hat{H}|\Psi\rangle = 0$ for any $|\Psi\rangle \to |\Psi\rangle + |\delta\Psi\rangle$ $= 0$
with $\langle\delta\Psi|\Psi\rangle = 0$

Now this can be done in the full space of theory get exact answer or in a <u>limited</u> trial space and get an approximate answer

consider a family of normalized states parameterized by some set of parameters

eg 1 parameter family

$|\psi(\alpha)\rangle$

where

$$\langle x|\psi(\alpha)\rangle = (\alpha\pi)^{-\frac{1}{4}} e^{-\frac{x^2}{2\alpha^2}}$$

Clearly this family of states does not span the entire space but we want to find the state in this family which <u>best</u> approximates the true ground state

impose some variational condition in limited family eg $\delta \langle \Psi(\alpha) | \hat{H} | \Psi(\alpha) \rangle = 0$

eg find value of α which minimize

$\langle \Psi(\alpha) | \hat{H} | \Psi(\alpha) \rangle$ that gives "best" approx to true wavefunction in limited class.

formally

$$\frac{\partial \langle \Psi(\alpha) | \hat{H} | \Psi(\alpha) \rangle}{\partial \alpha} = 0$$

gives equation for α
call solution α_0

$|\Psi(\alpha_0)\rangle$ is approx. wave function

$$E_g^{approx} = \langle \Psi(\alpha_0) | \hat{H} | \Psi(\alpha_0) \rangle$$

How good an approx is it?
well it depends on how close my family of states is true state