

4/25/96

No.

Date

1.

Approximate Methods

Few problems can be solved exactly in Quantum mechanics, $\therefore$ one needs to find approximation methods to solve problems. The followings are the three most common used ones.

A. Variational method.

Principles: $E[\psi] = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$ for any $|\psi\rangle$

$$|\psi\rangle = \sum_n |E_n\rangle \langle E_n | \psi \rangle$$

$$\therefore E[\psi] = \frac{\sum_n E_n |\langle E_n | \psi \rangle|^2}{\sum_n |\langle E_n | \psi \rangle|^2}$$

* $E[\psi] \geq E_0$, $E_0 =$ absolute minimum, $|\psi_0\rangle =$ absolute min point.

* $|E_n\rangle =$ extreme point; any deviation from $|E_n\rangle$ may be

written as $|\psi\rangle = (1+\alpha)|E_n\rangle + |\delta\psi_n\rangle$ $\langle \delta\psi_n | E_n \rangle = 0$

$$\begin{aligned} E[\psi_n] &= \frac{|1+\alpha|^2 E_n + \langle \delta\psi_n | H | \delta\psi_n \rangle}{|1+\alpha|^2 + \langle \delta\psi_n | \delta\psi_n \rangle} \\ &= \frac{E_n \left(1 + \frac{1}{E_n |1+\alpha|^2} \langle \delta\psi_n | H | \delta\psi_n \rangle \right)}{1 + \frac{1}{|1+\alpha|^2} \langle \delta\psi_n | \delta\psi_n \rangle} \\ &= E_n + O[(\delta\psi_n)^2] \end{aligned}$$

i.e., $\left. \frac{\delta E}{\delta \psi_n} \right|_{|\psi\rangle=|E_n\rangle} = 0$, $|E_n\rangle$ is an extreme point.

* Variational method yields more excellent approximation to the actual energy than to the wave function.

$$\therefore \delta E = O[(\psi_n)^2]$$

4/25/96

No.

Date

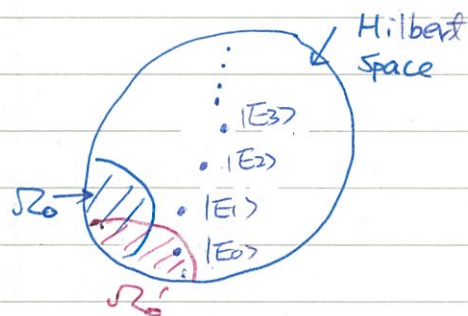
2.

e.g. $|\psi\rangle = |E_0\rangle + \frac{1}{100} |E_1\rangle$ 1% error

$$E[\psi] = \frac{E_0 + \frac{1}{100} \langle E_1 | H | E_1 \rangle}{1 + \frac{1}{100}} = \frac{E_0 + 0.01 E_1}{1.01}$$

$$\simeq 0.99 E_0 + 0.01 E_1, \quad \underline{1\%} \text{ "contamination" from } E_1$$

Scheme



usually, don't know $|E_0\rangle$,

$\therefore$ start from finding as accurately as possible of $|E_0\rangle$

trial wave function $\psi_0(\alpha, \beta, \gamma, \dots)$ by guessing $\alpha, \beta, \gamma, \dots \Rightarrow$ parameters define a subset of the whole Hilbert space as they vary!

Hopefully, Ω_0 covers as close to ψ_0 as possible!

e.g. Ω_0' is definitely better than Ω_0 .

Then, $E[\psi_0(\alpha, \beta, \gamma, \dots)] = f(\alpha, \beta, \gamma, \dots)$

$\Rightarrow$ minimizing: $\frac{\partial f}{\partial \alpha} = 0, \frac{\partial f}{\partial \beta} = 0, \dots \Rightarrow$ at $\alpha = \alpha_0, \beta = \beta_0, \gamma = \gamma_0, \dots$

$\therefore |E_0\rangle \simeq |\psi_0(\alpha_0, \beta_0, \gamma_0, \dots)\rangle$

$E_0 \simeq f(\alpha_0, \beta_0, \gamma_0, \dots), \quad E_0 \leq f(\alpha_0, \beta_0, \gamma_0, \dots)$

* if Ω_0 (as the case of Ω_0') accidentally covers

$|\psi_0\rangle$, then $|E_0\rangle = |\psi_0(\alpha_0, \beta_0, \gamma_0, \dots)\rangle$

$E_0 = f(\alpha_0, \beta_0, \gamma_0, \dots)$

example. $H = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \lambda x^4$, try $\psi_0(x) = e^{-\frac{\alpha x^2}{2}}$

4/25/96

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$$

No.

Date

3.

$$E[\alpha] = \frac{\hbar^2 \alpha}{4m} + \frac{3\lambda}{4\alpha^2}, \quad \text{min at } \alpha_0 = \left(\frac{6m\lambda}{\hbar^2}\right)^{\frac{1}{3}}$$

$$\therefore 0 \leq E_0 \leq E(\alpha_0) = \frac{3}{8} \left(\frac{6\hbar^4 \lambda}{m^2}\right)^{\frac{1}{3}}$$

* $E_1, E_2, E_3, \dots$ excited states

After finding $E(\alpha_0)$, we may want to ^{find} $|E_1\rangle$ & E_1 .

This is achieved by constructing $|\Psi_1(\alpha_1, \beta_1, \delta_1, \dots)\rangle$

such that $\langle \Psi_1(\alpha_1, \beta_1, \dots) | \Psi_0(\alpha_0, \beta_0, \delta_0, \dots) \rangle = 0$

(If $|\Psi_1\rangle$ doesn't satisfy this, we form $|\tilde{\Psi}_1\rangle = |\Psi_1\rangle - |\Psi_0(\alpha_0, \dots)\rangle \langle \Psi_0 | \Psi_1 \rangle$)

Then, minimizing $E[\Psi_1(\alpha_1, \beta_1, \dots)]$ w.r.t. $\alpha_1, \beta_1, \delta_1, \dots$

Similarly, to find $|E_2\rangle$ & E_2 , we construct

$|\Psi_2(\alpha_2, \beta_2, \delta_2, \dots)\rangle$ such that

$$\langle \Psi_2(\alpha_2, \beta_2, \delta_2, \dots) | \Psi_1(\alpha_1^0, \beta_1^0, \delta_1^0, \dots) \rangle = 0$$

↑ ↑ ↑

extreme points

$$\langle \Psi_2(\alpha_2, \beta_2, \delta_2, \dots) | \Psi_0(\alpha_0, \beta_0, \delta_0, \dots) \rangle = 0$$

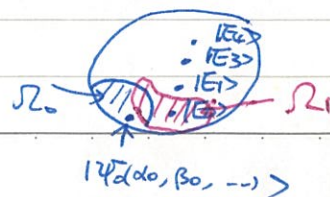
$$\Rightarrow \text{minimizing } E[\Psi_2(\alpha_2, \beta_2, \delta_2, \dots)] = 0.$$

⋮

* Apparently, as we go ^{to} higher states, the error increases too due to uncertainty of $|E_n\rangle$ at each step!

In fact, even at the level of E_1 , the subset formed by $|\Psi_1(\alpha, \beta, \dots)\rangle$ may accidentally cover $|E_0\rangle$, the state thus found does not represent $|\Psi_1\rangle$ at all!

⇒ see over



4/21/98

* Ground State Projection Method

Is there any way to check the guessed ground state / energy good or not?

The answer is yes:

Consider $|\psi^m\rangle = f^m(\hat{H}) |\psi\rangle$

$|\psi\rangle = \text{guessed ground state}$

$= \sum_n a_n |E_n\rangle$

$\therefore |\psi^m\rangle = \sum_n a_n f^m(E_n) |E_n\rangle$

$$\langle \hat{H} \rangle_m = \frac{\langle \psi^m | \hat{H} | \psi^m \rangle}{\langle \psi^m | \psi^m \rangle} = \frac{\sum_n |a_n|^2 |f^m(E_n)|^2 E_n}{\sum_n |a_n|^2 |f^m(E_n)|^2}$$

$$= \frac{\sum_n |a_n|^2 E_n \left| \frac{f^m(E_n)}{f^m(E_0)} \right|^2}{\sum_n |a_n|^2 \left| \frac{f^m(E_n)}{f^m(E_0)} \right|^2}$$

Now, let $m \rightarrow \infty$, if $\left| \frac{f(E_n)}{f(E_0)} \right| < 1, n > 0$

$$\lim_{m \rightarrow \infty} \left| \frac{f^m(E_n)}{f^m(E_0)} \right|^2 \rightarrow 0 \quad \text{for } n \neq 0$$

$$\therefore \lim_{m \rightarrow \infty} \langle \hat{H} \rangle_m = E_0$$

4/21/98

There are many ways to choose $f(H)$.

For example, $f(H) = e^{-\hat{H}}$

$$\left| \frac{f(E_n)}{f(E_0)} \right| = e^{-(E_n - E_0)} < 1$$

$$\left| \frac{f^m(E_n)}{f^m(E_0)} \right| = e^{-m(E_n - E_0)} = e^{-\frac{E_n - E_0}{T}}, \quad T = \frac{1}{m} \rightarrow 0$$

as $m \rightarrow \infty$

Another choice is $f(H) = W - \hat{H}$, $W = \text{some large \#}$

(good if $\hat{H}$ is upper bounded!)

In practice, one can't really go to $m = \infty$. One

always has to stop at some m_0 . In addition to this,

one can show that there is a numerical instability at large m . Therefore, one can't really go to very large m . However, by looking at

the trend of $\langle \hat{H} \rangle_m$, one can see whether

$|\Psi\rangle$ is good or not!

April 8, 1998.

* General variational principle.

What we said above, regarding the fact $|E_n\rangle =$ extreme point, can be stated differently.

The Schrödinger eq. $\hat{H}\psi = E\psi$

can be also obtained from the variational principle

$$\delta \int d\vec{r} \psi^* (\hat{H} - E) \psi = 0$$

$\because \psi = \text{Complex}$, we can vary $\delta\psi$, $\delta\psi^*$ independently, fix ψ we get

$$\delta \int \psi^* (\hat{H} - E) \psi = \int \delta\psi^* [(\hat{H} - E) \psi] = 0$$

$$\therefore (\hat{H} - E) \psi = 0 \quad \dots \quad (1)$$

The variation of ψ , $\delta\psi$, gives

$$\int \psi^* (\hat{H} - E) \delta\psi = \int \delta\psi (\hat{H}^* - E) \psi^* = 0$$

$\hat{H}^* = \text{Hermitian}$

$\int \psi^* \hat{H}^\dagger \delta\psi = \int \psi^* \hat{H} \delta\psi$
 $\hat{H}^\dagger = \hat{H}$

$$\therefore (\hat{H}^* - E) \psi^* = 0 \quad \text{which is identical to (1) !}$$

This can be stated in another way: $(\int \delta\psi^* \hat{H} \psi)^*$

$$\delta \int \psi^* \hat{H} \psi = 0$$

under the condition $\int d\vec{r} \psi^* \psi = 1$

In this case, $E = \text{Lagrangian multiplier}$!

4/8/18.

* If there is no magnetic field, ψ can be chosen to be real as ψ & ψ^* are both solutions to the same E !

In this case
$$\int \psi^* \hat{H} \psi = \int \pi d^3 \vec{r} \left[\sum_i \frac{\hbar^2}{2m_i} \psi \nabla_i^2 \psi + V \psi^2 \right]$$

$$= \int \pi d^3 \vec{r} \sum_i \left[\frac{\hbar^2}{2m_i} (\nabla_i \psi)^2 + V(r_1, \dots, r_N) \psi^2 \right]$$

↑
assume surface terms $\rightarrow 0$

* The min. energy of $\hat{H} \equiv E_0$, $\psi \rightarrow \psi_0 = \text{ground state}$.

$\psi_0 \neq 0$ for all $r_1, r_2, \dots, r_N$ $\rightarrow \psi_0 \neq 0 \Rightarrow \psi_0 = \text{ground state}$

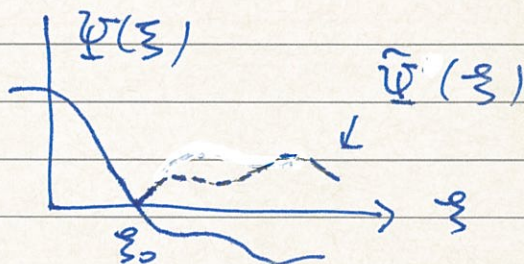
i.e. no node! (rigorous proof $\Rightarrow$ exercise)

Feynman's argument (if $\psi_0 = \text{ground state} \Rightarrow$ no node)

$$\psi_0(x_1, x_2, \dots, \xi, \dots) \equiv \Psi(\xi)$$

$\uparrow \quad \uparrow$
 fixed varied

if $\Psi(\xi)$ has a node $\Rightarrow$



4/8/18.

From $\Psi(x)$, one can form $\tilde{\Psi}(x)$ by reflection of $\Psi(x)$ for $x \geq x_0$

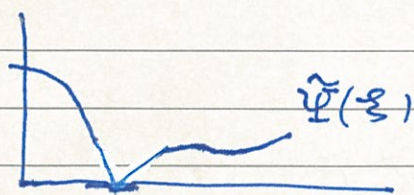
Obviously, $\left(\frac{d\Psi}{dx}\right)^2 = \left(\frac{d\tilde{\Psi}}{dx}\right)^2$

$$\left(\frac{d\Psi}{dx_i}\right)^2 = \left(\frac{d\tilde{\Psi}}{dx_i}\right)^2$$

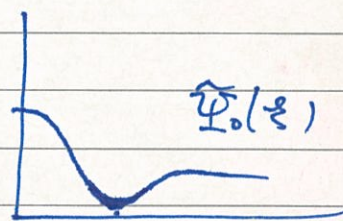
$$\Psi^2 = \tilde{\Psi}^2$$

$$\therefore \int \frac{\hbar^2}{2m} (\partial_i \Psi)^2 + V \Psi^2 = \int \frac{\hbar^2}{2m} (\partial_i \tilde{\Psi})^2 + V \tilde{\Psi}^2$$

$$\therefore E(\Psi) = E(\tilde{\Psi})$$



Smooth



$$|\hat{\Psi}_0(x)|^2 \sim |\tilde{\Psi}(x)|^2$$

$$\text{but } \left(\frac{d}{dx} \hat{\Psi}_0(x)\right)^2 < \left(\frac{d}{dx} \tilde{\Psi}(x)\right)^2 !$$

$$\text{i.e. } E(\hat{\Psi}_0(x)) < E(\tilde{\Psi})$$

* Ψ_0 is non degenerate : $\therefore$ if degenerate

$\Rightarrow \Psi_{01}, \Psi_{02}, \Psi = c_1 \Psi_{01} + c_2 \Psi_{02}$ can have nodes !!

$\therefore$ ground state : real, everywhere positive !

* identical particles:

if orbital part has definite symmetry (no spin-orbit interaction)

$\Rightarrow \psi_0$ must be ^{totally} symmetric; otherwise if

$$\psi_0(\dots r_1, \dots r_2, \dots) = -\psi_0(\dots r_2, \dots r_1, \dots)$$

$$\psi_0 = 0 \text{ when } r_1 = r_2$$

But when $n \geq 3$, for fermions, the

$\uparrow$
of particles $\rightarrow$ mixed symmetry

Spin part can't be ^{totally} antisymmetric, $\therefore$ orbital

part can't be totally symmetric.

$\therefore \psi_0$ to the Schrödinger eq is not admissible!

i.e. the smallest eigenvalue to the Schrödinger eq.

doesn't correspond to ~~the~~ ^{any} real state of identical

fermions (with $n \geq 3$)!

For bosons, however, totally symmetric ^{orbital} state is always possible!

4/25/96

No.

Date

4,

B. Time-independent perturbation theory

Suppose we have known the solutions to a Hamiltonian

$H_0: |n^0\rangle, E_n^0$, we can then use them to approximate

solutions to $H = H_0 + V$ if $V \ll H_0$.

The premise is the change from H_0 to H is not too dramatic!

* In the previous example, $H = \frac{p^2}{2m} + \lambda x^4$, if we take $H_0 = \frac{p^2}{2m}$, the eigenstates of H_0 are free particles (plane waves) which are delocalized, while the eigenstates to H must be localized. The change is so dramatic, so the perturbation theory is not suitable here.

In this case, normally, one tries the variational method since intuitively one knows that $|\psi_0\rangle$ is localized and can guess it at least.

In the case of $V \ll H$, we assume we can expand $|n\rangle$ & E_n , defined by $H|n\rangle = E_n|n\rangle$, as follows

$$|n\rangle = |n^0\rangle + |n^1\rangle + |n^2\rangle + \dots$$

$$E_n = E_n^0 + E_n^1 + E_n^2 + \dots$$

$$\begin{array}{cc} \uparrow & \uparrow \\ O(V) & O(V^2) \end{array}$$

Formally, one can introduce a "coupling" constant λ

such that $H = H_0 + \lambda V$, $0 \leq \lambda \leq 1$, $\lambda = 1$ recovers original problem. For a given λ , we denote the eigenvalues & eigenkets as $E_n(\lambda)$, $|n\rangle_\lambda$.

4/25/96

No.

Date

5.

As we change λ from 0 to 1 ("turn-on" the perturbation), we go from H_0 to $H_0 + V$, and from $|n^0\rangle$ to $|n\rangle$.

The requirement "change not too dramatic" means the changes are continuous w.r.t. λ !
& analytic.

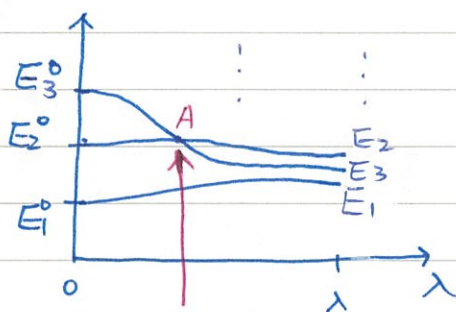
This is completely analogous to the Taylor

$$\text{expansion: } f(x+a) = f(x) + a f'(x) + \frac{a^2}{2!} f''(x) + \dots$$

evaluating in terms of $f(x)$, one requires analyticity of $f(x)$

$$\text{between } x \text{ \& } x+a! \quad E_n(\lambda) = E_n(0) + E_n'(0)\lambda + \frac{E_n''(0)}{2!}\lambda^2 + \dots$$

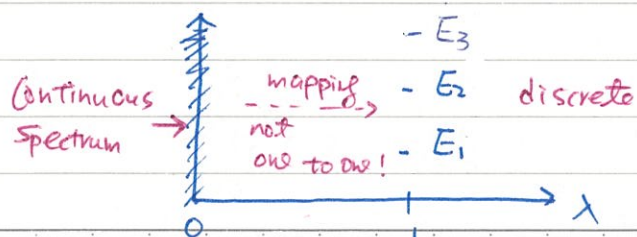
So, if we plot $E_n(\lambda)$, we do not want "level-crossing"



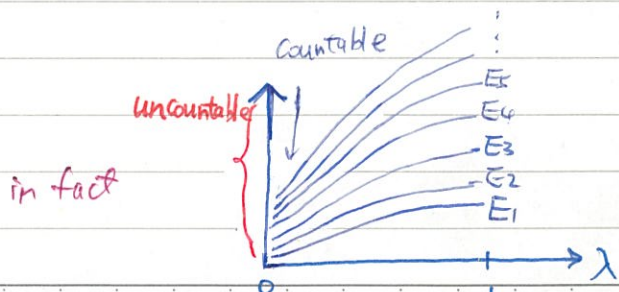
not good, $\frac{dE}{d\lambda}$ not well-defined here.

technically speaking, degenerate at point A.
 (will not happen in 1D!)

The example. $H_0 = \frac{p^2}{2m}$, $V = x^4$. apparently have this problem exactly:



change must not be analytic



$E_n(\lambda)$ not analytic in λ !

4/26/96

No.

Date

1-1

The Hellmann - Feynman theorem:

$H(\lambda)$ be a Hermitian operator (which needs not to be the Hamiltonian) which depends on a real parameter λ .

Let $|\psi(\lambda)\rangle$ be the normalized eigenket of $H(\lambda)$ with eigen value $E(\lambda)$:

$$H(\lambda)|\psi(\lambda)\rangle = E(\lambda)|\psi(\lambda)\rangle, \quad \langle\psi(\lambda)|\psi(\lambda)\rangle = 1$$

$$\Rightarrow \frac{dE(\lambda)}{d\lambda} = \langle\psi(\lambda)| \frac{dH(\lambda)}{d\lambda} |\psi(\lambda)\rangle$$

$$\text{pf: } \frac{dE(\lambda)}{d\lambda} = \frac{d}{d\lambda} \langle\psi(\lambda)| H(\lambda) |\psi(\lambda)\rangle$$

$$= \frac{d\langle\psi(\lambda)|}{d\lambda} H(\lambda) |\psi(\lambda)\rangle$$

$$+ \langle\psi(\lambda)| \frac{dH(\lambda)}{d\lambda} |\psi(\lambda)\rangle + \langle\psi(\lambda)| H(\lambda) \frac{d}{d\lambda} |\psi(\lambda)\rangle$$

$$= E(\lambda) \frac{d\langle\psi(\lambda)|}{d\lambda} |\psi(\lambda)\rangle + \langle\psi(\lambda)| \frac{dH(\lambda)}{d\lambda} |\psi(\lambda)\rangle$$

$$+ E(\lambda) \langle\psi(\lambda)| \frac{d|\psi(\lambda)\rangle}{d\lambda}$$

$$= E(\lambda) \left[\frac{d}{d\lambda} \langle\psi(\lambda)|\psi(\lambda)\rangle \right] + \langle\psi(\lambda)| \frac{dH(\lambda)}{d\lambda} |\psi(\lambda)\rangle$$

Usage: example 1. $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$. $E_n = (n + \frac{1}{2})\hbar\omega$

take ω as λ , $E_n(\lambda) = (n + \frac{1}{2})\hbar\lambda$

$$\therefore \frac{dE_n}{d\lambda} = (n + \frac{1}{2})\hbar = \left\langle \frac{dH}{d\omega} \right\rangle = m\omega \langle x^2 \rangle_n$$

$$\therefore \langle x^2 \rangle_n = \frac{1}{m\omega} (n + \frac{1}{2})\hbar$$

i.e. $\langle \frac{1}{2}m\omega^2 x^2 \rangle_n = \langle V \rangle_n = \frac{1}{2}E_n$

thus $\langle \frac{1}{2m} p^2 \rangle_n = \frac{1}{2}E_n = \langle V \rangle_n$

4/26/96

No.

Date

1-2

example 2. Virial theorem

$$H = \frac{p^2}{2m} + V(r), \quad U(\lambda r) = \lambda^n U(r)$$

$$\Rightarrow \langle T \rangle = \frac{n}{2} \langle V \rangle$$

pf: Consider $H(\lambda) = \frac{p^2}{2m} + U(\lambda r)$. $H = H(\lambda=1)$

$$\left. \frac{dE(\lambda)}{d\lambda} \right|_{\lambda=1} = \left\langle \frac{dU(\lambda r)}{d\lambda} \right\rangle_{\lambda=1} = n \langle V(r) \rangle$$

↑ with respect to $|\psi_E\rangle$
 $H|\psi_E\rangle = E|\psi_E\rangle$
 $E = E(\lambda=1)$

On the other hand, if we change variable:

$$\vec{r} = \lambda \vec{r}'$$

$$\vec{p} = \lambda \vec{p}'$$

$$\therefore H(\lambda) = \frac{\lambda^2 \vec{p}'^2}{2m} + V(r'), \quad H(\lambda=1) = H \text{ too!}$$

$$\therefore E(\lambda=1) \Rightarrow |\psi_E\rangle \text{ same wave function}$$

but now $\left. \frac{dE(\lambda)}{d\lambda} \right|_{\lambda=1} = \left\langle \frac{dH(\lambda)}{d\lambda} \right\rangle_{\lambda=1} = 2 \langle T \rangle$

$$\therefore \langle T \rangle = \frac{n}{2} \langle V(r) \rangle$$

example 3 Suppose $V_1(x) < V_2(x)$, and both potentials support only bound states

$$\left. \begin{array}{l} E_{1n}, n=1, 2, 3, \dots \\ E_{2m}, m=1, 2, 3, \dots \end{array} \right\} \Rightarrow E_{1n} < E_{2n}$$

pf. consider $U(\lambda, x) = (1-\lambda)V_1(x) + \lambda V_2(x)$, $\frac{dU(\lambda, x)}{d\lambda} = V_2 - V_1 \geq 0$

$$\frac{dE_n}{d\lambda} \geq 0$$

(g-fold)

degeneracy: If $H(\lambda)$ has degeneracy at λ_0 , then there are more than one $|\psi_n(\lambda_0)\rangle$ with the same $E_n(\lambda_0)$:

can be applied to 3D central potential.

$$E \leftarrow \frac{\ell(\ell+1)}{2mr^2} + V(r) > \frac{\ell(\ell+1)}{2mr^2} + V(r)$$

4/26/96

No.

Date

1-3

$$H(\lambda) |\psi_n^i(\lambda)\rangle = E_n^i(\lambda) |\psi_n^i(\lambda)\rangle, \quad i=1,2,3,\dots,g$$

$$E_n^i(\lambda_0) = E_n(\lambda_0), \quad \langle \psi_n^i(\lambda) | \psi_n^j(\lambda) \rangle = \delta_{ij}$$

In this case, the appropriate quantities one considers are

$$\begin{aligned} E_n^{ij}(\lambda) &\equiv \langle \psi_n^i(\lambda) | H(\lambda) | \psi_n^j(\lambda) \rangle \\ &= E_n^i(\lambda) \delta_{ij} \end{aligned}$$

$$\begin{aligned} \therefore \frac{\partial E_n^{ij}(\lambda)}{\partial \lambda} &= \langle \psi_n^i(\lambda) | \frac{\partial H(\lambda)}{\partial \lambda} | \psi_n^j(\lambda) \rangle \\ &\quad + E_n^i(\lambda) \langle \psi_n^i(\lambda) | \frac{\partial}{\partial \lambda} | \psi_n^j(\lambda) \rangle \\ &\quad + E_n^j(\lambda) \left(\frac{\partial}{\partial \lambda} \langle \psi_n^i(\lambda) | \right) | \psi_n^j(\lambda) \rangle \end{aligned}$$

The RHS simplifies when $\lambda = \lambda_0$:

$$\begin{aligned} \frac{\partial E_n^{ij}(\lambda_0)}{\partial \lambda_0} &= \langle \psi_n^i(\lambda_0) | \frac{\partial H(\lambda_0)}{\partial \lambda_0} | \psi_n^j(\lambda_0) \rangle \\ &\quad \parallel \\ &\delta_{ij} \frac{\partial E_n^i(\lambda_0)}{\partial \lambda_0} \end{aligned}$$

* This means if we use correct basis, $\frac{\partial E_n^{ij}(\lambda_0)}{\partial \lambda_0}$ is diagonalized and is equal to $\langle \psi_n^i(\lambda_0) | \frac{\partial H(\lambda_0)}{\partial \lambda_0} | \psi_n^j(\lambda_0) \rangle$

In general, if we start from arbitrary basis,

$$|\psi^i(\lambda)\rangle \quad i=1,2,3,\dots,g$$

$$\therefore |\psi^i(\lambda)\rangle = \sum_j U_{ij}^T(\lambda) |\psi_n^j(\lambda)\rangle, \quad U: \text{unitary so that } \langle \psi^i(\lambda) | \psi^j(\lambda) \rangle = \delta_{ij}$$

$$\begin{aligned} \tilde{E}^{ij}(\lambda) &\equiv \langle \psi^i(\lambda) | H(\lambda) | \psi^j(\lambda) \rangle \\ &= (U E(\lambda) U^\dagger)^{ij}, \quad E(\lambda) = \begin{pmatrix} E_1(\lambda) & 0 \\ 0 & \ddots E_g(\lambda) \end{pmatrix} \end{aligned}$$

4/26/96

1-4

i.e. $\tilde{E} = U E U^\dagger$

$$\begin{aligned} \therefore \frac{\partial \tilde{E}}{\partial \lambda} &= U \frac{\partial E}{\partial \lambda} U^\dagger + \frac{\partial U}{\partial \lambda} E U^\dagger + U E \frac{\partial U^\dagger}{\partial \lambda} \\ &= U \frac{\partial E}{\partial \lambda} U^\dagger - \left(U \frac{\partial U^\dagger}{\partial \lambda} \tilde{E} + \tilde{E} \left(\frac{\partial U}{\partial \lambda} U^\dagger \right) \right) \end{aligned}$$

$$\begin{cases} \frac{\partial}{\partial \lambda} (U U^\dagger) = 0 \\ \frac{\partial U}{\partial \lambda} U^\dagger + U \frac{\partial U^\dagger}{\partial \lambda} = 0 \end{cases} \Rightarrow \begin{aligned} \frac{\partial U}{\partial \lambda} &= -U \frac{\partial U^\dagger}{\partial \lambda} U \\ \frac{\partial U^\dagger}{\partial \lambda} &= -U^\dagger \frac{\partial U}{\partial \lambda} U \end{aligned}$$

$$= U \frac{\partial E}{\partial \lambda} U^\dagger - [U \frac{\partial U^\dagger}{\partial \lambda}, \tilde{E}]$$

(seem to ^{have} similar structure as Non-Abelian gauge)

At λ_0 , $E = E_h(\lambda_0) \mathbb{I}$

$$\therefore [U \frac{\partial U^\dagger}{\partial \lambda}, \tilde{E}] \Big|_{\lambda_0} = 0$$

$$\therefore \left. \frac{\partial \tilde{E}}{\partial \lambda} \right|_{\lambda=\lambda_0} = U(\lambda_0) \begin{pmatrix} \frac{\partial E_1}{\partial \lambda_0} & 0 \\ 0 & \frac{\partial E_3}{\partial \lambda_0} \end{pmatrix} U^\dagger(\lambda_0)$$

see more details in exercises.

(use $|n\rangle = |n_0\rangle + \dots$ from perturbation theory)

$$\begin{aligned} \langle n^0 | V | n \rangle &= \frac{\partial E_h}{\partial \lambda} = \frac{\langle n | V | n \rangle}{\langle n | n \rangle} \\ &+ \lambda \langle n^0 | V | \frac{\partial | n \rangle}{\partial \lambda} \end{aligned}$$

$$\int_0^1 \bar{U}(\lambda) d\lambda = \langle n^0 | V | n \rangle$$

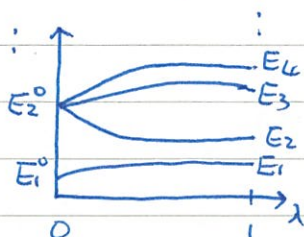
4/26/96

No.

Date

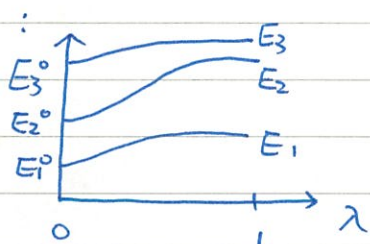
1.

Other pathological case:



will be handled differently.

Simplest case: non-degenerate (1D must be so!)



but usually, one does not know
a priori that there is no level-crossing
and simply assumes it does not happen!

* Hellmann - Feynman theorem: Before we go into the perturbation business,
let's mention the Hellmann - Feynman theorem
which is one of exactly known results. Non-degenerate

Formal expansion (Sakurai's book, Chapter 5 for other derivation)

$$\begin{aligned}
 |n\rangle &= |n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \lambda^3 |n^3\rangle + \dots \\
 E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \lambda^3 E_n^3 + \dots
 \end{aligned}$$

$(H_0 + \lambda V - E_n^0 - \lambda E_n^1 - \dots)$
 $(|n^0\rangle + \lambda |n^1\rangle + \dots) = 0$

$$\begin{aligned}
 \therefore H|n\rangle &= (H_0 + \lambda V) [|n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \lambda^3 |n^3\rangle + \dots] \\
 &= E_n |n\rangle = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \lambda^3 E_n^3 + \dots) [|n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \dots]
 \end{aligned}$$

$$O(\lambda^0): (H_0 - E_n^0) |n^0\rangle = 0 \quad \dots \quad (1)$$

$$O(\lambda^1): (H_0 - E_n^0) |n^1\rangle + (V - E_n^1) |n^0\rangle = 0 \quad \dots \quad (2)$$

$$O(\lambda^2): (H_0 - E_n^0) |n^2\rangle + (V - E_n^1) |n^1\rangle - E_n^2 |n^0\rangle = 0 \quad \dots \quad (3)$$

$$O(\lambda^3): (H_0 - E_n^0) |n^3\rangle + (V - E_n^1) |n^2\rangle - E_n^2 |n^1\rangle - E_n^3 |n^0\rangle = 0 \quad \dots \quad (4)$$

$$\begin{aligned}
 O(\lambda^m): & \underbrace{(H_0 - E_n^0)}_{O(\lambda^0)} \underbrace{|n^m\rangle}_{O(\lambda^m)} + \underbrace{(V - E_n^1)}_{O(\lambda^1)} \underbrace{|n^{m-1}\rangle}_{O(\lambda^{m-1})} - E_n^2 |n^{m-2}\rangle - \dots - E_n^m |n^0\rangle = 0 \quad (5)
 \end{aligned}$$

$\uparrow \quad \uparrow$
 $O(\lambda^m) \quad O(\lambda^0)$

4/26/96

No.

Date

2.

normalization: The usual normalization condition $\langle n|n \rangle = 1$ is not convenient here because at each order, say $O(\lambda^m)$, it involves too many $|n^k\rangle$'s and we have to set the coefficients of all $O(\lambda^m) = 0$!

A clever way is to realize, first, quite generally

$$|n_R\rangle = \alpha |n^0\rangle + |n^1\rangle, \text{ where } \langle n^0 | n^1 \rangle = 0$$

$$\langle n_R | n_R \rangle = 1 = |\alpha|^2 + \langle n^1 | n^1 \rangle$$

$$\therefore |\alpha| = \sqrt{1 - \langle n^1 | n^1 \rangle}$$

We may set $\alpha = |\alpha|$ by absorbing its phase to $|n^1\rangle$ & $|n_R\rangle$

If we define $\beta = \frac{1}{\alpha}$, then

$$|n_R\rangle = \frac{|n^0\rangle + \beta |n^1\rangle}{\beta} = \frac{|n\rangle}{\langle n|n \rangle} \quad \beta = \frac{1}{\sqrt{1 - \langle n^1 | n^1 \rangle}}$$

If we work on $|n\rangle = |n^0\rangle + \beta |n^1\rangle$ (instead $|n_R\rangle$),
(see over)

then the normalization: $\langle n^0 | n \rangle = 1$

which can be satisfied at each order simply by $\langle n^0 | n^m \rangle = 0$!

Then, after we find $|n\rangle$, we define $|n_R\rangle = \frac{|n\rangle}{\sqrt{\langle n|n \rangle}}$ to

go back to the true normalized $|n_R\rangle$!

$$\therefore \langle n^0 | \textcircled{3} \Rightarrow E_n^1 = \langle n^0 | V | n^0 \rangle$$

$$\langle n^0 | \textcircled{3} \Rightarrow E_n^2 = \langle n^0 | V | n^1 \rangle$$

⋮

$$E_n^m = \langle n^0 | V | n^m \rangle$$

$$\begin{aligned} \langle n|n \rangle &= \langle n^0 | n^0 \rangle + 2\langle n^0 | n^1 \rangle + \langle n^1 | n^1 \rangle \\ &= 1 + 2\langle n^0 | n^1 \rangle + \langle n^1 | n^1 \rangle \\ &= 1 + \frac{\langle n^1 | n^0 \rangle}{1 - \langle n^1 | n^1 \rangle} = \frac{1}{1 - \langle n^1 | n^1 \rangle} \\ &= \beta^2 \end{aligned}$$

4/26/96

red over
←No. _____
Date 3,To find $|n^m\rangle$, from eq. ⑤, we have

$$(E_n^0 - H_0) |n^m\rangle = (V - E_n^1) |n^{m-1}\rangle - E_n^2 |n^{m-2}\rangle - \dots - E_n^m |n^0\rangle \dots \textcircled{6}$$

Naively, one would simply invert $E_n^0 - H_0$ to get

$$|n^m\rangle = \frac{1}{E_n^0 - H_0} [(V - E_n^1) |n^{m-1}\rangle - \dots]$$

This is not correct because $\frac{1}{E_n^0 - H_0}$ is not well-defined when acting on $|n^0\rangle$.To avoid this, we first operate eq. ⑥ by $\Phi_n = \mathbb{I} - |n^0\rangle\langle n^0|$ (projection operator)

$$\Rightarrow \Phi_n (E_n^0 - H_0) |n^m\rangle = \Phi_n [(V - E_n^1) |n^{m-1}\rangle - E_n^2 |n^{m-2}\rangle - \dots - E_n^m |n^0\rangle]$$

$$\because \langle n^0 | n^m \rangle = 0, \therefore |n^m\rangle = \Phi_n |n^m\rangle$$

$$\Phi_n (E_n^0 - H_0) \Phi_n = E_n^0 - H_0$$

↑

$$\Phi_n^2 = \mathbb{I}$$

$$\Phi_n H_0 = \left(\sum_{k \neq n} E_k^0 |k^0\rangle\langle k^0| \right) = H_0 \Phi_n$$

Now, we can invert $E_n^0 - H_0$ since the RHS has no component along $|n^0\rangle$:

$$|n^m\rangle = \frac{1}{E_n^0 - H_0} \Phi_n [(V - E_n^1) |n^{m-1}\rangle - E_n^2 |n^{m-2}\rangle - \dots - E_n^m |n^0\rangle]$$

$$\text{where } \frac{1}{E_n^0 - H_0} \Phi_n = \sum_{k \neq n} \frac{1}{E_n^0 - E_k^0} |k^0\rangle\langle k^0| = \Phi_n \frac{1}{E_n^0 - H_0} \quad \text{--- ⑦}$$

$$= \Phi_n \frac{1}{E_n^0 - H_0} \Phi_n \equiv \frac{\Phi_n}{E_n^0 - H_0}$$

$$\therefore |n\rangle = |n^0\rangle + \sum_{m=1}^{\infty} \frac{\Phi_n}{E_n^0 - H_0} [(V - E_n^1) |n^{m-1}\rangle - E_n^2 |n^{m-2}\rangle - \dots - E_n^m |n^0\rangle] \lambda^m$$

4/26/96

No.

Date

4.

Recall that

$$\left[\underbrace{(V-E_n^1)}_{O(\lambda)} \underbrace{|n^{m-1}\rangle}_{O(\lambda^{m-1})} - \underbrace{E_n^2}_{O(\lambda^2)} \underbrace{|n^{m-2}\rangle}_{O(\lambda^{m-2})} - \dots - \underbrace{E_n^m}_{O(\lambda^m)} \underbrace{|n^0\rangle}_{O(\lambda^0)} \right] \lambda^m$$

$$= O(\lambda^m) \text{ of } [\lambda(V-E_n^1) - \lambda^2 E_n^2 - \dots - \lambda^m E_n^m - \dots]$$

$$\times [|n^0\rangle + \lambda |n^1\rangle + \dots + \lambda^{m-2} |n^{m-2}\rangle + \lambda^{m-1} |n^{m-1}\rangle + \dots]$$

$$\therefore |n\rangle = |n^0\rangle + \frac{\phi_n}{E_n^0 - H_0} [\lambda(V-E_n^1) - \lambda^2 E_n^2 - \dots - \lambda^m E_n^m - \dots]$$

$$\times [|n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \dots + \dots]$$

$$= |n^0\rangle + \frac{\phi_n}{E_n^0 - H_0} (\lambda V - \Delta_n) |n\rangle$$

$$\uparrow$$

$$E_n - E_n^0 = \lambda E_n^1 + \lambda^2 E_n^2 + \lambda^3 E_n^3 + \dots$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \lambda^3 E_n^3 + \dots$$

$$= E_n^0 + \lambda [\langle n^0 | V | n^0 \rangle + \langle n^0 | V \lambda | n^1 \rangle + \langle n^0 | V \lambda^2 | n^2 \rangle + \dots]$$

$$= E_n^0 + \lambda \langle n^0 | V | n \rangle$$

Example: $H = \underbrace{\frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2}_{H_0} - \underbrace{g E x}_{\lambda, V(x) = -x}$

$$H_0 = \hbar \omega (a^\dagger + \frac{1}{2}), |n^0\rangle$$

$$x = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} (a^\dagger + a), \quad V(x) = -\left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}} (a^\dagger + a)$$

$$E_n^1 = \langle n^0 | V(x) | n^0 \rangle = 0, \quad |n^1\rangle = \lambda \frac{\phi_n}{E_n^0 - H_0} V |n^0\rangle$$

$$= +gE \sum_m' \frac{|n^0\rangle \langle n^0 | V | n^0 \rangle}{E_n^0 - E_m^0}$$

4/26/96

No.

Date

5.

$$\langle m^0 | U | n^0 \rangle = -\frac{\hbar}{\sqrt{2m\hbar\omega}} \langle m^0 | a^\dagger + a | n^0 \rangle$$

$$= -\frac{\hbar}{\sqrt{2m\hbar\omega}} [\sqrt{n+1} \delta_{m,n+1} + \sqrt{n} \delta_{m,n-1}]$$

$$\therefore |n'\rangle = -8E \frac{\hbar}{\sqrt{2m\hbar\omega}} \left[\frac{\sqrt{n+1}}{-\hbar\omega} |(n+1)^0\rangle + \frac{\sqrt{n}}{\hbar\omega} |(n-1)^0\rangle \right]$$

$$\therefore |n\rangle = |n^0\rangle + 8E \frac{1}{\sqrt{2m\hbar\omega^3}} [\sqrt{n+1} |(n+1)^0\rangle - \sqrt{n} |(n-1)^0\rangle] \dots \infty$$

$$E_n^2 = \langle n^0 | U | n' \rangle$$

$$= 8E \frac{1}{\sqrt{2m\hbar\omega^3}} \left[\sqrt{n+1} \underbrace{\langle n^0 | U | (n+1)^0 \rangle}_{-\frac{\hbar}{\sqrt{2m\hbar\omega}} \sqrt{n+1}} - \sqrt{n} \underbrace{\langle n^0 | U | (n-1)^0 \rangle}_{-\frac{\hbar}{\sqrt{2m\hbar\omega}} \sqrt{n}} \right]$$

$$= 8E \frac{1}{\sqrt{2m\hbar\omega^3}} \sqrt{\frac{\hbar}{2m\hbar\omega}} [n - n - 1] = -\frac{8E}{2m\omega^2}$$

$$\therefore E_n \approx \hbar\omega(n + \frac{1}{2}) - \frac{(8E)^2}{2m\omega^2} \dots \textcircled{2}$$

Comparing to exact solution:

$$\langle x | \hat{T}(a) | \psi \rangle = \psi(x-a)$$

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 \left(x - \frac{8E}{m\omega^2}\right)^2 - \frac{1}{2} \frac{8^2 E^2}{m\omega^2} = H_0 \left(x - \frac{8E}{m\omega^2}\right) - \frac{1}{2} \frac{8^2 E^2}{m\omega^2}$$

$$\therefore E_n = \hbar\omega(n + \frac{1}{2}) - \frac{8^2 E^2}{2m\omega^2}$$

$$\hat{T}(a) = e^{\frac{i}{\hbar} a \hat{p}}$$

$$\hat{T}^\dagger(a) \hat{x} \hat{T}(a) = \hat{x} + a$$

$\therefore$ In fact, $\textcircled{2}$ is exact!

Since in H , x is shifted by $\frac{8E}{m\omega^2}$, i.e., $H_0(x - \frac{8E}{m\omega^2}) = \hat{T}^\dagger(a) H_0(x) \hat{T}(a)$

$$a = -\frac{8E}{m\omega^2}, \therefore |n\rangle = \hat{T}^\dagger(a) |n^0\rangle = e^{\frac{i}{\hbar} a \hat{p}} |n^0\rangle = e^{-\frac{i}{\hbar} \frac{8E}{m\omega^2} \hat{p}} |n^0\rangle \quad \text{(canonical transform)} \\ (a = -8E/m\omega^2)$$

$$\left(H_0 \left(x - \frac{8E}{m\omega^2} \right) \right) |n\rangle = \hat{T}^\dagger(a) H_0(x) \hat{T}(a) \hat{T}^\dagger(a) |n^0\rangle$$

$$= \hat{T}^\dagger(a) H_0(x) |n^0\rangle = \hbar\omega(n + \frac{1}{2}) \hat{T}^\dagger(a) |n^0\rangle \\ = \hbar\omega(n + \frac{1}{2}) |n\rangle$$

4/26/96

No.

Date

6.

$$\therefore p = i\sqrt{\frac{m\hbar\omega}{2}} (a^\dagger - a)$$

$$\therefore |n\rangle = \exp\left[\frac{gE}{\sqrt{2m\hbar\omega^3}} (a^\dagger - a)\right] |n^0\rangle$$

$$= |n^0\rangle + \frac{gE}{\sqrt{2m\hbar\omega^3}} [\sqrt{n+1} |(n+1)^0\rangle - \sqrt{n} |(n-1)^0\rangle] + \dots$$

Consistent with equation ①.

Summary: non-degenerate (always true in 1D)

$$E_n = E_n^0 + \lambda \langle n^0 | V | n \rangle = E_n^0 + \lambda \langle n^0 | V | n^0 \rangle + \lambda^2 \langle n^0 | V | n' \rangle + \dots$$

$$= E_n^0 + \lambda V_{nn} + \lambda^2 \sum_{k \neq n} \frac{|V_{nk}|^2}{E_n^0 - E_k^0} + \dots \quad \text{i.e., } E_n'(0) = V_{nn}$$

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

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

$$= |n^0\rangle + \lambda \underbrace{\sum_{k \neq n} \frac{V_{kn}}{E_n^0 - E_k^0} |k^0\rangle}_{|n'\rangle}$$

$$+ \lambda^2 \left[\sum_{k \neq n} \sum_{l \neq n} \frac{|k^0\rangle V_{kl} V_{ln}}{(E_n^0 - E_k^0)(E_n^0 - E_l^0)} - \sum_{k \neq n} \frac{|k^0\rangle V_{nn} V_{kn}}{(E_n^0 - E_k^0)^2} \right] + \dots$$

Expanding parameter $\left| \frac{\lambda V_{kn}}{E_n^0 - E_k^0} \right| \ll 1$ for convergence $\downarrow$
 can't be applied to degenerate case when $E_n^0 = E_k^0$

$\Rightarrow$ Known as Rayleigh - Schrödinger expansion (non-)

(in terms E_n^0 , unperturbed energy)

There exists another scheme known as Brillouin - Wigner expansion which expresses the perturbation in terms of the exact energy E_n !

4/26/96

No.

Date

7.

Brillouin-Wigner expansion: (converges more rapidly)

$$H|n\rangle = E_n|n\rangle, \quad H = H_0 + \lambda V$$

$$\Rightarrow (E_n - \hat{H}_0)|n\rangle = \lambda V|n\rangle$$

Use $\langle m^0|$ ($m \neq n$)

we get

$$(E_n - E_m^0) \langle m^0|n\rangle = \lambda \langle m^0|V|n\rangle$$

Now, $\langle n^0|n\rangle = 1$ implies

$$|n\rangle = |n^0\rangle + \sum_{m \neq n} |m^0\rangle \langle m^0|n\rangle$$

$$= |n^0\rangle + \sum_m' |m^0\rangle \frac{1}{E_n - E_m^0} \lambda \langle m^0|V|n\rangle$$

$$= |n^0\rangle + \lambda \sum_m' \frac{V_{mn}}{E_n - E_m^0} |m^0\rangle + \lambda^2 \sum_{\ell \neq n} \frac{V_{\ell n}}{E_n - E_\ell^0} \frac{V_{n\ell}}{E_n - E_m^0} |l^0\rangle$$

+ ...

$E_n \neq E_m^0$! avoid degeneracy problem!

(if one substitutes $E_n = E_n^0 + \lambda \langle n^0|V|n\rangle = E_n^0 + \lambda V_{nn} + \dots$

into above expression, one recovers Rayleigh-Schrödinger expansion)
the

Usually, one takes the approximated E_n from the variational calculation (since it is more accurate in calculating energy),

then feeds it into Brillouin-Wigner expansion to get

an approximation of $|n\rangle$!

5/8/96

- $\frac{p^2}{2m} E_n \neq E_n$ for discrete levels

No.

Date

1.

perturbation of the continuum spectrum: the Lippmann-Schwinger equation.

Nothing in previous derivations prevents us to set

E_n continuous. Here we consider the continuum spectrum

by letting E_n in Brillouin-Wigner expansion become continuous.

We will consider the special case:

use Brillouin-Wigner expansion

the spectrum of $H_0 \subset$ the spectrum of H .
(In this case, there is no need to expand E_n !)

In particular, we consider the case when $E_n = E_n^0$.

($\therefore E_n \neq E_n^0$ if $n \neq n^0$)

This is made possible by ① and is the most often encountered case. For example, in the elastic scattering problem, we have $H_0 = \frac{p^2}{2m}$, after scattering, $E = \frac{p^2}{2m}$!

According to Brillouin-Wigner expansion, we have

$$|n\rangle = |n^0\rangle + \sum_m \frac{1}{E_n - E_m^0} |m^0\rangle \langle m^0|U|n\rangle \quad (\text{we have set } U|n\rangle = U|n^0\rangle) \quad \text{--- ②}$$

$$E_n = E_n^0 \text{ implies } \begin{cases} \langle n^0|U|n\rangle = 0 & (\because E_n = E_n^0 + \langle n^0|U|n\rangle) \\ \text{and inclusion of } |n^0\rangle \text{ in ②!} \end{cases}$$

In the continuum limit, ② becomes
 $\sum'_m$ becomes $\int dm$

$$|n\rangle = |n^0\rangle + \int dm \frac{1}{E_n - E_m^0} |m^0\rangle \langle m^0|U|n\rangle \quad \text{--- ③}$$

$$\therefore P \frac{1}{E_n - E_m^0} = \frac{1}{E_n - E_m^0 \pm i\epsilon} \pm i\pi \delta(E_n - E_m^0) \quad (\text{exercise})$$

$$\int dm \delta(E_n - E_m^0) |m^0\rangle \langle m^0|U|n\rangle = |n^0\rangle \underbrace{\langle n^0|U|n\rangle}_{=0} = 0$$

5/8/96

No.

Date

2

 $\therefore$ Eq. (3) becomes

$$\begin{aligned}
 |n^\pm\rangle &= |n^0\rangle + \int dm \frac{1}{E_n - E_m^0 \pm i\varepsilon} |m^0\rangle \langle m^0| V |n^\pm\rangle \\
 &= |n^0\rangle + \int dm \frac{1}{E_n - H^0 \pm i\varepsilon} |m^0\rangle \langle m^0| V |n^\pm\rangle \\
 &= |n^0\rangle + \frac{1}{E_n - H^0 \pm i\varepsilon} V |n^\pm\rangle
 \end{aligned}$$

By setting $|n^0\rangle = |\phi\rangle$, $|n^\pm\rangle = |\psi^\pm\rangle$, $E_n \rightarrow E$, we get the usual form of Lippmann-Schwinger eq.:

$$|\psi^\pm\rangle = |\phi\rangle + \frac{1}{E - H^0 \pm i\varepsilon} V |\psi^\pm\rangle \quad \text{--- (4)}$$

The " $\pm$ " bears some explanations here.

In the elastic scattering problem, one has

$$\langle x | \phi \rangle = \frac{1}{\sqrt{(2\pi\hbar)^3}} e^{i\frac{\vec{p} \cdot \vec{x}}{\hbar}} \quad (\text{plane wave, "incident" wave!})$$

Eq. (4) becomes

$$\psi^\pm(\vec{r}) = \phi(\vec{r}) + \int d^3\vec{r}' \langle \vec{r} | \frac{1}{E - H^0 \pm i\varepsilon} | \vec{r}' \rangle V(\vec{r}') \psi^\pm(\vec{r}')$$

$$\text{Let } G^\pm(\vec{r}, \vec{r}') \equiv \langle \vec{r} | \frac{1}{E - H^0 \pm i\varepsilon} | \vec{r}' \rangle \quad (\text{Green's function}) \quad \leftarrow \text{習題}$$

$$\begin{aligned}
 &= \int d\vec{p} \int d\vec{p}' \underbrace{\langle \vec{r} | \vec{p} \rangle}_{\frac{e^{i\vec{p} \cdot \vec{r}}}{(2\pi\hbar)^{3/2}}} \underbrace{\langle \vec{p} | \frac{1}{E - H^0 \pm i\varepsilon} | \vec{p}' \rangle}_{\frac{1}{E - \frac{p^2}{2m} \pm i\varepsilon} \delta(\vec{p} - \vec{p}')} \langle \vec{p}' | \vec{r}' \rangle \\
 &= \int \frac{d^3\vec{p}}{(2\pi\hbar)^3} \frac{e^{i\vec{p} \cdot (\vec{r} - \vec{r}')/\hbar}}{E - \frac{p^2}{2m} \pm i\varepsilon}, \quad G^\pm \text{ satisfies } \underline{\left(\frac{\hbar^2}{2m} \nabla^2 + E \right) G^\pm(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}')}
 \end{aligned}$$

5/8/96

No.

Date

3

If we write $E = \frac{\hbar^2 k^2}{2m}$, we get ($\vec{p} = \hbar \vec{g}$)

$$G^{\pm}(\vec{r}-\vec{r}') = \frac{2m}{\hbar^2} \int \frac{d^3 \vec{g}}{(2\pi)^3} \frac{e^{i\vec{g} \cdot (\vec{r}-\vec{r}')}}{k^2 - g^2 \pm i\epsilon}$$

$$= \frac{2m}{\hbar^2} \frac{1}{(2\pi)^3} \int_0^\infty g^2 dg \int_0^{2\pi} d\phi \int_{-1}^1 d\cos\theta \frac{e^{i g |\vec{r}-\vec{r}'| \cos\theta}}{k^2 - g^2 \pm i\epsilon}$$

$$= \frac{2m}{\hbar^2} \frac{1}{(2\pi)^3} \times 2\pi \times \frac{1}{i|\vec{r}-\vec{r}'|} \int_0^\infty g dg \frac{e^{i g |\vec{r}-\vec{r}'|} - e^{-i g |\vec{r}-\vec{r}'|}}{k^2 - g^2 \pm i\epsilon}$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} z dz \frac{e^{i z |\vec{r}-\vec{r}'|} - e^{-i z |\vec{r}-\vec{r}'|}}{z^2 - k^2 \pm i\epsilon}$$

$$= -\frac{2m}{\hbar^2} \frac{e^{\pm i k |\vec{r}-\vec{r}'|}}{4\pi |\vec{r}-\vec{r}'|} \left\{ \begin{array}{l} + \text{ out going} \\ - \text{ incoming} \end{array} \right.$$

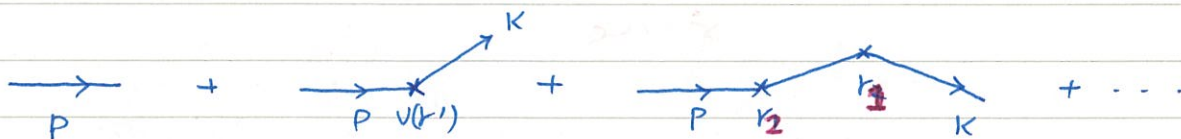
$$\therefore \psi^{\pm}(\vec{r}) = \phi_{\vec{p}}(\vec{r}) - \frac{2m}{\hbar^2} \int d^3 \vec{r}' \frac{e^{\pm i k |\vec{r}-\vec{r}'|}}{4\pi |\vec{r}-\vec{r}'|} V(r') \psi^{\pm}(\vec{r}') \quad |\vec{p}| = |\vec{k}|$$

For out going waves, one has

$$\begin{aligned} \psi^+(\vec{r}) &= \phi_{\vec{p}}(\vec{r}) - \frac{2m}{\hbar^2} \int d^3 \vec{r}' \frac{e^{i k |\vec{r}-\vec{r}'|}}{4\pi |\vec{r}-\vec{r}'|} V(r') \psi^+(\vec{r}') \\ &= \phi_{\vec{p}}(\vec{r}) - \frac{2m}{\hbar^2} \int d\vec{r}' \frac{e^{i k |\vec{r}-\vec{r}'|}}{4\pi |\vec{r}-\vec{r}'|} V(r') \phi_{\vec{p}}(\vec{r}') + \left(\frac{2m}{\hbar^2}\right)^2 \int d\vec{r}_1 \int d\vec{r}_2 \frac{e^{i k |\vec{r}-\vec{r}_1|}}{4\pi |\vec{r}-\vec{r}_1|} \frac{e^{i k |\vec{r}_1-\vec{r}_2|}}{4\pi |\vec{r}_1-\vec{r}_2|} V(r_1) V(r_2) \end{aligned}$$

$$+ \dots$$

Pictorial representation:



(prototype of Feynman diagrams)

→ see over

5/13/96

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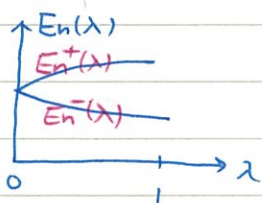
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1.

Degenerate perturbation theory

Suppose that in the absence of $V(x)$ ($\lambda=0$), H_0 is degenerate, say, $E_n^0 = E_k^0$, then the above expansion scheme fails because $\frac{\langle K^0 | V | n^0 \rangle}{E_n^0 - E_k^0}$ is ill-defined (can't $\ll 1$!), unless $\langle K^0 | V | n^0 \rangle$ can be made to vanish!

The apparent catastrophe: $\left. \frac{\partial E_n}{\partial \lambda} \right|_{\lambda=0}$ doesn't exist, in fact, is



not that serious if one realizes that in this case, one has to introduce another label for degeneracy.

That is, $E_n(\lambda) \rightarrow E_{n(\alpha)}(\lambda)$, $\alpha=1, 2, \dots, g$. (suppose g -fold degeneracy!)

$\left. \frac{\partial E_{n(\alpha)}(\lambda)}{\partial \lambda} \right|_{\lambda=0}$ then exists !!

At $\lambda=0$, $E_{n(1)}(0) = E_{n(2)}(0) = \dots = E_{n(g)}(0)$. The eigenkets $|n_i^0\rangle$ ($i=1, \dots, g$) all have the same energy.

When $\lambda \neq 0$, $E_{n(\alpha)}(\lambda)$ usually don't equate to each other.

We say that the degeneracy is lifted!

* Since $|n_i^0(\lambda)\rangle$, $0 \leq \lambda \leq 1$, are uniquely defined (when no further degeneracy is found in $E_{n(\alpha)}(\lambda)$, one can't start arbitrary state at $\lambda=0$ and must start from $|n_i^0(0)\rangle$ determined by V ($\text{all } E_n^0 = \frac{13.6}{2^2} \text{ eV}$))

For example, if one perturbs $|2p, m\rangle$, $m=1, 0, -1$, of the H atom, $|2p, m\rangle$ may not be good starting point! (one has to use linear combination of $|2p, m\rangle$!)

5/13/96

No.

Date

2.

To get a feeling of how to solve the problem in this case, consider a system that has only g states

$$|\tilde{n}_1^0\rangle, |\tilde{n}_2^0\rangle, \dots, |\tilde{n}_g^0\rangle.$$

$$\text{When } \lambda=0, \quad E_{n_1}(0) = E_{n_2}(0) = \dots = E_{n_g}(0) \equiv \varepsilon$$

$$\text{i.e. } H_0 |\tilde{n}_i^0\rangle = \varepsilon |\tilde{n}_i^0\rangle, \quad \langle \tilde{n}_i^0 | \tilde{n}_j^0 \rangle = \delta_{ij}$$

Note that

$|\tilde{n}_i^0\rangle$ may not be the final eigenkets!

Now, the problem is to solve

$$H|\Psi\rangle = E|\Psi\rangle, \quad H = H_0 + \lambda V \quad \text{--- } \textcircled{1}$$

Since $|\Psi\rangle$ resides on a finite dimensional space

($d=g$), this is an eigenvalue problem for a matrix ($g \times g$).

If we write $|\Psi\rangle = \sum_i c_i |\tilde{n}_i^0\rangle$, eq. $\textcircled{1}$ becomes

$$\sum_i \underbrace{\langle \tilde{n}_j^0 | H | \tilde{n}_i^0 \rangle}_H c_i = E c_j \quad (\lambda=1)$$

$$\varepsilon \delta_{ij} + V_{ji} \quad , \quad V_{ij} \equiv \langle \tilde{n}_i^0 | V | \tilde{n}_j^0 \rangle$$

$$\therefore \begin{pmatrix} \varepsilon + V_{11} & V_{12} & V_{13} & \dots & V_{1g} \\ V_{21} & \varepsilon + V_{22} & V_{23} & \dots & V_{2g} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ V_{g1} & V_{g2} & V_{g3} & \dots & \varepsilon + V_{gg} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_g \end{pmatrix} = E \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_g \end{pmatrix}$$

To solve E , we solve the secular equation:

$$\begin{vmatrix} \varepsilon + V_{11} - E & V_{12} & V_{13} & \dots & V_{1g} \\ V_{21} & \varepsilon + V_{22} - E & V_{23} & \dots & V_{2g} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ V_{g1} & V_{g2} & V_{g3} & \dots & \varepsilon + V_{gg} - E \end{vmatrix} = 0$$

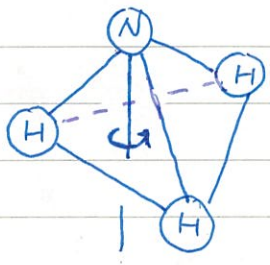
5/3/96

and get $E_{n_1}^0, E_{n_2}^0, \dots, E_{n_g}^0 \triangleq |n_1\rangle, |n_2\rangle, \dots, |n_g\rangle$

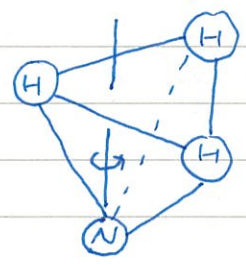
* In terms of $|n_1\rangle, |n_2\rangle, \dots, |n_g\rangle$, $E_{n_\alpha}^0 \equiv \langle n_\alpha | H | n_\alpha \rangle$, $\therefore \Delta_\alpha = E_{n_\alpha}^0 - E = \langle n_\alpha | V | n_\alpha \rangle = 0(V)$

example: Two-state system

The ammonia molecule: two ^{possible} configurations if we consider only the degree of freedom that allows the molecule spin around the axis of symmetry.



$|11\rangle$



$|12\rangle$

(see Feynman's Lecture III for more details.)

N tunnels through  plane to go from $|11\rangle$ to $|12\rangle$.

If these two configurations can't be switched,

$$H^0 = E_0 |11\rangle\langle 11| + E_0 |12\rangle\langle 12| = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix}, \quad |11\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |12\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

i.e., if an ammonia molecule is in the state $|11\rangle$, it will stay in $|11\rangle$ forever: $|11\rangle e^{-\frac{i}{\hbar} E_0 t}$.

Allowing switching from $|11\rangle$ to $|12\rangle$ means: if

$$|\psi\rangle = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}, \quad i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle$$

$$\left. \begin{aligned} i\hbar \frac{dC_1}{dt} &= H_{11} C_1 + H_{12} C_2, & H_{12} &\neq 0 \\ i\hbar \frac{dC_2}{dt} &= H_{21} C_1 + H_{22} C_2, & \underline{H_{21} \neq 0} \end{aligned} \right\} H_{12} = H_{21}^*$$

$$\begin{aligned} \therefore H &= E_0 |11\rangle\langle 11| + E_0 |12\rangle\langle 12| + \lambda V |11\rangle\langle 12| + \lambda V^* |12\rangle\langle 11| \\ &= \begin{pmatrix} E_0 & \lambda V \\ \lambda V^* & E_0 \end{pmatrix} \end{aligned}$$

The final eigenkets are thus neither $|11\rangle$ nor $|12\rangle$.

5/13/96

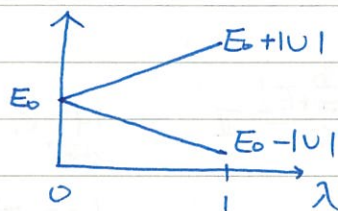
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Date

4

$$\begin{vmatrix} E_0 - E & \lambda V \\ \lambda V^* & E_0 - E \end{vmatrix} = (E - E_0)^2 - \lambda^2 |V|^2 = 0$$

$$\therefore E = E_0 \pm \lambda |V|$$



$$| \pm \rangle = \frac{1}{\sqrt{2}} \left(\frac{\pm V}{|V|} |1\rangle + |2\rangle \right)$$

Note that if initially, $H^0 = E_1^0 |1\rangle\langle 1| + E_2^0 |2\rangle\langle 2|$, $E_1^0 \neq E_2^0$, we get

$$E = \frac{E_1^0 + E_2^0}{2} \pm \sqrt{\left(\frac{E_1^0 - E_2^0}{2}\right)^2 + \lambda^2 |V|^2}$$

Expanding E , one gets

$$E = \frac{E_1^0 + E_2^0}{2} \pm \frac{|E_1^0 - E_2^0|}{2} \left(1 + \left(\frac{2\lambda |V|}{E_1^0 - E_2^0} \right)^2 + \dots \right)$$

which is the perturbation series one would get from non-degenerate perturbation theory. One can see that it fails when

$$E_1^0 = E_2^0!$$

$\Rightarrow$ {more about 2-level system Page 4-1, 2...
another point of view of 2-state system (see over)}

Including other states:

H_0	$O(V^0)$	$O(V)$
$E_1^0 \quad 1\rangle$	$ 1\rangle$	?
$E_2^0 \quad 2\rangle$	$ 2\rangle$	? $E=?$
$\vdots$	$\vdots$	
$ \tilde{h}_1^0\rangle, \tilde{h}_2^0\rangle, \dots, \tilde{h}_g^0\rangle$	$ \tilde{h}_1^0\rangle, \tilde{h}_2^0\rangle, \dots, \tilde{h}_g^0\rangle$	? $E_{n\alpha}^0 = E + \langle \tilde{h}_\alpha^0 V \tilde{h}_\alpha^0 \rangle$
$\vdots$	$\vdots$	
$E_m^0 \quad m\rangle$	$ m\rangle$	? $E=?$
	$\uparrow$ correct basis	

5/3, 2001

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4-1

Level crossing or repulsion?

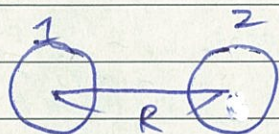
In the above two-level system,

$$\lambda V = \langle 1 | H | 2 \rangle = H_{12}$$

$$\lambda V^* = H_{21}$$

$$\therefore E = \frac{E_1^0 + E_2^0}{2} \pm \sqrt{\left(\frac{E_1^0 - E_2^0}{2}\right)^2 + |H_{12}|^2}$$

A good example is to consider two electronic configuration of two atoms separated by R :



$$H = \frac{p^2}{2m} + \underbrace{\left(\frac{ze}{|r - R_1 \hat{x}|} + \frac{ze}{|r + R_2 \hat{x}|} \right)}_{V(R, r)}$$

$E_1^0(R), E_2^0(R)$ are two electronic states $\downarrow$
to $H_0(R)$

$\rightarrow$ localized at each atom at $R \rightarrow \infty$

$$H(R \rightarrow \infty) = H(R)$$

as R decreases $|E_1^0(R) - E_2^0(R)|$ decreases.

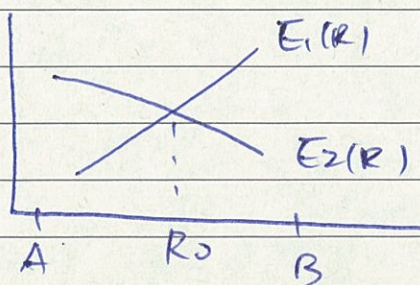
$$+V_0(R/2R) - V_0(R)$$

$$\equiv H_0(R) + V$$

Eventually $E_1^0(R) = E_2^0(R)$ at some R_0

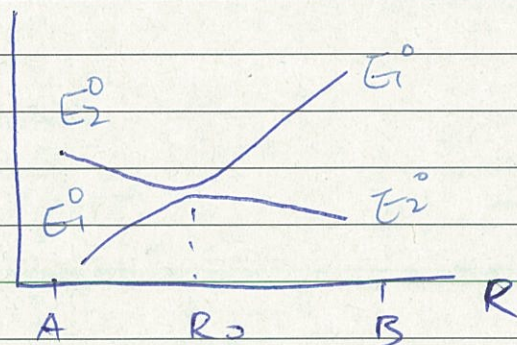
(two nuclei $\simeq$ one nuclei)

if $H_{12}(R) = 0$ at R_0 , then we get



they cross

Otherwise $H_{12}(R_0) \neq 0$ they repulse!



$\therefore$ whether one has level crossing or repulsion depends on $\langle 1 | H | 2 \rangle = 0$ or not!

Usually, this is dictated by symmetry.

(say, $|1\rangle$ & $|2\rangle$ have different m (choose R as

the z axis) so that H is ϕ independent

Furthermore, Suppose the eigenstate

$$|\psi\rangle = a|1\rangle + b|2\rangle. \quad \text{we have}$$

$$\begin{cases} (E_1^0 - E)a + H_{12}b = 0 & \text{--- ①} \\ H_{21}a + (E_2^0 - E)b = 0 & \text{--- ②} \end{cases}$$

$$\therefore a = H_{12}, \quad b = E - E_1^0 = \frac{E_2^0 - E_1^0}{2} \pm \sqrt{\left(\frac{E_2^0 - E_1^0}{2}\right)^2 + |H_{12}|^2}$$

(unnormalized)

$$\therefore |\psi_+\rangle = H_{12}|1\rangle + \left(\frac{E_2^0 - E_1^0}{2} + \sqrt{\left(\frac{E_2^0 - E_1^0}{2}\right)^2 + |H_{12}|^2}\right)|2\rangle$$

$$|\psi_-\rangle = H_{12}|1\rangle + \left(\frac{E_2^0 - E_1^0}{2} - \sqrt{\left(\frac{E_2^0 - E_1^0}{2}\right)^2 + |H_{12}|^2}\right)|2\rangle$$

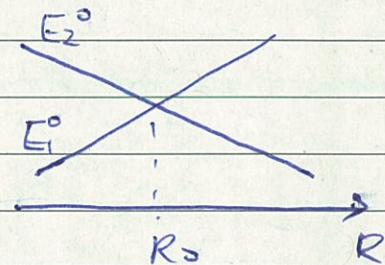
After normalization :

$$\frac{\Delta}{2} + \sqrt{\left(\frac{\Delta}{2}\right)^2 + |H_{12}|^2}$$

$$|\psi_+\rangle = \frac{H_{12}|1\rangle + \left(\left(\frac{E_2^0 - E_1^0}{2}\right) + \sqrt{\left(\frac{E_2^0 - E_1^0}{2}\right)^2 + |H_{12}|^2}\right)|2\rangle}{\sqrt{|H_{12}|^2 + \left(\frac{\Delta}{2} + \sqrt{\left(\frac{\Delta}{2}\right)^2 + |H_{12}|^2}\right)^2}}$$

Far left to R_0 ,

$$|\Delta| = |E_2^0 - E_1^0| \gg |H_{12}|$$

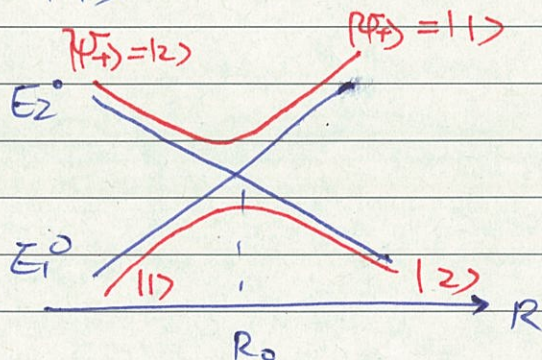


$$\therefore |\psi_+\rangle \rightarrow |2\rangle \quad \Delta \rightarrow \infty$$

Far right to R_0 , $\Delta \rightarrow -\infty$

$$\begin{aligned} \therefore \sqrt{\left(\frac{\Delta}{2}\right)^2 + |H_{12}|^2} - \frac{|\Delta|}{2} &= \frac{|\Delta|}{2} \left(1 + \frac{4|H_{12}|^2}{\Delta^2}\right)^{\frac{1}{2}} - \frac{|\Delta|}{2} \\ &= \frac{|\Delta|}{2} \left(1 + \left(\frac{1}{2} \cdot \frac{4|H_{12}|^2}{\Delta^2} + \dots\right)\right) - \frac{|\Delta|}{2} \\ &\rightarrow 0 \end{aligned}$$

$$\therefore |\psi_+\rangle \rightarrow |1\rangle$$



Similarly, $|\psi_-\rangle \rightarrow |1\rangle$ $R \ll R_0$

$|\psi_-\rangle \rightarrow |2\rangle$ $R \gg R_0$

$\therefore$ Even though there is no energy crossing, levels do cross to each other.

As a result, an ~~electron~~ originally at $|2\rangle$ will transfer to $|1\rangle$ when two nuclei come across each other! $\Rightarrow$ Landau-Zener effect.

The transfer probability can be shown to be given by the Landau-Zener formula:

$$H = \frac{1}{2} v x (|1\rangle\langle 1| - |2\rangle\langle 2|)$$

$$+ \Delta |1\rangle\langle 2| + \Delta |2\rangle\langle 1|$$

$$\begin{array}{l} t \rightarrow +\infty \quad |\psi\rangle = |2\rangle \\ t \rightarrow -\infty \quad |\psi\rangle = |1\rangle \end{array} \quad \Rightarrow \quad |\langle 2| \psi(+\infty) \rangle|^2 = 1 - e^{-\frac{2\pi\Delta^2}{\hbar v}}$$

5/13/96

No.

Date

5.

The trick is to write $U = (P_D + \Phi_D) U (P_D + \Phi_D)$

$$\equiv P_D U P_D + \tilde{U} \Rightarrow \text{see over for a pictorial interpretation}$$

Where $\Phi_D \equiv 1 - P_D$, $P_D \equiv \sum_{\alpha} |n_{\alpha}^0\rangle \langle n_{\alpha}^0|$, $|n_{\alpha}^0\rangle$ form the D subspace and $\tilde{U} \equiv P_D U \Phi_D + \Phi_D U P_D + \Phi_D U \Phi_D$.

$$\therefore H = H_0 + P_D U P_D + \tilde{U} \Rightarrow \tilde{H}_0 + \lambda \tilde{U}$$

$$\tilde{H}_0 = H_0 + P_D U P_D$$

$|n_{\alpha}^0\rangle$, $\alpha=1, 2, \dots, g$, & $|k^0\rangle$ ($k \notin D$) are now non-degenerate eigenkets of $\tilde{H}_0$ with the eigenvalues $E_{n_{\alpha}}^0$, $\alpha=1, 2, \dots, g$, E_k^0 , $k \notin D$.

$\therefore$ The problem of including $\tilde{U}$ is exactly the same as the non-degenerate perturbation theory!!

$\therefore$ We have

$$|k\rangle = |k^0\rangle + \frac{1}{E_k^0 - \tilde{H}_0} \Phi_k (\lambda \tilde{U} - \Delta_k) |k\rangle$$

$$= |k^0\rangle + \lambda \sum_{m \neq k} \frac{1}{E_k^0 - E_m^0} \tilde{V}_{mk} |m^0\rangle + \dots$$

for $k \notin D$

$$\Phi_D U P_D |k^0\rangle = 0$$

(where m include n_{α}^0 , $\alpha=1, 2, \dots, g$!)

where

$$\begin{aligned} \tilde{V}_{mk} &= \langle m^0 | \tilde{U} | k^0 \rangle = \langle m^0 | P_D U \Phi_D + \Phi_D U P_D | k^0 \rangle = \langle m^0 | U \Phi_D | k^0 \rangle \\ &= \begin{cases} \langle m^0 | U | k^0 \rangle & m^0 \in D \\ \langle m^0 | \Phi_D U \Phi_D | k^0 \rangle = \langle m^0 | U | k^0 \rangle, & m^0 \notin D \end{cases} = V_{mk} \end{aligned}$$

$$\begin{aligned} \therefore E_k &= E_k^0 + \lambda \langle k^0 | \tilde{U} | k^0 \rangle = E_k^0 + \lambda \langle k^0 | \tilde{U} | k^0 \rangle + \lambda^2 \sum_{m \neq k} \frac{|\tilde{V}_{mk}|^2}{E_m^0 - E_k^0} + \dots \\ &= E_k^0 + \lambda \langle k^0 | U | k^0 \rangle + \lambda^2 \sum_{m \neq k} \frac{|V_{mk}|^2}{E_m^0 - E_k^0} + \dots \quad (k \notin D) \end{aligned}$$

When $K=n_\alpha$, we get

$$\begin{aligned}
 |n_\alpha\rangle &= |n_\alpha^0\rangle + \frac{1}{E_{n_\alpha}^0 - E_0} \Phi_{n_\alpha} (\lambda \tilde{V} - \Delta_{n_\alpha}) |n_\alpha\rangle \\
 &= |n_\alpha^0\rangle + \lambda \sum_{m \neq n_\alpha} \frac{1}{E_{n_\alpha}^0 - E_m^0} \tilde{V}_{mn_\alpha} |m^0\rangle + \dots \quad (2)
 \end{aligned}$$

$$\tilde{V}_{mn_\alpha} = \langle m^0 | \tilde{V} | n_\alpha^0 \rangle$$

$$= \langle m^0 | \Phi_D V P_D | n_\alpha^0 \rangle$$

$$= \langle m^0 | \Phi_D V | n_\alpha^0 \rangle = \langle m^0 | V | n_\alpha^0 \rangle, \quad m \notin D$$

$$= 0 \quad \text{if } m \in D$$

$$\therefore (2) \text{ becomes } |n_\alpha\rangle = |n_\alpha^0\rangle + \lambda \sum_{m \notin D} \frac{1}{E_{n_\alpha}^0 - E_m^0} \tilde{V}_{mn_\alpha} |m^0\rangle + \dots$$

$$\text{Similarly, } E_{n_\alpha} = E_{n_\alpha}^0 + \lambda \langle n_\alpha^0 | \tilde{V} | n_\alpha^0 \rangle + \lambda^2 \sum_{m \notin D} \frac{|\tilde{V}_{mn_\alpha}|^2}{E_m^0 - E_{n_\alpha}^0} + \dots \quad (3)$$

$\therefore$ To $O(\lambda^2)$, $|n_\alpha\rangle$ becomes

$$|n_\alpha\rangle = |n_\alpha^0\rangle + \lambda \sum_{m \notin D} \frac{1}{E_{n_\alpha}^0 - E_m^0} \tilde{V}_{mn_\alpha} |m^0\rangle$$

$$\Phi_{n_\alpha} \lambda^2 E_{n_\alpha}^2 |n_\alpha\rangle = 0$$

$$+ \lambda^2 \sum_{m \neq n_\alpha} \frac{1}{E_{n_\alpha}^0 - E_m^0} |m^0\rangle \langle m^0 | \tilde{V} \sum_{l \notin D} \frac{1}{E_{n_\alpha}^0 - E_l^0} \tilde{V}_{ln_\alpha} |l^0\rangle + \dots$$

$$\begin{aligned}
 &\sum_{m \neq n_\alpha} \sum_{l \notin D} \frac{1}{E_{n_\alpha}^0 - E_m^0} \frac{\tilde{V}_{ln_\alpha}}{E_{n_\alpha}^0 - E_l^0} |m^0\rangle \underbrace{\langle m^0 | \tilde{V} | l^0 \rangle}_{\langle m^0 | P_D V P_D | l^0 \rangle} \\
 &\sum_{\beta \neq n_\alpha} \sum_{l \notin D} \frac{\tilde{V}_{n_\alpha l} \tilde{V}_{l \beta}}{(E_{n_\alpha}^0 - E_\beta^0)(E_{n_\alpha}^0 - E_l^0)} |n_\beta^0\rangle \dots \quad (4)
 \end{aligned}$$

5/13/96

No.

Date

6.

complications: The above formulation works only if there is no degeneracy in the roots of the secular equation. When there is degeneracy, it becomes (see eg. ④!) more complicated!

see Gottfried's book for more details.

(or my notes) page 5/20/96 1-4

C. WKB method (Reviewed)

To $O(\hbar)$, $\psi(x) = e^{\frac{i}{\hbar}\phi(x)}$, expand $\phi(x)$ in terms of $\hbar$.

$$= \psi(x_0) \sqrt{\frac{p(x_0)}{p(x)}} \exp\left[\pm \frac{i}{\hbar} \int_{x_0}^x p(x') dx'\right]$$

$$p(x) = \sqrt{2m(E - V(x))}$$

For bound states, $\int_{x_1}^{x_2} p(x) dx = (n + \frac{1}{2})\pi\hbar$

x_i = turning points.

Useful for estimating E_n !

D. Time-dependent perturbation theory

When the perturbation V depends on time, one has to solve the time-dependent Schrödinger eq.

$$i\hbar \frac{d|\psi\rangle}{dt} = (H_0 + V(t)) |\psi\rangle$$

instead of time independent Schrödinger eq. $(H_0 + V)|\psi\rangle = E|\psi\rangle$.

5/20/0

2nd order degenerate perturbation theory

It's quite often that $\langle n^0 | V | m^0 \rangle = 0$.

Examples include many important problems such as models of high temperature superconductors ... etc.

In this case, one has

$$H = H_0 + V$$

$$= \underbrace{\begin{pmatrix} E_1^0 & & 0 \\ & E_2^0 & \\ 0 & \ddots & \boxed{\begin{matrix} \varepsilon & 0 \\ 0 & \varepsilon \end{matrix}} \end{pmatrix}}_{\parallel} + \begin{pmatrix} 0 & 0 \\ & A \end{pmatrix}$$

$$\begin{pmatrix} E^0 & & 0 \\ & E_2^0 & \\ 0 & \ddots & \varepsilon \end{pmatrix} + \underbrace{\begin{pmatrix} \times & \times \\ & \times & 0 \end{pmatrix}}$$

To be able to do perturbation, one needs to include effect of $\hat{V}$ on ε to remove their degeneracy. This is done by

5/20/96

2nd method
 add a few other states
 to g states ^{data} remove the degeneracy. 1.

Perturbation scheme for the case when the secular

equation does not remove the degeneracy:

(but degeneracy is removed by other states!)

Consider $H = H_0 + V$

$$|K\rangle, |K^0\rangle, \quad H|K\rangle = E_K|K\rangle, \quad H_0|K^0\rangle = E_K^0|K^0\rangle, \quad \text{as before}$$

$$\Delta_K \equiv E_K - E_K^0$$

$$P_K = |K^0\rangle\langle K^0|, \quad Q_K = 1 - P_K$$

When $|K^0\rangle$ are g-fold degenerate, we denote:

$$|K_i^0\rangle, \quad i=1, 2, 3, \dots, g. \quad \langle K_i^0 | K_j^0 \rangle = \delta_{ij}$$

$$P_K = \sum_{i=1}^g |K_i^0\rangle\langle K_i^0|, \quad Q_K = 1 - P_K, \quad |K\rangle \rightarrow |K_i\rangle, \quad E_K \rightarrow E_{K_i}$$

(The following treatment basically just tries to separate $P_K|K\rangle$ & $Q_K|K\rangle$!)

First, we have $\underbrace{P_K(H - H_0)|K\rangle}_{P_K V |K\rangle} = (E_K - E_K^0) P_K |K\rangle$

↓
 (derive closed
 eq. for $P_K|K\rangle$
 & $Q_K|K\rangle$ separately)

$$\therefore P_K V |K\rangle = \Delta_K P_K |K\rangle \quad \dots \quad (1)$$

Next, starting from $(H_0 + V)|K\rangle = E_K|K\rangle$,

we have

$$(E_K^0 - H_0)|K\rangle = (V - \Delta_K)|K\rangle$$

Q_K acts on it, we get

$$(E_K^0 - H_0) Q_K |K\rangle = Q_K (V - \Delta_K) |K\rangle$$

$\therefore$ we can invert it, we get

$$\underbrace{Q_K |K\rangle}_{||} = \frac{Q_K}{E_K^0 - H_0} (V - \Delta_K) |K\rangle$$

$$|K\rangle - P_K |K\rangle$$

$$\therefore \left(1 + \frac{Q_K}{E_K^0 - H_0} (\Delta_K - V)\right) |K\rangle = P_K |K\rangle \quad \dots \quad (2)$$

(this is equivalent to $|n\rangle = |n^0\rangle + \frac{\phi_n}{E_n^0 - H_0} (1 - P_n) |n\rangle$
 on page 4/26/96, 4)

5/20/96

No.

Date

2

From eq. ②, one gets

$$|K\rangle = \frac{1}{1 + \frac{Q_K}{E_K^0 - H_0} (\Delta K - V)} P_K |K\rangle$$

Substituting it into eq. ①, we get

$$P_K V \frac{1}{1 + \frac{Q_K}{E_K^0 - H_0} (\Delta K - V)} \underline{P_K |K\rangle} = \Delta K P_K |K\rangle \quad \dots \text{③}$$

In the non-degenerate case, one has

$$|K^0\rangle \langle K^0| V \frac{1}{1 + \frac{Q_K}{E_K^0 - H_0} (\Delta K - V)} |K^0\rangle \langle K^0| K\rangle = \Delta K |K^0\rangle \langle K^0| K\rangle$$

$$\therefore \Delta K = \langle K^0| V \frac{1}{1 + \frac{Q_K}{E_K^0 - H_0} (\Delta K - V)} |K^0\rangle \underset{\substack{\uparrow \\ \text{eq. ②}}}{=} \langle K^0| V |K\rangle$$

consistent with previous results!

For degenerate case, eq. ③ becomes $|K\rangle \rightarrow |K_\alpha\rangle$, $\Delta K \rightarrow \Delta K_\alpha$

$$\sum_{i,j} |K_i^0\rangle \langle K_i^0| V \frac{1}{1 + \frac{Q_K}{E_K^0 - H_0} (\Delta K_\alpha - V)} |K_j^0\rangle \langle K_j^0| K_\alpha\rangle = \sum_i \Delta K_\alpha |K_i^0\rangle \langle K_i^0| K_\alpha\rangle$$

$$\therefore \sum_{j=1}^g \underbrace{\langle K_i^0| V \frac{1}{1 + \frac{Q_K}{E_K^0 - H_0} (\Delta K_\alpha - V)} |K_j^0\rangle \langle K_j^0| K_\alpha\rangle}_{\text{III}} = \Delta K_\alpha \langle K_i^0| K_\alpha\rangle \quad \dots \text{④}$$

$$\text{III} \\ \langle K_i^0| V^R |K_j^0\rangle$$

The secular equation becomes

$$\begin{vmatrix} U_{11}^R - \Delta & U_{12}^R & U_{13}^R & \dots & U_{1g}^R \\ U_{21}^R & U_{22}^R - \Delta & U_{23}^R & \dots & U_{2g}^R \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ U_{g1}^R & U_{g2}^R & U_{g3}^R & \dots & U_{gg}^R - \Delta \end{vmatrix} = 0 \quad \dots (5)$$

$\Delta_{k\alpha}$ can also be evaluated perturbatively:

Using
$$\frac{1}{1 + \frac{\partial K}{\partial E_k^0 - H_0} (\Delta_{k\alpha} - U)} = 1 - \frac{\partial K}{\partial E_k^0 - H_0} (\Delta_{k\alpha} - U) + \dots$$

and expanding $\Delta_{k\alpha} = \Delta_{k\alpha}^{(1)} + \Delta_{k\alpha}^{(2)} + \dots$, we get
($\Delta_{k\alpha}^{(0)} = 0$)

$$O(V): \sum_{j=1}^g \langle k_i^0 | V | k_j^0 \rangle \langle k_j^0 | k_\alpha \rangle = \Delta_{k\alpha}^{(1)} \langle k_i^0 | k_\alpha \rangle$$

$\Rightarrow$ solve the secular eq. as before

Here, one could get $\Delta_{k\alpha}^{(1)} = 0$!

i.e. degeneracy is ^{not} removed within the secular eq.

$$O(V^2): - \sum_{j=1}^g \sum_{n \neq k} \frac{\langle k_i^0 | V | n \rangle \langle n | \Delta_{k\alpha}^{(1)} - U | k_j^0 \rangle}{E_k^0 - E_n^0} \langle k_j^0 | k_\alpha \rangle = \Delta_{k\alpha}^{(2)} \langle k_i^0 | k_\alpha \rangle$$

in the case when $\Delta_{k\alpha}^{(1)} = 0$, one has to solve

$$\sum_{j=1}^g \left(\sum_{n \neq k} \frac{\langle k_i^0 | V | n \rangle \langle n | V | k_j^0 \rangle}{E_k^0 - E_n^0} \right) \langle k_j^0 | k_\alpha \rangle = \Delta_{k\alpha}^{(2)} \langle k_i^0 | k_\alpha \rangle \quad \dots (6)$$

which is also reduced to solve a secular eq. !

5/20/96

No.

Date

4.

example: $g=2$, the secular eq. of eq. (6) becomes

$$\begin{vmatrix} M_{11} - \Delta & M_{12} \\ M_{21} & M_{22} - \Delta \end{vmatrix} = 0$$

$$M_{ij} = \sum_{n \neq k} \frac{\langle K_i^0 | V | n \rangle \langle n | V | K_j^0 \rangle}{E_k^0 - E_n^0} = M_{ji}^*$$

$$\therefore (\Delta - M_{11})(\Delta - M_{22}) = |M_{12}|^2$$

The above only discusses the evaluation of components of $|K\rangle$ that lie in the subspace formed by $|K_i^0\rangle$ ($\equiv D$)

For components outside D , we start from

$$\begin{aligned} (E_k - H_0) \Theta_k |K\rangle &= \Theta_k V |K\rangle \\ &= \Theta_k V \Theta_k |K\rangle + \Theta_k V P_k |K\rangle \end{aligned}$$

$$\therefore (E_k - H_0 - \Theta_k V \Theta_k) \Theta_k |K\rangle = \Theta_k V P_k |K\rangle$$

$$\therefore \Theta_k |K\rangle = \frac{1}{E_k - H_0 - \Theta_k V \Theta_k} \Theta_k V P_k |K\rangle$$

then feed results from calculation of $P_k |K\rangle$

(including $E_k = E_k^0 + \Delta_k$)

e.g. if we write $|K_\alpha\rangle = |K_\alpha^{(0)}\rangle + \overset{\downarrow O(V)}{|K_\alpha^{(1)}\rangle} + \dots$

$\uparrow$
solution to scalar eq. (quite often, indept. of V)

$$O(V): \Theta_k |\hat{K}_\alpha^{(1)}\rangle = \sum_{n \notin D} \frac{1}{E_k^{(0)} - E_n^{(0)}} |n^0\rangle \langle n^0 | V | \hat{K}_\alpha^{(0)}\rangle$$

5/14/96

No.

Date

1.

The typical question one asks in this problem is:

at $t=0$ (or $-\infty$) $|\psi\rangle = |n^0\rangle$, what is the amplitude (probability) of finding the system in the state $|m^0\rangle$ at a later time?

Obviously, without $V(t)$, the answer is δ_{mn} because

$|\psi(t)\rangle = |n^0\rangle e^{-\frac{i}{\hbar} E_n^0 t}$, $\therefore$ the effect of $V(t)$ starts after this δ_{mn} .

Matrix formulation & the interaction picture:

Let the eigenkets of H_0 be $|n\rangle$: $\hat{H}_0 |n\rangle = E_n^0 |n\rangle$

We want to solve $i\hbar \frac{d}{dt} |\psi(t)\rangle = (\hat{H}_0 + \hat{V}(t)) |\psi(t)\rangle$.

For this purpose, one may expand $|\psi(t)\rangle$:

$$|\psi(t)\rangle = \sum_n C_n(t) |n\rangle. \quad \therefore i\hbar \dot{C}_n(t) = \sum_m (E_n^0 \delta_{nm} + V_{nm}(t)) C_m(t)$$

L --- ①

Where $V_{nm}(t) = \langle n | V(t) | m \rangle$.

In the absence of $V(t)$, $C_n(t) = e^{-\frac{i}{\hbar} E_n^0 t}$. This suggests

that E_n^0 in ① can be shifted away by the transformation:

$$C_n(t) \rightarrow C_n(t) e^{-\frac{i}{\hbar} E_n^0 t},$$

then eq. ① becomes

$$i\hbar \dot{C}_n(t) = \sum_m V_{nm} e^{i W_{nm} t} C_m(t). \quad W_{nm} \equiv \frac{1}{\hbar} (E_n^0 - E_m^0)$$

L --- ②

5/14/96

No.

Date

2.

This transformation rewrites

$$\begin{aligned}
 |\psi(t)\rangle &= \sum_n e^{-\frac{i}{\hbar} E_n^0 t} c_n(t) |n\rangle \\
 &= e^{-\frac{i}{\hbar} \hat{H}_0 t} \sum_n c_n(t) |n\rangle \equiv e^{-\frac{i}{\hbar} \hat{H}_0 t} |\psi(t)\rangle_I
 \end{aligned}$$

This defines $|\psi\rangle$ in the so-called interaction picture $|\psi(t)\rangle_I$.

Since $|\psi(t)\rangle_I = e^{\frac{i}{\hbar} \hat{H}_0 t} |\psi(t)\rangle$

$$\begin{aligned}
 \therefore i\hbar \frac{d}{dt} |\psi(t)\rangle_I &= -\hat{H}_0 |\psi(t)\rangle_I + e^{\frac{i}{\hbar} \hat{H}_0 t} (\hat{H}_0 + V(t)) e^{-\frac{i}{\hbar} \hat{H}_0 t} |\psi(t)\rangle_I \\
 &= [-\hat{H}_0 + e^{\frac{i}{\hbar} \hat{H}_0 t} (\hat{H}_0 + V(t)) e^{-\frac{i}{\hbar} \hat{H}_0 t}] |\psi(t)\rangle_I \\
 &\equiv \hat{U}_I(t) |\psi(t)\rangle_I
 \end{aligned}$$

where $\hat{U}_I(t) = e^{\frac{i}{\hbar} \hat{H}_0 t} V(t) e^{-\frac{i}{\hbar} \hat{H}_0 t}$.

$\therefore$ In the interaction picture, $\hat{H}_0$ is hidden. The evolution is determined by $\hat{U}_I(t)$. (see over for a discussion)

The following is a comparison of various

	Heisenberg	Interaction	Schrödinger
ket	$ \psi\rangle$ (indep. of time)	$ \psi(t)\rangle_I$	$ \psi(t)\rangle$
evolution of $ \psi\rangle$	no change	$\hat{U}_I(t)$	H
observable	$\frac{dA_H}{dt} = \frac{i}{\hbar} [A_H, H]$ by H	$\frac{dA_I}{dt} = \frac{i}{\hbar} [A_I, H_0]$ by H_0 $A_I = e^{\frac{i}{\hbar} H_0 t} A e^{-\frac{i}{\hbar} H_0 t}$	no change A indep. of t.

Now, if we write out eq. (2), it is

$$i\hbar \begin{pmatrix} \dot{C}_1 \\ \dot{C}_2 \\ \dot{C}_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}e^{i\omega_2 t} & - & - & - \\ V_{21}e^{i\omega_2 t} & V_{22} & - & - & - \\ & & V_{33} & - & - \\ & & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \end{pmatrix}$$

This is a system of coupled differential equation of infinite dimension. Unless further approximations such as

truncation are made, analytic solutions are impossible.

example $H = -\vec{u} \cdot \vec{B}$ $\Leftarrow$ only probes finite degrees of freedom of the system.

$$\vec{B} = B_0 \hat{z} + B_1 [\hat{x} \cos \omega t + \hat{y} \sin \omega t]$$

$$\vec{u} = \frac{e}{mc} \vec{S}$$

$$\Rightarrow \text{---} \omega_2$$

$$\omega_2 \omega_2$$

$$\therefore H = -\frac{eB_0}{mc} S_z - \frac{eB_1}{mc} (\cos \omega t S_x + \sin \omega t S_y)$$

$$= -\frac{e\hbar B_0}{2mc} [1+\rangle\langle +1 -1-\rangle\langle -1] - \frac{eB_1\hbar}{2mc} [\cos \omega t (1+\rangle\langle -1 +1-\rangle\langle +1) + \sin \omega t (-i1+\rangle\langle -1 +i1-\rangle\langle +1)]$$

$$\Rightarrow \frac{+e\hbar B_0}{2mc} [11\rangle\langle 11 - 12\rangle\langle 21] + \delta e^{i\omega t} 11\rangle\langle 21 + \delta e^{-i\omega t} 12\rangle\langle 11$$

$$1-\rangle\langle 11\rangle$$

$$1+\rangle\langle 12\rangle$$

$$\text{where } \delta = \frac{-eB_1\hbar}{2mc}$$

$$= \begin{pmatrix} \frac{e\hbar B_0}{2mc} & \delta e^{i\omega t} \\ \delta e^{-i\omega t} & -\frac{e\hbar B_0}{2mc} \end{pmatrix}$$

$$V_{11} = V_{22} = 0$$

$$H_0 = \begin{pmatrix} \frac{e\hbar B_0}{2mc} & 0 \\ 0 & -\frac{e\hbar B_0}{2mc} \end{pmatrix}$$

$$V_{12} = \delta e^{i\omega t}, \quad V_{21} = V_{12}^* = \delta e^{-i\omega t}$$

5/14/96

$$\therefore i\hbar \begin{pmatrix} \dot{C}_1 \\ \dot{C}_2 \end{pmatrix} = \begin{pmatrix} 0 & e^{i(\omega_{12} + \omega)t} \\ e^{i(\omega_{21} - \omega)t} & 0 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}$$

Similar to Ex 14.4.3
go to rotating frame (ω)
but here go to rotating frame with $\omega = \omega_0$

$$\omega_{12} = \frac{1}{\hbar} \frac{e\hbar B_0}{2m_{ec}} \times 2 = \frac{eB_0}{m_{ec}} = -\omega_{21}$$

Solve C_1 & C_2 (eliminate C_2 in terms of C_1), we find
if $C_1(0)=1, C_2(0)=0$

$$|C_2(t)|^2 = \frac{\delta^2/\hbar^2}{\delta^2/\hbar^2 + (\omega - \omega_{21})^2/4} \sin^2 \left\{ \left[\frac{\delta^2}{\hbar^2} + \frac{(\omega - \omega_{21})^2}{4} \right]^{1/2} t \right\}$$

if $\omega \gg \omega_{21}$
or $\omega \ll \omega_{21}$

$$\Rightarrow \boxed{C_2 \approx 0} \quad |C_1(t)|^2 = 1 - |C_2(t)|^2 \quad (\text{exercise})$$

see over for a comparison

Formal perturbation series: Dyson series

Since we are interested in the "transition" amplitude of going from $|n^0\rangle$ to $|m^0\rangle$, this is entirely encoded in the evolution operator: $U_I(t, t_0)$ defined below.

$$|\psi(t)\rangle_I = U_I(t, t_0) |\psi(t_0)\rangle_I \quad \left(\begin{array}{l} \text{obviously} \\ U_I(t_0, t_0) = I \end{array} \right)$$

$$\therefore i\hbar \frac{d}{dt} |\psi(t)\rangle_I = V_I(t) |\psi(t)\rangle_I$$

We get $i\hbar \frac{dU_I(t, t_0)}{dt} = V_I(t) U_I(t, t_0)$

This equation can not be solved in the usual way:

$$\frac{dy}{dx} = \alpha(x) y(x), \quad \frac{dy(x)}{y(x)} = \alpha(x) dx$$

$$\int^x \frac{dy(x)}{y(x)} = \int^x \alpha(x) dx \quad \therefore y(x) = y(x_0) e^{\int_{x_0}^x \alpha(t) dt}$$

because one does not know $U_I^{-1}(t, t_0) U_I(t) U_I(t, t_0) !!$

5/14/86

No.

Date

5

To solve it, we convert it to an integral equation:

$$i\hbar \int_{t_0}^t \frac{dU_I(t', t_0)}{dt'} dt' = \int_{t_0}^t V_I(t') U_I(t', t_0) dt'$$

$$\therefore U_I(t, t_0) = \mathbb{I} - \frac{i}{\hbar} \int_{t_0}^t V_I(t') U_I(t', t_0) dt'$$

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

$$+ \left(\frac{-i}{\hbar}\right)^3 \int_{t_0}^t \int_{t_0}^{t'} \int_{t_0}^{t''} dt' dt'' dt''' V_I(t') U_I(t'', t_0) U_I(t''', t_0) + \dots$$

by successive substituting U_I on RHS.

This is known as the Dyson series!

Note that the orderings in the integrands are important.

Since $[V_I(t), V_I(t')] \neq 0$ for $t \neq t'$!! (see over)

Suppose that initially $|\psi(t_0)\rangle_I = |n^0\rangle$.

$$\therefore |\psi(t)\rangle_I = \sum_m C_m(t) |m^0\rangle$$

$$\& \text{ on the other hand, } |\psi(t)\rangle_I = U_I(t, t_0) |\psi(t_0)\rangle_I$$

$$= U_I(t, t_0) |n^0\rangle$$

$$= \sum_m \langle m^0 | U_I(t, t_0) | n^0 \rangle |m^0\rangle$$

$$\therefore C_m(t) = \langle m^0 | U_I(t, t_0) | n^0 \rangle$$

$$O(V^0): C_m^{(0)}(t) = \langle m^0 | n^0 \rangle = \delta_{mn}$$

$$O(V): C_m^{(1)}(t) = \frac{-i}{\hbar} \int_{t_0}^t \langle m^0 | V_I(t') | n^0 \rangle dt' = \frac{-i}{\hbar} \int_{t_0}^t e^{i\omega_{mn}t'} V_{mn}(t') dt'$$

$$\omega_{mn} \equiv \frac{1}{\hbar} (E_m^0 - E_n^0), \quad V_{mn}(t') = \langle m^0 | V(t') | n^0 \rangle$$

5/14/96

No.

Date

6

$$C_m^{(2)}(t) = \left(\frac{-i}{\hbar}\right)^2 \sum_k \int_{t_0}^t \int_{t_0}^{t'} dt' dt'' e^{i\omega_{mk}t'} V_{mk}(t') e^{i\omega_{kn}t''} V_{kn}(t'')$$

$$\vdots$$

$$\vdots$$

The transition probability for $|n^0\rangle \rightarrow |m^0\rangle$ is

$$P(n \rightarrow m) = |C_m^{(1)}(t) + C_m^{(2)}(t) + \dots|^2$$

$$R(n \rightarrow m) \text{ (transition rate)} = \left. \frac{dP(n \rightarrow m)}{dt} \right|_{t=0}, \quad \sum_m R(n \rightarrow m) = \frac{1}{\tau_n}$$

The harmonic perturbation:

$$|C_n(t)|^2 = e^{-t/\tau_n} \text{ for } t \approx 0 \quad \text{life time}$$

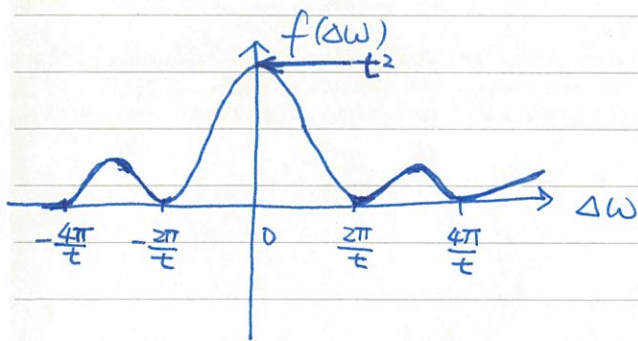
$V(t) = V e^{-i\omega t}$, the system is under this perturbation starting at $t=0$.

$$C_m^{(1)}(t) = \frac{-i}{\hbar} \int_0^t \langle m^0 | V | n^0 \rangle e^{i(\omega_{mn} - \omega)t'} dt'$$

$$= \frac{-i}{\hbar} \langle m^0 | V | n^0 \rangle \frac{e^{i(\omega_{mn} - \omega)t} - 1}{i(\omega_{mn} - \omega)}$$

$$P(n \rightarrow m) = \frac{1}{\hbar^2} |\langle m^0 | V | n^0 \rangle|^2 \frac{4 \sin^2\left(\frac{\omega_{mn} - \omega}{2} t\right)}{(\omega_{mn} - \omega)^2}$$

Let $\Delta\omega = \omega_{mn} - \omega$, $f(\Delta\omega) \equiv \frac{4 \sin^2\left(\frac{\Delta\omega t}{2}\right)}{\Delta\omega^2}$, we have



As $t \rightarrow \infty$, $f(\Delta\omega)$ at $\Delta\omega = 0$ goes to ∞ . $\therefore f(\Delta\omega) \sim \delta(\Delta\omega)$

In fact, one has the identity:

$$\lim_{t \rightarrow \infty} \frac{1}{t\pi} \frac{\sin^2 tx}{x^2} = \delta(x)$$

5/14/96

No.

Date

7.

(note: $\frac{1}{n\pi} \int_{-\infty}^{\infty} \frac{\sin^2 nx}{x^2} dx = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\sin^2 y}{y^2} dy = \frac{1}{\pi} \times \pi = 1$)

$\therefore$ As $t \rightarrow \infty$, $f(\Delta\omega) = \frac{4}{\Delta\omega^2} \left(\frac{\Delta\omega}{2}\right)^2 \cdot t \pi \delta\left(\frac{\Delta\omega}{2}\right)$ ($x = \frac{\Delta\omega}{2}$, $t = n$)

$$= 2\pi t \delta(\Delta\omega)$$

problem: shouldn't

$\downarrow$ $P(n \rightarrow m) < 1$?

$\therefore P(n \rightarrow m) = \frac{2\pi}{\hbar^2} |\langle m^0 | V | n^0 \rangle|^2 \delta(\underbrace{\omega_{mn} - \omega}_{\frac{1}{\hbar}(E_m^0 - E_n^0 - \hbar\omega)}) \cdot t$ ($\Leftarrow$ must appear

$\therefore$ the average transition rate $R(n \rightarrow m)$ in the integral

$$= \frac{P(n \rightarrow m)}{t} = \frac{2\pi}{\hbar} \delta(E_m^0 - E_n^0 - \hbar\omega) |\langle m^0 | V | n^0 \rangle|^2$$

$\Rightarrow$ Fermi's golden rule! $\Rightarrow$ see over

Note that: only at $t \rightarrow \infty$, $E_m^0 = E_n^0 + \hbar\omega$ is restricted! Otherwise, for a finite t , transitions to other states are also possible.

Density of final state

In some situations, we consider transitions to a group of states of nearby energies.

This is always encountered when one considers transitions to states of continuous spectrum or E_n is in fact degenerate!

In this case, we are interested in

$$\sum_{m, E_m^0 \approx E_n^0 + \hbar\omega} P(n \rightarrow m) \quad \text{or} \quad \sum_{m, E_m^0 \approx E_n^0 + \hbar\omega} R(n \rightarrow m)$$

Another derivation of ^{the} Fermi Golden rule

adiabatically turning on

$$H = H_0 + V e^{-i\omega t} e^{\eta t} \quad (+ V^+ e^{i\omega t} e^{\eta t})$$

at $t=0$, $V = V e^{-i\omega t}$

$$|\psi(t)\rangle_I = \sum_m C_m(t) |m^0\rangle$$

$$= |n^0\rangle - \frac{i}{\hbar} \sum_m \int_{-\infty}^t e^{i\omega_{mn}t'} V_{mn}(t') dt' |m^0\rangle$$

$\frac{1}{\hbar}(E_m^0 - E_n^0)$

$$\therefore |\psi(t)\rangle = e^{\frac{i}{\hbar} H_0 t} |\psi(t)\rangle_I$$

$$= e^{-\frac{i}{\hbar} H_0 t} |n^0\rangle$$

$$- \frac{i}{\hbar} \sum_m \int_{-\infty}^t e^{-\frac{i}{\hbar} E_n^0 t'} \underbrace{e^{\frac{i}{\hbar} E_m^0 (t'-t)}}_{\langle m^0 | V | n^0 \rangle e^{-i\omega t'} e^{\eta t'} dt' |m^0\rangle}$$

+ ...

$$= e^{-\frac{i}{\hbar} E_n^0 t} |n^0\rangle - \frac{i}{\hbar} \sum_m \langle m^0 | V | n^0 \rangle |m^0\rangle \frac{e^{i(\omega_{mn} - \omega - i\eta)t}}{i(\omega_{mn} - \omega - i\eta)} e^{\frac{i}{\hbar} E_n^0 t}$$

$$= e^{-\frac{i}{\hbar} E_n^0 t} \left\{ |n^0\rangle - \frac{1}{\hbar} \sum_m \frac{\langle m^0 | V | n^0 \rangle}{\omega_{mn} - \omega - i\eta} e^{-i\omega t} e^{\eta t} |m^0\rangle \right\}$$

∴ transition rate to m

$$= \frac{d}{dt} \frac{1}{\hbar^2} \left| \frac{\langle m^0 | V | n^0 \rangle}{\omega_{mn} - \omega - i\eta} \right|^2 \frac{d}{dt} e^{2\eta t} \Big|_{t=0}$$

$$= \frac{2}{\hbar^2} |\langle m^0 | V | n^0 \rangle|^2 \frac{\eta}{(\omega_{mn} - \omega)^2 + \eta^2}$$

$$= \frac{2}{\hbar^2} |\langle m^0 | V | n^0 \rangle|^2 \text{Im} \frac{1}{\omega_{mn} - \omega - i\eta}$$

$$\text{but } \text{Im} \frac{1}{\omega_{mn} - \omega - i\eta} = \pi \delta(\omega_{mn} - \omega)$$

$$\therefore \text{rate} = \frac{2\pi}{\hbar^2} |\langle m^0 | V | n^0 \rangle|^2 \delta(\omega_{mn} - \omega) !$$

5/14/96

No.

Date

P.

One usually introduces $\rho(E)$: # of states within $(E, E+dE)$
 i.e. $\rho(E)dE = \# \text{ of states within } (E, E+dE)$

$$\text{Hence, } \sum_{E_m^0 \approx E_n^0 + \hbar\omega} R(n \rightarrow m) = \int dE_m^0 \underbrace{\frac{2\pi}{\hbar} \delta(E_m^0 - E_n^0 - \hbar\omega)}_{\rho(E_m^0)} |\langle m^0 | \hat{U} | n^0 \rangle|^2$$

$$= \frac{2\pi}{\hbar} \rho(E_n^0 + \hbar\omega) |\langle m^0 | \hat{U} | n^0 \rangle|^2$$

$$\uparrow \\ m^0 \Rightarrow E_m^0 = E_n^0 + \hbar\omega$$

i.e. we say, $R(n \rightarrow m) = \frac{2\pi}{\hbar} \rho(E_m^0) |\langle m^0 | \hat{U} | n^0 \rangle|^2 \Big|_{E_m^0 = E_n^0 + \hbar\omega}$
 In particular, for real potentials, $\Downarrow$ may be replaced by $|V_{mn}|^2$
 it implies

emission rate for $n \rightarrow m$

density of final states m

= absorption rate for $m \rightarrow n$
density of ... n

$\Rightarrow$ detailed balance!

... means averaging over similar m^0 !

$$\vec{K} = \frac{2\pi}{L} (n_x, n_y, n_z)$$

example: $E = \frac{p^2}{2m}$, $p = \hbar k$, $E = \frac{\hbar^2}{2m} k^2$

$$\rho(E) dE = V \frac{4\pi k^2 dk}{(2\pi)^3} \quad \left(V \frac{d^3 \vec{k}}{(2\pi)^3} \right) \Leftrightarrow \sum_{E_m^0 \approx E_n^0 + \hbar\omega} R(n \rightarrow m) = \sum_{\vec{k}} (-)$$

$V = \text{Volume}$

$$\therefore \frac{\rho(E)}{V} = \frac{4\pi k^2}{(2\pi)^3} \frac{dk}{dE} = \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{E} = V \frac{d^3 \vec{k}}{(2\pi)^3} \frac{2\pi}{\hbar} \delta(E_k - E_g - \hbar\omega) |\langle \vec{k} | V | \vec{g} \rangle|^2$$

$$|V_{pg}|^2 = \frac{1}{4\pi} \int d^3 r_p \overline{| \langle p | \hat{U} | g \rangle |^2}$$

$$\int \sin \theta_p d\theta_p d\phi_p$$

$\Rightarrow$ interaction with the E.M. field.

Sudden Approximation (quenched dynamics)

Suppose the Hamiltonian H is changed from H_0 at t_0 to $H_0 + V$ at t_1 .

5/14/96

No.

Date

9.

Let $T = t_1 - t_0$.Then $T \rightarrow 0$ is called **Sudden change**. (a pulse!) $T \rightarrow \infty$ " " **Adiabatic change**It's convenient to reparametrize t :

$$s \equiv \frac{t-t_0}{T}, \quad t=t_0 \Rightarrow s=0 \quad H(t) \rightarrow H(s)$$

$$t=t_1, \quad s=1$$

$$\therefore H(0) = H_0, \quad H(1) = H_0 + V$$

$$U(t, t_0) \rightarrow U_T(s)$$

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle = U_T(s) |\psi(t_0)\rangle$$

$$i\hbar \frac{dU(t, t_0)}{dt} = H(t) U(t, t_0) \Rightarrow \frac{i\hbar}{T} \frac{dU_T(s)}{ds} = H(s) U_T(s)$$

$$\therefore U_T(s) = \mathbb{I} - \frac{i}{\hbar} T \int_0^s H(s') U_T(s') ds'$$

$$T \rightarrow 0 \quad U_T(s) \rightarrow \mathbb{I}$$

$$\therefore |\psi_{\text{after}}\rangle = \mathbb{I} |\psi_{\text{initial}}\rangle = |\psi_{\text{initial}}\rangle$$

X In the case of a sudden jump

Sudden Approximation: ($T \neq 0$) $\xrightarrow{t=t_0} H(t)$, it tells us that we can use $|\psi(t_0)\rangle$ as the initial condition for $t > 0$!

Approximate $U_T(1) \simeq \mathbb{I}$

$$\therefore |\psi(t_1)\rangle = U(t_1, t_0) |\psi(t_0)\rangle \simeq |\psi(t_0)\rangle$$

Let $P_0 \equiv \mathbb{I} - |\phi_0\rangle\langle\phi_0|$. $\therefore$ In sudden approximation,

$$\langle\psi(t_1)|P_0|\psi(t_1)\rangle \simeq 0 \quad \text{Since } |\psi(t_1)\rangle \simeq |\psi(t_0)\rangle$$

is approximately unperturbed! $\xrightarrow{\text{same as ①}}$

$\therefore$ To measure how good this approximation is, one measures the deviation of $|\psi(t_1)\rangle$ from $|\psi(t_0)\rangle$!

5/14/96

No.

Date

10

 $\therefore$ one measures

$$\tilde{\Delta} \equiv \langle \psi(t_0) | U^\dagger(t_1, t_0) P_0 U(t_1, t_0) | \psi(t_0) \rangle$$

$$= \langle \psi(t_0) | U_T^\dagger(1) P_0 U_T(1) | \psi(t_0) \rangle \quad \text{--- (1)}$$

$$\therefore U_T(1) = 1 - \frac{iT}{\hbar} \underbrace{\int_0^1 H(s) ds}_{\equiv \bar{H}} + \left(\frac{iT}{\hbar}\right)^2 \int_0^1 ds_1 \int_0^{s_1} ds_2 H(s_1) H(s_2) + \dots$$

$$\bar{H} = \frac{1}{T} \int_{t_0}^{t_1} H(t) dt$$

$$O(T^0) \text{ in } \tilde{\Delta} = 0$$

$$O(T) \text{ in } \tilde{\Delta} = \frac{iT}{\hbar} \langle \psi(t_0) | \bar{H} \underbrace{P_0}_{\uparrow 0} | \psi(t_0) \rangle$$

$$- \frac{iT}{\hbar} \underbrace{\langle \psi(t_0) | P_0}_{\downarrow 0} \bar{H} | \psi(t_0) \rangle$$

$$= 0 \quad \because P_0 | \psi(t_0) \rangle = 0$$

$$O(T^2) \text{ in } \tilde{\Delta} = \left(\frac{T}{\hbar}\right)^2 \langle \psi(t_0) | \bar{H} P_0 \bar{H} | \psi(t_0) \rangle$$

$$= \left(\frac{T}{\hbar}\right)^2 \left[\langle \psi(t_0) | \bar{H}^2 | \psi(t_0) \rangle - (\langle \psi(t_0) | \bar{H} | \psi(t_0) \rangle)^2 \right]$$

$$= \left(\frac{T}{\hbar}\right)^2 (\Delta \bar{H})^2 \left(\underbrace{\langle \psi(t_0) | P_0}_{=0} \int_0^1 ds_1 \int_0^{s_1} ds_2 H(s_1) H(s_2) \dots \right)$$

$\therefore$ For sudden approximation to be good, one requires

$$T \ll \frac{\hbar}{\Delta \bar{H}} \quad \bar{H} = \frac{1}{T} \int_{t_0}^{t_1} H(t) dt.$$

Adiabatic approximation, adiabatic theorem & Berry phase

$T \rightarrow \infty \Rightarrow$ adiabatic change.

What do we mean by $T \rightarrow \infty$?

5/14/96

No.

Date

11

In practical situations, " $T \rightarrow \infty$ " means $T \gg \min$ characteristic timescale^($T_{\min}$) in the system. (Recall the result of periodic perturbation $\hbar\omega$ has to be $E_n - E_m$ to cause transition, $\therefore$ if $\hbar\omega \rightarrow 0$ ($T \rightarrow \infty$), no transition!)

For example, if the length of the box (L) that confines a particle expands slowly to $L(t)$,

$$T_{\min} \approx \frac{L}{v_{\text{particle}}} = \frac{mL}{p} \approx \frac{mL^2}{\hbar} \approx \frac{1}{\omega_{\min}}$$

$$\omega_{\min} = \frac{1}{\hbar} \left[\frac{\hbar^2 \pi^2}{2mL^2} - \frac{\hbar^2 \pi^2}{2mL^2} \right] = \frac{3\hbar \pi^2}{2mL^2}$$

$$T \approx \frac{L}{\left| \frac{dL}{dt} \right|} \gg T_{\min} \Rightarrow \frac{mL}{\hbar} \left| \frac{dL}{dt} \right| \ll 1$$

e.g. $\frac{v_{\text{wall}}}{v_{\text{particle}}} \ll 1$

$$\approx \frac{1}{v_{\text{particle}}}$$

instantaneous eigenket

Adiabatic theorem: Let $H(s) |\psi_n(s)\rangle = E_n(s) |\psi_n(s)\rangle$, $0 \leq s \leq 1$
 $\phi_n(s) = |\psi_n(s)\rangle \langle \psi_n(s)|$

Assuming (i) no level-crossing, i.e., for $0 \leq s \leq 1$

$$E_n(s) \neq E_m(s) \text{ for any } n \neq m$$

(ii) $\frac{d\phi_n(s)}{ds}$ & $\frac{d^2\phi_n(s)}{ds^2}$ are well-defined &

piece-wise continuous

(When $T \rightarrow \infty$, i.e., turn on the perturbation too rapid, these could be violated!)

$$\Rightarrow \lim_{T \rightarrow \infty} U_T(s) \phi_n(0) = \phi_n(s) \lim_{T \rightarrow \infty} U_T(s) \quad (\text{see Messiah's book Chapter XVII or exercise})$$

i.e., if $|\psi(0)\rangle$ is an eigenket of $H(0)$ with $E = E_n(0)$,

then at time t , i.e., $s = \frac{t-t_0}{T}$, $|\psi(s)\rangle \equiv U_T(s) |\psi(0)\rangle$,

$|\psi(s)\rangle$ is an eigenket of $H(s)$: $H(s) |\psi(s)\rangle = E_n(s) |\psi(s)\rangle$!

i.e. $|\psi(s)\rangle$ is an instantaneous eigenket.

5/14/96

example: particle confined in a box ($L(t)$)

if $\frac{mL}{\hbar} \left| \frac{dL}{dt} \right| \ll 1$ is satisfied, $\psi(0) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$

at time t , $\psi(t) \propto \sqrt{\frac{2}{L(t)}} \sin \frac{n\pi x}{L(t)}$ where $L \equiv L(0)$
(not equal!)

Usually, the adiabatic condition ($T \gg T_{\min}$) is achieved by so-called adiabatically switch on:

by setting $H(t) = H_0 + e^{\epsilon t} V(\vec{r})$, $\epsilon \rightarrow 0^+$, $-\infty \leq t \leq 0$
($T = \frac{1}{\epsilon} \rightarrow \infty$)

The adiabatic theorem tells us that starting $|n^0\rangle$ at $t = -\infty$, the system will evolve into $|n\rangle$ of $H(0) = H_0 + V(\vec{r})$ at $t = 0$.

Thus, the time-dependent perturbation theory should recover the time-independent perturbation theory in this case ($\epsilon \rightarrow 0^+$)!

This is indeed true as one can verify to $O(V)$ below.

Recovering time-independent perturbation theory in the long width:

$H(t) = H_0 + e^{\epsilon t} V(\vec{r})$, $\epsilon \rightarrow 0^+$, $-\infty \leq t \leq 0$, $\epsilon \equiv \frac{1}{T}$

$$c'_k(t=0) = \frac{-i}{\hbar} \int_{-\infty}^0 \langle k^0 | V | n^0 \rangle e^{\frac{\epsilon}{\hbar} t'} e^{i\omega_{kn} t'} dt', \quad \omega_{kn} = \frac{1}{\hbar} (E_k^0 - E_n^0)$$

$$= \frac{-i}{\hbar} \frac{\langle k^0 | V | n^0 \rangle}{\frac{1}{T} + i\omega_{kn}}$$

$$\rightarrow \begin{cases} \frac{-i}{\hbar} \frac{V_{kn}}{\omega_{kn}} = \frac{V_{kn}}{E_n^0 - E_k^0} & k \neq n \\ \frac{-i}{\hbar} \frac{V_{nn}}{\epsilon} & k = n \end{cases}$$

$$\therefore |n_R\rangle = \left(1 - \frac{i}{\hbar} \frac{V_{nn}}{\epsilon}\right) |n^0\rangle + \sum_{k \neq n} \frac{V_{kn}}{E_n^0 - E_k^0} |k^0\rangle + \dots = \left(1 - \frac{i}{\hbar} \frac{V_{nn}}{\epsilon}\right) \left[|n^0\rangle + \sum_{k \neq n} \frac{V_{kn}}{E_n^0 - E_k^0} |k^0\rangle \right]$$

$+ O(V^2)$ $\uparrow$ normalization factor. In $|n\rangle$ accurate to $O(V)$

5/16/96

No.

Date

1.

(Note that at $t=0$, $|\psi(0)\rangle_I = |\psi(0)\rangle$, $\therefore |n\rangle_I = |n\rangle$)

There is also a related theorem in Quantum Field theory by Gell-man and Low, which states that the ground state $|\phi_0\rangle$ of H_0 will evolve into
 $\rightarrow$ but usually is
 some eigenket (not necessarily the ground state) of H

if $\frac{U_\epsilon(0, -\infty)|\phi_0\rangle}{\langle\phi_0|U_\epsilon(0, -\infty)|\phi_0\rangle}$ ($\epsilon \rightarrow 0^+$) exists to all orders in perturbation theory.

See Quantum Theory of Many-particle systems by Fetter & Walecka.

* Adiabatic Approximation & the Berry phase:

The adiabatic theorem states that starting from an eigenket of $H(0)$, $|n^0\rangle$, the state

$$|\psi(t)\rangle \equiv \lim_{T \rightarrow \infty} U_T(t, 0) |n^0\rangle \quad \text{is an eigenket}$$

$$\text{of } H(t): \quad H(t) |\psi(t)\rangle = E_n(t) |\psi(t)\rangle. \quad \dots \textcircled{1}$$

Of course, $\therefore i\hbar \frac{d}{dt} U_T(t, 0) = H(t) U_T(t, 0)$

$$\therefore i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle, \quad |\psi(t)\rangle \text{ is}$$

a solution to the Schrödinger eq.

5/16/96

$\therefore$ The solution thus constructed satisfies both the Schrödinger eq. and the eigenvalue eq. ①.

For example, if $H(t)$ is indept. of t , $H(t) = H$,

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

$$\begin{cases} i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H} |\psi(t)\rangle \\ \hat{H} |\psi(t)\rangle = E_n |\psi(t)\rangle \end{cases}$$

But, by no means, any solution to ① is a solution of the Schrödinger eq.!!

e.g. $|\psi(t)\rangle = |n^0\rangle \Rightarrow i\hbar \frac{d|\psi(t)\rangle}{dt} \neq \hat{H} |\psi(t)\rangle !!$
(H time independent)

One sees that the phase (e.g. $e^{-\frac{i}{\hbar} E_n t}$) plays an important role here. (even though $\hat{H}(t)$ is non-degenerate, the eigenket is specified only up to a phase!)

It is this phase which makes the whole thing non-trivial: because solving $i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$

does not reduce to solving $H(t) |\psi(t)\rangle = E_n(t) |\psi(t)\rangle$
as what happens for time-independent problems. (not separable)

* Fortunately, the adiabatic theorem also says that

5/16/96

No.

Date

3.

When $T \rightarrow \infty$, the problem can be solved as
in the time-independent situation:

One first solves: $H(t) |n(t)\rangle = E_n(t) |n(t)\rangle$

to get a set time-varying basis $|n(t)\rangle$ (normalized)
and corresponding eigenvalues $E_n(t)$

then $\lim_{T \rightarrow \infty} |\psi(t)\rangle_T = \sum_n a_n e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle \dots \textcircled{2}$
 $\uparrow$
 indept. of time.

In particular, for $H(t) = H$ (indept. of t), $T = \infty$ of

course. In this case $|\psi(t)\rangle = \sum_n a_n e^{-\frac{i}{\hbar} E_n t} \underbrace{|n(t)\rangle}_{|n^0\rangle}$

Consistent with $\textcircled{1}$!

Note that $e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'}$ is a generalization
of $e^{-\frac{i}{\hbar} E_n t}$. It is an accumulation of phase
due to change of E_n v.s. time just as that in

WKB approximation: $\psi(x) = \psi(x_0) e^{\pm \frac{i}{\hbar} \int_{x_0}^x p(x') dx'}$

$$\frac{1}{\hbar} p(x') dx' = 2\pi \frac{dx'}{\lambda(x')}$$

$$\Leftrightarrow \frac{1}{\hbar} E_n(t') dt' = 2\pi \frac{dt'}{T_n(t')}$$

In general, T is finite. $\therefore \textcircled{2}$ is not exact.

If one approximates $|\psi(t)\rangle$ by $\sum_n a_n e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle$

, this is the adiabatic approximation!! An indept. of time!
(Zeroth order, see below)

5/16/96

No.

Date

4.

One can also view eq. (2) as the success of method of separation of variables in the limit of $T \rightarrow \infty$:

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}(x,t) \psi(x,t)$$

try $\psi(x,t) = T(t) \psi(x)$

We get
$$i\hbar \frac{T'(t)}{T(t)} = \frac{\hat{H}(x,t) \psi(x)}{\psi(x)} \quad \text{--- (1)}$$

$\therefore \frac{\hat{H}(x,t) \psi(x)}{\psi(x)} = E_n(t)$ (function of t only).

This is actually not quite right because one can't find a time-indep. of $\psi(x)$ to satisfy $\hat{H}(x,t) \psi(x) = E_n(t) \psi(x)$

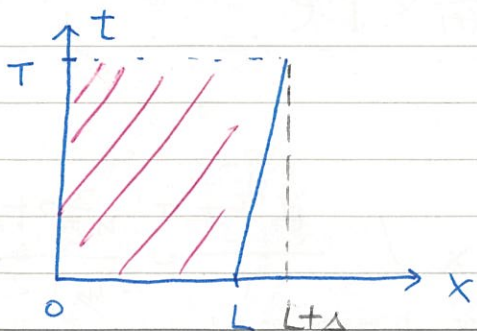
$\therefore \psi(x)$ should be rewritten as $u_n(x,t)$, but then what do we mean by the separation: $\psi(x,t) = T_n(t) u_n(x,t)$?

The separation basically just separates different speed of change: "fast variable" $u_n(x,t)$, "slow variable" $T_n(t)$!

(Because we know that $\delta E_n(t) = O([\delta u_n(x,t)]^2)$!)

As an example, consider a particle confined in a box of $L(t)$ i.e. when u_n rapidly changes, E_n can be hardly changed so that (1) is satisfied

$L(t) = L_0 + \frac{t}{T} \Delta$, $0 \leq t \leq T$. The boundaries are shown below:



Obviously, as $T \rightarrow \infty$, the boundaries approach a rectangular stripe!

The problem becomes separable!!

see over ($H = H(x)$!)

5/18/96

No.

Date

/

* Full adiabatic expansion:

The actual solution for a finite T is of course not in the form of eq. (2), but it can be put in the form:

$$|\psi(t)\rangle = \sum_n a_n(t) e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle \dots (3)$$

With time-dependent $a(t)$!!

dynamical phase

As $T \rightarrow \infty$, (3) reduces to

$$\sum_n a_n(0) e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle$$

which, for a finite T , is the adiabatic approximation.

As we will see, this is actually zeroth order of the full adiabatic approximation.

$$\text{Let } \hat{H}(t) = \hat{H}_0 + \hat{U}(t)$$

$$\therefore i\hbar \frac{d}{dt} |\psi(t)\rangle = \sum_n \left[(i\hbar \dot{a}_n(t) + E_n(t)) |n(t)\rangle + a_n(t) \underbrace{i\hbar \frac{d}{dt} |n(t)\rangle}_{i\hbar \dot{|n(t)\rangle}} \right] e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'}$$

$$= \hat{H} |\psi\rangle = \sum_n a_n E_n(t) |n(t)\rangle e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'}$$

$$\therefore \sum_n \dot{a}_n(t) e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle = - \sum_m a_m(t) e^{-\frac{i}{\hbar} \int_0^t E_m(t') dt'} |m(t)\rangle$$

$$\therefore \dot{a}_n(t) = - \sum_m a_m(t) e^{-\frac{i}{\hbar} \int_0^t (E_m(t') - E_n(t')) dt'} \langle n(t) | \dot{m}(t) \rangle \dots (4)$$

$$\text{Now, } \because \langle n(t) | n(t) \rangle = 1 \Rightarrow \underbrace{\langle \dot{n}(t) | n(t) \rangle}_{\langle n(t) | \dot{n}(t) \rangle^*} + \langle n(t) | \dot{n}(t) \rangle = 0$$

$$\therefore \text{Re } \langle n(t) | \dot{n}(t) \rangle = 0$$

5/18 196

$\therefore \langle n(t) | \dot{n}(t) \rangle$ is purely imaginary

$\therefore$ One sets $\langle n(t) | i(t) \rangle = i \alpha_n(t)$.

We can make $\alpha(t)$ zero by changing $\ln f(t)$:
(as we see later, this is not always true!)

$$|h(t)\rangle = e^{i\delta_n(t)} |n(t)\rangle$$

$$\langle \hat{n}(+) | \dot{\hat{n}}(+) \rangle = \langle n(+) | \dot{n}(+) \rangle + i \dot{\gamma}_n(+) = i [\dot{\alpha}_n(+) + \dot{\gamma}_n(+)]$$

$\therefore$ if we choose $k_n(t) = -\int_0^t \alpha_n(t') dt'$, $\langle \tilde{n}(t) | \dot{\tilde{n}}(t) \rangle = 0$

That is, if we start from $|n(t_1)\rangle \rightarrow \underbrace{e^{-i\int_{t_0}^{t_1} \Delta n(t) dt}}_{|\tilde{n}(t_1)\rangle} |n(t_1)\rangle$ in eq. ③, we end up with

$$\dot{a}_n(t) = - \sum_{\substack{m \\ m \neq n}}' a_m(t) e^{-\frac{i}{\hbar} \int_0^t [E_m(t') - E_n(t')] dt'} \quad \langle n(t) | \dot{m}(t) \rangle \dots (5)$$

Now, $\therefore \hat{H}|m(t)\rangle = E_m(t)|m(t)\rangle$

$$\therefore \underbrace{\frac{d}{dt} \hat{H}(t) |m(t)\rangle}_{II} = \dot{E}_m(t) |m(t)\rangle + E_m(t) |\dot{m}(t)\rangle$$

$$\therefore \langle n(t) | \dot{U}(t) | m(t) \rangle + E_n(t) \langle n(t) | \dot{m}(t) \rangle = E_m(t) \langle n(t) | \dot{m}(t) \rangle$$

$$\therefore \langle n(t) | \dot{n}(t) \rangle = \frac{\langle n(t) | \dot{U}(t) | n(t) \rangle}{E_m(t) - E_n(t)}$$

Hence, $\dot{a}_n(t) = \sum_m' a_m(t) \exp\left[\frac{-i}{\hbar} \int_0^t [E_m(t') - E_n(t')] dt'\right] \frac{\langle n(t) | \dot{V}(t) | m(t) \rangle}{E_n(t) - E_m(t)} \quad \text{--- (6)}$

The effort to remove $m=n$ is clear now. because there is $\frac{1}{E_n - E_m}$ factor in (6)!

5/18/96, 5/23/96 (revision)

No.

Date

3.

Integrating eq. (6), one gets

$$\begin{aligned}
 a_n(t) &= a_n(0) + \sum_m' \int_0^t dt' \exp \left[\frac{-i}{\hbar} \int_0^{t'} dt'' (E_m(t'') - E_n(t'')) \right] \\
 &\quad \times \frac{\langle n(t') | \dot{V}(t') | m(t') \rangle}{E_n(t') - E_m(t')} a_m(t') \\
 &= a_n(0) + \sum_m' a_m(0) \int_0^t dt' \frac{\langle n(t') | \dot{V}(t') | m(t') \rangle}{E_n(t') - E_m(t')} \exp \left[\frac{-i}{\hbar} \int_0^{t'} dt'' (E_m(t'') - E_n(t'')) \right] \\
 &\quad + \dots \quad (7)
 \end{aligned}$$

This is the full adiabatic expansion which is valid

if $r = \left| \int_0^t dt' \frac{\langle n(t') | \dot{V}(t') | m(t') \rangle}{E_n(t') - E_m(t')} e^{\frac{-i}{\hbar} \int_0^{t'} dt'' (E_m(t'') - E_n(t''))} \right|$

$$\sim \left| \int_0^t dt' \frac{1}{\Delta E} \langle n(t') | \dot{V}(t') | m(t') \rangle e^{\frac{-i}{\hbar} \Delta E t'} \right| \ll 1$$

ΔE = Characteristic energy scale in the system

$\therefore \langle n(t') | \dot{V}(t') | m(t') \rangle$ is a smooth function, we can take it outside of the integral:

$$\therefore r = \left| \langle n \left| \dot{V}(t) \right| m \right\rangle \int_0^t dt' \frac{1}{\Delta E} e^{\frac{-i}{\hbar} \Delta E t'} \right| \ll 1$$

$$\Rightarrow \left| \frac{2\hbar}{\Delta E^2} \right| \left| \langle n | \dot{V}(t) | m \rangle \right| \left| \sin\left(\frac{T \Delta E}{2\hbar}\right) \right| \ll 1$$

$$\therefore \left| \frac{1}{\omega_{nm}} \frac{d}{dt} \langle n | V(t) | m \rangle \right| \ll |\Delta E_{nm}|$$

$$\therefore \langle n | \dot{V}(t) | m \rangle \sim O\left(\frac{U_0}{T}\right) \sim O\left(\frac{\Delta E}{T}\right) \Rightarrow \frac{\hbar}{T \Delta E} \ll 1$$

$\therefore T \Delta E / \hbar \gg 1$ for eq. (7) to be valid.

i.e. the timescale of changing $V \gg$ characteristic timescale

In particular, as $T \rightarrow \infty$, $a_n(t) = a_n(0)$ of the system.

Full adiabatic expansion & Berry phase

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

write $|\psi(t)\rangle = \sum_n a_n(t) e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle$

$|\psi(t)\rangle$ satisfies $i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$

$$\sum_n \left\{ (i\hbar \dot{a}_n(t) + E_n(t) a_n(t)) |n(t)\rangle + a_n i\hbar |\dot{n}(t)\rangle \right\} e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'}$$

$$= \hat{H} |\psi(t)\rangle = \sum_n a_n E_n(t) |n(t)\rangle e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'}$$

$$\therefore \sum_n \dot{a}_n(t) e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n\rangle = - \sum_m a_m(t) e^{\frac{i}{\hbar} \int_0^t E_m(t') dt'} |\dot{m}(t)\rangle$$

$$\therefore \dot{a}_n(t) = - \sum_m a_m(t) e^{-\frac{i}{\hbar} \int_0^t [E_m(t') - E_n(t')] dt'} \langle n(t) | \dot{m}(t) \rangle \quad \text{--- (1)}$$

(i) $m \neq n \quad \therefore \hat{H} |m(t)\rangle = E_m(t) |m(t)\rangle$

$$\therefore \frac{d}{dt} \hat{H} |m(t)\rangle = \dot{E}_m(t) |m(t)\rangle + E_m(t) |\dot{m}(t)\rangle$$

$$\underbrace{\frac{d}{dt} \hat{H}}_V(t) |m(t)\rangle + \underbrace{E_m(t)}_{\hat{H}} |\dot{m}(t)\rangle$$

$$\therefore \langle n(t) | \dot{V}(t) |m(t)\rangle = (E_m(t) - E_n(t)) \langle n | \dot{m} \rangle$$

$$\therefore \langle n | \dot{m} \rangle = \frac{\langle n | \dot{V} | m \rangle}{E_m(t) - E_n(t)}$$

$$(ii) m=n \quad \therefore \langle n(t) | n(t) \rangle = 1$$

$$\Rightarrow \underbrace{\langle \dot{n}(t) | n(t) \rangle + \langle n(t) | \dot{n}(t) \rangle}_{\langle n(t) | \dot{n}(t) \rangle^*} = 0$$

$$\therefore \text{Re } \langle n(t) | \dot{n}(t) \rangle = 0 \quad \langle n(t) | \dot{n}(t) \rangle = i\alpha_n(t) \quad \alpha_n = \text{real}$$

$$\text{or } \alpha_n(t) = -i \langle n | \dot{n} \rangle$$

$$\therefore \textcircled{1} \Rightarrow \dot{a}_n(t) = -i\alpha_n(t) a_n(t) + \sum_{m \neq n} a_m(t) \frac{\langle n(t) | \dot{V} | m(t) \rangle}{E_n(t) - E_m(t)} e^{\frac{-i}{\hbar} \int_0^t (E_n(t') - E_m(t')) dt'}$$

just like interaction picture, we try to remove idn term, by defining $a_n(t) = e^{\frac{-i \int_0^t \alpha_n(t') dt'}{i\hbar}} b_n(t)$

$$\therefore \dot{b}_n(t) = \sum_{m \neq n} e^{-i(E_n(t) - E_m(t))} b_m(t) \frac{\langle n(t) | \dot{V} | m(t) \rangle}{E_n(t) - E_m(t)} e^{\frac{-i}{\hbar} \int_0^t (E_n(t') - E_m(t')) dt'}$$

$$b_n(t) = \underbrace{b_n(0)}_{a_n(0)} + \sum_{m \neq n} \int_0^t dt' b_m(t') \frac{\langle \tilde{n}(t') | \dot{V} | \tilde{m}(t') \rangle}{E_n(t') - E_m(t')} e^{\frac{-i}{\hbar} \int_0^t (E_n(t'') - E_m(t'')) dt''}$$

That is, one can absorb $e^{i\alpha_n(t)}$ into $|n(t)\rangle$

$$\text{so that } |\tilde{n}(t)\rangle \equiv e^{i\alpha_n(t)} |n(t)\rangle$$

the expansion coefficient is then $b_n(t)$.

We get

$$b_n(t) = \underbrace{b_n(0)}_{a_n(0)} + \sum_{m \neq n} b_m(0) \int_0^t dt' \frac{\langle \tilde{n}(t') | \dot{V} | \tilde{m}(t') \rangle}{E_n(t') - E_m(t')} e^{\frac{-i}{\hbar} \int_0^t (E_n(t'') - E_m(t'')) dt''}$$

+ . .

$\Rightarrow$ d'Alambert adiabatic expansion!

$$\therefore \dot{b}_n(t) \leq a_n(0)$$

$$\text{if } \sigma \equiv \left| \int_0^t dt' e^{\frac{i}{\hbar} \int_0^{t'} dt'' (E_n(t'') - E_m(t''))} \frac{\langle \hat{n}(t') | \dot{V} | \hat{m}(t') \rangle}{E_n - E_m(t')} \right|$$

$$\sim \left| \int_0^t dt' \frac{1}{\Delta E} e^{\frac{i}{\hbar} \Delta E t'} \langle \hat{n}(t') | \dot{V}(t') | \hat{m}(t') \rangle \right| \ll 1$$

$\Delta E = \text{characteristic energy scale}$

$\therefore \langle \hat{n}(t) | \dot{V}(t) | \hat{m}(t) \rangle$ is a smooth function

$$\therefore \sigma \sim \left| \langle \hat{n}(t) | \dot{V}(t) | \hat{m}(t) \rangle \right| \left| \int_0^t dt' \frac{e^{\frac{i}{\hbar} \Delta E t'}}{\Delta E} \right| \ll 1$$

$$\Rightarrow \left| \frac{2\hbar}{\Delta E^2} \right| \left| \langle n | \dot{V} | m \rangle \right| \underbrace{\left| \sin\left(\frac{\Delta E}{2\hbar} t\right) \right|}_{<1} \ll 1$$

$$\therefore \left| \frac{1}{\omega_{nm}} \frac{d}{dt} \langle \hat{n} | V(t) | \hat{m} \rangle \right| \ll |\Delta E_{nm}|$$

$$\therefore \langle \hat{n} | \dot{V} | \hat{m} \rangle \sim O\left(\frac{V_0}{T}\right) \sim O\left(\frac{\Delta E}{T}\right) \Rightarrow \frac{\hbar}{T \Delta E} \ll 1$$

$$\text{i.e. } \dot{V} \rightarrow 0 \quad b_n(t) \rightarrow a_n(0)$$

The above is fine as long as $H(t)$ doesn't go back to $H(0)$!

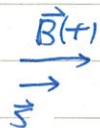
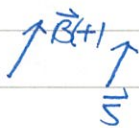
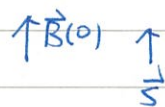
if $H(t) = H(0)$ then obviously, $H(t) |\hat{n}(t)\rangle = E(t) |\hat{n}(t)\rangle$, the basis has to satisfy $|\hat{n}(t)\rangle = |\hat{n}(0)\rangle$ which

can't be true for $|\hat{n}(t)\rangle$! $\therefore$ we have to keep $e^{-i\hbar}$

$$\therefore a_n(t) = a_n(0) e^{-i\hbar(t)}$$

5/18/96

example: $S = \frac{1}{2}$, $H = -\vec{\mu} \cdot \vec{B}(t)$, $\Delta E = 2\mu B$, $|\vec{B}(t)| = B$
 indept. of t !

 $t=0$

provided $T \gg \frac{\hbar}{2\mu B}$!

(may be achieved by restricting the particle on a sphere while the magnetic field is fixed!)

In this case, one can alter the directions of spins

* Berry phase: In the above, it seems the phase $\chi_n(t)$ can be always made to disappear?
 Is the phase $\chi_n(t)$ always a redundant?

The answer is no! (Michael Berry, 1984)

In the special case when $H(T) = H(0)$, we ^{must} have

$|n(T)\rangle = |n(0)\rangle$ (by construction) for any set of basis $\hat{H}(t)|n(t)\rangle = E(t)|n(t)\rangle$

$$\therefore \chi_n(T) = i \int_0^T \langle n(t') | \frac{d}{dt'} | n(t') \rangle dt'$$

$$= i \oint \langle n(t) | \frac{d}{dt} | n(t) \rangle dt \quad \text{close-loop integral in } t\text{-space.}$$

& Since the integrand is not a total derivative,

$\therefore \chi_n(T) \neq 0$!! i.e., one can't make it vanishing by redefining $|n(t)\rangle \Rightarrow e^{i\chi_n(t)} |n(t)\rangle \equiv |\hat{n}(t)\rangle$ because

Such a redefinition does not obey single-valued

requirement in general: $|\hat{n}(T)\rangle = e^{i\chi_n(T)} |n(T)\rangle = e^{i\chi_n(T)} |n(0)\rangle$

$\Rightarrow |\hat{n}(t)$ is not an acceptable basis of $\hat{H}(t)$ $| \hat{n}(t) \rangle = |n(0)\rangle$ only when $\chi_n(T) = 0$!! (or, $2k\pi$)
 $= E(t) |\hat{n}(t)\rangle$!

5/18/96

No.

Date

5.

$\gamma_n(T)$ is called the Berry phase! (geometrical phase)

This phase is universal in the sense that

$e^{i\gamma_n(T)}$ does not depend on the basis $|n(t)\rangle$ one chooses.

Why?

Suppose we start from another basis $|n'(t)\rangle$.

Quite generally, we can write $|n'(t)\rangle = e^{i\chi(t)} |n(t)\rangle$, where $\chi(t)$ is a phase that may depend on time.

By construction, one also requires $|n'(T)\rangle = |n'(0)\rangle$

$$\therefore e^{i\chi(T)} |n(T)\rangle = e^{i\chi(0)} |n(0)\rangle$$

$$\therefore |n(T)\rangle = |n(0)\rangle \therefore e^{i\chi(T) - i\chi(0)} = 1$$

$$\text{Now, } \gamma_n'(T) = i \oint dt \langle n'(t) | \frac{d}{dt} | n'(t) \rangle$$

$$= i \int_0^T dt \, i \frac{d\chi(t)}{dt} + i \oint dt \langle n(t) | \frac{d}{dt} | n(t) \rangle$$

$$= \gamma_n(T) - (\chi(T) - \chi(0))$$

$$\therefore e^{i\gamma_n'(T)} = e^{i\gamma_n(T)} e^{-i(\chi(T) - \chi(0))} = e^{i\gamma_n(T)}$$

* Now, suppose that initially, $|\psi(0)\rangle = |n(0)\rangle$, then in the adiabatic approximation, one has

$$H(t) |\psi(t)\rangle = E_n(t) |\psi(t)\rangle$$

$$\therefore |\psi(t)\rangle \propto |n(t)\rangle \quad \therefore \langle \psi(t) | \psi(t) \rangle = 1$$

$\therefore$ The proportional factor must be a phase term!

$$\Rightarrow |\psi(t)\rangle = \underbrace{a_n(t)}_{\text{adiabatic approx. other m do not enter!}} e^{\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle \quad (a_n(0) = 1)$$

5/18/96

$$\dot{Q}_n = -Q_n(t) \langle n_0 | \dot{n} \rangle \quad \text{eq. (4)}$$

Date

6.

This phase term is just $e^{i\gamma_n(t)} e^{\frac{i}{\hbar} \int_0^t E_n(t') dt'}$

$\therefore$ In the adiabatic approximation, we have

$$\begin{aligned} |\psi(t)\rangle &= U(t, 0) |n(0)\rangle \\ &= e^{i\gamma_n(t)} e^{\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle \end{aligned}$$

$$\begin{aligned} \text{If at } t=T, \quad H(T) &= H(0), \quad |\psi(T)\rangle = e^{i\gamma_n(T)} e^{\frac{i}{\hbar} \int_0^T E_n(t') dt'} |n(T)\rangle \\ &= e^{i\gamma_n(T)} e^{\frac{i}{\hbar} \int_0^T E_n(t') dt'} |n(0)\rangle \end{aligned}$$

Which is not equal to $|n(0)\rangle$, i.e., $|\psi(t)\rangle$ does not return to original state!

Thus, if we prepare two systems, one is under the perturbation $V(t)$, the other is not. At $t=T$, we bring two systems together. The Berry phase will cause interference between two systems each other and hence is observable!

example: $H = -\vec{\mu} \cdot \vec{B}(t), \quad |\vec{B}(t)| = B$

$$\therefore \vec{B}(t) = B \hat{n}(t), \quad \hat{n}(t) = \begin{pmatrix} \sin\theta(t) \cos\phi(t) \\ \sin\theta(t) \sin\phi(t) \\ \cos\theta(t) \end{pmatrix}, \quad \begin{aligned} &\text{take } \theta(t) = \theta \\ &\phi(t) = \omega t \end{aligned}$$

Take $|+, t\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} e^{i\omega t} \end{pmatrix}$ (to be single-valued! the

one $\begin{pmatrix} \cos\frac{\theta}{2} e^{-i\frac{1}{2}\phi(t)} \\ \sin\frac{\theta}{2} e^{i\frac{1}{2}\phi(t)} \end{pmatrix}$ we used is not!)

Let $\omega = \frac{2\pi}{T}$, Suppose $|\psi(T, 0)\rangle = |+, 0\rangle$.

5/18/96

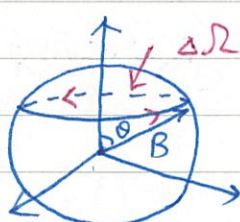
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Date

7.

$$\gamma_+ = i \int_0^T \langle +, t | \frac{d}{dt} | +, t \rangle dt$$

$$= -\omega T \sin^2 \frac{\theta}{2} = -2\pi \frac{1 - \cos \theta}{2} = -\pi(1 - \cos \theta)$$



$$\Delta\Omega = \text{solid angle} = 2\pi(1 - \cos \theta) \therefore \gamma_+ = -\frac{1}{2} \Delta\Omega$$

for



$$\gamma_+ = \pi(1 - \cos \theta) = \frac{1}{2} \Delta\Omega$$

$$\therefore \gamma_+ = \pm \frac{1}{2} \Delta\Omega$$

This can be verified by directly solving

$$H = -\mu B \begin{pmatrix} \cos \theta & \sin \theta e^{-i\omega t} \\ \sin \theta e^{i\omega t} & -\cos \theta \end{pmatrix} \quad H(T) = H(0)$$

$$|\psi(0)\rangle = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}$$

$$|\psi(t)\rangle = \begin{pmatrix} G(t) \\ G(t) \end{pmatrix}$$

(Hw. 6.
Ex 1a)

To find more about the Berry phase, see

Chapter 21, pages 592 - 607.

⇒ Emphasize "non-dynamical" origin of the

Berry phase ⇒ see 5/12/96 notes page 2-3

use flux tube as another example

2006/6/2

*

For general s ,

$$\text{one has } k_{\pm} = \pm ms \Delta\Omega$$

In particular, when $\theta = \pi/2$, $\Delta\Omega = 2\pi(1 - \cos\theta)$

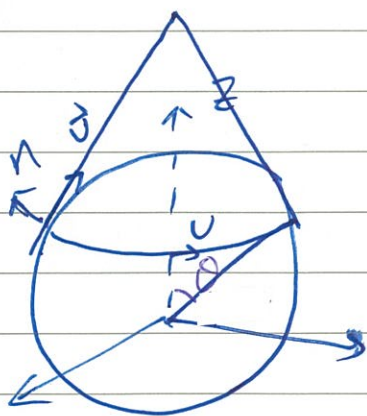
$$\therefore k_{\pm} = \pm\pi$$

therefor $\psi \rightarrow -\psi$, this is consistent with

the previous result: $s = 1/2$, particles charges $3/2, \dots$ wavefunction

sign after being rotated by 360° !

* The above is in contrast to the parallel transport of ordinary vector:



locally $\vec{U}$ does not

twist around $\hat{n}$

after one circle

$\vec{U}$ changes by α

$$\alpha = 2\pi(1 - \cos\theta) \text{ which is}$$

$$2k_{\pm}!$$

see Ong's argument in the next page

2006/6/2

No.

Date

1

More about the Berry phase:

1. for real & non-degenerate H .

ψ can also change into $\pm \psi$

$\therefore \theta = 0 \text{ or } \pi$

2.

$$\gamma_n^{(C)} = i \oint_C \langle n(R) | D n(R) \rangle \cdot d\vec{R}$$

$$= i \int_S D \times \langle n | D n \rangle \cdot d^2 S$$

$\Rightarrow$ Berry curvature

$$= i \int_S \underbrace{\langle D n | \times | D n \rangle}_{\text{II}} d^2 S$$

$$\int d^3 R \sum_n D_n^*(R) \times D_n(R)$$

$$\langle D n | \times | D n \rangle$$

$$= \sum_{m \neq n} \langle D n | m \rangle \times \langle m | D n \rangle$$

$$\langle D n | m \rangle \times \langle m | D n \rangle = \langle n | D m \rangle^* \times \langle n | D m \rangle$$

$$= 0 \quad (\because \langle n | D m \rangle \text{ is purely}$$

$$\text{imaginary, } \therefore \langle n | D m \rangle^* \propto \langle n | D m \rangle)$$

Now, $\therefore H|n\rangle = E_n(R)|n\rangle$

$$\therefore (D H)|n\rangle + H(D n) = (D E_n)|n\rangle + E_n(D n)$$

$$\therefore \langle m | D H | n \rangle = D E_n \langle m | n \rangle + (E_n - E_m) \langle m | D n \rangle$$

$$\therefore \langle m | D n \rangle = \frac{\langle m | D H | n \rangle}{E_n - E_m}$$

$$\therefore \gamma_n(dS) = i \int_S \sum_{m \neq n} \frac{\langle n | D H | m \rangle \langle m | D H | n \rangle}{(E_n - E_m)^2} \cdot d^2 S$$

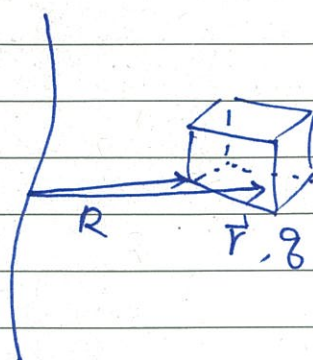
the Berry phase equation.

$\therefore$ when there is a degeneracy, $\gamma_n(dS)$ can

be non-vanishing!

↓
as singular
point

Berry's example AB effect



$$A=0.$$

$$H_0 = \frac{\hat{p}^2}{2m} + V(r-R)$$

$$H(\hat{p}, r-R) |n_0(R)\rangle$$

$$= E_n |n_0(R)\rangle$$

↳ independent of $\vec{R}$

$$A \neq 0.$$

$$H = \frac{1}{2m} (\hat{p} - \frac{q}{c} \vec{A})^2 + V(r-R)$$

$$H |n(R)\rangle = E_n |n(R)\rangle$$

from $\vec{R}$ to $\vec{R}'$, there is no singularity

$$\langle \vec{R}' | n(R) \rangle = e^{\frac{iq}{\hbar c} \int_{\vec{R}}^{\vec{R}'} d\vec{r}' \cdot \vec{A}(\vec{r}')} \langle \vec{r}' | n_0(R) \rangle$$

$$\gamma_n = i \oint \underbrace{\langle n | d\vec{R} | n \rangle}_{||} \cdot d\vec{R}$$

even though the point is that the lower end of the integral needs not to be $\vec{R}$, it can be some other point $\vec{R}_1$, but $\vec{R}_1$ must go with $\vec{R}$ in the same speed

$$\int d\vec{R}' \langle n(R) | \vec{r}' \rangle \underbrace{\langle \vec{r}' | d\vec{R} | n \rangle}_{||}$$

$$d\vec{R} e^{\frac{iq}{\hbar c} \int_{\vec{R}}^{\vec{R}'} d\vec{r}' \cdot \vec{A}(\vec{r}')} \langle \vec{r}' | n_0 \rangle$$

$$= \frac{iq}{\hbar c} \vec{A}(\vec{R}) \langle \vec{r}' | n_0 \rangle e^{\frac{iq}{\hbar c} \int_{\vec{R}}^{\vec{R}'} d\vec{r}' \cdot \vec{A}(\vec{r}')} + e^{\frac{iq}{\hbar c} \int_{\vec{R}}^{\vec{R}'} d\vec{r}' \cdot \vec{A}(\vec{r}')} d\vec{R} \langle \vec{r}' | n_0(R) \rangle$$

$$= 2\pi \frac{q}{\hbar c} \oint \vec{A} \cdot d\vec{R} + i \oint \underbrace{\langle n_0 | d\vec{R} | n_0 \rangle}_{||} \cdot d\vec{R}$$

Note if $\vec{R}$ is replaced by $\vec{R}'$,

$$\therefore \frac{d}{dt} e^{\frac{i q}{\hbar c} \int_{R_1}^R d\vec{r}' \cdot \vec{A}(\vec{r}')} = \nabla_{R_1} (\quad) \cdot \frac{d\vec{R}_1}{dt}$$

$$\stackrel{||}{=} \frac{d\vec{R}}{dt}$$

$$\Rightarrow \oint \vec{A}(\vec{R}) \cdot d\vec{R} = \oint \vec{A}(\vec{R}) \cdot d\vec{R}$$

$k_n^0 = 0$ $\therefore H_0$ is real, $\therefore \langle \vec{r} | H_0(R) \rangle$ can be
chosen to be real!

$$\therefore \nabla_R \underbrace{\langle H_0 | H_0 \rangle}_{=1} = 0$$

$$\nabla_R |H_0(R, r)|^2 = 0$$

$$H_0(R, r) \nabla_R H_0(R, r) = 0$$

$$\therefore k_n = 2\pi \frac{\Phi}{\Phi_0} \quad \Phi_0 = \frac{hc}{q}$$

5/12/18

Transparent derivation of the Berry phaseif $H =$ time independent

$$H|n\rangle = E_n|n\rangle \Rightarrow \psi(t) = e^{\frac{i}{\hbar} E_n t} |n\rangle$$

Similarly, if $H =$ time dependent,

$$\text{one tries } \psi(t) = e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle \quad \text{--- (separable) --- } \textcircled{1}$$

$$\text{With } H(t)|n(t)\rangle = E_n(t)|n(t)\rangle$$

But in principle, one can put a phase in. $\textcircled{1}$

$$\psi(t) = e^{i\gamma_n(t)} e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle$$

$$\text{Substituting into } i\hbar \frac{d\psi}{dt} = \hat{H} \psi$$

$$\begin{aligned} \Rightarrow i\hbar \left[e^{i\gamma_n} e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} \frac{d}{dt} |n(t)\rangle - \frac{i}{\hbar} E_n(t) e^{i\gamma_n(t)} e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} \right. \\ \left. \times |n(t)\rangle + i\dot{\gamma}_n(t) e^{i\gamma_n(t)} e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle \right] \\ = E_n e^{i\gamma_n} e^{-\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n\rangle \end{aligned}$$

$$\therefore \frac{d}{dt} |n(t)\rangle + i\dot{\gamma}_n(t) |n\rangle = 0 \quad \therefore \text{--- } \textcircled{2}$$

$$\therefore \dot{\gamma}_n(t) = i \int_0^t \langle n(t') | \dot{n}(t') \rangle dt'$$

Note that $\textcircled{2}$ is not rigorous right, it's only valid when $T \rightarrow \infty$ because in general,

5/2/18

2.

$$\langle m(t) | \frac{d}{dt} | n(t) \rangle \neq 0 \quad \dots \quad (i)$$

along other component^{≠0}

in fact, as we have seen,

$$\langle m | \dot{n} \rangle = \frac{\langle m(t) | \dot{U}(t) | n(t) \rangle}{E_n(t) - E_m(t)} \lesssim \frac{1}{T} \rightarrow 0 \text{ as } T \rightarrow \infty$$

$\Uparrow$
 $\dot{U} \lesssim \frac{\Delta E}{T}$

$$\therefore T \rightarrow \infty \quad \psi(t) = e^{i\gamma_n(t)} e^{\frac{i}{\hbar} \int_0^t E_n(t') dt'} |n(t)\rangle$$

$\Uparrow$ Berry phase
 $\Uparrow$ dynamical phase
 (geometrical phase)

$\hookrightarrow$ dependent on path

If the time dependence of $H(t)$ is resulted

from the change of some coordinate $\vec{R}(t)$, we

then have $\frac{d}{dt} |n(t)\rangle = \frac{\partial}{\partial \vec{R}} |n(\vec{R})\rangle \dot{\vec{R}}(t)$

$$\therefore \gamma_n = i \int_0^t \langle n(\vec{R}) | \frac{\partial}{\partial \vec{R}} | n(\vec{R}) \rangle \dot{\vec{R}}(t') dt'$$

$$= i \int_{R_i}^{R_f} \langle n(\vec{R}') | \frac{\partial}{\partial \vec{R}} | n(\vec{R}') \rangle d\vec{R}'$$

$$= i \int_{R_i}^{R_f} \langle n(\vec{R}) | \frac{\partial n}{\partial \vec{R}} \rangle d\vec{R}$$

$$\vec{R} \rightarrow \oint \langle n(\vec{R}) | \frac{\partial n}{\partial \vec{R}} \rangle d\vec{R} \quad \dots \quad (2)$$

if $\vec{R}_i = \vec{R}_f$

5/12/98

if R is a vector $\vec{R}$, ③ becomes

$$\gamma_n(t) = i \int_{R_i}^{R_f} \langle n | \nabla n \rangle \cdot d\vec{R}$$

$$= i \oint \langle n | \nabla_R n \rangle \cdot d\vec{R}$$

if $R_f = R_i$

$$(\because \frac{d}{dt} |n\rangle = \int \frac{d}{d\vec{e}_i} |n\rangle \dot{R}_i)$$

This reminds us the vector potential $\vec{A}$

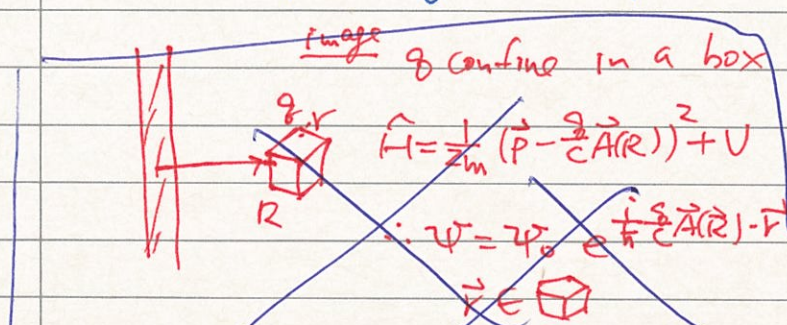
$$i \langle n | \nabla_R n \rangle \Leftrightarrow \vec{A}, \quad \gamma_n(t) \Leftrightarrow \text{flux}$$

$\therefore i \langle n | \nabla_R n \rangle$ is often termed "Berry potential"

Indeed, in the case of AB effect, it can be regarded as a Berry phase.

In that case, $\langle n | \nabla_R n \rangle \propto$ real $\vec{A} !!$

(see Berry's original paper!)



Confine particle in a box & move a circle around the flux tube.

$$\gamma_n = \frac{-iq}{\hbar c} \oint \vec{A} \cdot d\vec{R} = -\frac{q}{\hbar c} \Phi = -\frac{q}{\hbar c} \left(\frac{\Phi}{\Phi_0} \right) \Phi_0$$

$\Phi_0 = \frac{hc}{q}$

$\frac{q\Phi}{\hbar c} = \frac{\Phi}{\Phi_0}$

$q = 2e, \frac{\hbar c}{2e} = \Phi_0$

5/5/98

historical origin of

Born - Oppenheimer approximation & Berry phase

$$H(R, r, p)$$

 $\uparrow \quad \times$

nuclear
(slow)

electronic (fast)

Assume $\Psi(R, r) = \Phi(R) \phi(R, r)$

Born -
Oppenheimer

Approximation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(R, r) \right] \phi(R, r) = E(R) \phi(R, r)$$

$$\left[-\frac{\hbar^2}{2M} \nabla^2 + E(R) \right] \Phi(R) = E \Phi(R)$$

neglect $\frac{\hbar^2}{2M} \nabla^2 \Phi(R) \cdot \nabla^2 \phi(R, r) + \frac{\hbar^2}{2M} \Phi(R) \nabla^2 \phi(R, r)$

$$\ll \frac{\hbar^2}{2m} \Phi(R) \nabla^2 \phi(R, r)$$

$$(\because M \gg m)$$

It was first noticed by Herzberg & Longuet-Higgins
in 1963 (Discuss. Faraday Soc. 35, 77 (1963))

that if $\vec{R}$ traverses a circuit within
which the state is degenerate with another,
then $\phi(R, r) \rightarrow -\phi(R, r)$ after coming back

i.e. $\delta = \pi$ extra phase $\Rightarrow$ Berry phase.

This phase implies $\Phi(R)$ must also change
sign as $\vec{R}$ traverses a circuit as $\phi(R, r)$
has to be single valued!

5/5/98

This result tells us that the quantum # of $\vec{R}$ can take on fractional values! (even in the absence of spins!)

For example, for rotations

$$\vec{R} \rightarrow (R, \phi) \quad e^{im\phi}$$

usually, $m = \text{integers}$

but now, $m = \text{half integers}$

$$\therefore m = -l, -l+1, \dots, l$$

$$\therefore E = \frac{l(l+1)}{2I} \quad l = \text{half integers!}$$

~~It also imposes some selection rules:~~

~~vibration~~

The phenomenon of the Berry phase is quite ubiquitous. Along the change of $\vec{R}$, $\phi(R, r)$

changes conforming to $U(R, r)$, we say $\phi(R, r)$ is "parallel transported".

A system does not return to its original state when transported along a closed loop.

is said to be nonholonomic!

An example is to transport the tangent vector
along



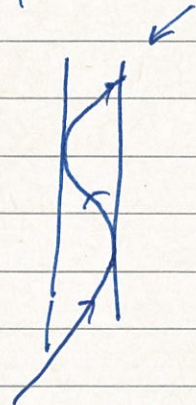
on a sphere

Classical counterpart to Berry phase

⇒ Hannay angle

Example (a) Foucault pendulum

(b) optical fiber PRL 57, P37-P40 (1986)



k -space



↻ circular polarized
or linearly polarized

the final phase
would not be
the same!

5/14/97

Interaction of atoms with electromagnetic radiation* Semi-classical treatment:

treat $\vec{E}, \vec{B}$ classically but ψ quantum-mechanically!
radiation fields (no charges, & current!)

$$\begin{cases} \nabla \cdot \vec{E} = 0 \\ \nabla \cdot \vec{B} = 0 \Rightarrow \vec{B} = \nabla \times \vec{A} \\ \nabla \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0 \Rightarrow \vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t} - \nabla \phi \\ \nabla \times \vec{B} - \frac{1}{c} \frac{\partial \vec{E}}{\partial t} = 0 \end{cases}$$

$$\nabla \cdot \vec{E} = 0 \Rightarrow \nabla^2 \phi + \frac{1}{c} \frac{\partial}{\partial t} \nabla \cdot \vec{A} = 0 \quad \text{--- ①}$$

$$\nabla \times \vec{B} - \frac{1}{c} \frac{\partial \vec{E}}{\partial t} = 0 \Rightarrow \nabla^2 \vec{A} - \frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} - \nabla [\nabla \cdot \vec{A} + \frac{1}{c} \frac{\partial \phi}{\partial t}] = 0 \quad \text{--- ②}$$

These two equations decide $\vec{A}$ & ϕ which in turn determine $\vec{E}$ & $\vec{B}$.

Note that ① & ② can be combined in a more concise form: $\square A^\alpha - \partial^\alpha \partial_\beta A^\beta = 0$

$$\square = -\nabla^2 + \frac{1}{c^2} \frac{\partial^2}{\partial t^2}, \quad \partial^0 = \frac{1}{c} \frac{\partial}{\partial t}$$

Gauge invariance:

$$\vec{A}_{\text{new}}^0 = \vec{A}_{\text{old}} + \nabla \Lambda$$

$$\phi_{\text{new}}^0 = \phi_{\text{old}} - \frac{1}{c} \frac{\partial \Lambda}{\partial t}$$

$\vec{E}, \vec{B}$ not changed
 i.e. ① ② are satisfied for any $\vec{A}, \phi \rightarrow \vec{E}, \vec{B}$ same

but if we choose Λ such that

$$\nabla^2 \Lambda - \frac{1}{c^2} \frac{\partial^2 \Lambda}{\partial t^2} = -\nabla \cdot \vec{A}_{\text{old}} - \frac{1}{c} \frac{\partial \phi_{\text{old}}}{\partial t}$$

$\vec{A}_{\text{new}}^0$ & ϕ_{new}^0 satisfy $\nabla \cdot \vec{A}_{\text{new}}^0 + \frac{1}{c} \frac{\partial \phi_{\text{new}}^0}{\partial t} = 0$
 (Lorentz condition)

5/14/P1

if one sticks with the Lorentz condition
and write $D \cdot \vec{A}_{new} = -\frac{1}{c} \frac{\partial}{\partial t} \Phi_{new}$

No.

$$\Rightarrow (D^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) \vec{A}_{new} = 0 \quad (D^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) \Phi_{new} = 0$$

then $\vec{A}_{new}$ decouples from Φ (eq. ②) : Lorentz gauge

$$\begin{cases} D^2 \Phi_{new} + \frac{1}{c} \frac{\partial}{\partial t} D \cdot \vec{A}_{new} = D^2 \Phi_{old} + \frac{1}{c} \frac{\partial}{\partial t} D \cdot \vec{A}_{old} \\ -\frac{1}{c} \frac{\partial}{\partial t} D^2 \chi + \frac{1}{c} \frac{\partial}{\partial t} D^2 \chi = 0 \\ D^2 \vec{A}_{new} - \frac{1}{c^2} \frac{\partial^2 \vec{A}_{new}}{\partial t^2} = 0 \end{cases}$$

① & ② are satisfied for both new & old since
 $\vec{E} = -D\Phi_{old} - \frac{\partial}{\partial t} \vec{A}_{old} = -D\Phi_{new} - \frac{\partial}{\partial t} \vec{A}_{new}$

Even under the Lorentz condition, we still have freedom to choose $\vec{A}_{new}$ & Φ_{new} :

$$\vec{A}_{new} = \vec{A}_{new}^0 + D\chi$$

$$\Phi_{new} = \Phi_{new}^0 - \frac{1}{c} \frac{\partial \chi}{\partial t} \quad (\because \text{Now } D \cdot \vec{A} + \frac{1}{c} \frac{\partial \Phi}{\partial t} = 0 \text{ is satisfied})$$

as long as χ satisfies $D^2 \chi - \frac{1}{c^2} \frac{\partial^2 \chi}{\partial t^2} = 0$ (require)

so that $D \cdot \vec{A}_{new} + \frac{1}{c} \frac{\partial \Phi_{new}}{\partial t} = 0$ is still obeyed!

$$\begin{cases} D^2 \Phi_{new} + \frac{1}{c} \frac{\partial}{\partial t} D \cdot \vec{A}_{new} = 0 \quad \dots \text{③} \\ (D^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) \vec{A}_{new} = 0 \quad \dots \text{④} \end{cases}$$

can be satisfied by many $(\Phi, \vec{A})$ but connected by the gauge χ .

Coulomb gauge : choose χ such that

$$D^2 \chi = -D \cdot \vec{A}_{new} \quad (\vec{A}_{new} = \vec{A}_{new}^0 + D\chi) \\ \Rightarrow D \cdot \vec{A}_{new} = 0 !$$

Since

$$D^2 \Phi_{new}^0 + \frac{1}{c} \frac{\partial}{\partial t} D \cdot \vec{A}_{new}^0 = 0$$

$$\text{i.e. } D^2 \Phi_{new}^0 = -\frac{1}{c} \frac{\partial}{\partial t} D \cdot \vec{A}_{new}^0 = -D \cdot \left[\frac{1}{c} \frac{\partial \vec{A}_{new}^0}{\partial t} \right] \\ \Rightarrow \frac{1}{c} D^2 \frac{\partial \chi}{\partial t} = -D \cdot \left(\frac{1}{c} \frac{\partial \vec{A}_{new}^0}{\partial t} \right)$$

$\therefore$ In particular, we can choose $\chi = c \int dt \Phi_{\text{new}}^0$

(because of the Lorentz condition,

$$\therefore \Phi_{\text{new}} = \Phi_{\text{new}}^0 - \frac{1}{c} \frac{\partial \chi}{\partial t} = 0$$

$$(\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}) \vec{A}_{\text{new}} = 0$$

$$\nabla \cdot \vec{A}_{\text{new}} = 0$$

in the Coulomb gauge!

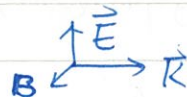
$$\begin{aligned} \nabla^2 \chi - \frac{1}{c^2} \frac{\partial^2 \chi}{\partial t^2} &= -\nabla \cdot \vec{A}_{\text{new}} - \frac{1}{c} \frac{\partial \Phi_{\text{new}}^0}{\partial t} = 0 \\ &\text{automatically!} \end{aligned}$$

Now, we will drop "new".

$\therefore$ In the Coulomb gauge, the radiation fields are described by

$$\begin{cases} \vec{A} = \vec{A}_0 \cos(\vec{k} \cdot \vec{r} - \omega t) \\ \omega^2 = k^2 c^2 \\ \nabla \cdot \vec{A} = 0 \Rightarrow \vec{k} \cdot \vec{A}_0 = 0 \\ \vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t} = -\frac{\omega}{c} \vec{A}_0 \sin(\vec{k} \cdot \vec{r} - \omega t) \\ \vec{B} = \nabla \times \vec{A} = -\vec{k} \times \vec{A}_0 \sin(\vec{k} \cdot \vec{r} - \omega t) \end{cases}$$

matter:



$$\frac{1}{2m} \left(p - \frac{e}{c} \vec{A} \right)^2 \psi = i \hbar \frac{\partial \psi}{\partial t} \quad \text{in the Coulomb gauge} \quad (e < 0)$$

neglect $O(A^2)$, we have

$$\textcircled{1} \quad \nabla^2 \phi + \frac{1}{c} \frac{\partial}{\partial t} \nabla \cdot \vec{A} = -4\pi \rho$$

Superposition

$$H = \frac{p^2}{2m} - \frac{e}{mc} \vec{A} \cdot \vec{p} \quad (\nabla \cdot \vec{A} = 0) \rightarrow$$

$\downarrow$ In the presence of a static charge (such as the charge of the nucleus), $\textcircled{3}$ becomes $\nabla^2 \phi_{\text{new}} = -4\pi \rho \quad \therefore \phi_{\text{new}} \neq 0$

in the Coulomb gauge. (one can't choose $\chi = c \int dt \Phi_{\text{new}}^0$ to make χ satisfy $\nabla^2 \chi = -\nabla \cdot \vec{A}_{\text{new}}$ any more!)

$$\text{one has to solve } \frac{1}{c^2} \frac{\partial^2 \chi}{\partial t^2} = \nabla^2 \chi = -\nabla \cdot \vec{A}_{\text{new}}$$

5/14/99

No.

Date

4.

then, we have

$$H = \frac{p^2}{2m} - \frac{e}{mc} \vec{A} \cdot \vec{p} + e\phi(\vec{r}) \equiv H_0 - \frac{e}{mc} \vec{A} \cdot \vec{p}$$

In any case, we treat $-\frac{e}{mc} \vec{A} \cdot \vec{p}$ as the perturbation:

$$V(t) = \frac{-e}{mc} \cos(\vec{k} \cdot \vec{r} - \omega t) \vec{A}_0 \cdot \vec{p}$$

$$= \frac{|e|}{2mc} [e^{i(\vec{k} \cdot \vec{r} - \omega t)} + e^{-i(\vec{k} \cdot \vec{r} - \omega t)}] \vec{A}_0 \cdot \vec{p}$$

For absorptions, it is suffice to consider

$$V(t) = \underbrace{\frac{|e|}{2mc} e^{i\vec{k} \cdot \vec{r}} \vec{A}_0 \cdot \vec{p}}_{\hat{V}} e^{-i\omega t}$$

$$\therefore R_{n \rightarrow m} = \frac{2\pi}{\hbar} \frac{e^2}{4mc^2} |\vec{A}_0 \cdot \langle m^0 | e^{i\vec{k} \cdot \vec{r}} \vec{p} | n^0 \rangle|^2$$

$$\times \delta(E_m^0 - E_n^0 - \hbar\omega) \quad \text{--- (5)}$$

Δ dipole approximation

$$\therefore \hbar\omega = E_m^0 - E_n^0 \sim \frac{e^2}{a_0} \quad \text{for atoms levels } E_n \text{ and } E_m$$

$$\therefore \hbar k = \hbar \frac{\omega}{c} \simeq \frac{e^2}{a_0 c}$$

$\therefore \langle m^0 | e^{i\vec{k} \cdot \vec{r}} \vec{p} | n^0 \rangle$ is appreciable only when $r \sim a_0$

$$\therefore \vec{k} \cdot \vec{r} \sim k a_0 \sim \frac{e^2}{\hbar c} \simeq \frac{1}{137} \ll 1$$

$\therefore$ We can approximate $e^{i\vec{k} \cdot \vec{r}}$ by 1.

5/4/17

No.

Date

5.

Such approximation leads to

$$\langle m^0 | e^{i\vec{k} \cdot \vec{r}} \vec{p} | n^0 \rangle \cong \langle m^0 | \vec{p} | n^0 \rangle$$

$$\therefore [x, H_0] = [x, \frac{p^2}{2m} + e\phi] = \frac{i\hbar}{m} p_x$$

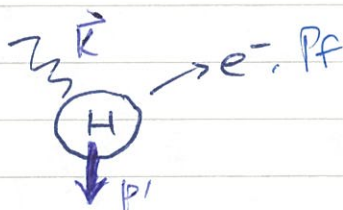
$$\therefore \langle m^0 | \vec{p} | n^0 \rangle = \frac{m}{i\hbar} \langle m^0 | [\vec{r}, H_0] | n^0 \rangle$$

$$= im W_{mn} \underbrace{\langle m^0 | \vec{r} | n^0 \rangle}_{\text{xe} = \text{dipole}}$$

$\Rightarrow$ so is the name "dipole approximation"!

$$\therefore R_{n \rightarrow m} = \frac{2\pi}{\hbar} \frac{e^2}{4c^2} (W_{mn})^2 |\vec{A}_0 \cdot \langle m^0 | \vec{r} | n^0 \rangle|^2 \times \delta(E_m^0 - E_n^0 - \hbar\omega)$$

Δ photo-electric effect



$$|n^0\rangle = |0\rangle$$

$$\langle m^0 | = \langle f | \cong \langle \vec{p}' | \quad (\text{dipole approx. is no longer valid})$$

(see Shankar's discussion p.500)

$$\vec{A}_0 \cdot \langle m^0 | \vec{p} | n^0 \rangle = \frac{1}{\sqrt{V}} \left(\frac{1}{\pi a_0^3} \right)^{\frac{1}{2}} \quad \vec{p} = \vec{p}' + \hbar\vec{k}, \quad \vec{r} - \vec{r}_f = \vec{p}'$$

$$\times \int d^3r \, e^{-i\frac{\vec{p}}{\hbar} \cdot \vec{r}} \vec{A}_0 \cdot \frac{1}{i} \nabla e^{-r/a_0}$$

$$\cong \frac{1}{\sqrt{V}} \left(\frac{1}{\pi a_0^3} \right)^{\frac{1}{2}} \underbrace{\vec{A}_0 \cdot \vec{p}_f}_{\substack{|| \\ (-\vec{A}_0 \cdot \vec{p}')}} \underbrace{\int d^3r \, e^{-r/a_0} e^{-i\vec{r} \cdot \vec{p}'/\hbar}}_{\substack{|| \\ (\because \vec{r} \cdot \vec{A}_0) \\ = 0}}$$

integration by parts

form factor of the ground state!

$$= \frac{1}{\sqrt{V}} \left(\frac{1}{\pi a_0^3} \right)^{\frac{1}{2}} \frac{8\pi/a_0}{\left[\left(\frac{1}{a_0} \right)^2 + (P_f/\hbar)^2 \right]^2} (\vec{A}_0 \cdot \vec{P}_f)$$

$$\Rightarrow R = \frac{2\pi}{\hbar} \left(\frac{e}{2mc} \right)^2 \left(\frac{1}{\sqrt{V}} \right)^2 \frac{1}{\pi a_0^3} \frac{|\vec{A}_0 \cdot \vec{P}_f|^2 \cdot 64\pi^2 a_0^6}{[1 + (P_f a_0/\hbar)^2]^4}$$

$$\times \delta(E_f^0 - E_i^0 - \hbar\omega)$$

$$\uparrow \uparrow$$

$$\frac{P_f^2}{2m}$$

$$\begin{cases} \Delta k_x = \frac{2\pi}{L} \\ L^3 \frac{\delta^3 k}{(2\pi)^3} = 1 \end{cases} \downarrow$$

$$V \frac{d^3 k}{(2\pi)^3} = \rho(E) dE$$

$$\frac{d^3 k}{(2\pi)^3}$$

replacing $\delta(E_f^0 - E_i^0 - \hbar\omega)$ by $\rho(E)$, we get:

$\left(\frac{1}{V} \right)$ gets cancelled

$$R_{0 \rightarrow d\Omega} = \frac{2\pi}{\hbar} \left(\frac{e}{2mc} \right)^2 \frac{1}{(2\pi\hbar)^3} \frac{1}{\pi a_0^3} \frac{|\vec{A}_0 \cdot \vec{P}_f|^2 \cdot 64\pi^2 a_0^6}{[1 + (P_f a_0/\hbar)^2]^4} \cdot d\Omega \cdot \underbrace{\frac{P_f^2 dP_f}{\hbar dE_f}}_{m P_f}$$

$$= \frac{4a_0^3 e^2 P_f |\vec{A}_0 \cdot \vec{P}_f|^2}{m\pi \hbar^4 c^2 [1 + (P_f a_0/\hbar)^2]^4} d\Omega$$

* the need for field quantization:

Classically, vacuum (free space) : $A=0$ (really free!) , no any transition can occur!

However, we do observe the spontaneous

decay of atoms. e.g. $H : |2, l, m\rangle \rightarrow |1, 0, 0\rangle!$

$(R \approx 10^8 \text{ seconds})$

5/14/97

No.

Date

7.

This implies ^{real} $A \neq 0$!

What is happening then?

analogy: Oscillator $\Rightarrow$ classically: ground state $x=p=0$

quantum: only $\langle x \rangle = 0$, $\langle p \rangle = 0$

$\Delta x^2, \Delta p^2 \neq 0$!

$\therefore$ To escape from the conclusion $A=0$, we

need to promote $A \rightarrow \hat{A}$ (operator) so that

$$\langle A \rangle = 0, \quad \Delta A^2 \neq 0! \Rightarrow \therefore \langle A^2 \rangle = \langle 0 | \hat{A} \hat{A} | 0 \rangle$$

Since $A(r)$ is $\vec{r}$ -dependent, $\hat{A}(\vec{r})$ is a "field operator" $\Rightarrow$ field quantization.

When combined with the treatment on $\mathcal{H}$ involve relativistic

$\Rightarrow$ QED.

EM fields as harmonic oscillators

take $\hat{R} \parallel \hat{x}$ $\hat{A}_0 \parallel \hat{y}$

$$E = E_0 \sin(kx - \omega t), \quad (E_0 = -\frac{\omega}{c} A_0)$$

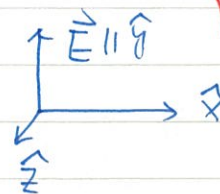
$$B = B_0 \sin(kx - \omega t), \quad (B_0 = A_0 k = -E_0)$$

$$E(x, t) = E_0 [\cos \omega t \sin kx - \sin \omega t \cos kx]$$

$$\equiv \omega q(t) \sin kx + p(t) \cos kx$$

$$q(t) = \frac{E_0}{\omega} \cos \omega t$$

$$p(t) = -E_0 \sin \omega t = \dot{q}(t)$$



$\langle m | \hat{A} | m \rangle$
complete set

matrix element
 $\langle m | \hat{A} | 0 \rangle$
Compared to
 $\langle A \rangle = \langle 0 | \hat{A} | 0 \rangle = 0!$

5/14/99

This is to be compared with the elastic waves one learned in the classical mechanics!

For a finite size, $0 \leq x \leq L$, periodic boundary

conditions: $k = \frac{2\pi n}{L}$, $n = 0, \pm 1, \pm 2, \dots$

$H =$ energy per area (in y - z plane)

$$= \frac{1}{2} \int_0^L dx \left[\frac{E^2}{8\pi} + \frac{B^2}{8\pi} \right]$$

$$= \frac{1}{8\pi} \int_0^L dx E^2$$

$$= \frac{L}{16\pi} [\omega^2 q^2(t) + p^2(t)]$$

Let $Q = \sqrt{\frac{L}{8\pi}} q$, $P = \sqrt{\frac{L}{8\pi}} p$ ($P = \dot{Q}$ is still correct)

$\therefore H = \frac{1}{2} (P^2 + \omega^2 Q^2)$ is precisely the Hamiltonian for an oscillator!

$\therefore$ quantization $[P, Q] = \frac{\hbar}{i}$ (canonical quantization)

$$\hat{H} = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) \quad \hat{Q} = \frac{1}{\sqrt{2\hbar\omega}} (\omega \hat{Q} + i \hat{P})$$

(Note that this is actually in the Heisenberg picture, $\therefore a(t) = a e^{-i\omega t}$!)

In general, there are many $\vec{R}$, $\checkmark$ for each $\vec{R}$, $\vec{E}$

5/14/19

can be either $\parallel \hat{y}$ or $\parallel \hat{z}$ $\Rightarrow$ two polarization

$$\Rightarrow \hat{H} = \sum_{\lambda=1,2} \int d^3\vec{R} \hbar \omega(\vec{k}) \left[a_{\lambda}^{\dagger}(\vec{k}) a_{\lambda}(\vec{k}) + \frac{1}{2} \right]$$

↑
polarization

Now, $\therefore a = \frac{1}{\sqrt{2\hbar\omega}} (\omega Q + i P)$

$$a^{\dagger} = \frac{1}{\sqrt{2\hbar\omega}} (\omega Q - i P)$$

$$\therefore Q = \sqrt{\frac{\hbar}{2\omega}} (a + a^{\dagger}) = \sqrt{\frac{L}{8\pi}} q = \sqrt{\frac{L}{8\pi}} \frac{A_0}{c} \cos \omega t$$

$$P = \sqrt{\frac{\hbar\omega}{2}} \frac{1}{i} (a - a^{\dagger}) = \sqrt{\frac{L}{8\pi}} p = \sqrt{\frac{L}{8\pi}} \frac{-\omega A_0}{c} \sin \omega t$$

$$\therefore A = A_0 \cos(\omega Kx - \omega t)$$

$$= A_0 \cos Kx \cos \omega t + A_0 \sin Kx \sin \omega t$$

$$= -c q \cos Kx - \frac{c}{\omega} p \sin Kx$$

$$= -c \sqrt{\frac{8\pi}{L}} \sqrt{\frac{\hbar}{2\omega}} \left[a e^{iKx} + e^{iKx} a^{\dagger} \right] \quad \leftarrow \begin{array}{l} \text{as expected} \\ \because A = \text{real} \end{array}$$

In general, $c \sqrt{\frac{\hbar}{2\omega}} = \sqrt{\frac{\hbar c^2}{2\omega}}$

$$\vec{A} = \sum_{\lambda=1,2} \int \frac{\sqrt{\hbar c^2}}{\sqrt{4\pi^2 \omega}} d^3\vec{R} \left[a_{\lambda}(\vec{R}) \hat{\epsilon}_{\lambda}(\vec{R}) e^{i\vec{R} \cdot \vec{r}} + a_{\lambda}^{\dagger}(\vec{R}) \hat{\epsilon}_{\lambda}(\vec{R}) e^{-i\vec{R} \cdot \vec{r}} \right] \quad (\vec{A}^{\dagger} = \vec{A})$$

(see Shaker's book 518.5 for more details)

5/14/99

No.

Date

10.

where $[a_\lambda(\vec{k}), a_{\lambda'}^\dagger(\vec{k}')] = \delta_{\lambda\lambda'} \delta^3(\vec{k}-\vec{k}')$

In this approach, the spontaneous decay goes

like:

$$V = \frac{-e}{mc} \vec{A} \cdot \vec{p}$$

$\uparrow$
 operator acting on fields state

$\nwarrow$ acting on matter state

initial: $|i\rangle = |2\ell m\rangle \otimes |0\rangle$

$\because a_{\vec{k}\lambda}^\dagger |0\rangle = \sqrt{\frac{1}{2\pi\hbar\omega}} |1_{\vec{k}\lambda}\rangle$
 so it is more likely to emit the

$\uparrow$
 vacuum of E.M.

final: $|f\rangle = |100\rangle \otimes |0, 0, \dots, 1, 0, \dots\rangle$

same photon

$\uparrow$
 one quanta in the state $|1_{\vec{k}\lambda}\rangle$

$$\equiv |100\rangle \otimes |1_{\vec{k}\lambda}\rangle$$

thus produce coherent light!

$$\therefore \langle f | V | i \rangle = \langle 2\ell m | \underbrace{\langle 1_{\vec{k}\lambda} | \vec{A} | 0 \rangle}_{\sqrt{\frac{\hbar c^2}{4\pi^2 \omega}} \hat{\epsilon}_\lambda(\vec{k}) e^{i\vec{k} \cdot \vec{r}}} \cdot \vec{p} | 100 \rangle \frac{-e}{mc}$$

$$\approx \frac{-e}{mc} \sqrt{\frac{\hbar c^2}{4\pi^2 \omega}} \hat{\epsilon}_\lambda \cdot \int d^3r \psi_{100}^* \frac{1}{i} \vec{\nabla} \psi_{2\ell m}$$

(dipole approximation)

= -- $\Rightarrow$ see Shkar's book Chapter 18 for more details.

Here we just demonstrate the principle of calculation!

$$\therefore \int d^3r \psi_{100}^* \frac{1}{r} \psi_{2em}$$

$$= im \omega_{mn} \int d^3r \psi_{100}^* \hat{r} \psi_{2em} \quad \omega_{mn} = \frac{E_2 - E_1}{\hbar} \equiv \omega$$

$$\therefore \langle f | V | i \rangle = \frac{-e}{mc} \frac{\sqrt{\hbar c^2}}{\sqrt{4\pi\omega}} im \omega \int \psi_{100}^* \hat{\Sigma} \cdot \vec{r} \psi_{2em} d^3r$$

$$\hat{\Sigma} \cdot \vec{r} = \Sigma_x r_x + \Sigma_y r_y + \Sigma_z r_z$$

$$(\Sigma_{\pm} = \mp \frac{\Sigma_x \pm i \Sigma_y}{\sqrt{2}})$$

$$r_{\pm} = \sqrt{\frac{4\pi}{3}} r Y_{\pm 1}$$

$$z = \sqrt{\frac{4\pi}{3}} r Y_0$$

$$\therefore \int \psi_{100}^* \hat{\Sigma} \cdot \vec{r} \psi_{2em} d^3r$$

$$= \sqrt{\frac{4\pi}{3}} \int_0^{\infty} R_{10} r R_{21} r^2 dr$$

$$\times \int d\Omega Y_0^* [-\Sigma_+ Y_{-1} + \Sigma_z Y_0 - \Sigma_- Y_1] Y_1 d\Omega$$

$$= \sqrt{\frac{3}{2}} \frac{2^{\frac{1}{2}}}{3^{\frac{1}{2}}} \frac{a_0}{\sqrt{3}} (\Sigma_+ \delta_{m,-1} + \Sigma_z \delta_{m,0} + \Sigma_- \delta_{m,1})$$

$$|\langle f | \vec{r} | i \rangle|^2 = \frac{2^{\frac{1}{2}}}{3^{1/2}} a_0^2 [|\Sigma_+|^2 \delta_{m,-1} + |\Sigma_z|^2 \delta_{m,0} + |\Sigma_-|^2 \delta_{m,1}]$$

Averaging over m , one gets

$$= \frac{2^{\frac{1}{2}}}{3^{1/2}} a_0^2 \times \frac{1}{3} (|\Sigma_x|^2 + |\Sigma_y|^2 + |\Sigma_z|^2) = \frac{2^{\frac{1}{2}}}{3^{1/2}} a_0^2$$

$$R_{10} = \frac{2}{\pi} \frac{1}{a_0} \frac{1}{r} \frac{1}{\sqrt{2}} \frac{2^{\frac{1}{2}}}{3^{1/2}} a_0^2 f(R_{10} + \hbar \omega - E_{2em})$$

Now, i is the initial state including the photon state.

If we sum over all possible photon momentum and two possible polarizations, we get

$$\int \delta(E_{00} + \hbar\omega - E_{em}) k^2 dk d\Omega = \frac{4\pi k^2}{\hbar c}$$

where $k = \frac{\omega}{c} = \frac{E_{em} - E_{00}}{\hbar c} = \frac{e^2}{20.4e} \times \frac{3}{4}$

$$\therefore R_{i \rightarrow all} = \left(\frac{2}{3}\right)^4 \alpha^5 \frac{mc^2}{\hbar}$$

+
sum
over
photon
states

$$\alpha = \frac{1}{137} = \frac{e^2}{\hbar c}$$

$$\frac{mc^2}{\hbar} = 10^{21} \text{ sec}^{-1}$$

$$R_{i \rightarrow all} \approx 0.6 \times 10^9 \text{ sec}^{-1}$$

$$\tau = \frac{1}{R} \approx 1.6 \times 10^{-9} \text{ sec}$$

agrees with expt.