TIME DEPENDENT (PERTURBATION) THEORY

HOW DOES $\psi(t)$ EVOLVE IN QUANTUM THEORY?

SCHRÖDINGER: $i\hbar\dot{\psi} = H\psi$

HAMILTONIAN, DIMENSIONS OF ENERGY

FORMAL SOLUTION: $\psi(t) = e^{-\frac{i}{\hbar}\int H(t)dt}\psi_0$ ONLY OCCASIONALLY USEFUL

H TIME INDEPENDENT: $\psi(t) = e^{-\frac{iHt}{\hbar}}\psi_0$

[USED BY VON NEUMANN (1932) IN HIS FAMOUS "EXPLANATION" OF MEASUREMENT]

NARROWER QUESTION: WHAT IS THE <u>RATE</u> OF TRANSITIONS $\psi_i \to \psi_f$?

[DIRAC 1926, PRSLA 112, 661]

ANSWER CAN BE PUT IN A FORM MORE GENERAL THAN THE "USUAL" DERIVATIONS

FERMI: "THE GOLDEN RULE" (~1950)

RATE HAS DIMENSION $\frac{1}{t}$ AND SEEMS RELATED TO $|\langle f|H|i\rangle|^2$

BUT $\langle f|H|i\rangle \sim E$ (IF STATES NORMALIZED TO 1).

QUANTUM RELATION $\Delta E\Delta t \sim \hbar$

SO ALSO, ENERGY SHOULD BE CONSERVED (OVER LONG TIMES

$\Rightarrow$ RATE FORMULA SHOULD INCLUDE $\delta(E_f - E_i)$

NOTE: δ FUNCTION HAS DIMENSION 1/DIMENSIONS OF ARGUMENT

$\delta(E_f - E_i)$ HAS DIMENSIONS $\frac{1}{E}$

$$\Rightarrow \text{RATE} = \frac{2\pi}{\hbar}|\langle f|H|i\rangle|^2\,\delta(E_f - E_i)$$ <u>GOLDEN RULE</u>

ONLY THE 2π NOT EVIDENT FROM DIMENSIONAL ANALYSIS

APPLICATION TO FINAL-STATE CONTINUUM

MAYBE E_f CONTINUOUS, AND MANY MICROSTATES IN A NARROW ENERGY RANGE dE. i.e. $\rho = dN/dE$ KNOWN

THEN $\text{RATE} = \frac{2\pi}{\hbar}|\langle f|H|i\rangle|^2\frac{dN}{dE}$ <u>GOLDEN RULE FOR CONTINUUM</u>

$$\text{RATE} = \frac{2\pi}{\hbar}\int|\langle f|H|i\rangle|^2\,\delta(E_f - E_i)\,\rho(E_f)\,dE_f$$

PERTURBATION THEORY DERIVATION [FERMI, QM, 1954, p99]

$H = H_0 + \mathcal{H}(t)$ H_0 TIME INDEPENDENT

$i\hbar \dot{\psi}_0 = H_0 \psi_0$

WITH EXPANSION $\psi_0 = \sum a_n(0)\, u_0^{(n)} e^{-\frac{i}{\hbar} E_0^{(n)} t}$

$u_0^{(n)}$ = BASIS FUNCTIONS $\quad H_0 u_0^{(n)} = E_0^{(n)} u_0^{(n)}$; $\quad \langle u_0^{(m)} | u_0^{(n)} \rangle = \delta_{mn}$

TRY $\psi = \sum a_n(t)\, u_0^{(n)} e^{-\frac{i}{\hbar} E_0^{(n)} t}$ IN GENERAL EQ $i\hbar\dot{\psi} = H\psi = (H_0 + \mathcal{H})\psi$

$$u_0^{(m)+} i\hbar\dot{\psi} = i\hbar \sum_n \left(-\frac{i a_n E_0^{(n)}}{\hbar} + \dot{a}_n\right) \underbrace{\langle u_0^{(m)} | u_0^{(n)} \rangle}_{\delta_{mn}} e^{-\frac{i}{\hbar} E_0^{(n)} t} = \sum_n \Big[\underbrace{\langle u_0^{(m)} H_0 | u_0^{(n)} \rangle}_{E_0^{n}\, \delta_{mn}} + \langle u_0^{(m)} | \mathcal{H} | u_0^{n} \rangle \Big] e^{-\frac{i}{\hbar} E_0^{(n)} t} a_n$$

CANCEL

$$\dot{a}_m = -\frac{i}{\hbar} \sum_n a_n \langle m | \mathcal{H} | n \rangle e^{\frac{i}{\hbar}(E_0^{(m)} - E_0^{(n)})t}$$

APPROXIMATION $a_n(t) \approx a_n(0)$

$$a_m(t) = a_m(0) - \frac{i}{\hbar} \sum_n a_n(0) \int_0^t \langle m | \mathcal{H}(t) | n \rangle e^{\frac{i}{\hbar}(E_0^{(m)} - E_0^{(n)})t} dt$$

EXAMPLE: AT $t = 0$, $\psi = u_0^{(n)} \Rightarrow a_m(0) = 0$ FOR $m \neq n$

THEN $$a_m(t) = -\frac{i}{\hbar} \int_0^t \langle m | \mathcal{H}(t) | n \rangle e^{\frac{i}{\hbar}(E_0^{(m)} - E_0^{(n)})t} dt \qquad m \neq n$$

SUPPOSE ALSO A CONTINUUM OF FINAL STATES

AND THAT $\mathcal{H}$ IS INDEPENDENT OF TIME

$n \longrightarrow m$

$$\Rightarrow a_m(t) = -\frac{i}{\hbar} \langle m | \mathcal{H} | n \rangle \frac{e^{\frac{i}{\hbar}(E_0^{(m)} - E_0^{(n)})t} - 1}{\frac{i}{\hbar}(E_0^{(m)} - E_0^{(n)})}$$

$$= -2i \langle m | \mathcal{H} | n \rangle \frac{e^{\frac{i}{2\hbar}(E_0^{(m)} - E_0^{(n)})t}}{E_0^{(m)} - E_0^{(n)}} \cdot \frac{e^{\frac{i}{2\hbar}(E_0^{(m)} - E_0^{(n)})t} - e^{-\frac{i}{2\hbar}(\ )t}}{2i}$$

$$= -2i \langle m | \mathcal{H} | n \rangle \frac{e^{\frac{i}{2\hbar}(E_0^{(m)} - E_0^{(n)})t}}{E_0^{(m)} - E_0^{(n)}} \sin\left[\frac{(E_0^{(m)} - E_0^{(n)})t}{2\hbar}\right]$$

$$|a_m(t)|^2 = 4 |\langle m | \mathcal{H} | n \rangle|^2 \frac{\sin^2 (E_0^{(m)} - E_0^{(n)}) \frac{t}{2\hbar}}{(E_0^{(m)} - E_0^{(n)})^2}$$

PROB OF TRANSITION TO A NARROW RANGE OF FINAL STATE dE

$$P(t) = \sum_{\text{RANGE}} |a_n(t)|^2 \sim 4\,|\langle m|\mathcal{H}|n\rangle|^2_{\text{AVE}} \sum \frac{\sin^2 (E^{(m)} - E^{(n)})\frac{t}{2\hbar}}{(E_0^{(m)} - E_0^{(n)})^2}$$

$$\sim 4\,|\langle m|\mathcal{H}|n\rangle|^2_{\text{AVE}} \int dE\, \rho(E) \frac{\sin^2 (E - E_0^{(n)})\frac{t}{2\hbar}}{(E - E_0^{(n)})^2}.$$

$\rho(E) = \frac{dN}{dE} \longleftrightarrow$ DENSITY OF STATES

$$\sim 4\,\langle m|\mathcal{H}|n\rangle|^2_{\text{AVE}}\; \rho_{\text{AVE}}(E) \int dE \frac{\sin^2 (E - E_0^{(n)})\frac{t}{2\hbar}}{(E - E_0^{(n)})^2}$$

CAN CHANGE TO $d(E - E_0^{(n)})$

$$\sim t \cdot \frac{2\pi}{\hbar} \underbrace{|\langle m|\mathcal{H}|n\rangle|^2 \rho(E)}_{\text{FOR } E \sim E_n}$$

$$\int \frac{\sin^2 (x \frac{t}{2\hbar})}{x^2} = \frac{\pi t}{2\hbar}$$

$$\text{RATE} = \frac{P(t)}{t} = \frac{2\pi}{\hbar} |\langle m|\mathcal{H}|n\rangle|^2 \rho(E_n)$$

CLASSIC APPLICATIONS: EMISSION & ABSORPTION OF RADIATION BY ATOMS (DIRAC, 26), HERE "RADIATION" = PLANE WAVES WITH NO TIME DEPENDENCE

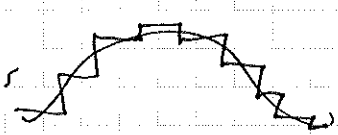
ALSO: SCATTERING BY A TIME-INDEPENDENT POTENTIAL, EX: RUTHERFORD SCAT.

SUCH APPLICATIONS INVOKE THE ABOVE FORMALISM, WHICH INCLUDED TIME,

BUT WE MADE THE ASSUMPTION THAT $\mathcal{H}$ WAS TIME INDEPENDENT, SO WE HAVE FALLEN SHORT OF A FULL THEORY OF TIME DEPENDENT PERTURBATIONS.

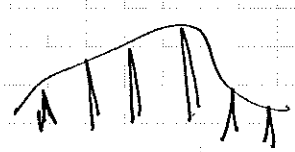
? HOW TO MAKE THE ANALYSIS "MORE TIME DEPENDENT"?

COULD IMAGINE THAT $\mathcal{H}(t)$ IS MADE UP OF CONSTANT STEPS



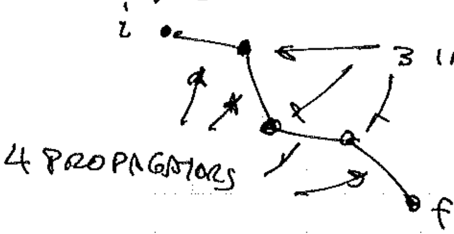
AND USE SPIRIT OF ABOVE ANALYSIS FOR EACH STEP ....
(SPIRIT OF HEAVISIDE)

OR, MAYBE IMAGINE THAT $\mathcal{H}(t)$ IS A SERIES OF DELTA FUNCTIONS
(SPIRIT OF GREEN)



THE FIRST APPROACH IS SOMEWHAT IMPLIED BY DIRAC, WHILE THE 2ND APPROACH WAS MORE SYSTEMATICALLY DEVELOPED BY FEYNMAN - WHO SPOKE OF

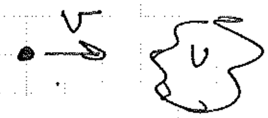
$\mathcal{H}(t)$ AS CONSISTING OF "PROPAGATORS" + BRIEF INTERACTIONS



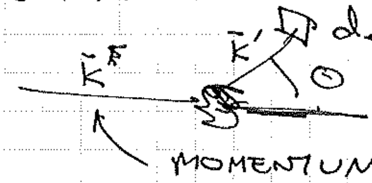
$$\Longrightarrow \langle f|\mathcal{H}|i\rangle \sim V_{fi} + \sum_m V_{fm} \frac{1}{E_f - E_k + i\epsilon} V_{ki} + \sum_{m,n} V_{fm} \frac{1}{E_f - E_m + i\epsilon} V_{mn} \frac{1}{E_m - E_n + i\epsilon} V_{ni} + \cdots$$

POTENTIAL SCATTERING IN BORN APPROX.

σ = SCATTERING CROSS SECTION, AN AREA



$$\text{RATE} = \frac{v\,\sigma}{\text{Volume}}$$ IF ONE BEAM PARTICLE & ONE TARGET PARTICLE PER VOLUME V



DIFFERENTIAL CROSS SECTION

$$\text{RATE INTO } d\Omega = \frac{v}{V}\boxed{\frac{d\sigma}{d\Omega}}\,d\Omega$$

$$\psi_i = \frac{e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}}}{\sqrt{V}} \qquad \psi_f = \frac{e^{\frac{i}{\hbar}\vec{p}'\cdot\vec{x}}}{\sqrt{V}}$$ $\leftarrow$ STATES NORMALIZED TO 1 PER VOLUME V

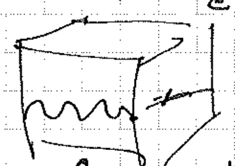
$\mathcal{H} = U(x)$ = SCATTERING POTENTIAL - TIME INDEPENDENT

$$\langle f|\mathcal{H}|i\rangle = \frac{1}{V}\int U(x)\,e^{\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{x}}\,d^3\vec{x} \equiv \frac{U_{\vec{p}-\vec{p}'}}{V}$$ $\leftarrow$ FOURIER TRANSFORM

NEED DENSITY OF FINAL STATES IN SOLID ANGLE $d\Omega$

$$dE = v\,dp$$ $\left[E = \frac{1}{2}mv^2 \Rightarrow dE = mv\,dv\ ;\ E^2 = m^2c^4 + p^2c^2 \Rightarrow 2E\,dE = 2pc^2\,dp\ \ \&\ v = \frac{pc}{E} \Rightarrow dE = v\,dp\right]$

$$dN = \frac{V p^2\,dp\,d\Omega}{(2\pi\hbar)^3}$$



$\sin k_x x$ VANISH AT WALLS

NEED $k_x \frac{\ell}{2} = n_x \pi \qquad n_x = \frac{k_x \ell}{2\pi} = \frac{p_x \ell}{2\pi\hbar}$

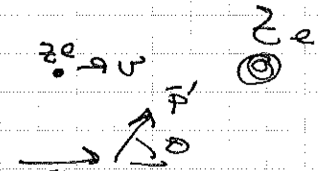
$N = n_x n_y n_z = \frac{p_x p_y p_z}{(2\pi\hbar)^3} V$

$$\rho = \frac{dN}{dE} = \frac{V\,d\Omega}{(2\pi\hbar)^3}\frac{p^2\,dp}{v\,dp} = \frac{V p^2\,d\Omega}{8\pi^3\hbar^3 v}$$

$$\frac{v}{V}\frac{d\sigma}{d\Omega}d\Omega = \text{RATE} = \frac{2\pi}{\hbar}|\langle f|\mathcal{H}|i\rangle|^2\rho = \frac{2\pi}{\hbar}\frac{|U_{\vec{p}-\vec{p}'}|^2}{V^2}\cdot\frac{V p^2\,d\Omega}{8\pi^3\hbar^3 v}$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2\hbar^4}\frac{p^2}{v^2}|U_{\vec{p}-\vec{p}'}|^2$$

COULOMB SCATTERING $\quad U = \frac{zZe^2}{r}$



$$U_{\vec{p}-\vec{p}'} = zZe^2\int\frac{e^{\frac{i}{\hbar}(\vec{p}-\vec{p}')\cdot\vec{x}}}{r}\,\underset{2\pi r^2\,dr\,d\cos\phi}{d^3\vec{x}}$$

$$\cancel{= 2\pi zZe^2\int r\,dr}$$

$$(\vec{p}-\vec{p}')^2 = 2p^2(1-\cos\theta) = 4p^2\sin^2\frac{\theta}{2}$$

$$|\vec{p}-\vec{p}'| = 2p\sin\theta/2$$

TRICK (WENTZEL 1927)

TAKE $U = zZe^2\frac{e^{-\alpha r}}{r}$ AND LATER PUT $\alpha \to 0$! $\qquad K = \frac{i|\vec{p}-\vec{p}'|}{\hbar}$

$$U_{\vec{p}-\vec{p}'} = zZe^2\,2\pi\int r^2\,dr\,\frac{e^{-\alpha r}}{r}\int_{-1}^{1}d\cos\phi\ e^{\frac{i}{\hbar}|\vec{p}-\vec{p}'|\,r\cos\phi} = 2\pi zZe^2\int r\,dr\,e^{-\alpha r}\int_{-1}^{1}d\cos\phi\ e^{iKr\cos\phi}$$

$$\cancel{= 4\pi zZe^2\int_0^\infty r^2\,dr\,\frac{e^{-\alpha r}}{r}\,\frac{\hbar\sin\frac{1}{\hbar}|\vec{p}-\vec{p}'|r}{|\vec{p}-\vec{p}'|r}} \qquad = 2\pi zZe^2\int r\,dr\,e^{-\alpha r}\,\frac{e^{iKr}-e^{-iKr}}{iKr}$$

$$U_{\bar p-\bar p'} = \frac{2\pi z Z^2 e^2}{K}\int_0^\infty dr\left[e^{(-\alpha+k)r} - e^{(-\alpha-k)r}\right]$$

$$= \frac{2\pi z Z^2 e^2}{K}\left[\frac{-1}{-\alpha+k} - \frac{-1}{-\alpha-K}\right]$$

$$\frac{+\alpha+k+(-\alpha+k)}{-(k^2-\alpha^2)} = \frac{2K}{-(k^2-\alpha^2)} \xrightarrow{\alpha\to 0} \frac{-2}{K}$$

$$= \frac{-4\pi z Z e^2}{K^2} = \frac{\pi z Z e^2 \hbar^2}{p^2 \sin^2\theta/2} \qquad K = \frac{i}{\hbar}|\bar p-\bar p'|,\quad k^2 = \frac{-|\bar p-\bar p'|^2}{\hbar^2} = \frac{-4p^2\sin^2\theta/2}{\hbar^2}$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{4\pi^2\hbar^4}\frac{p^2}{v^2}\left|U_{\bar p-\bar p}\right|^2 = \frac{z^2 Z^2 e^4}{4v^2p^2\sin^4\theta/2}$$ RUTHERFORD

SINUSOIDAL PERTURBATION

$$\mathcal{H} = eEz\cos\omega t \qquad \text{FOR } \bar E \text{ ALONG } \hat z$$

$t=0$, ONLY $a_n(0)=1$. THEN FROM MIDDLE OF P. 2 (BEFORE ASSUMED $\mathcal{H}$ IND. OF t)

$$a_m(t) \sim -\frac{i}{\hbar}\int_0^t \langle m|\mathcal{H}(t)|n\rangle e^{i\omega_{mn}t}\,dt$$ WHERE NOW DEFINE $\omega_{mn} = \frac{E_0^{(m)}-E_0^{(n)}}{\hbar}$

$$eE\langle m|z|n\rangle\cos\omega t = eE\,z_{mn}\,\frac{e^{i\omega t}+e^{-i\omega t}}{2}$$

WE EXPECT AN EFFECT MAINLY FOR ω SUCH THAT ENERGY IS CONSERVED, $\omega \sim \omega_{mn}$

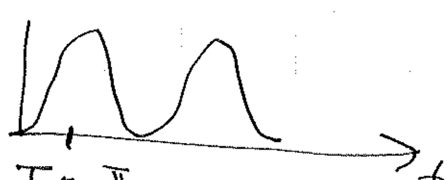
MATHEMATICALLY, THIS MEANS THAT ONLY THE TERM $e^{-i\omega t}$ IS IMPORTANT

$$a_m(t) \sim -\frac{i\,eE z_{mn}}{2\hbar}\int_0^t e^{i(\omega_{mn}-\omega)t}\,dt = -\frac{i\,eE z_{mn}}{2\hbar}\,\frac{e^{i(\omega_{mn}-\omega)t}-1}{i(\omega_{mn}-\omega)}$$

$$\sim \frac{eE z_{mn}}{\hbar}\,\frac{\sin(\omega_{mn}-\omega)\frac{t}{2}}{\omega_{mn}-\omega}$$

$$P_m(t) = |a_m(t)|^2 \sim \frac{e^2E^2|z_{mn}|^2}{\hbar^2}\,\frac{\sin^2(\omega_{mn}-\omega)\frac{t}{2}}{(\omega_{mn}-\omega)^2}$$

P(t)



$T = \frac{\pi}{\omega_{mn}-\omega}$

IF WANT TO "FORCE" A TRANSITION, TURN ON THE PERTURBATION JUST FOR TIME T.

SPINTRONICS (CAN SOLVE "EXACT" SOLUTION & DON'T REALLY NEED "PERTURBATION" THEORY. PROB 19, PH 410)