

# TIME-DEPENDENT PERTURBATION THEORY

①

WE ARE INTERESTED IN PROBLEMS SUCH THAT

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

THE FORMAL SOLUTION IS VIA THE TIME DEVELOPMENT OPERATOR

$$U(t, t_0) \quad \text{SINCE} \quad |\Psi_s(t)\rangle = U(t, t_0) |\Psi_s(t_0)\rangle$$

(SUB INDEX S DENOTES THE SCHRÖDINGER REPRESENTATION)

AND  $U(t, t_0)$  IS DETERMINED BY  $H(t)$ :

$$i\hbar \frac{d}{dt} U(t, t_0) = H(t) U(t, t_0) \Rightarrow U(t, t_0) = 1 + \frac{1}{i\hbar} \int_{t_0}^t dt' H(t') U(t', t_0)$$

$$\text{WHERE } U(t_0, t_0) = 1$$

THIS EQUATION CAN BE SOLVED ITERATIVELY:

$$U(t, t_0) = 1 + \frac{1}{i\hbar} \int_{t_0}^t dt_1 H(t_1) + \left(\frac{1}{i\hbar}\right)^2 \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 H(t_1) H(t_2) + \dots$$

$$= \sum_{n=0}^{\infty} \left(\frac{1}{i\hbar}\right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \dots \int_{t_0}^{t_{n-1}} dt_n H(t_1) H(t_2) \dots H(t_n)$$

\* NOTE THAT  $t > t_1 > t_2 > \dots > t_n > t_0$  AND  $[H(t_i), H(t_j)] \neq 0$

THERE IS A COMPACT WAY OF WRITING THE ABOVE RESULT

$$U(t, t_0) = T \left\{ \exp \left( \frac{1}{i\hbar} \int_{t_0}^t H(t') dt' \right) \right\}$$

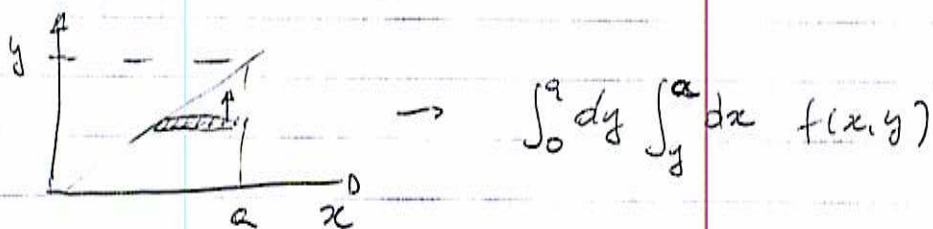
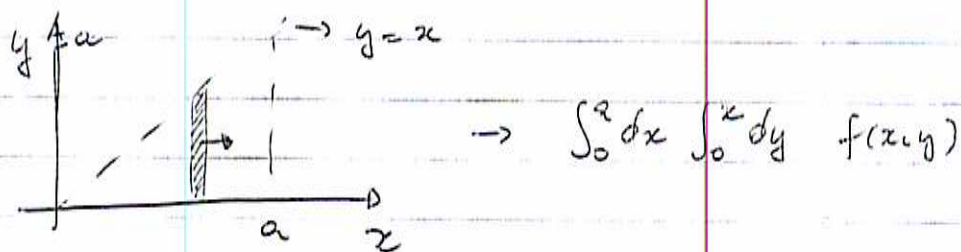
WHERE  $T \equiv$  TIME ORDERING OPERATOR

$$\begin{aligned} \text{EXAMPLE: } T \{ H(t_1) H(t_2) \} &= \begin{cases} H(t_1) H(t_2), & \text{if } t_1 > t_2 \\ H(t_2) H(t_1), & \text{if } t_1 \leq t_2 \end{cases} \\ &= \Theta(t_1 - t_2) H(t_1) H(t_2) + \Theta(t_2 - t_1) H(t_2) H(t_1) \end{aligned}$$

HOW DO WE ARRIVE AT THIS RESULT?

(2)

CONSIDER  $I = \int_0^a dx \int_0^x dy f(x,y)$



$$\begin{aligned}
 I &= \frac{1}{2} \int_0^a dx \int_0^x dy f(x,y) + \frac{1}{2} \int_0^a dy \int_y^a dx f(x,y) && \left. \begin{array}{l} \updownarrow \\ x \leftrightarrow y \end{array} \right\} \\
 &= \frac{1}{2} \int_0^a dx \int_0^x dy f(x,y) + \frac{1}{2} \int_0^a dx \int_x^a dy f(y,x) \\
 &= \frac{1}{2} \int_0^a dx \int_0^a dy \Theta(x-y) f(x,y) + \Theta(y-x) f(y,x) \\
 &= T \left\{ \frac{1}{2} \int_0^a dx \int_0^a dy f(x,y) \right\}
 \end{aligned}$$

SAME FOR  $f(x_1, x_2, \dots)$  AND SO ON

$$\begin{aligned}
 \Rightarrow \sum_{n=0}^{\infty} \int_0^x dx_1 \int_0^{x_1} dx_2 \dots \int_0^{x_{n-1}} dx_n f(x_1, x_2, \dots, x_n) \\
 = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^x dx_1 \dots \int_0^x dx_n T \{ f(x_1, \dots, x_n) \}
 \end{aligned}$$

FOR  $f(x_1, \dots, x_n) = f(x_1) \dots f(x_n)$

$$\begin{aligned}
 &= \sum_{n=0}^{\infty} \frac{1}{n!} T \left( \int_0^x dx' f(x') \right)^n = T \left\{ \sum_{n=0}^{\infty} \frac{1}{n!} \left[ \int_0^x f(x') dx' \right]^n \right\} \\
 &= T \left\{ e^{\int_0^x f(x') dx'} \right\}
 \end{aligned}$$

USUALLY, IT IS HARD TO INTEGRATE (OR IMPOSSIBLE) ANALYTICALLY (OR EVEN NUMERICALLY)  $\int_{t_0}^t dt' H(t')$

(3)

AND, AT THE SAME TIME, PERFORM THE TIME ORDERING

WHAT DO WE DO? ~~ANSWER:~~ ANSWER: PERTURBATION THEORY

- EXPAND  $U(t, t_0)$  UP TO SOME ORDER
- IN MANY CASES  $H = H_0 + V(t)$  WITH  $V(t) \ll H_0$   
(GAPS IN THE SPECTRUM OF  $V(t)$   $\ll$  GAPS OF SPECTRUM OF  $H_0$ )
- ⇒ TREAT  $V(t)$  PERTURBATIVELY

IN OTHER WORDS, WE INVESTIGATE HOW THE DYNAMICS OF A SYSTEM GOVERNED BY  $H_0$  IS AFFECTED BY  $V(t)$

IN THIS WAY, THE INTERACTION REPRESENTATION IS VERY CONVENIENT, THE DYNAMICS OF  $H_0$  IS EASILY INCORPORATED IN THE OPERATORS WHILE THE EFFECTS OF  $V(t)$  IS ENCODED IN THE STATE VECTORS WHICH WE OBTAIN PERTURBATIVELY.

RECALL:  $i\hbar \frac{d}{dt} |\psi_s\rangle = (H_0 + V) |\psi_s\rangle$ ,  $|\psi_I(t)\rangle = e^{i\frac{H_0 t}{\hbar}} |\psi_s(t)\rangle = T_0^+(t) |\psi_s(t)\rangle$   
 $i\hbar \frac{d}{dt} U_I(t, t_0) = V_I(t) U_I(t, t_0)$ ,  $V_I = T_0^+(t) V T_0(t)$   
 $|\psi_I(t)\rangle = U_I(t, t_0) |\psi_I(t_0)\rangle$

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

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

THIS EQUATION IS THE BASIS OF OUR FORMALISM FOR THE PERTURBATION THEORY

WE WILL BE INTERESTED IN THE TRANSITION AMPLITUDES BETWEEN STATES OF  $H_0$ :

$H_0 |m\rangle = E_m |m\rangle \rightarrow |m(t)\rangle = U_S(t, t_0) |m(t_0)\rangle = U_S(t, t_0) |m\rangle$

TRANSITION AMPLITUDE:  $\langle m | m(t) \rangle = \langle m | U_S(t, t_0) | m \rangle = C_{m,m}$



USING THAT  $U_S(t, t_0) = T_0(t) U_I(t, t_0) T_0^\dagger(t_0)$   
 $= e^{-\frac{i}{\hbar} H_0 t} U_I(t, t_0) e^{\frac{i}{\hbar} H_0 t_0}$

$\Rightarrow C_{m,m} = \langle m | T_0(t) U_I(t, t_0) T_0^\dagger(t_0) | m \rangle$

$C_{m,m} = \langle m | T_0(t) T_0^\dagger(t_0) | m \rangle + \frac{1}{i\hbar} \int_{t_0}^t dt_1 \langle m | T_0(t) V_I(t_1) T_0^\dagger(t_0) | m \rangle + \dots$   
 $= \langle m | U_0(t, t_0) | m \rangle + \frac{1}{i\hbar} \int_{t_0}^t dt_1 \langle m | T_0(t) T_0^\dagger(t_1) V(t_1) T_0(t_1) T_0^\dagger(t_0) | m \rangle + \dots$   
 $= \langle m | U_0(t, t_0) | m \rangle + \frac{1}{i\hbar} \int_{t_0}^t dt_1 \langle m | U_0(t, t_1) V(t_1) U_0(t_1, t_0) | m \rangle +$   
 $(\frac{1}{i\hbar})^2 \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \langle m | U_0(t, t_1) V(t_1) U_0(t_1, t_2) V(t_2) U_0(t_2, t_0) | m \rangle + \dots$

$\Rightarrow C_{m,m} = \langle m | U_0(t, t_0) + \sum_{n=1}^{\infty} \int_{t_0}^t dt_1 \dots \int_{t_0}^{t_{n-1}} dt_n U_0(t, t_1) V(t_1) U_0(t_1, t_2) V(t_2) \dots U_0(t_{n-1}, t_n) V(t_n) U_0(t_n, t_0) | m \rangle$

VARIOUS ORDERS OF PERTURBATION:

0th:  $C_{m,m}^{(0)} = \delta_{m,m} e^{-\frac{i}{\hbar} E_m(t-t_0)} = \delta_{m,m} e^{\frac{-iE_m t}{\hbar}} e^{\frac{iE_m t_0}{\hbar}}$

1st:  $C_{m,m}^{(1)} = \frac{1}{i\hbar} \int dt_1 \langle m | U_0(t_0, t_1) V(t_1) \sum_{k \neq m} |k\rangle \langle k| U_0(t_1, t_0) | m \rangle$   
 $= \frac{1}{i\hbar} \sum_k \int dt_1 e^{-\frac{iE_m}{\hbar}(t-t_1)} V_{mk}(t_1) e^{-\frac{iE_k}{\hbar}(t_1-t_0)} \delta_{k,m}$   
 $= e^{\frac{-iE_m t}{\hbar}} e^{\frac{iE_m t_0}{\hbar}} * \frac{1}{i\hbar} \int_{t_0}^t dt_1 e^{iW_{mm} t_1} V_{mm}(t_1)$

FOURIER TRANSFORM OF  $V_{mm}$

WHERE  $\hbar W_{mm} = E_m - E_m$

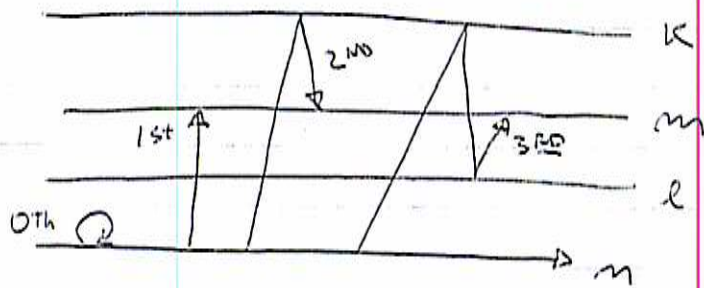
2ND:  $C_{m,m}^{(2)} = (\frac{1}{i\hbar})^2 \int dt_1 dt_2 \sum_{k \neq l} e^{-\frac{iE_m}{\hbar}(t-t_1)} V_{mk}(t_1) e^{-\frac{iE_k}{\hbar}(t_1-t_2)} V_{kl}(t_2) e^{-\frac{iE_l}{\hbar}(t_2-t_0)} \delta_{l,m}$   
 $= e^{\frac{-iE_m t}{\hbar}} e^{\frac{iE_m t_0}{\hbar}} * (\frac{1}{i\hbar})^2 \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \sum_k e^{iW_{mk} t_1} V_{mk}(t_1) e^{iW_{kl} t_2} V_{kl}(t_2)$

SAME PHASE

# GRAPHIC INTERPRETATION (DIAGRAMS)

(5)

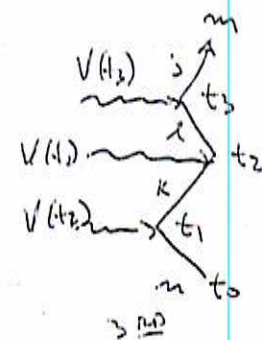
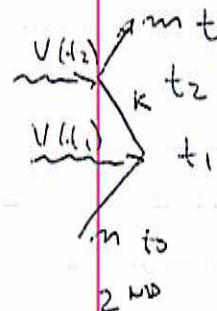
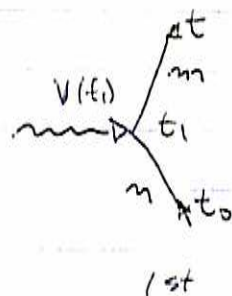
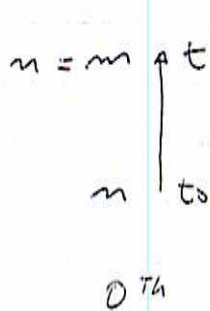
A SIMPLE GRAPHIC VISUALIZATION REFERS TO THE STRING OF OPERATORS THAT APPEARS IN THE VARIOUS ORDERS OF PERT. THEORY:  $V_{mk} V_{kl} V_{ls} \dots V_{im}$



VIRTUAL TRANSITIONS BEFORE REACHING THE FINAL ~~STATE~~ STATE

ANOTHER, AND MORE INTUITIVE, DESCRIPTION IS VIA DIAGRAMS

TIME ↑



~~~~~ = INTERACTION (CAN CARRY ENERGY AND MOMENTUM)  
 ——— = "FREE" PROPAGATION (ACCORDING TO  $H_0$ ) UNPERTURBED

THUS, IT IS LIKE THE SYSTEM'S DYNAMICS IS DICTATED BY  $H_0$  AND OCCASIONALLY,  $V$  ENTERS IN THE GAME (ON INSTANTS  $t_1, t_2, t_3, \dots$ )

THE GENERAL PROBLEM ONE MAY BE CONCERNED IS THE TRANSITION FROM A GENERIC STATE  $|\psi_0\rangle = \sum_i \alpha_i |i\rangle$  AT  $t = t_0$  TO ANOTHER STATE  $|\psi\rangle = \sum_j \beta_j |j\rangle$  AT TIME  $t = t$ . THEN ONE HAS TO GO OVER THE SIMPLE ALGEBRA

$$\langle \psi | U_S | \psi_0 \rangle = \sum_{ij} \alpha_i \beta_j^* \langle j | U_S | i \rangle = \sum_{ij} \alpha_i \beta_j^* c_{ji}$$

WHERE THE COEFFICIENTS  $c_{ji}$  WERE CALCULATED IN ORDERS OF PERTURBATION



EXAMPLE : TIME INDEPENDENT PERTURBATION

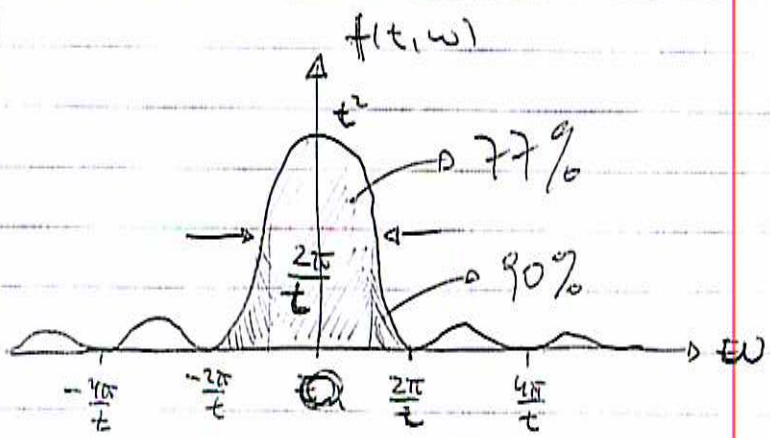
$V(t) = V \Theta(t) \rightarrow$  PERTURBATION IS SWITCHED ON INSTANTLY AT  $t=0$

TRANSITION PROBABILITY =  $P_{m,m}(t) = |c_{m,m}(t)|^2$   
 UP TO 1ST ORDER  $\Rightarrow P_{m,m} = |s_{m,m} + \frac{1}{i\hbar} \int_0^t dt' e^{i\omega_{mm}t'} V_{mm}|^2$

FOR  $m \neq m$ , IT SIMPLIFIES TO

$$P_{m,m} = \frac{1}{\hbar^2} |\langle m|V|m \rangle|^2 \left| \frac{1}{i\omega_{mm}} (e^{i\omega_{mm}t} - 1) \right|^2 = \frac{4|V_{mm}|^2}{(\hbar\omega_{mm})^2} \left( \sin \frac{\omega_{mm}t}{2} \right)^2$$
  
 YIELDS TO SELECTION RULES  $= \frac{1}{\hbar^2} |V_{mm}|^2 f(t, \omega_{mm})$

LET US ANALYZE  $f(t, \omega) = \frac{4 \sin^2(\omega t/2)}{\omega^2}$



NOTICE THAT  
 $\lim_{t \rightarrow \infty} f(t, \omega) = t^2 \delta(\omega)$

WIDTH:  
 $\Delta \omega$  IS SUBSTANTIAL  
 $f(\omega, t) \approx t^2$

~~...~~ SINCE THE 1ST MINIMUM IS OF ORDER  $2\pi/t \Rightarrow$  WIDTH  $\approx \frac{2\pi}{t}$

SINCE THE PEAK GROWS  $\sim t^2$  AND THE WIDTH DIMINISHES  $\sim 1/t \Rightarrow$  THE AREA OF THE CENTER GROWS  $\sim t \Rightarrow$  FOR LARGE  $t$ , ALL TRANSITIONS REMAIN CLOSE TO THE INITIAL STATE

PRECISELY  $\int_{-\frac{2\pi}{t}}^{\frac{2\pi}{t}} \frac{4 \sin^2(\omega t/2)}{\omega^2} d\omega \approx 4.86 t$  /  $\int_{-\frac{2\pi}{t}}^{\frac{2\pi}{t}} f(t, \omega) d\omega = 5.6t$

NOTICE THAT  $\int_{-\infty}^{\infty} \frac{4 \sin^2(\omega t/2)}{\omega^2} d\omega = 2\pi t = 6.28 t$   $\frac{5.6t}{6.28} \approx 0.9$

$\Rightarrow \frac{4.86 t}{6.28 t} \approx 0.77 \Rightarrow$  77% OF THE TRANSITION STATES ARE WITHIN  $-\frac{2\pi}{t} < \omega < \frac{2\pi}{t}$

CONCLUSIONS:

(a) FOR  $\omega t \ll 1 \Rightarrow P_{m,m} \sim t^2$  (GROWS RAPIDLY)

(b) THE MOST IMPORTANT TRANSITIONS ARE SUCH THAT

$|V_{mm}| \frac{2\pi}{t} \Rightarrow \frac{|E_m - E_m| t}{2\pi \hbar} \rightarrow \Delta E \Delta t \approx 2\pi \hbar = \hbar$   
 (WE DUBBLED THE CENTRAL PEAK IS) LOOKS LIKE AN UNCERTAINTY RELATION

BUT RECALL IT IS NOT.  $t$  IS NOT AN OPERATOR

$\Delta E \equiv$  UNCERTAINTY ON THE SYSTEM ENERGY

$t \Delta t \equiv$  TIME THAT THE SYSTEM IS UNDER  $V$

(c) SYSTEM'S ENERGY IS CONSERVED WITHIN THE ERROR  $\frac{2\pi \hbar}{t}$   
(THE ERROR IS DUE TO THE INTERACTION  $V$  WHICH IS CAUSED BY AN EXTERNAL AGENT)

REWRITE  $P_{m,m} = \frac{4 |V_{mm}|^2 t^2 \sin^2(\frac{\omega_{mm} t}{2})}{(\hbar \omega_{mm} t)^2}$ , call  $\theta = \frac{\omega_{mm} t}{2}$

$\Rightarrow P_{m,m} = t^2 \left| \frac{V_{mm}}{\hbar} \right|^2 \left( \frac{\sin \theta}{\theta} \right)^2$

\* LIMIT CASE  $\theta \ll 1 \Rightarrow |\omega_{mm} t| \ll 1 \Rightarrow P_{m,m} \approx \left( \frac{V_{mm}}{\hbar} \right)^2 t^2$

TRANSITION RATE (IN 1ST ORDER)  $\Gamma_{m,m} = \frac{P_{m,m}}{t} = \left( \frac{V_{mm}}{\hbar} \right)^2 t$

$\Rightarrow$  TRANSITION RATE GROWS LINEARLY IN TIME

\* LIMIT CASE  $\theta \gg 1 \Rightarrow |\omega_{mm} t| \gg 1$ , THE MAJORITY OF TRANSITIONS ARE SUCH THAT  $|E_m - E_m| < \frac{2\pi \hbar}{t}$

THIS IS VALID AS LONG AS  $P_{m,m} \ll 1$ , OTHERWISE HIGHER ORDER CONTRIBUTIONS ARE NEEDED



WHILE

THIS LIMIT IS VALID, THEN

(8)

WE USE THAT  $\frac{1}{\omega_{mn}^2 t} \sin^2\left(\frac{\omega_{mn} t}{2}\right) \xrightarrow{t \rightarrow \infty} \frac{\pi}{2} \delta(\omega_{mn})$

THIS COMES FROM  $\int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2} dx = \pi$

$$\Rightarrow \lim_{\alpha \rightarrow 0} \frac{1}{\pi} \frac{\sin^2 \alpha x}{\alpha x^2} = \delta(x)$$

$$\Rightarrow P_{m,m} = 4 \left| \frac{V_{m,m}}{\hbar} \right|^2 \left( \frac{\sin^2 \omega_{mn} t / 2}{\omega_{mn} t} \right) t \rightarrow 2\pi \left| \frac{V_{m,m}}{\hbar} \right|^2 \delta(\omega_{mn}) t$$
$$= \Gamma_{m,m} t, \quad \Gamma_{m,m} = \frac{2\pi}{\hbar} |V_{m,m}|^2 \delta(\omega_{mn})$$

$$\boxed{\Gamma_{m,m} = \frac{2\pi}{\hbar} |V_{m,m}|^2 \delta(E_m - E_m)}$$

APPLICATION: DECAY TO A CONTINUUM (AND AUGER EFFECT)

SUPPOSE THERE IS A CONTINUUM OF STATES IN WHICH  $V$  CONNECTS THE INITIAL STATE  $|m\rangle$



QUESTION: WHAT IS THE DECAY PROBABILITY?

$$P_m(t) = \sum_m P_{m,m}(t)$$

FOR A CONTINUUM  $\sum_m \rightarrow \int dE_m p(E_m)$

$\hookrightarrow$  DENSITY OF STATES

$$\Rightarrow P_m(t) \rightarrow \int dE_m p(E_m) \frac{2\pi}{\hbar} |V_{m,m}|^2 \delta(E_m - E_m) t$$
$$= \frac{2\pi}{\hbar} |V_{m,m}|^2 p(E_m) t = \Gamma_m t \rightarrow \text{LINEAR IN } t$$

$$\boxed{\Gamma_m \equiv \text{TRANSITION RATE} = \frac{2\pi}{\hbar} |\langle m|V|m\rangle|^2 p(E_m)}$$

(RECALL THE FIRST PEAK INTEGRAL  $\sim t^2 \times \frac{1}{t} \sim t$ )

FERMI'S GOLDEN RULE



"FORMAL" DERIVATION:

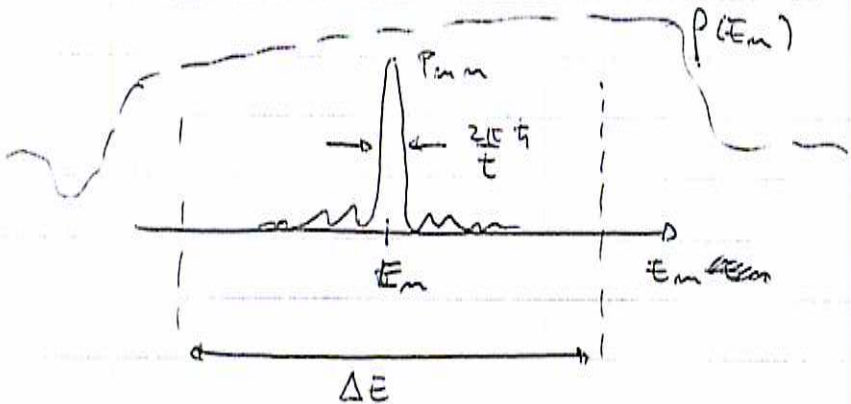
$$P_m = \int dE_m \rho(E_m) \frac{|V_{mm}|^2 4 \sin^2 \left( \frac{\Delta(E_m - E_m)t}{2\hbar} \right)}{(E_m - E_m)^2}$$

ASSUMPTIONS:  $\left\{ \begin{array}{l} \rho(E_m) \text{ VARIES SLOWLY AROUND THE FINAL STATES} \\ |V_{mm}|^2 \text{ VARIES WEAKLY ACROSS THE FINAL STATES} \end{array} \right.$

$$\Rightarrow P_m \approx \rho |V_{mm}|^2 \int_{-\infty}^{\infty} dE_m \frac{4 \sin^2(\dots)}{(E_m - E_m)^2}$$

(THE LIMITS OF INTEGRATION ARE OK AS LONG AS  $\frac{\sin^2}{\Delta E^2}$  VANISHES SUFFICIENTLY RAPID

$$\Rightarrow P_m(t) = \rho |V_{mm}|^2 * 2\pi \frac{t}{\hbar}$$



VALIDITY: ~~1st ORDER~~ VALID WHEN  $\frac{\Gamma_m}{E_m - E_m} \ll 1$

- ①  $P_m(t) = \Gamma_m t \Rightarrow t \ll \frac{1}{\Gamma_m} = \text{"LIFE TIME"}$
- ②  $\frac{2\pi\hbar}{t} \gg \delta E \Rightarrow t \ll \frac{\hbar}{\delta E}$  (CONTINUUM LIMIT EXISTS)
- ③  $\Delta E \gg \Gamma_m t$  (SHARP TRANSITION)  
IT ENSURES THE SYSTEM GOES TO THE CONTINUUM AND DO NOT COME BACK TO  $|m\rangle$

# ANOTHER DERIVATION

(10)

$$\Gamma_m = \frac{d}{dt} P_m(t) = \frac{d}{dt} \left[ \int d\tilde{E}_m p(\tilde{E}_m) \frac{1}{\hbar^2} \left| \int_0^t V_{mm} e^{i\omega_{mm}t'} dt' \right|^2 \right]$$

$$= \frac{d}{dt} \left[ \int d\tilde{E}_m \frac{p(\tilde{E}_m)}{\hbar^2} \int_0^t dt_1 \int_0^{t_1} dt_2 \langle m | V(t_1) | m \rangle \langle m | V(t_2) | m \rangle e^{i\omega_{mm}(t_1-t_2)} \right]$$

FOR  $p(\tilde{E}_m)$  AND  $\langle m | V(t) | m \rangle$  SLOWLY VARYING WITH RESPECT TO  $e^{i\omega_{mm}(t_1-t_2)}$   $\Rightarrow$  INTEGRATE OVER  $d\tilde{E}_m$

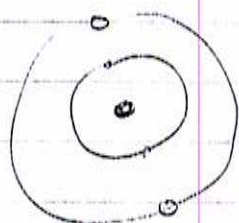
$$\int_{-\infty}^{\infty} \frac{d\tilde{E}_m}{\hbar} e^{i \frac{\tilde{E}_m - \tilde{E}_m}{\hbar} (t_1 - t_2)} = \int_{-\infty}^{\infty} dx e^{ix(t_1-t_2)} = 2\pi \delta(t_1-t_2)$$

DOES NOT DEPEND ON  $t$

$$\Rightarrow \Gamma_m = \frac{d}{dt} \int_0^t dt_1 \left[ \langle m | V(t_1) | m \rangle \right]^2 \frac{2\pi}{\hbar} p(\tilde{E}_m)$$

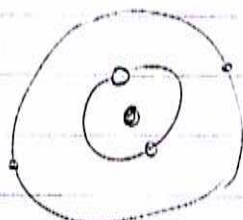
$$\Rightarrow \boxed{\Gamma_m = \frac{2\pi}{\hbar} \langle m | V | m \rangle^2 p(\tilde{E}_m)}$$

## AUGER EFFECT FOR He



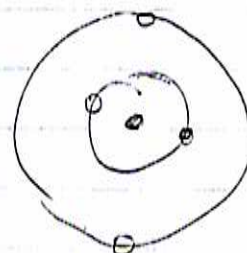
$$\bar{E} = -108 \text{ eV}$$

$$n_1 = n_2 = 1$$



$$\bar{E} = -27 \text{ eV}$$

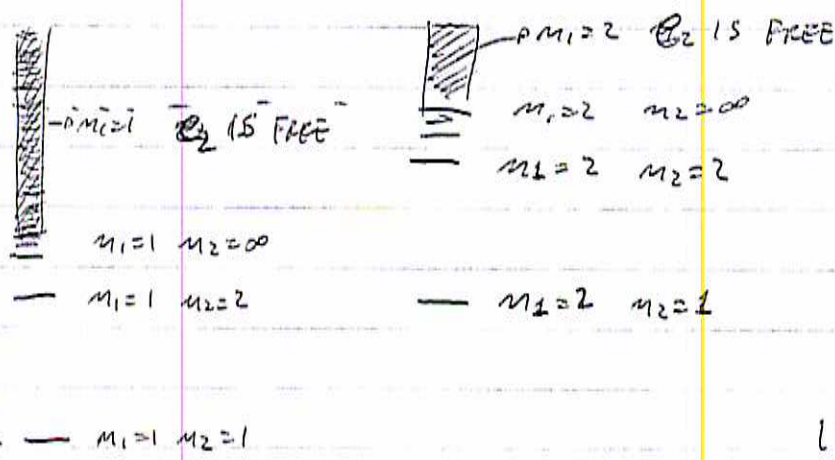
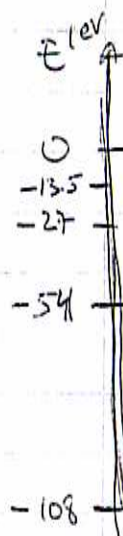
$$n_1 = n_2 = 2$$



$$\bar{E} = -54 \text{ eV}$$

$$n_1 = 1, n_2 = \infty$$

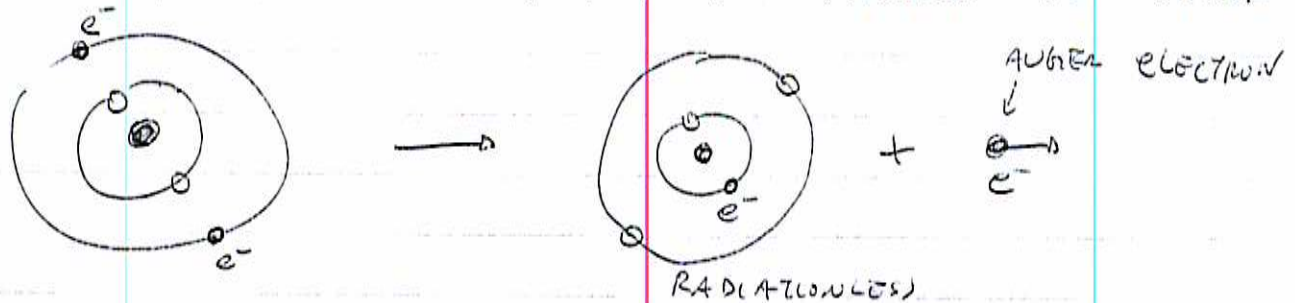
+  $e^-$  LIVRE



NOTICE THAT THE STATE  $|n_1=2, n_2=2\rangle = |m\rangle$  CAN DECAY INTO A CONTINUUM IN WHICH  $|m\rangle = |n_1=1\rangle \otimes |k_2\rangle$  PLANE WAVES



THEREFORE, THERE IS A PHYSICAL PROCESS IN WHICH



$$H_0 = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{ze^2}{r_1} - \frac{ze^2}{r_2}$$

$V = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$  → COULOMB REPULSION IS SUFFICIENT TO PROMOTE THE DECAY

THE TRANSITION  $|2s, 2s\rangle \rightarrow |1s, 2s\rangle + \gamma$   
 $\rightarrow |1s, 1s\rangle + 2\gamma$   
 ARE POSSIBLE, BUT MUCH LESS PROBABLE

LATER, WE WILL COME BACK TO THE CALCULATION OF THE TRANSITION RATE  $|2s, 2s\rangle \rightarrow |1s\rangle + |\bar{\nu}_e\rangle$

NOW, WE WANT TO GENERALIZE THE FERMIS GOLDEN RULE TO PERTURBATION THAT DEPENDS ON TIME IN A HARMONIC FASHION

$$V(t) = V_0 \cos(\omega t + \phi) = \frac{1}{2} (V_0 e^{i\omega t} + V_0^* e^{-i\omega t}) \Theta(t)$$

1st ORDER:  $P_{mn}(t) = \frac{| \langle m | V_0 | n \rangle |^2}{\hbar^2} \left| \int_0^t \frac{e^{i(\omega + \omega_{mn})t'} + e^{i(\omega_{mn} - \omega)t'}}{2} dt' \right|^2$

(CROSS TERM WILL GIVE  $\delta(\omega_{mn} - \omega) \delta(\omega_{mn} + \omega)$  → VERY SMALL)

$$= \frac{2 |V_{nm}|^2}{\hbar^2} \left[ \frac{\sin^2(\omega_{mn} + \omega) \frac{t}{2}}{(\omega_{mn} + \omega)^2} + \frac{\sin^2(\omega_{mn} - \omega) \frac{t}{2}}{(\omega_{mn} - \omega)^2} \right]$$

SAME ANALYSIS AS BEFORE BUT WE HAVE TO TAKE INTO ACCOUNT TWO PEAK AT  $\omega_{mn} = \omega_n + \omega$  AND  $\omega_{mn} = \omega_n - \omega$

$$I = \int_0^t e^{iAt} + e^{iBt} dt = \frac{1}{iA} (e^{iAt} - 1) + \frac{1}{iB} (e^{iBt} - 1)$$

$$|I|^2 = \left| 2 e^{i \frac{A+B}{2} t} \frac{\sin \frac{(A-B)t}{2}}{A} + 2 e^{i \frac{A-B}{2} t} \frac{\sin \frac{Bt}{2}}{B} \right|^2$$

$$= \frac{4 \sin^2 \frac{At}{2}}{A^2} + \frac{4 \sin^2 \frac{Bt}{2}}{B^2} \pm \frac{8 \sin \frac{At}{2} \sin \frac{Bt}{2} \cos \frac{(A-B)t}{2}}{A-B}$$

$$|e^{i\theta} A + e^{i\gamma} B|^2 = |A \cos \theta + B \cos \gamma + i(A \sin \theta + B \sin \gamma)|^2$$

$$= \frac{A^2 \cos^2 \theta + B^2 \cos^2 \gamma}{A^2 + B^2} + \frac{2AB (\cos \theta \cos \gamma + \sin \theta \sin \gamma)}{A^2 + B^2}$$

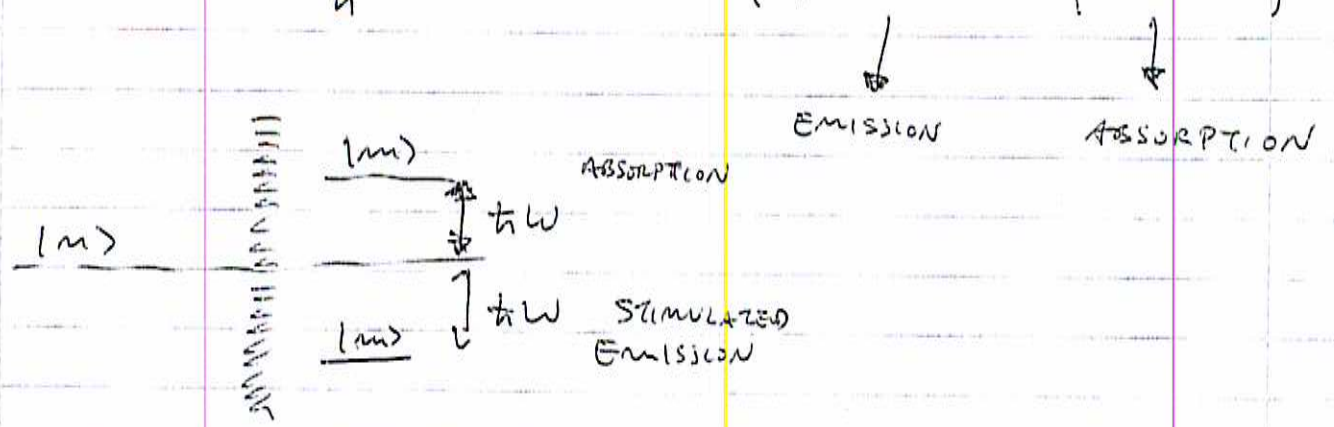
$$\pm \frac{2AB \sin(\theta - \gamma)}{A^2 + B^2}$$

$$\frac{\sin^2 \frac{(\omega_{max} + \omega)t}{2}}{(\omega_{max} + \omega)^2} + \frac{\sin^2 \frac{(\omega_{min} - \omega)t}{2}}{(\omega_{min} - \omega)^2} \pm \frac{2 \sin \frac{(\omega_{max} + \omega)t}{2} \sin \frac{(\omega_{min} - \omega)t}{2} \cos \omega t}{\omega_{max}^2 - \omega^2}$$



FOR TRANSITIONS INTO THE CONTINUUM LIMIT

$$\Rightarrow T_m = \frac{\pi}{\hbar} |\langle m | V_0 | n \rangle|^2 \left\{ \rho(E_n - \omega) + \rho(E_n + \omega) \right\}$$



EXAMPLE: PHOTOELECTRIC EFFECT (WE WILL COME BACK TO THIS LATER)

EXPONENTIAL DECAY

FOR STOCHASTIC PROCESSES, WE CAN COMPUTE THE PROBABILITY THAT THE SYSTEM IS IN STATE  $|m\rangle$  GIVEN THAT IT'S DECAY RATE IS  $\Gamma$

$$P_m(t+dt) = P_m(t) (1 - \Gamma dt) + \sum_{m \neq n} P_n(t) \Gamma_{nm} dt$$

$\downarrow$  PROBABILITY OF NOT DECAYING       $\downarrow$  PROBABILITY TO RETURN TO  $|m\rangle$

$$\Rightarrow P_m(t+dt) = P_m(t) + \frac{dP_m}{dt} dt = P_m(t) - P_m(t) \Gamma dt$$

(LET'S NEGLECT IT) IRREVERSIBLE DECAY

$$\Rightarrow \frac{dP_m}{dt} = -P_m \Gamma \Rightarrow \boxed{P_m(t) = P_m(0) e^{-\Gamma t}}$$

EXPONENTIAL DECAY LAW

OBSERVATIONS: (a) THE FACT THE STATE  $|m\rangle$  IS NOT REPLENISHED IS NECESSARY HOW DOES IT APPLY TO Q.M. PROBLEMS?

(b) IT IS ALSO NECESSARY THAT THE DETERMINATION (OR MEASUREMENT) ~~THE STATE~~ OF  $P_m$  AT TIME  $t$  DOES NOT AFFECT  $P_m$  AT  $t+dt$ .

OF COURSE, OBSERVATION (b) IS NOT SATISFIED IN Q.M. SINCE ~~THE~~ MEASUREMENT OF THE SYSTEM IS INDEED IN (M) NECESSARILY IMPLIES THAT  $P_S(t) = 1$  (THIS IS DUE TO THE WAVE FUNCTION COLLAPSE) NATURALLY, IT APPLIES TO Q.M. PROBLEMS IF A MEASUREMENT BETWEEN THE INITIAL AND FINAL TIMES IS NOT PERFORMED.

IRREVERSIBLE DECAY AND Q.M

IF IRREV. DECAY IS TO TAKE PLACE, THEN

$$P_m(t+dt) = P_m(t) (1 - \Gamma_m dt)$$

$$\Rightarrow |\langle m | U_{\pm}(t+dt, t_0) | m \rangle|^2 = |\langle m | U_{\pm}(t, t_0) | m \rangle|^2 (1 - \Gamma_m dt)$$

THERE IS NO REASON, A PRIORI, THAT THIS SHOULD HOLD HOWEVER, THE SAME CONDITIONS THAT ENSURE THE FERMI'S GOLDEN RULE ENSURE THIS RELATION

IN ORDER TO SEE THIS, LET'S FOCUS ON

$$\begin{aligned} i\hbar \frac{d}{dt} \langle m | U_{\pm}(t, t_0) | m \rangle &= i\hbar \langle m | \frac{d}{dt} U_{\pm} | m \rangle = \langle m | V_{\pm}(t) U_{\pm}(t, t_0) | m \rangle \\ &= \sum_k \langle m | V_{\pm}(t) | k \rangle \langle k | U_{\pm}(t, t_0) | m \rangle \\ &= \sum_k e^{i\omega_{km} t} \langle m | V(t) | k \rangle \langle k | U_{\pm}(t, t_0) | m \rangle \end{aligned}$$

① FOR  $k \neq m \rightarrow$  GREATEST CONTRIBUTION IS FROM  $k=m$  BECAUSE  $\langle k \neq m | U_{\pm}(t, t_0) | m \rangle \ll \langle m | U_{\pm}(t, t_0) | m \rangle$  FOR SHORT TIMES

$$\Rightarrow i\hbar \frac{d}{dt} \langle m | U_{\pm}(t, t_0) | m \rangle \approx e^{i\omega_{mm} t} \langle m | V(t) | m \rangle \langle m | U_{\pm}(t, t_0) | m \rangle$$

FOR CONSTANT IN TIME  $V(t) \equiv V$

$$\Rightarrow \langle m | U_{\pm}(t, t_0) | m \rangle = \frac{1}{i\hbar} \langle m | V | m \rangle \int_{t_0}^t dt' e^{i\omega_{mm} t'} \langle m | U_{\pm}(t', t_0) | m \rangle$$

② FOR  $m=n$

$$\Rightarrow i\hbar \frac{d}{dt} \langle m | U_{\pm} | m \rangle = \langle m | V | m \rangle \langle m | U_{\pm} | m \rangle + \sum_{k \neq m} e^{i\omega_{km} t} \langle m | V | k \rangle \langle k | U_{\pm} | m \rangle$$

NOW USE THE RESULT OF ①

$$\Rightarrow i\hbar \frac{d}{dt} \langle m | U_{\pm} | m \rangle = \langle m | V | m \rangle \langle m | U_{\pm} | m \rangle - \frac{1}{i\hbar} \sum_{k \neq m} \langle m | V | k \rangle \langle k | V | m \rangle \int_{t_0}^t dt' e^{i\omega_{mm}(t-t')} \langle m | U_{\pm}(t', t_0) | m \rangle$$



CASE  $\langle m | U_{\pm}(t', t_0) | m \rangle$  VARIES SLOWLY COMPARED (14)  
 $T_0 e^{i\omega_{km}(t'-t_0)}$  IN THE TIME INTERVAL  $t_0 < t < t_0 + T_0$

$$\Rightarrow i\hbar \frac{d}{dt} \langle m | U_{\pm}(t) | m \rangle \approx \left[ \langle m | V | m \rangle + \frac{1}{i\hbar} \sum_{k \neq m} |\langle k | V | m \rangle|^2 \int_0^t dt' e^{i\omega_{km}(t-t')} \right] \langle m | U_{\pm}(t) | m \rangle$$

THIS ASSUMPTION IS TRUE WHEN  $|\omega_{km}(t-t)| \gg 1$   
~~IN THE TIME INTERVAL~~ IN WHICH WE USE

$$I = \int_{t_0}^t dt' e^{i\omega_{km}(t-t')} \rightarrow \pi \delta(\omega_{km}) + i \mathcal{P} \left( \frac{1}{\omega} \right)$$

$$I = \int_{t_0}^t dt' e^{i\omega_{km}(t-t')} = \int_{t-t}^0 dx e^{i\omega_{km}x} \rightarrow \int_{-\infty}^0 dx e^{i\omega x}$$

$$\lim_{\epsilon \rightarrow 0^+} \int_{-\infty}^0 dx e^{i(\omega - i\epsilon)x} = \lim_{\epsilon \rightarrow 0^+} \frac{1}{i\omega + \epsilon} = \pi \delta(\omega) - i \mathcal{P} \left( \frac{1}{\omega} \right)$$

↓  
CAUCHY'S PRINCIPLE VALUE

$$\Rightarrow i\hbar \frac{d}{dt} \langle m | U_{\pm}(t) | m \rangle = \left[ \langle m | V | m \rangle + \frac{1}{i\hbar} \sum_{k \neq m} |\langle k | V | m \rangle|^2 \left( \pi \delta(\omega_{km}) + i \mathcal{P}(\omega_{km}) \right) \right] \langle m | U_{\pm}(t) | m \rangle$$

$$\Rightarrow \frac{d}{dt} \langle m | U_{\pm}(t) | m \rangle = \left[ -\frac{\pi}{\hbar^2} \sum_{k \neq m} |V_{km}|^2 \delta(\omega_{km}) - \frac{i}{\hbar} \left( \langle m | V | m \rangle + \sum_{k \neq m} |V_{km}|^2 \frac{1}{\omega_{km}} \right) \right] \langle m | U_{\pm}(t) | m \rangle$$

$$= \left[ -\frac{\omega}{2} - \frac{i}{\hbar} \Delta E_m \right] \langle m | U_{\pm}(t) | m \rangle$$

THIS LOOKS LIKE  $dP_m(t) = (A - \Gamma_m dt) P_m(t)$

SOLVING =  $\langle m | U_{\pm}(t, t_0) | m \rangle = e^{-\left(\frac{\omega}{2} + i \frac{\Delta E_m}{\hbar}\right)t}$

WHERE  $\omega = \frac{2\pi}{\hbar^2} \sum_{k \neq m} |V_{km}|^2 \delta(\omega_{km}) = \frac{2\pi}{\hbar} \sum_{k \neq m} |V_{km}|^2 \delta(E_{km})$

$\rightarrow \frac{2\pi}{\hbar} |\langle k | V | m \rangle|^2 \rho(E_m)$  FERMI'S GOLDEN RULE

$$\Delta E_m = \sum_{k \neq m} \frac{|V_{km}|^2}{\hbar \omega_{km}} + V_{mm} = V_{mm} + \sum_{k \neq m} \frac{|\langle k | V | m \rangle|^2}{E_k - E_m}$$

= ENERGY SHIFT OF STATE  $|m\rangle$

UP TO 2ND ORDER IN PERT. THEORY

FWARDLY,  $P_{mm}(t) = |\langle n | U_{\pm}(t) | m \rangle|^2 = e^{-\omega t}$

(15)

THAT'S THE EXPONENTIAL DECAY OF AN UNSTABLE STATE

EXAMPLE: RADIOACTIVE EXPONENTIAL DECAY.

IT IS TRUE THAT WE NEED Q.M. IN ORDER TO HAVE TUNNELING, AND THUS, THE DECAY. HOWEVER THE EXPONENTIAL DECAY IS A CONSEQUENCE THAT THE INITIAL STATE IS COUPLED TO MANY (A LARGE NUMBER) OF FINAL (TARGET) STATES WITH SIMILAR ENERGY.

IN THIS MANNER, THE EXPONENTIAL DECAY IS POSSIBLE DUE TO A SERIES OF DELICATE APPROXIMATIONS.

COMING BACK TO THE  $m \rightarrow n$  CASE

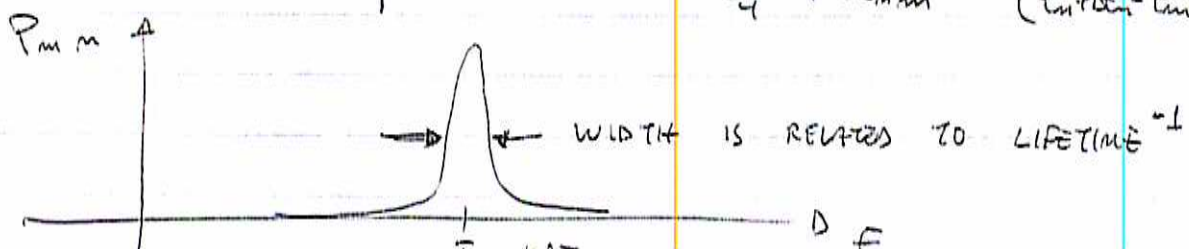
$$\begin{aligned} \langle n | U_{\pm}(t) | m \rangle &\approx \frac{1}{i\hbar} \langle n | V | m \rangle \int_0^t dt' e^{i\omega_{nm}t'} \langle m | U_{\pm}(t') | m \rangle \\ &= \frac{1}{i\hbar} V_{nm} \int dt' e^{i\omega_{nm}t'} e^{-(\frac{\omega}{2} + i\frac{\Delta E_n}{\hbar})t'} \\ &= \frac{1}{i\hbar} V_{nm} \left[ \frac{e^{-\frac{\omega}{2}t} e^{i(\frac{\Delta E_n}{\hbar} - \omega_{nm})t}}{-\frac{\omega}{2} - i(\frac{\Delta E_n}{\hbar} - \omega_{nm})} - 1 \right] \end{aligned}$$

$$\Rightarrow P_{mm}(t) = \frac{|\langle n | V | m \rangle|^2}{\hbar^2} \left( \frac{1 - 2 \cos \Omega_{nm} t e^{-\frac{\omega t}{2}} + e^{-\omega t}}{\Omega_{nm}^2 + \omega^2/4} \right)$$

Where  $\hbar \Omega_{nm} = E_n + \Delta E_n - E_m \equiv$  ENERGY DIFFERENCE

FOR LONG TIMES  $\omega t \gg 1$

$$\Rightarrow P_{mm} \rightarrow \left| \frac{\langle n | V | m \rangle}{\hbar} \right|^2 \frac{1}{\frac{\omega^2}{4} + \Omega_{nm}^2} = \frac{|\langle n | V | m \rangle|^2}{(E_n + \Delta E_n - E_m)^2 + (\hbar\omega)^2/4}$$





~~PROBAB~~ ZENO'S PARADOX

• HOW DOES A STATE DECAY IF IT IS CONTINUOUSLY MEASURED?

$P_N(t) \equiv \left( |\langle \psi(0) | \psi(t/N) \rangle|^2 \right)^N$ 
PROBABILITY OF BEING AT  $|\psi\rangle$  AFTER N MEASUREMENTS EQUALLY SPACED IN THE TIME INTERVAL  $[0, t]$   
 $\hookrightarrow$  N MEASUREMENT IN THE INTERVAL  $[0, t]$

$= \left( \langle \psi_0 | U(t/N) | \psi_0 \rangle \langle \psi_0 | U^\dagger(t/N) | \psi_0 \rangle \right)^N$

AS  $U(t/N) = 1 + \frac{i}{\hbar} \frac{t}{N} H + \frac{1}{2} \left( \frac{i}{\hbar} \right)^2 \left( \frac{t}{N} \right)^2 H^2 + \dots$   
 $\downarrow$  RECALL THE TIME ORDERING  
 FOR  $\frac{t}{N} \ll 1$

$\Rightarrow P_N \approx \left( \left| 1 + \frac{i}{\hbar} \left( \frac{t}{N} \right) \langle \psi_0 | H | \psi_0 \rangle + \frac{1}{2} \left( \frac{i}{\hbar} \right)^2 \left( \frac{t}{N} \right)^2 \langle \psi_0 | H^2 | \psi_0 \rangle + \dots \right|^2 \right)^N$   
 $= \left( 1 + \frac{1}{\hbar^2} \langle H^2 \rangle \left( \frac{t}{N} \right)^2 - 2 * \frac{1}{2} \frac{1}{\hbar^2} \langle H^2 \rangle \left( \frac{t}{N} \right)^2 + \dots \right)^N \equiv$  CUMULANT EXPANSION

(NOTICE THE LINEAR TERM VANISHES  $\frac{1}{\hbar} \langle H \rangle \left( \frac{t}{N} \right) + \left( \frac{1}{\hbar} \langle H \rangle \frac{t}{N} \right)^* = 0$ )

$\Rightarrow P_N \approx 1 - N \frac{\langle \Delta H \rangle^2}{\hbar^2} \left( \frac{t}{N} \right)^2 + O\left(\frac{t}{N^3}\right)$  ,  $\langle \Delta H \rangle^2 = \langle H^2 \rangle - \langle H \rangle^2$   
 $\Rightarrow \lim_{N \rightarrow \infty} P_N = 1 - \frac{\langle \Delta H \rangle^2}{\hbar^2} \frac{t^2}{N} \rightarrow 1$  = 2ND CUMULANT

$\Rightarrow$  THE STATE DOES NOT DECAY (NO PERTURBATION THEORY NEEDED)

\* IN CLASSICAL MECHANICS

$P_N(t) = \left( \langle \psi_0 | \psi\left(\frac{t}{N}\right) \rangle \right)^N$  , NO SQUARE NEEDED SINCE  $\langle \psi_0 | \psi \rangle$  IS ALREADY THE PROBABILITY

$\Rightarrow P_N \approx \left( 1 + \frac{d\psi}{dE} \frac{t}{N} + \dots \right)^N \approx 1 + \left( \frac{d\psi}{dE} \right)^* t < 1$   
 $\downarrow$   
 $\Rightarrow$  STATE DECAYS  $\psi'(t) < 0$

EXAMPLE (APPLICATIONS):

~~PARTICLE~~ PARTICLE IN A FIELD (NEGLECT SPIN)

(17)

$$H = \frac{1}{2m} (\vec{p} - q\vec{A})^2 + q\phi$$

COULOMB GAUGE:  $\phi = 0$ ,  $\nabla \cdot \vec{A} = 0 \Rightarrow \nabla^2 \vec{A} = -\frac{1}{c^2} \frac{\partial^2 \vec{A}}{\partial t^2} = 0$

$$\Rightarrow H = \frac{p^2}{2m} - \frac{q}{2m} (\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}) + \frac{q^2}{2m} A^2$$

IN THIS GAUGE  $[\vec{p}, \vec{A}] = 0$

$$\vec{p} \cdot \vec{A} |\psi\rangle = -i\hbar \nabla \cdot (\vec{A} |\psi\rangle) = -i\hbar [(\nabla \cdot \vec{A}) |\psi\rangle + \vec{A} \cdot \nabla |\psi\rangle] = \vec{A} \cdot (i\hbar \nabla |\psi\rangle) = \vec{A} \cdot \vec{p} |\psi\rangle$$

$$\Rightarrow H = \frac{p^2}{2m} - \frac{q}{m} \vec{A} \cdot \vec{p} + O(A^2) \quad \text{(SMALL)}$$

PARTICLE IN A E.M. FIELD + ~~EXTERNAL~~ EXTERNAL POTENTIAL

$$\Rightarrow H = \frac{p^2}{2m} + V_0 - \frac{q}{m} \vec{A} \cdot \vec{p}$$

HYDROGEN ATOM, FOR INSTANCE

DEFINING THE VECTOR POTENTIAL (RADIATION FIELD)

$$A(\vec{r}, t) = \int_{-\infty}^{\infty} d\omega \vec{A}(\omega) e^{-i\omega(t - \frac{\hat{n} \cdot \vec{r}}{c})}$$

where  $\begin{cases} \hat{n} \equiv \text{DIRECTION OF PROPAGATION} \\ \vec{A} \cdot \hat{n} = 0 \end{cases}$

$$A(\vec{r}, t) \in \mathbb{R} \Rightarrow \vec{A}^*(\omega) = \vec{A}(-\omega)$$

EXAMPLE:  $\hat{n} = \hat{z}$ ,  $\vec{A}(\omega) = A_0 [\delta(\omega - \omega_0) + \delta(\omega + \omega_0)] \hat{x}$

$$\Rightarrow \begin{cases} \vec{E}(\vec{r}, t) = -\frac{\partial}{\partial t} \vec{A} = \omega A_0 \sin(\omega t - \frac{\omega}{c} z) \hat{x} \\ \vec{B}(\vec{r}, t) = \nabla \times \vec{A} = \frac{\omega}{c} A_0 \sin(\omega t - \frac{\omega}{c} z) \hat{y} \end{cases}$$

POYNTING VECTOR:  $\vec{N} = \frac{1}{\mu_0} \vec{E} \times \vec{B} = \frac{1}{\mu_0} \frac{\partial}{\partial t} \vec{A} \times (\nabla \times \vec{A}) = \frac{\omega^2 A_0^2}{\mu_0 c} \sin^2(\dots) \hat{z}$



# TRANSITION PROBABILITY

(18)

$$C_{fi} = \frac{\langle f | V_I (-\infty, \infty) | i \rangle}{i\hbar}$$

1st ORDER IN  
PERTURBATION THEORY

$$= \frac{1}{i\hbar} \int_{-\infty}^{\infty} dt V_{fi}(t) e^{i\omega_{fi}t} \equiv \text{FOURIER TRANSFORM OF THE PERTURBATION}$$

WITH  $V(t) = -\frac{q}{m} \int_{-\infty}^{\infty} d\omega' e^{-i\omega'(t - \frac{\hat{n} \cdot \vec{r}}{c})} \vec{A}(\omega') \cdot \vec{p}$

INTEGRATING OVER TIME:

$$\int_{-\infty}^{\infty} dt e^{i(\omega_{fi} - \omega')t} = 2\pi \delta(\omega_{fi} - \omega')$$

$$\Rightarrow C_{fi} = \frac{-2\pi q}{i m \hbar} \langle f | e^{i\omega_{fi} \frac{\hat{n} \cdot \vec{r}}{c}} \vec{A}(\omega_{fi}) \cdot \vec{p} | i \rangle$$

LET  $\vec{A}(\omega_{fi}) = A(\omega_{fi}) \hat{e}$ , WITH  $\hat{e} \cdot \hat{n} = 0$

$$\Rightarrow P_{f \leftarrow i} = \frac{4\pi^2 q^2}{m^2 \hbar^2} |A(\omega_{fi})|^2 |\langle f | e^{i\omega_{fi} \frac{\hat{n} \cdot \vec{r}}{c}} \hat{p} \cdot \hat{e} | i \rangle|^2$$

THIS CAN BE RELATED TO THE POYNTING VECTOR

$$\vec{N} = -\frac{1}{\mu_0} \left( \frac{\partial}{\partial t} \vec{A} \right) \times (\nabla \times \vec{A})$$

$$= -\frac{1}{\mu_0} \left[ \int_{-\infty}^{\infty} d\omega' (-i\omega') \vec{A}(\omega') \hat{e} e^{-i\omega'(t - \frac{\hat{n} \cdot \vec{r}}{c})} \right] \times \left[ \int_{-\infty}^{\infty} d\omega'' \left( \frac{i\omega''}{c} \right) A(\omega'') e^{-i\omega''(t - \frac{\hat{n} \cdot \vec{r}}{c})} \hat{n} \times \hat{e} \right]$$

WHERE WE USE THAT  $\nabla \times (f \vec{c}) = f \nabla \times \vec{c} + \nabla f \times \vec{c}$

NOW WE USE  $\hat{e} \times (\hat{n} \times \hat{e}) = (\hat{e} \cdot \hat{e}) \hat{n} - (\hat{e} \cdot \hat{n}) \hat{e} = \hat{n}$

$$\Rightarrow \vec{N} = -\frac{\hat{n}}{\mu_0 c} \int_{-\infty}^{\infty} d\omega' d\omega'' A(\omega') A(\omega'') e^{-i(\omega' + \omega'')(t - \frac{\hat{n} \cdot \vec{r}}{c})} \omega' \omega''$$

RADIATION PRESSURE  $\equiv \frac{\vec{N} \cdot \hat{n}}{c} = \frac{\text{ENERGY}}{\text{VOLUME}}$

DEFINITION:  $c \int_{-\infty}^{\infty} \frac{\vec{N} \cdot \hat{n}}{c} dt \equiv \int_{\odot}^{\infty} \tilde{N}(\omega) d\omega$

WHAT IS  $\tilde{N}(\omega)$ ?

$$[\tilde{N}] = \frac{\text{ENERGY}}{\text{VOLUME}} \times \frac{\text{LENGTH}}{\text{TIME}} \times \frac{\text{TIME}}{\text{FREQUENCY}} = \frac{\text{ENERGY}}{\text{AREA} \times \text{FREQUENCY}}$$

$$\int_{-\infty}^{\infty} N(\omega) d\omega = \frac{-1}{\mu_0 c} \int_{-\infty}^{\infty} d\omega' d\omega'' A(\omega') A(\omega'') \omega' \omega'' \underbrace{\int_{-\infty}^{\infty} dt e^{-i(\omega'+\omega'')(t-\frac{\hat{n}\cdot\vec{r}}{c})}}_{2\pi \delta(\omega'+\omega'')}$$

$$= \frac{2\pi}{\mu_0 c} \int_{-\infty}^{\infty} d\omega A(\omega) A(-\omega) \omega^2$$

AS  $A(\omega) = A^*(-\omega)$

$$\Rightarrow \boxed{N(\omega) = \frac{4\pi\omega^4}{\mu_0 c} |A(\omega)|^2}$$

THUS,  $P_{f \rightarrow i} = \frac{\pi \tilde{f}^2}{m^2 \hbar^2} \mu_0 c \frac{N(\omega)}{\omega^2} |\langle f | e^{i\omega \hat{n} \cdot \vec{r} / c} | \hat{p} \cdot \hat{e} | i \rangle|^2$

ABSORBING CROSS SECTION:  $\int_0^{\infty} \sigma(\omega) N(\omega) d\omega \equiv \text{ABSORBED ENERGY}$

$[\sigma(\omega)] \equiv \frac{\text{ABSORBED ENERGY}}{\text{INCIDENT ENERGY / AREA}}$

$N(\omega) \equiv \frac{\text{INCIDENT ENERGY}}{\text{AREA} \times \text{FREQ}}$

$$\Rightarrow \int_0^{\infty} \sigma(\omega) N(\omega) d\omega = \int_0^{\infty} \underbrace{\hbar \omega}_{\text{INCIDENT ENERGY}} \underbrace{P_{f \rightarrow i}}_{\text{ABSORPTION PROBABILITY}} d\omega$$

$$\Rightarrow \sigma(\omega) = \frac{\pi \tilde{f}^2 \mu_0 c}{m^2 \hbar^2} \frac{\hbar \omega}{\omega^2} |\langle f | e^{i\omega \hat{n} \cdot \vec{r} / c} | \hat{p} \cdot \hat{e} | i \rangle|^2$$

FINE STRUCTURE CONSTANT  $\alpha \equiv \frac{\tilde{f}^2}{4\pi\epsilon_0} \times \frac{1}{\hbar c} \approx \frac{1}{137} = \frac{1}{137.035999074(44)}$

$$\Rightarrow \boxed{\sigma_{fi}(\omega) = \frac{4\pi^2}{m^2 \omega_{fi}} \alpha |\langle f | e^{i\omega_{fi} \frac{\hat{n} \cdot \vec{r}}{c}} | \hat{p} \cdot \hat{e} | i \rangle|^2}$$



# COMPUTING THE MATRIX ELEMENT

WE NEED TO EXPAND  $e^{i \frac{\omega_{fi}}{c} \vec{m} \cdot \vec{r}} = 1 + i \omega_{fi} \frac{\vec{m} \cdot \vec{r}}{c} + \dots$

TYPICALLY,  $\frac{\omega_{fi}}{c} \vec{m} \cdot \vec{r} = \frac{\text{IONIZATION FREQ} \times \text{ATOM RADIUS}}{c}$

$$= \frac{1}{\hbar} \left( \frac{z^2 q^2}{4\pi\epsilon_0 (2a_0)} \right) \times \left( \frac{a_0}{z c} \right), \quad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e q^2} = \frac{\hbar}{m_e \alpha}$$

$$= \frac{z q^2}{2 \cdot 4\pi\epsilon_0 \hbar c} = \frac{1}{2} z \alpha \equiv \frac{z}{2 \times 137}$$

$\Rightarrow$  THE SERIES EXPANSION CONVERGES AS LONG AS  $z \ll 137$

1st TERM: ELECTRIC DIPOLE

$$\langle f | \vec{p} | i \rangle = \vec{e}$$

RECALL THAT  $H_0 = \frac{p^2}{2m} + V(\vec{r})$

$$\Rightarrow [\vec{r}, H_0] = \frac{1}{2m} [\vec{r}, p^2] = i \hbar / m \vec{p}$$

$$\Rightarrow \langle f | \vec{p} | i \rangle = \frac{m}{i \hbar} \langle f | [\vec{r}, H_0] | i \rangle = \frac{m}{i \hbar} \omega_{fi} \langle f | \vec{r} | i \rangle = i m \omega_{fi} \langle f | \vec{r} | i \rangle$$

THEREFORE, ONLY TRANSITIONS IN WHICH  $\langle f | \vec{r} | i \rangle \neq 0$  ARE ALLOWED (SELECTION RULES)

IN GENERAL, THE SELECTION RULES COMES FROM INTEGRALS

OF TYPE

$$\int_{-\infty}^{\infty} \psi_f^* \mathcal{O} \psi_i d\vec{r}$$

WITH  $\mathcal{O}$  BEING THE "TRANSITION" OPERATOR

IT IS THEN USEFUL TO USE THE SYMMETRIES OF  $\psi_{i,f}$  IN ORDER TO KNOW THE ALLOWED TRANSITIONS

EXAMPLE: INITIAL STATE =  $|l\rangle = |1s\rangle$

FINAL STATE =  $|f\rangle = |n\ell m\rangle =$  GENERIC STATE OF HYDROGEN ATOM

(21)

$$\langle \vec{r} | 1s \rangle = \frac{1}{\sqrt{\pi}} \left( \frac{1}{a_0} \right)^{3/2} e^{-r/a_0} = \langle \vec{r} | 100 \rangle$$

$$\langle \vec{r} | n\ell m \rangle = \left[ \left( \frac{2}{na_0} \right)^3 \frac{(n-\ell-1)!}{2m(m+\ell)!} \right]^{1/2} e^{-\frac{1}{2}\rho} L_{n-\ell-1}^{2\ell+1}(\rho) Y_{\ell}^m(\theta, \varphi)$$

where  $\rho = \frac{2r}{na_0}$

SELECTION RULES:

LET  $\vec{A} \cdot \hat{e} = z = r \cos\theta = r \sqrt{\frac{4\pi}{3}} Y_{10}(\theta, \varphi)$

↓  
ELECTRIC FIELD POLARIZATION

$$\Rightarrow \langle n\ell m | z | 100 \rangle = \int d\Omega Y_{\ell}^{m*}(\theta, \varphi) Y_{10}(\theta, \varphi) Y_0^0(\theta, \varphi)$$

↓  
RADIAL INTEGRAL

USING THE ORTHOGONALITY PROPERTIES OF  $Y_{\ell}^m$ , WE CONCLUDE THAT ONLY WHEN  $\ell=1$  AND  $m=0$ , THE TRANSITION MATRIX IS DIFFERENT FROM ZERO

IF WE HAD CHOSEN  $\hat{e} = \hat{x} \Rightarrow \vec{A} \cdot \hat{e} = x = r \sin\theta \cos\varphi = \sqrt{\frac{4\pi}{3}} r (Y_1^{+1} + Y_1^{-1})$

⇒ ALLOWED TRANSITIONS WOULD BE  $\ell=1$  AND  $m=\pm 1$

(SAME FOR  $\hat{y} = \hat{e}$ ,  $y = r \sin\theta \sin\varphi = \sqrt{\frac{4\pi}{3}} r (Y_1^{+1} - Y_1^{-1})$ )

IN GENERAL THE DIPOLE ELECTRIC TRANSITIONS ARE SUCH THAT  $\Delta\ell = \pm 1$  AND  $\Delta m = -1, 0, +1$

ANOTHER EXAMPLE: AUGER EFFECT

$$H = \underbrace{\frac{1}{2m} P_1^2 + \frac{1}{2m} P_2^2 + V(1\text{-NUCLEUS}) + V(2\text{-NUCLEUS})}_{H_0} + \frac{p_{\text{NUCLEUS}}^2}{2M} + V(1 \leftrightarrow 2)$$

$$V(1 \leftrightarrow 2) = \frac{q^2}{4\pi\epsilon_0} \frac{1}{|\vec{r}_1 - \vec{r}_2|} = \frac{q^2}{4\pi\epsilon_0} * 4\pi \sum_{\ell=0}^{\infty} \frac{r_{<}^{\ell}}{r_{>}^{2\ell+1}} \frac{1}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell}^{m*}(\hat{r}_1) Y_{\ell}^m(\hat{r}_2)$$



INITIAL STATE  $\equiv |i\rangle = |2s, 2s\rangle$

FINAL STATE  $\equiv |f\rangle = |1s, \vec{k}\rangle = |1s\rangle \otimes (\text{PLANE WAVE})$

1st ORDER :  $\langle 100, \vec{k} | V(1+2) | 200, 200 \rangle$

$$\langle \vec{r} | m l m \rangle = R_{nl}(r) Y_{lm}(\hat{r})$$

$$\langle \vec{r} | \vec{r} \rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} = \frac{4\pi}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{1}{r^l} j_l(kr) Y_{lm}^*(\hat{r}) Y_{lm}(\hat{r})$$

FERMI'S GOLDEN RULE :  $\bar{E}_i = \bar{E}_f \Rightarrow 2E_{2s} = E_{1s} + \frac{\hbar^2 k^2}{2m}$

$$\text{RECALL THAT } E_n = -\frac{Z^2 m e^4}{2\hbar^2} \left( \frac{1}{4\pi\epsilon_0} \right)^2 \frac{1}{n^2} = -\frac{Z^2}{n^2} \times 13.6 \text{ eV}$$

$$\Rightarrow \frac{\hbar^2 k^2}{2m} = 2E_{2s} - E_{1s} = -2^2 \left( 2 \times \frac{1}{4} - 1 \right) \times 13.6 \text{ eV}$$

$$= 27.2 \text{ eV} = \frac{1}{2} E_{\text{IONIZATION}} = \frac{1}{2} \frac{Z^2 m^2 c^4 \alpha^2}{2}$$

$$\Rightarrow k^2 = \frac{Z^2 m^2 c^4 \alpha^2}{2\hbar^2} \Rightarrow \boxed{k = \frac{Z m c \alpha}{\sqrt{2} \hbar}} = 2.7 \times 10^{-10} \text{ m}^{-1} \Rightarrow \lambda = 2.3 \text{ \AA}$$

SELECTION RULES:

$\langle 100 | V | 200 \rangle \rightarrow$  SELECTS  $l=0$  IN  $V(1-2)$

$$\Rightarrow V(1-2) \rightarrow \frac{q^2}{4\pi\epsilon_0} + \frac{4\pi}{r_2} \underbrace{Y_{00}^*(\hat{r}_1) Y_{00}(\hat{r}_2)}_{\frac{1}{4\pi}}$$

$\langle \vec{k} | V | 100 \rangle \rightarrow$  SELECTS THE  $l=0$

COMPONENT OF THE  $\vec{k}$ -WAVE

$$\Rightarrow \langle \vec{k} | \vec{r}_2 \rangle \rightarrow \frac{4\pi}{\sqrt{V}} j_0(kr_2) \underbrace{Y_{00}^*(\hat{r}) Y_{00}(\hat{r}_2)}_{1/4\pi}$$

DECAY RATE:

$$W = \frac{2\pi}{\hbar} |\langle 1s, \vec{k} | V(1-2) | 2s, 2s \rangle|^2 \rho(E_k)$$

$$\hookrightarrow \frac{q^2}{4\pi\epsilon_0} \left( \int d\Omega_1 d\Omega_2 \int r_1^2 r_2^2 \frac{1}{r_1 r_2} R_{10}(r_1) R_{20}(r_2) j_0(kr_2) R_{10}(r_1) \right)^2 \int d\Omega_1 d\Omega_2 |Y_{00}(\hat{r}_1)|^2 |Y_{00}(\hat{r}_2)|^2$$

NOW WE USE THAT

(23)

$$\begin{cases} R_{10}(r) = 2 \left(\frac{r}{a_0}\right)^{3/2} e^{-\frac{r}{a_0}} \\ R_{20}(r) = \left(\frac{r}{2a_0}\right)^{3/2} \left(2 - \frac{r}{a_0}\right) e^{-\frac{r}{2a_0}} \end{cases}$$

A RECALL THAT

$$\frac{d^3k}{(2\pi)^3} = \rho(E) d\Omega dE$$

AND  $\rho(E_k) = \frac{V m \sqrt{2m E_k}}{(2\pi \hbar)^3}$

$4 \cdot 10^{16} \frac{1}{\text{SEC}}$

$$\Rightarrow W = \frac{2\pi}{\hbar} \left| \int_{\text{three}} \dots \right|^2 \frac{V m \sqrt{2m E_k}}{(2\pi \hbar)^3} \approx 10^{-3} \frac{m}{\hbar^3} \left(\frac{\hbar^2}{4m e_0}\right)^2$$

SELECTION RULES (RELOADS)

CONSIDER THE ATOMIC TRANSITIONS VIA ELECTRIC DIPOLE

WHEN  $\langle m' l' m' | \vec{r} | m l m \rangle \neq 0$

- LETS FOCUS ON  $L_z$  AND  $z : L_z |m l m\rangle = m \hbar |m l m\rangle$

RECALL THAT  $[L_z, z] = 0$

$$\Rightarrow \langle f | [L_z, z] | i \rangle = 0 = \hbar (m' - m) \langle m' l' m' | z | m l m \rangle$$

$$\Rightarrow \langle m' l' m' | z | m l m \rangle \neq 0 \text{ ONLY WHEN } m = m' \Rightarrow \Delta m = 0$$

NOW FOCUS ON  $L_{\pm} = x \mp i y$

$$\Rightarrow [L_z, L_{\pm}] = [x p_y - y p_x, x \mp i y] = \pm \hbar L_{\pm}$$

$$\Rightarrow \langle f | [L_z, L_{\pm}] | i \rangle = \pm \hbar \langle f | L_{\pm} | i \rangle = 0 = \hbar [m' - (m \pm 1)] \langle m' l' m' | L_{\pm} | m l m \rangle$$

$\Rightarrow$  ALLOWED TRANSITIONS ARE SUCH THAT  $\Delta m = \pm 1$

WHAT CAN BE SAID ABOUT  $l$  AND  $l'$ ?

THE STRATEGY IS TO USE  $L^2 : L^2 |m l m\rangle = l(l+1) \hbar^2 |m l m\rangle$

$$[L^2, z] = 2i \hbar (x L_y - L_x y)$$

ON THE RHS,  $L^2$  OR  $z$  DID NOT APPEAR  $\Rightarrow$  COMMUTE

ONCE MORE :

$$[L^2, [L^2, z]] = 2 \hbar^2 \{L^2, z\}$$

$\Rightarrow$  ALLOWED TRANSITIONS ARE SUCH THAT  $\Delta l = \pm 1$  AND  $\Delta m = 0, \pm 1$



→ CLASSICAL ELECTRON RADIUS

$$r_0 = \frac{q^2}{4\pi\epsilon_0} \times \frac{1}{mc^2} = \frac{q^2}{4\pi\epsilon_0 \hbar} \times \frac{\hbar}{mc} = \alpha \frac{\hbar}{mc}$$

$$\Rightarrow \int_f \sigma(\omega_{fi}) = \text{TOTAL CROSS SECTION} = 2\pi^2 r_0 c$$

# ELECTRIC QUADRUPOLE

(24)

$$\langle f | x y, x z, y z, x^2, y^2, z^2 | i \rangle$$

- $[L_z, z^2] = 0 \Rightarrow \Delta m = 0$
- $[L_z, r_{\pm}^2] = \pm 2 \hbar r_{\pm}^2 \Rightarrow \Delta m = \pm 2$
- $[L_z, r_{\pm} z] = \pm \hbar r_{\pm} z \Rightarrow \Delta m = \pm 1$

FOR THE QUANTUM NUMBER  $l \Rightarrow$  COMPUTE  $[L^2, [L^2, z^2]]$  AND THE OTHERS

## SUM RULES:

SOMETIMES IT IS VERY USEFUL

$$LET \quad H_0 = \frac{p^2}{2m} + V(\vec{r})$$

$$\Rightarrow [H_0, x] = \frac{1}{2m} (p_x [p_x, x] + [p_x, x] p_x) = -\frac{i\hbar}{m} p_x$$

$$\Rightarrow [x, [H_0, x]] = \frac{\hbar^2}{m}$$

$$\Rightarrow \langle i | [x, [H_0, x]] | i \rangle = \frac{\hbar^2}{m} = \langle i | x H_0 x - x H_0 x - H_0 x x + x H_0 x | i \rangle$$

$$= 2 \left( \langle i | x H_0 x | i \rangle - E_i \langle i | x x | i \rangle \right)$$

$$\uparrow \qquad \qquad \qquad \uparrow$$

$$\sum_f |f\rangle \langle f| \qquad \qquad \qquad \sum_f |f\rangle \langle f|$$

$$= 2 \sum_f (E_f - E_i) |\langle f | x | i \rangle|^2 = 2\hbar \sum_f \omega_{fi} |\langle f | x | i \rangle|^2$$

$$\Rightarrow \sum_f \sigma(\omega_{fi}) \approx \sum_f \frac{4\pi^2}{m^2 \omega_{fi}^2} \alpha |\langle f | \underbrace{e^{i\omega_{fi} \vec{r}}}_{\approx 1} \vec{p} \cdot \vec{e} | i \rangle|^2$$

$$= 4\pi^2 \alpha \sum_f \omega_{fi} |\langle f | \vec{r} \cdot \vec{e} | i \rangle|^2$$

$$\Rightarrow \sum_f \sigma(\omega_{fi}) \approx \sum_f 4\pi^2 \alpha \omega_{fi} |\langle f | x | i \rangle|^2$$

TOTAL CROSS SECTION / FREQUENCY

$$= 4\pi^2 \alpha \frac{\hbar^2}{m} \times \frac{1}{2\hbar} = \left[ \frac{2\pi^2 \hbar \alpha}{m} = \sum_f \sigma(\omega_{fi}) \right]$$



SUDDEN AND ADIABATIC APPROXIMATIONS

MESSEIAH (QUANTUM MECHANICS) - CHAP XXVII (VOL 2)

GALINSO & PASCHAL (QUANTUM MECHANICS) CHAP 33 (VOL 2)

LEVIN (INTROD. TO Q.M.) CHAP 16

SUDDEN APPROXIMATION

IN THIS CASE, THE SITUATION IS SIMPLIFIED TO

$$H(t) = \begin{cases} H_1, & t < t_0 \\ H_2, & t > t_0 \end{cases}$$

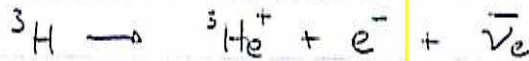
where  $H_1$  AND  $H_2$  ARE TIME INDEPENDENT

THUS, THE TIME EVOLUTION IS SIMPLE

FOR  $t < t_0 \rightarrow |\psi(t)\rangle = e^{-iH_1 t/\hbar} |\psi_0\rangle$

FOR  $t > t_0 \rightarrow |\psi(t)\rangle = e^{-iH_2(t-t_0)/\hbar} e^{-iH_1 t_0/\hbar} |\psi_0\rangle$

EXAMPLE:  $\beta$ -DECAY OF TRITIUM



INITIAL STATE: NEUTRAL  $\Delta e^-$  AND  $\Delta p$  ( $z=1$ ) + 2 NEUTRONS

FINAL STATE: CHARGED He ATOM:  $2p + \Delta e^-$  ( $z=2$ ) + 1 NEUTRON +  $\Delta e^- + \Delta \bar{\nu}_e$   
FREE

LET'S FOCUS ONLY IN THE BOUNDED ELECTRON

$$\Rightarrow \begin{cases} |i\rangle = |100\rangle_{z=1} \\ H_1 = \frac{p^2}{2m} + V_{z=1}(r) \end{cases}$$

JUST AFTER THE DECAY,  $H_2 = \frac{p^2}{2m} + V_{z=2}(r)$

$$\Rightarrow |f(t)\rangle = \sum_{n, l, m} c_{n, l, m} e^{-\frac{i}{\hbar} E_n t} |n, l, m\rangle_{z=2}$$

JUST AFTER THE DECAY, THE STATE OF  ${}^3\text{He}^+$  IS MEASURED  
WHAT IS THE PROBABILITY IT IS FOUND IN  $|f\rangle = |100\rangle_{z=2}$  ?

$$\Rightarrow P = |\langle 100_{z=2} | 100_{z=1} \rangle|^2 = \left| \int_0^\infty dr r^2 \underbrace{\left(\frac{2}{a_0}\right)^{3/2} 2e^{-\frac{2r}{a_0}}}_{R_{10}(r)|_{z=2}} \times \underbrace{\left(\frac{1}{a_0}\right)^{3/2} 2e^{-\frac{r}{a_0}}}_{R_{10}(r)|_{z=1}} \right|^2$$

$$= \left| \frac{16\sqrt{2}}{27} \right|^2 = 70,23\%$$

## ADIABATIC APPROXIMATION

(26)

THIS IS THE OPPOSITE OF THE SUDDEN CHANGE

HERE,  $H_1(t_0) \rightarrow H_2(t_1)$  EVOLVES VERY SMOOTHLY,  $\tau = t_1 - t_0 \rightarrow \infty$

FOR  $\tau \rightarrow \infty$  WE WILL HAVE THAT  $|\psi(\vec{r}, t_0)|^2 \neq |\psi(\vec{r}, t_1)|^2$   
AS WE HAVE SEEN IN THE SUDDEN CHANGE CASE,  $|\psi(\vec{r}, t_0)|^2 = |\psi(\vec{r}, t_1)|^2$

THE "ADIABATIC" TERM IS USED IN THERMODYNAMICS <sup>LOW ORDER</sup> TO DESIGNATE PROCESSES THAT DO NOT EXCHANGE HEAT. HERE, IN Q.M., THE CHANGE  $H_1 \rightarrow H_2$  IN TIME  $\tau \rightarrow \infty$  IS MORE RELATED TO THE QUASISTATIC PROCESS, AND ITS RELATION TO HEAT EXCHANGE IS NOT SO CLEAR.

• INSTANTANEOUS <sup>EIGEN</sup> BASIS: ~~QUASISTATIC~~  $H(t) |\varphi_m(t)\rangle = E_m(t) |\varphi_m(t)\rangle$

\*  $|\varphi_m\rangle$  IS NOT SOLUTION OF THE TIME-DEPENDENT SCHRÖDINGER EQUATION:  $i\hbar \frac{\partial}{\partial t} |\varphi_m\rangle = H(t) |\varphi_m\rangle$

LETS USE THE INSTANTANEOUS <sup>EIGEN</sup> BASIS TO EXPRESS THE TRUE STATE

$$|\psi(t)\rangle = \sum_m c_m(t) |\varphi_m(t)\rangle$$

$$\Rightarrow (\text{SCHROD. EQ}) \sum_m i\hbar \left( \dot{c}_m |\varphi_m\rangle + c_m \left( \frac{\partial}{\partial t} |\varphi_m\rangle \right) \right) = \sum_m c_m(t) E_m(t) |\varphi_m(t)\rangle$$

$$\Rightarrow \langle \varphi_k | \left( i\hbar \dot{c}_k - E_k c_k = -i\hbar \sum_m \langle \varphi_k | \frac{\partial}{\partial t} |\varphi_m\rangle c_m \right) | \varphi_m \rangle$$

LETS INVESTIGATE  $\langle \varphi_k | \frac{\partial}{\partial t} |\varphi_m\rangle$

$$\begin{aligned} \bullet H|\varphi_m\rangle = E_m|\varphi_m\rangle &\Rightarrow \left( \frac{\partial H}{\partial t} |\varphi_m\rangle + H \left( \frac{\partial}{\partial t} |\varphi_m\rangle \right) \right) = \dot{E}_m |\varphi_m\rangle + E_m \left( \frac{\partial}{\partial t} |\varphi_m\rangle \right) \\ \langle \varphi_k | \Rightarrow \langle \varphi_k | \frac{\partial}{\partial t} |\varphi_m\rangle &= \frac{\langle \varphi_k | \left( \frac{\partial H}{\partial t} |\varphi_m\rangle \right)}{E_m - E_k} - \frac{\dot{E}_m}{E_m - E_k} \delta_{mk} \end{aligned}$$

\(\Rightarrow\) FOR  $m \neq k$

$$\langle \varphi_k | \frac{\partial}{\partial t} |\varphi_m\rangle = \frac{\langle \varphi_k | \frac{\partial H}{\partial t} |\varphi_m\rangle}{E_m - E_k}$$



FOR  $n=k \Rightarrow$  ~~USE~~ THERE IS NO USE OF THE PREVIOUS CALCULATION  
 HOWEVER, THINGS ARE MUCH SIMPLER

NOTICE THAT  $\frac{\partial}{\partial t} \langle \psi_n | \psi_n \rangle = 0 = \left( \frac{\partial}{\partial t} \langle \psi_n | \right) | \psi_n \rangle + \langle \psi_n | \left( \frac{\partial}{\partial t} | \psi_n \rangle \right)$   
 $= 2 \operatorname{Re} \{ \langle \psi_n | \left( \frac{\partial}{\partial t} | \psi_n \rangle \right) \}$

THUS, WE CONCLUDE THAT  $\langle \psi_n | \frac{\partial}{\partial t} | \psi_n \rangle$  IS PURE IMAGINARY  $\equiv i \alpha_n(t)$   
 WITH  $\alpha_n \in \mathbb{R}$

COMING BACK TO THE EQUATION FOR  $C_k$ :

$$i\hbar \dot{C}_k - E_k C_k = -i\hbar \left\{ i \alpha_k C_k + \sum_{m \neq k} \langle \psi_k | \frac{\partial}{\partial t} | \psi_m \rangle C_m \right\}$$

$$= -i\hbar \left\{ i \alpha_k C_k + \sum_{m \neq k} \frac{\langle \psi_k | \frac{\partial \hat{H}}{\partial t} | \psi_m \rangle C_m}{E_m - E_k} \right\}$$

NEW DEFINITION:  $\tilde{C}_k(t) = C_k(t) * e^{\int_t^t -\frac{1}{i\hbar} (E_k + \hbar \alpha_k) dt}$

$$\Rightarrow C_k = \tilde{C}_k(t) e^{\frac{1}{i\hbar} \int_t^t (E_k(t') + \hbar \alpha_k(t')) dt'}$$

$$\Rightarrow i\hbar \dot{\tilde{C}}_k e^{\frac{1}{i\hbar} \int_t^t (E_k + \hbar \alpha_k)} + \tilde{C}_k (E_k + \hbar \alpha_k) e^{\frac{1}{i\hbar} \int_t^t (E_k + \hbar \alpha_k)} - E_k \tilde{C}_k e^{\frac{1}{i\hbar} \int_t^t (E_k + \hbar \alpha_k)} = \hbar \alpha_k \tilde{C}_k e^{\frac{1}{i\hbar} \int_t^t (E_k + \hbar \alpha_k)} - i\hbar \sum_{m \neq k} \frac{\langle \psi_k | \dot{\hat{H}} | \psi_m \rangle}{E_m - E_k} \tilde{C}_m e^{\frac{1}{i\hbar} \int_t^t (E_k + \hbar \alpha_k)}$$

$$\Rightarrow \dot{\tilde{C}}_k = \sum_{m \neq k} \frac{\langle \psi_k | \dot{\hat{H}} | \psi_m \rangle}{E_k - E_m} \tilde{C}_m e^{\frac{1}{i\hbar} \int_t^t dt' [E_m + \hbar \alpha_m - (E_k + \hbar \alpha_k)]}$$

NEW DEFINITION:  $|\tilde{\psi}_n\rangle \equiv |\psi_n\rangle e^{\frac{1}{i\hbar} \int_t^t dt' E_n + \hbar \alpha_n}$   
 ADIABATIC EIGENBASIS  $\Rightarrow |\psi_n\rangle = |\tilde{\psi}_n\rangle e^{-\frac{1}{i\hbar} \int_t^t dt' E_n + \hbar \alpha_n}$

$$\Rightarrow \dot{\tilde{C}}_k = \sum_{m \neq k} \frac{\langle \tilde{\psi}_k | \dot{\hat{H}} | \tilde{\psi}_m \rangle}{E_k - E_m} \tilde{C}_m$$

SOLUTION:  $\tilde{C}_k(t) = \tilde{C}_k(t_0) + \sum_{m \neq k} \int_{t_0}^t dt' \frac{\langle \tilde{\psi}_k(t') | \dot{\hat{H}}(t') | \tilde{\psi}_m(t') \rangle}{E_k(t') - E_m(t')} \tilde{C}_m(t')$

WE NOW CAN COMPUTE  $\tilde{C}_k$  IN A DYSON'S SERIES

1st ORDER : 
$$\tilde{c}_k(t) = \tilde{c}_k(t_0) + \sum_{m \neq k} \tilde{c}_m(t_0) \int_{t_0}^t \frac{\langle \tilde{\psi}_k | \dot{H} | \tilde{\psi}_m \rangle}{E_k - E_m} dt'$$

MOREOVER  $\tilde{c}_j(t_0) = c_j(t_0) \rightarrow$  (NO NEED)

$$\tilde{c}_k(t) = c_k(t_0) + \sum_{m \neq k} c_m(t_0) \int_{t_0}^t dt' \frac{\langle \tilde{\psi}_k | \dot{H} | \tilde{\psi}_m \rangle}{E_k - E_m}$$

THE SERIES CONVERGES AS LONG AS  $\tau \frac{\hbar \dot{H}_{km}}{E_k - E_m} \ll 1$   
 WITH  $\tau = t - t_0$

$$\frac{\hbar \dot{H}_{km}}{\hbar \omega_{km}} \ll 1$$

\* NOTICE THAT  $|\psi\rangle$  CAN BE EXPANDED IN THE "ADIABATIC" EIGEN BASIS

$$|\psi(t)\rangle = \sum_n c_n(t) |\psi_n(t)\rangle = \sum_n \tilde{c}_n(t) |\tilde{\psi}_n(t)\rangle$$

INTERPRETATION:

SUPPOSE WE HAVE THAT  $\tilde{c}_n \cong \text{CONST}$  IN TIME

$$\Rightarrow |\psi(t)\rangle = |\tilde{\psi}_n(t)\rangle = e^{\underbrace{\frac{i}{\hbar} \int_{t_0}^t dt' E_n(t')}_{\text{USUAL DYNAMICAL PHASE}}} \times e^{\underbrace{i \gamma_n(t)}_{\text{BERRY'S PHASE}}} |\psi_n(t)\rangle$$

$-\gamma_n = \int_{t_0}^t \alpha_n(t') dt'$

BERRY'S PHASE IS AN ADDITIONAL PHASE PREVIOUSLY UNNOTICED UNTIL 1984  $\in \mathbb{R}$

WHAT IS ITS SIGNIFICANCE? IS IT OBSERVABLE?

- THE DYNAMICAL PHASE  $e^{\frac{iEt}{\hbar}}$  IS UNOBSERVABLE, BUT THE BERRY'S PHASE IS IT YIELDS OBSERVABLE EFFECTS

MORE ON THIS LATER



BEFORE GOING INTO EXAMPLES, LET'S DISCUSS A BIT MORE ON WHAT MEANS ADIABATICITY

WE HAVE THAT  $|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle = U(t, t_0) |\varphi_n(t_0)\rangle$

WHERE WE USED THE INITIAL CONDITION  $|\psi(t_0)\rangle = |\varphi_n(t_0)\rangle$

$$\Rightarrow |\psi(t)\rangle = \sum_k |\varphi_k(t)\rangle \langle \varphi_k(t) | U(t, t_0) | \varphi_n(t_0) \rangle$$

THE ADIABATIC APPROXIMATION MEANS THAT  $\langle \varphi_k(t) | U(t, t_0) | \varphi_n(t_0) \rangle \cong e^{i\varphi_n(t, t_0)} \delta_{kn}$

WHICH IS : AFTER THE EVOLUTION IN A STATE  $|\varphi_n\rangle$  THE SYSTEM STAY IN STATE  $|\varphi_n\rangle = |\varphi_n\rangle$

### ADIABATIC THEOREM :

GIVEN THE INSTANTANEOUS EIGEN BASIS :  $H(t) |\varphi_n(t)\rangle = E_n(t) |\varphi_n(t)\rangle$

LET THE PROJECTORS  $P_n(t) = |\varphi_n(t)\rangle \langle \varphi_n(t)|$

- HYPOTHESIS :  $E_i(t) \neq E_j(t) \quad \forall i, j, t \in [t_0, t_0 + \tau]$

$\frac{d}{dt} P_j(t)$  AND  $\frac{d^2}{dt^2} P_j(t)$  ARE WELL DEFINED FUNCTIONS AND BOUNDED

$$\Rightarrow U(\tau + t_0, t_0) P_j(t_0) - P_j(t_0 + \tau) U(\tau + t_0, t_0) = O\left(\frac{1}{\tau}\right)$$

FOR  $\tau \rightarrow \infty$  THIS MEANS THAT A STATE <sup>DURING ITS EVOLUTION</sup> DOES NOT LEAVE THE SUBSPACE EXPANDED BY THE INITIAL STATE

$$\underbrace{U(\tau + t_0, t_0) P_j(t_0) |\varphi_j(t_0)\rangle}_{|\varphi_j(\tau + t_0)\rangle} = P_j(t_0 + \tau) \underbrace{U(\tau + t_0, t_0) |\varphi_j(t_0)\rangle}_{|\varphi_j(\tau + t_0)\rangle} \quad \text{FOR } \tau \rightarrow \infty$$

$$\underbrace{|\varphi_j(\tau + t_0)\rangle}_{\langle \varphi_j(\tau + t_0) | \varphi_j(\tau + t_0) \rangle} = 1$$

$$\Rightarrow \langle \varphi_j(\tau + t_0) | \varphi_j(\tau + t_0) \rangle = 1$$



IF AT  $t_0$ ,  $|\psi\rangle = |\varphi_1\rangle \Rightarrow$  AT  $t_0 + \tau$   $|\psi\rangle = |\varphi_1\rangle$   
 " " "  $|\psi\rangle = A|\varphi_1\rangle + B|\varphi_2\rangle \Rightarrow$  "  $|\psi\rangle = A'|\varphi_1\rangle + B'|\varphi_2\rangle$

MORE ON THE VALIDITY OF THIS THEOREM AND THAT ADIABATIC APPROXIMATION

LET  $S = \langle \varphi(t_0) | U^\dagger(t_0 + \tau, t_0) U(t_0 + \tau, t_0) | \varphi(t_0) \rangle - \langle \varphi(t_0) | U^\dagger(t_0 + \tau, t_0) | \varphi(t_0) \rangle \langle \varphi(t_0) | U(t_0 + \tau, t_0) | \varphi(t_0) \rangle$

DYSON'S SERIES:  $U = 1 + \frac{1}{i\hbar} \int_{t_0}^{t_0 + \tau} dt H(t) + \dots$

KEEP ONLY 1st ORDER

$$\begin{aligned} \Rightarrow S &\approx \langle 0 | (1 - \frac{1}{i\hbar} \int H) (1 + \frac{1}{i\hbar} \int H) | 0 \rangle - \langle 0 | 1 - \frac{1}{i\hbar} \int H | 0 \rangle \langle 0 | 1 + \frac{1}{i\hbar} \int H | 0 \rangle \\ &= 1 - \left(\frac{1}{i\hbar}\right)^2 \tau^2 \langle H^2 \rangle - \left(1 - \left(\frac{1}{i\hbar}\right) \tau^2 \langle H \rangle^2\right) \\ &= \frac{\tau^2}{\hbar^2} \left( \langle H^2 \rangle - \langle H \rangle^2 \right) = \frac{\tau^2 \Delta H^2}{\hbar^2} \end{aligned}$$

$S \ll 1 \rightarrow$  SUDDEN APPROXIMATION

$S \gg 1 \rightarrow$  ADIABATIC "



EXAMPLE 1: 1D HARMONIC OSCILLATOR

(31)

$$H(t) = \frac{1}{2m} P^2 + \frac{1}{2} m \omega^2 (x - \bar{x})^2 \quad \text{WITH} \quad \bar{x} = v_0 t$$

RECALL THAT  $Q = \sqrt{\frac{m\omega}{2\hbar}} (x + \frac{i}{m\omega} P)$ ,  $Q^\dagger = \sqrt{\frac{m\omega}{2\hbar}} (x - \frac{i}{m\omega} P)$

INSTANTANEOUS BASIS:  $|\psi_m\rangle \rightarrow \langle x | \psi_m(t) \rangle = \psi_m(x - \bar{x}) \equiv$  HARMONIC OSCILLATOR WAVE FUNCTION CENTERED AT  $\bar{x} = v_0 t$

AND 
$$\psi_m(x) = \sqrt{\frac{1}{2^m m!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega}{2\hbar} x^2\right\} H_m\left(-\sqrt{\frac{m\omega}{\hbar}} x\right)$$

$$= \frac{1}{\sqrt{2^m m!}} \frac{1}{\pi^{1/4}} \frac{1}{x_0^{m+1/2}} \left(x - x_0^2 \frac{d}{dx}\right)^m \exp\left\{-\frac{1}{2} \left(\frac{x}{x_0}\right)^2\right\}$$

$E_m = \hbar\omega(m + \frac{1}{2}) \equiv$  CONSTANT IN TIME WITH  $x_0 = \sqrt{\frac{\hbar}{m\omega}}$

ADIABATIC BASIS:  $|\tilde{\psi}_m\rangle = e^{\frac{i}{\hbar} \int_0^t (E_m + \hbar\alpha_m) dt'} |\psi_m\rangle$

NOTICE THAT  $i\alpha_m = \langle \psi_m | \frac{\partial}{\partial t} | \psi_m \rangle$  WHICH IS PURE IMAGINARY AS  $\langle \psi | \psi \rangle \in \mathbb{R} \Rightarrow \alpha_m = 0 \rightarrow$  TYPICAL OF 1D PROBLEMS

$\Rightarrow |\tilde{\psi}_m\rangle = e^{\frac{i}{\hbar} E_m t} |\psi_m\rangle$  (ONLY THE DYNAMICAL PHASE)

1st ORDER:

$$\tilde{C}_k(t) = \tilde{C}_k(0) + \sum_{m \neq k} \tilde{C}_m(0) \int_0^t dt' \frac{\langle \tilde{\psi}_k | \dot{H} | \tilde{\psi}_m \rangle}{E_k(t') - E_m(t')}$$

$$\dot{H} = m\omega^2 (x - \bar{x}) \dot{\bar{x}} = m\omega v_0 (x - v_0 t)$$

$$\Rightarrow \langle \tilde{\psi}_k | \dot{H} | \tilde{\psi}_m \rangle = m\omega^2 v_0 \langle \tilde{\psi}_k | x | \tilde{\psi}_m \rangle = m\omega^2 v_0 x_0 \frac{1}{\sqrt{2}} \langle \tilde{\psi}_k | Q + Q^\dagger | \tilde{\psi}_m \rangle$$

$$= m\omega^2 v_0 x_0 \frac{1}{\sqrt{2}} \left( \sqrt{m\hbar} \delta_{k,m-1} + \sqrt{m\hbar} \delta_{k,m+1} \right)$$

$$\Rightarrow \tilde{C}_k(t) = \tilde{C}_k(0) + \sum_{m \neq k} \tilde{C}_m(0) \frac{m\omega^2 v_0 x_0}{\sqrt{2}} \frac{1}{(k-m)\hbar\omega} \int_0^t e^{i(k-m)\omega t'} dt'$$

$$\frac{-2e^{i(k-m)\omega t}}{(k-m)\omega} \frac{\sin((k-m)\omega t)}{2}$$

INITIAL CONDITIONS:  $\tilde{c}_k(0) = \begin{cases} 1, & k=j \\ 0, & k \neq j \end{cases}$

(32)

$$\Rightarrow \begin{cases} \ddot{c}_{j+1}(t) = -x_0 \frac{\sqrt{j+1}}{\hbar \omega^2} \sin\left(\frac{\omega t}{2}\right) e^{i\frac{\omega t}{2}} \times m\omega^2 v_0 \sqrt{2} \\ \ddot{c}_{j-1}(t) = x_0 \frac{\sqrt{j}}{\hbar \omega^2} \sin\left(\frac{\omega t}{2}\right) e^{-i\frac{\omega t}{2}} \times m\omega^2 v_0 \sqrt{2} \end{cases}$$

TRANSITION PROBABILITY:

$$P_{j+1}(t) = |\tilde{c}_{j+1}(t)|^2 = \frac{x_0^2 m \omega^4}{\hbar^2 \omega^3} \times 4 \times \frac{\frac{1}{2} m v_0^2}{\hbar \omega} \times \sin^2\left(\frac{\omega t}{2}\right) \cdot (j+1)$$
$$= 4(j+1) \left( \frac{\frac{1}{2} m v_0^2}{\hbar \omega} \right) \sin^2\left(\frac{\omega t}{2}\right)$$

$$P_{j-1}(t) = 4j \left( \frac{\frac{1}{2} m v_0^2}{\hbar \omega} \right) \sin^2\left(\frac{\omega t}{2}\right)$$

THE APPROXIMATION IS GOOD WHEN

$\frac{\frac{1}{2} m v_0^2}{\hbar \omega} \ll 1$  WHICH IS KINETIC ENERGY OF THE PARTICLE

TYPICAL ENERGY OF THE H.O.

$$\hookrightarrow v_0 \ll \sqrt{\frac{\hbar \omega}{m}}$$

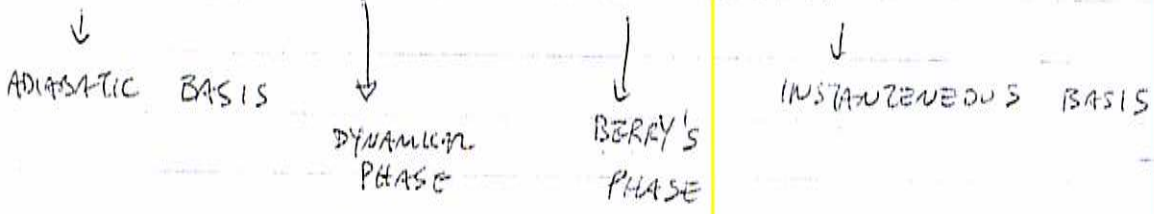


EXAMPLE: SPIN IN A MAGNETIC FIELD

BERRY'S PHASE (M.V. BERRY, PROC. ROY. SOC. LOND. A, 392, 45 (1984))

RECALL  $|\Psi(t)\rangle = \sum_m \tilde{c}_m(t) |\tilde{\varphi}_m(t)\rangle$

$|\tilde{\varphi}_m(t)\rangle = e^{\frac{i}{\hbar} \int_0^t \tilde{c}_m(t') dt'} e^{i\gamma_m(t)} |\varphi_m(t)\rangle$

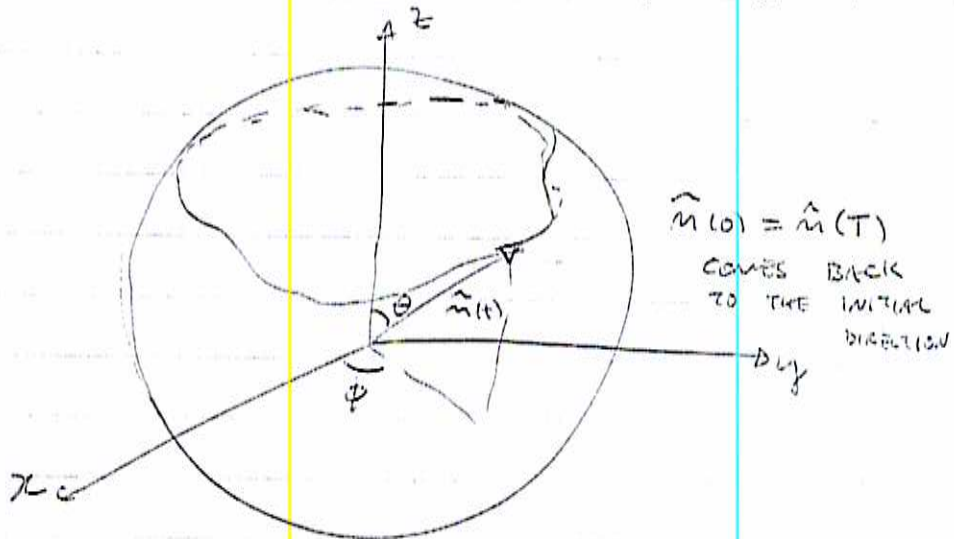


$\gamma_m(t) = i \int_0^t \langle \varphi_m(t') | \frac{\partial}{\partial t'} | \varphi_m(t') \rangle dt' = -\text{Im} \int_0^t \langle \varphi_m | \frac{\partial}{\partial t} | \varphi_m \rangle dt'$

$H = -\frac{g\mu_B}{\hbar} \vec{S} \cdot \vec{B}(t)$

SUPPOSE  $\vec{B}(t) = B_0 \hat{n}(t)$

$\Rightarrow H = -\omega \vec{S} \cdot \hat{n}$   
with  $\omega = \frac{g\mu_B B_0}{\hbar}$



$\hat{n}(t) = \sin\theta(t) \cos\phi(t) \hat{x} + \sin\theta(t) \sin\phi(t) \hat{y} + \cos\theta(t) \hat{z}$

• COMPUTE BERRY'S PHASE: 1st METHOD: PEDESTRIAN ONE  
INSTANTANEOUS BASIS:  $|m, \hat{n}\rangle$ :  $H(t) |m, \hat{n}(t)\rangle = m\hbar\omega |m, \hat{n}(t)\rangle$

HOW DO WE RELATE  $|m, \hat{n}\rangle$  TO  $|m, \hat{z}\rangle$ ?

ANSWER: GET  $|m, \hat{z}\rangle \rightarrow$  ROTATE  $\theta$  OVER  $\hat{y} \rightarrow$  ROTATE  $\phi$  OVER  $\hat{z}$   
 $\Rightarrow |m, \hat{n}\rangle = \exp\left\{-\frac{i}{\hbar} S_z \phi(t)\right\} \exp\left\{-\frac{i}{\hbar} S_y \theta(t)\right\} |m, \hat{z}\rangle$

THUS, WE HAVE TO COMPUTE

$\langle m, \hat{n} | \frac{\partial}{\partial t} | m, \hat{n} \rangle = \langle m, \hat{z} | e^{\frac{iS_z\phi}{\hbar}} e^{\frac{iS_y\theta}{\hbar}} \frac{\partial}{\partial t} \left( e^{-\frac{iS_z\phi}{\hbar}} e^{-\frac{iS_y\theta}{\hbar}} |m, \hat{z}\rangle \right)$   
 $= \frac{-i}{\hbar} \langle m, \hat{z} | e^{\frac{iS_z\phi}{\hbar}} e^{\frac{iS_y\theta}{\hbar}} \left( S_z \dot{\phi} e^{-\frac{iS_z\phi}{\hbar}} e^{-\frac{iS_y\theta}{\hbar}} + e^{-\frac{iS_z\phi}{\hbar}} S_y \dot{\theta} e^{-\frac{iS_y\theta}{\hbar}} \right) |m, \hat{z}\rangle$   
 $= \frac{-i}{\hbar} \left( \langle m, \hat{z} | \tilde{S}_z \dot{\phi} |m, \hat{z}\rangle + \langle m, \hat{z} | S_y \dot{\theta} |m, \hat{z}\rangle \right)$

33.5



$$\Rightarrow V_m = -m \cdot \Omega + \left( m \right)$$

EXT.  
PIVOT  
COMPY  
WITH  
NEXT R:  
BY DO  
OF S

IS THERE A PHYSICAL DIFFERENCE?  $\rightarrow$   $V_m$  IS NOT  
WITH ANOTHER  $\rightarrow$  WHAT IS DIFFERENCE



RECALL  $S^+ \sim (S^+ - S^-) \Rightarrow \langle m | S^+ | m \rangle \sim \langle m | m+1 \rangle + \langle m | m-1 \rangle$

(34)

NOW, WE HAVE TO COMPUTE

$$\tilde{S}_z = e^{i \frac{S_y \theta}{\hbar}} S_z e^{-i \frac{S_y \theta}{\hbar}}$$

WE USE  $e^{iG\lambda} A e^{-iG\lambda} = A + i\lambda [G, A] + \frac{(i\lambda)^2}{2!} [G, [G, A]] + \frac{(i\lambda)^3}{3!} [G, [G, [G, A]]] + \dots$

$$\begin{aligned} \Rightarrow \tilde{S}_z &= S_z + \frac{i\theta}{\hbar} [S_y, S_z] + \frac{(i\theta)^2}{2! \hbar^2} [S_y, [S_y, S_z]] + \frac{(i\theta)^3}{3! \hbar^3} [S_y, [S_y, [S_y, S_z]]] + \frac{(i\theta)^4}{4! \hbar^4} [S_y, [S_y, [S_y, [S_y, S_z]]]] + \dots \\ &= S_z \left( 1 - \frac{i^4 \theta^2}{2!} + \frac{i^8 \theta^4}{4!} - \dots \right) + i^2 S_x \left( \theta - \frac{i^4 \theta^3}{3!} + \frac{i^8 \theta^5}{5!} - \dots \right) \\ &= S_z \cos \theta - S_x \sin \theta \end{aligned}$$

$$\begin{aligned} \Rightarrow \langle m, \hat{n} | \frac{\partial}{\partial t} | m, \hat{n} \rangle &= -\frac{i}{\hbar} \dot{\phi} \langle m, \hat{n} | S_z \cos \theta - S_x \sin \theta | m, \hat{n} \rangle \\ &= -\frac{i}{\hbar} \dot{\phi} \cos \theta \times m \hbar = -i \dot{\phi} \cos \theta \times m \end{aligned}$$

$\Rightarrow$  BERRY'S PHASE =  $\gamma_m = \oint_{\text{PATH}} \dot{\phi}(t) \cos \theta(t) dt$

NOTICE THAT IT DEPENDS ONLY ON THE TRAJECTORY

$\gamma_m = m \times \oint_{\text{PATH}} \cos \theta(\phi) d\phi \rightarrow$  TIME IS ELIMINATED

$m = -m (-2\pi \cos \theta)$   
 $\Rightarrow$  AS LONG AS IT IS SUFFICIENTLY SLOW TO GUARANTEE ADIABATICITY  $\Rightarrow$  IT DOES NOT MATTER HOW FAST  $\hat{n}$  CHANGES

$\gamma_m = m \times \frac{\Omega}{2}$ ,  $\Omega \equiv$  SOLID ANGLE

2ND METHOD: BERRY'S METHOD

$$\gamma_m = -\text{Im} \int_0^T \langle \psi_m | \frac{\partial}{\partial t} | \psi_m \rangle dt = -\text{Im} \oint \langle \psi_m | \frac{\partial}{\partial \vec{B}} | \psi_m \rangle \cdot \frac{d\vec{B}}{dt} dt$$

$$= -\text{Im} \oint_{\text{PATH}} \langle \psi_m | \nabla_{\vec{B}} | \psi_m \rangle \cdot d\vec{B} \Rightarrow \text{IT DEPENDS ON THE "GEOMETRY" OF THE PATH OF } \vec{B}$$

THE TRICKS

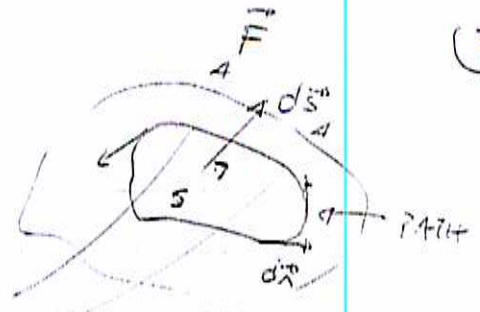
THE PATH OF  $\vec{B}$

IS THEOREM

IRREVERSIBLE, IN LTB ONE NEEDS TO DO INTERFERENCE

STOKES THEOREM:

$$\iint_S \nabla \times \vec{F} \cdot d\vec{S} = \oint_{\text{PATH}} \vec{F} \cdot d\vec{r}$$



(35)

$$\Rightarrow \gamma_m = -I_m \iint_S \vec{V}_m(\vec{B}) \cdot d\vec{S}$$

$$\begin{aligned} \text{where } \vec{V}_m(\vec{B}) &= \nabla_B \times (\langle \psi_m | \nabla_B | \psi_m \rangle) = \nabla_B \times \langle \psi_m | \nabla_B \psi_m \rangle \\ &= \langle \psi_m | \underbrace{(\nabla_B \times \nabla_B \psi_m)}_{=0} \rangle + \langle \nabla_B \psi_m | \times | \nabla_B \psi_m \rangle \end{aligned}$$

$$\begin{aligned} \Rightarrow \gamma_m &= -I_m \iint_S \sum_K \langle \nabla_B \psi_m | \times | \psi_K \rangle \langle \psi_K | \nabla_B | \psi_m \rangle \\ &= -I_m \iint_S \sum_K \langle \nabla_B \psi_m | \psi_K \rangle \times \langle \psi_K | \nabla_B \psi_m \rangle \end{aligned}$$

FOR  $K=M \Rightarrow \langle \psi_m | \nabla_B | \psi_m \rangle$  WHICH IS PURE IMAGINARY

$$\Rightarrow \gamma_m = -I_m \sum_{K \neq m} \iint_S \langle \nabla_B \psi_m | \psi_K \rangle \times \langle \psi_K | \nabla_B \psi_m \rangle$$

NOW, WE WANT TO INTRODUCE THE HAMILTONIAN INTO PLAY:

$$- \text{AS } H(t) | \psi_m \rangle = E_m(t) | \psi_m \rangle$$

$$\Rightarrow \nabla_B (H | \psi_m \rangle) + H | \nabla_B \psi_m \rangle = (\nabla_B E_m) | \psi_m \rangle + E_m | \nabla_B \psi_m \rangle$$

$\Rightarrow \langle \psi_K |$  WITH  $K \neq m$

$$\Rightarrow \langle \psi_K | \nabla_B H | \psi_m \rangle + E_K \langle \psi_K | \nabla_B \psi_m \rangle = \nabla_B E_m \delta_{K,m} + E_m \langle \psi_K | \nabla_B \psi_m \rangle$$

$$(K \neq m) \Rightarrow \langle \psi_K | \nabla_B \psi_m \rangle = \frac{\langle \psi_K | \nabla_B H | \psi_m \rangle}{E_m - E_K}$$

$$\begin{aligned} \Rightarrow \gamma_m &= -I_m \sum_{K \neq m} \iint_S d\vec{S} \cdot \frac{\langle \psi_m | \nabla_B H | \psi_K \rangle \times \langle \psi_K | \nabla_B H | \psi_m \rangle}{(E_m - E_K)^2} \\ &= - \iint_S d\vec{S} \cdot \vec{V}_m(\vec{B}) \end{aligned}$$



WITH  $\vec{V}_m = I_m \sum_{k \neq m} \frac{\langle \psi_m | \nabla_B H | \psi_k \rangle \times \langle \psi_k | \nabla_B H | \psi_m \rangle}{(E_m - E_k)^2}$

AS  $H = -\frac{\gamma \mu_B}{\hbar} \vec{B} \cdot \vec{S} \Rightarrow \nabla_B H = -\frac{\gamma \mu_B}{\hbar} \vec{S}$

RECALL  $S_{\pm} = S_x \pm i S_y \Rightarrow S_x = \frac{1}{2}(S_+ + S_-)$ ,  $S_y = \frac{1}{2i}(S_+ - S_-)$

$\begin{cases} S_+ |m\rangle = \hbar \sqrt{S(S+1) - m(m+1)} |m+1\rangle \\ S_- |m\rangle = \hbar \sqrt{S(S+1) - m(m-1)} |m-1\rangle \end{cases}$

$\Rightarrow \langle \psi_k | \nabla_B H | \psi_m \rangle = -\frac{\gamma \mu_B}{2\hbar} \left( \sqrt{m+1} \delta_{k,m+1} + \sqrt{-m} \delta_{k,m-1}, \frac{\sqrt{m+1} \delta_{k,m+1} - \sqrt{-m} \delta_{k,m-1}}{i}, 2 \delta_{k,m} \right)$

$\Rightarrow \vec{V}_m = I_m \left\{ \frac{\left(-\frac{\gamma \mu_B}{2}\right)^2 \left[ \frac{\sqrt{S(S+1) - (m+1)m} (1, i, 0) \times \sqrt{S(S+1) - m(m+1)} (1, -i, 0)}{\left(\frac{\gamma \mu_B B_0}{\hbar} \times \hbar\right)^2} \right. \right. \\ \left. \left. + \frac{\sqrt{S(S+1) - (m-1)m} (1, -i, 0) \times \sqrt{S(S+1) - m(m-1)} (1, i, 0)}{(S \mu_B B_0)^2} \right] \right\}$

$\vec{V}_m = I_m \left\{ \frac{1}{4B_0^2} \left[ (S(S+1) - m(m+1)) (-2i \hat{z}) + (S(S+1) - m(m-1)) (2i \hat{z}) \right] \right\}$   
 $= I_m \left\{ \frac{1}{4B_0^2} 2i \hat{z} (m(m+1) - m(m-1)) \right\} = I_m \left\{ \frac{im \hat{z}}{B_0^2} \right\}$

$\Rightarrow \vec{V}_m = \frac{m}{B_0} \hat{z} \rightarrow$  THIS IS COMPUTED IN THE INSTANTANEOUS BASIS WHERE  $\hat{z} \cdot \hat{n}$  IS ALWAYS POINTING PARALLEL TO  $\vec{B}$  IN THE LAB

$\vec{V}_m = m \frac{\vec{B}}{B_0^3}$  WHICH IS SINGULAR AT  $B=0$  (NOTICE THIS IS A MONOPOLE FIELD  $\sim \frac{\vec{R}}{R^2}$ )

$\gamma_m = - \iint \vec{V}_m \cdot d\vec{S}^3$ , WITH  $d\vec{S}^3 = d\vec{B}_0 = \hat{n} B_0^2 d\Omega_B$

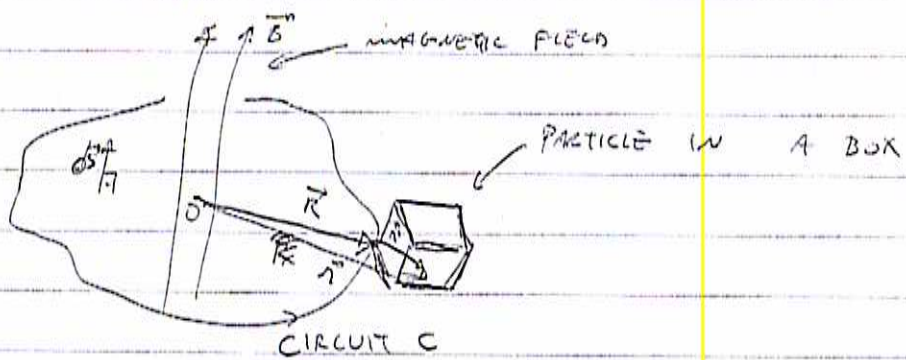
$\Rightarrow \gamma_m = - \iint m \frac{\vec{B}}{B_0^3} \cdot \hat{n} B_0^2 d\Omega_B = -m \Omega_B$   
 $\hookrightarrow$  TO SOLID ANGLE

DOES NOT DEPEND ON THE DYNAMICS OF THE FIELD, ONLY ON THE "GEOMETRY"

\* CLASSICAL ANALOGUE: FAULT PENDULUM (PARALLEL TRANSPORT)

# AHARONOV - BOHM EFFECT

THE PHASE ACQUIRED BY A CHARGED PARTICLE WHEN WINDING A MAGNETIC FLUX CAN BE VIEWED AS A GEOMETRICAL PHASE



STOKES

$$\text{MAGNETIC FLUX} = \Phi = \iint_S \vec{B} \cdot d\vec{s} = \iint_S \nabla \times \vec{A} \cdot d\vec{s} = \oint_C \vec{A} \cdot d\vec{R}$$

EVEN THOUGH THE MAGNETIC FIELD IS ZERO AT THE CIRCUIT C. THE PARTICLE "DOES NOT KNOW" ABOUT THE MAGNETIC FIELD IN THE INNER REGION. HOWEVER A PHASE IS ACQUIRED !! IT MEANS THAT THE VECTOR POTENTIAL HAS A PHYSICAL SIGNIFICANCE.

FOR  $\vec{A} = 0 \rightarrow$  PARTICLE IN A BOX (OR LOCALIZED PARTICLE AROUND  $\vec{r}$ ) WAVE FUNCTIONS  $\psi_m(\vec{r}) = \psi(\vec{r} - \vec{r}_0)$

AND  $H = \frac{1}{2m} p^2 + V(\vec{r}) = H(\vec{p}, \vec{r} - \vec{r}_0)$

$$H|\psi_m\rangle = E_m|\psi_m\rangle$$

FOR  $\vec{A} \neq 0$  : INSTANTANEOUS BASIS:

$$H(\vec{p} - q\vec{A}, \vec{r} - \vec{r}_0) |m(\vec{r})\rangle = E_m |m(\vec{r})\rangle$$

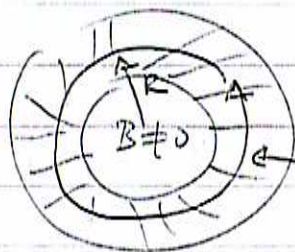
WHERE  $\langle \vec{r} | m(\vec{r}) \rangle = e^{\frac{i}{\hbar} \int_{\vec{r}_0}^{\vec{r}} d\vec{x} \cdot (-q\vec{A}(x))} \psi_m(\vec{r} - \vec{r}_0)$

LIKE AN ADDITIONAL PHASE

$$e^{\frac{i}{\hbar} \vec{p} \cdot (\vec{r} - \vec{r}_0)} \rightarrow e^{\frac{i}{\hbar} \int_{\vec{r}_0}^{\vec{r}} d\vec{x} \cdot (\vec{p}(x) - q\vec{A}(x))}$$



### FLUX QUANTIZATION IN SUPER CONDUCTORS



TRAPPED FLUX IN A CIRCULAR SUPER CONDUCTOR WHERE A DISSIPATIONLESS CURRENT FLOWS

$$\Rightarrow \frac{2\pi}{h} \oint \vec{A} \cdot d\vec{R} = \frac{2\pi}{h} \phi = 2\pi m \quad m = 0, 1, 2, \dots$$

$$\hookrightarrow \phi_0 = \frac{2\pi h}{2\pi} = \frac{h}{2\pi} = 2.07 \times 10^{-7} \text{ Gauss} \cdot \text{cm}$$

NOTICE THE ENERGIES ARE UNAFFECTED BY  $A(\vec{r})$

FOR INSTANCE, IF  $\psi_m(\vec{r})$  ARE PLANE WAVES

$\rightarrow \psi_m = e^{i\vec{k}_m \cdot \vec{r}}$   
 $H = \frac{1}{2m} (\vec{p} - q\vec{A})^2 \rightarrow H = e^{i\vec{k}_m \cdot \vec{r}} \int_{\vec{r}} d\vec{x} \cdot [\vec{k}_m - q\vec{A}(\vec{x})] = E_m(\mu(\vec{r}))$

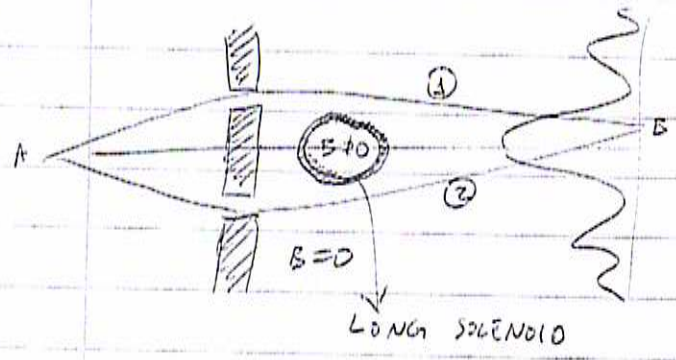
NOW LET THE BOX BE TRANSPORTED ALONG THE CIRCUIT C (NO NEED TO BE ADIABATICALLY TRANSPORTED)

$\Rightarrow \gamma_m = i \oint_C \langle m(\vec{r}) | \nabla_{\vec{r}} | m(\vec{r}) \rangle \cdot d\vec{r}$

WHERE  $\langle m(\vec{r}) | \nabla_{\vec{r}} | m(\vec{r}) \rangle = \int d^3r \psi_m^*(\vec{r}-\vec{r}') \cdot e^{-\frac{i}{\hbar} \int_{\vec{r}'}^{\vec{r}} d\vec{x} \cdot (-q\vec{A}(\vec{x}))} \nabla_{\vec{r}} \left( \psi_m(\vec{r}-\vec{r}') e^{\frac{i}{\hbar} \int_{\vec{r}'}^{\vec{r}} d\vec{x} \cdot (-q\vec{A}(\vec{x}))} \right)$   
 $= \int d^3r \psi_m^*(\vec{r}-\vec{r}') e^{-i(\vec{A} \cdot \text{phase})} \left[ (\nabla_{\vec{r}} \psi_m(\vec{r}-\vec{r}')) e^{i(\vec{A} \cdot \text{phase})} + \left( \frac{-1}{i\hbar} (-q\vec{A}(\vec{r})) \right) \psi_m(\vec{r}-\vec{r}') e^{i(\vec{A} \cdot \text{phase})} \right]$   
 $= \nabla_{\vec{r}} \int d^3r \psi_m^*(\vec{r}-\vec{r}') \psi_m(\vec{r}-\vec{r}') + \int d^3r \psi_m^*(\vec{r}-\vec{r}') \psi_m(\vec{r}-\vec{r}') \left( \frac{-i}{\hbar} q\vec{A}(\vec{r}) \right)$   
 $= 0 - iq\vec{A}(\vec{r})/\hbar$

$\Rightarrow \gamma_m = i \oint_C \frac{-iq}{\hbar} \vec{A}(\vec{r}) \cdot d\vec{r} = \frac{q}{\hbar} \Phi$ , INDEPENDS ON  $m$  AND  $C$

DOUBLE-SLIT EXPERIMENT



INTERFERENCE PATTERN DEPENDS ON THE ADDITIONAL PHASE  $\gamma_m$

$\Rightarrow$  AS THE FIELD IS INCREASED THE INTERFERENCE PATTERN CHANGES PERIODICALLY WITH

A FUNDAMENTAL UNITY OF  $A$

QUANTUM OF MAGNETIC FLUX:  $\frac{q}{\hbar} \Phi_0 = 2\pi \rightarrow \Phi_0 = \frac{2\pi\hbar}{q} \approx 4 \cdot 10^{15} \text{ Wb}$   
 $\frac{q}{\hbar} = 4 \cdot 10^7 \text{ GAUSS/cm}$

\* PHASE DIFFERENCE  $\Delta\theta \equiv \frac{q}{\hbar} \int_A^B \vec{A} \cdot d\vec{r} = \frac{q}{\hbar} \int_A^B \vec{A} \cdot d\vec{r} = \frac{q}{\hbar} \oint \vec{A} \cdot d\vec{r} = \frac{q}{\hbar} \Phi$

ALSO IN SUPER CONDUCTORS:

