TIME - DEPENDENT PERTURBATION THEORY

⇝ STUDY OF TIME - DEPENDENT PERTURBATIONS

⇒ TWO - LEVEL SYSTEMS

- H^0 UNPERTURBED HAMILTONIAN

↳ 2 STATES $|\psi_a\rangle$ $\quad H^0|\psi_a\rangle = E_a|\psi_a\rangle$

$|\psi_b\rangle$ $\quad H^0|\psi_b\rangle = E_b|\psi_b\rangle$

$$\langle\psi_a|\psi_b\rangle = \delta_{ab}$$

ANY STATE $|\Psi(t=0)\rangle = c_a|\psi_a\rangle + c_b|\psi_b\rangle$

$$|c_a|^2 + |c_b|^2 = 1$$

$$|\Psi(t)\rangle = c_a e^{-\frac{i}{\hbar}E_a t}|\psi_a\rangle + c_b e^{-\frac{i}{\hbar}E_b t}|\psi_b\rangle$$

c_a, c_b CONSTANTS

ALL TIME DEPENDENCE is in $e^{-\frac{i}{\hbar}Et}$ FOR STATIONARY STATES

• TIME-DEPENDENT PERTURBATION

↳ $H'(t)$

$\{ |\psi_a\rangle, |\psi_b\rangle \}$ FORM A COMPLETE SET

↓

WF AT TIME t CAN STILL BE EXPRESSED AS LINEAR COMBINATION OF $|\psi_a\rangle$ & $|\psi_b\rangle$

$$|\Psi(t)\rangle = c_a(t)\, e^{-\frac{i}{\hbar}E_a t}\,|\psi_a\rangle + c_b(t)\, e^{-\frac{i}{\hbar}E_b t}\,|\psi_b\rangle$$

COEFFICIENTS CAN NOW DEPEND ON TIME

$H'(t)$ CAN INDUCE TRANSITIONS BETWEEN a & b

e.g. $c_a(t=0) = 1$, $c_b(t=0) = 0$ $\overset{H'(t)}{\Longrightarrow}$ $c_a(t_1) = 0$, $c_b(t_1) = 1$

$(t_1 > 0)$

↳ $c_a(t),\ c_b(t)$?

$$H = H^0 + H'(t)$$

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

$$\downarrow \qquad |\Psi(t)\rangle = c_a(t)\, e^{-\frac{i}{\hbar}E_a t}\, |\psi_a\rangle + c_b(t)\, e^{-\frac{i}{\hbar}E_b t}\, |\psi_b\rangle$$

$$\cancel{c_a e^{-\frac{i}{\hbar}E_a t} H^0 |\psi_a\rangle}^{E_a} + \cancel{c_b e^{-\frac{i}{\hbar}E_b t} H^0 |\psi_b\rangle}^{E_b}$$

$$+ c_a e^{-\frac{i}{\hbar}E_a t} H' |\psi_a\rangle + c_b e^{-\frac{i}{\hbar}E_b t} H' |\psi_b\rangle$$

$$= i\hbar \left[\dot{c}_a e^{-\frac{i}{\hbar}E_a t} |\psi_a\rangle + \dot{c}_b e^{-\frac{i}{\hbar}E_b t} |\psi_b\rangle \right]$$

$$+ \cancel{c_a E_a e^{-\frac{i}{\hbar}E_a t} |\psi_a\rangle} + \cancel{c_b E_b e^{-\frac{i}{\hbar}E_b t} |\psi_b\rangle}$$

$$\Downarrow$$

$$c_a e^{-\frac{i}{\hbar}E_a t} H' |\psi_a\rangle + c_b e^{-\frac{i}{\hbar}E_b t} H' |\psi_b\rangle$$

$$= i\hbar \left[\dot{c}_a e^{-\frac{i}{\hbar}E_a t} |\psi_a\rangle + \dot{c}_b e^{-\frac{i}{\hbar}E_b t} |\psi_b\rangle \right]$$

$$\Downarrow \qquad \langle \psi_a |$$

$$c_a e^{-\frac{i}{\hbar}E_a t} \langle \psi_a | H' | \psi_a \rangle + c_b e^{-\frac{i}{\hbar}E_b t} \langle \psi_a | H' | \psi_b \rangle$$

$$= i\hbar\, \dot{c}_a e^{-\frac{i}{\hbar}E_a t}$$

DEFINE

$$\boxed{H'_{ab} \equiv \langle \psi_a | H' | \psi_b \rangle}$$

$$H'^{\dagger} = H' \qquad \text{(HERMITIAN)}$$

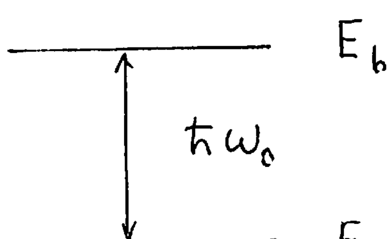
$$H'_{ba} = \left(H'_{ab} \right)^*$$

$$\boxed{\dot{c}_a = -\frac{i}{\hbar} \left[c_a H'_{aa} + c_b e^{-\frac{i}{\hbar}(E_b - E_a)t} H'_{ab} \right]}$$

ANALOGOUSLY

$$\boxed{\dot{c}_b = -\frac{i}{\hbar} \left[c_b H'_{bb} + c_a e^{-\frac{i}{\hbar}(E_a - E_b)t} H'_{ba} \right]}$$

- IMPORTANT SPECIAL CASE : $H'_{aa} = H'_{bb} = 0$



$$\hbar \omega_0 \equiv E_b - E_a$$

$$(E_b > E_a)$$

$$\boxed{\begin{aligned} \dot{c}_a &= -\frac{i}{\hbar} c_b e^{-i\omega_0 t} H'_{ab} \\ \dot{c}_b &= -\frac{i}{\hbar} c_a e^{+i\omega_0 t} H'_{ba} \end{aligned}}$$

• PERTURBATION THEORY

H' SMALL

↳ SUPPOSE AT $t=0$ SYSTEM IS IN STATE a

$$c_a(t=0) = 1$$
$$c_b(t=0) = 0$$

↳ ZERO ORDER : $H' = 0$

$$c_a^{(0)}(t) = 1$$
$$c_b^{(0)}(t) = 0$$

↳ FIRST ORDER

$$\dot{c}_a^{(1)} = 0 \quad \Rightarrow \quad c_a^{(1)}(t) = 1$$

$$\dot{c}_b^{(1)} = -\frac{i}{\hbar}\, c_a^{(0)}\, e^{i\omega_0 t}\, H'_{ba}(t)$$

$$\downarrow$$

$$c_b^{(1)}(t) = -\frac{i}{\hbar}\int_0^t dt'\, c_a^{(0)}(t')\, e^{i\omega_0 t'}\, H'_{ba}(t')$$

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

↳ SECOND ORDER

$$\dot{c}_a^{(2)} = -\frac{i}{\hbar}\, c_b^{(1)}\, e^{-i\omega_0 t}\, H'_{ab}(t)$$

$$c_a^{(2)}(t) - \underbrace{c_a^{(2)}(0)}_{1} = -\frac{i}{\hbar}\int_0^t dt'\, c_b^{(1)}(t')\, e^{-i\omega_0 t'}\, H'_{ab}(t')$$

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

$$c_b^{(2)}(t) = c_b^{(1)}(t)$$

⋮

ITERATIVE PROCEDURE

↳ NORMALIZATION

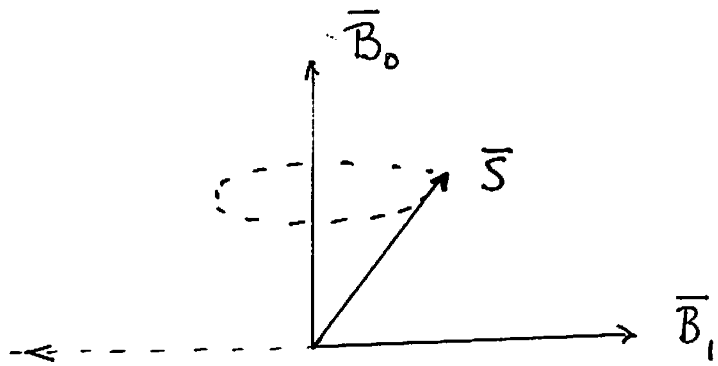
$$|c_a(t)|^2 + |c_b(t)|^2 = 1$$

WILL BE APPROXIMATE
TO THE GIVEN ORDER IN H'

$$\underbrace{|c_a^{(1)}(t)|^2}_{1} + \underbrace{|c_b^{(1)}(t)|^2}_{O(H'^2)} \cong 1 + O(H'^2)$$

• SINUSOIDAL PERTURBATION

↳

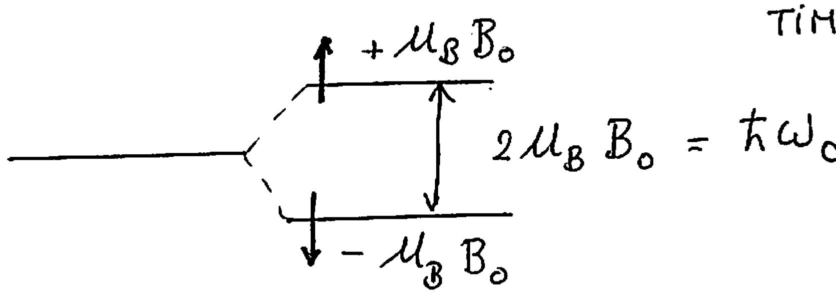


$$\bar{B} = B_0\,\hat{e}_z + B_1 \sin\omega t\;\hat{e}_x$$

$$H^0 = +\frac{e\hbar}{2m} B_0\,\sigma_z = \mu_B B_0\,\sigma_z$$

$$H' = \frac{e\hbar}{2m} B_1 \sin\omega t\;\sigma_x = \underbrace{\mu_B B_1\,\sigma_x}_{\hat{V}} \sin\omega t$$

$\Uparrow$ TIME INDEPENDENT



↳ $$H'_{ab} = \langle \psi_a | \hat{V} | \psi_b \rangle \sin\omega t$$

FOR $\hat{V} = \mu_B B_1 \sigma_x$

$$\langle \uparrow | \hat{V} | \uparrow \rangle = 0$$

$$\langle \downarrow | \hat{V} | \downarrow \rangle = 0$$

$$V_{\uparrow\downarrow} \equiv \langle \uparrow | \hat{V} | \downarrow \rangle = \langle \downarrow | \hat{V} | \uparrow \rangle = \mu_B B_1$$

$\hookrightarrow$ 1° ORDER

$$|\psi_a\rangle = |\downarrow\rangle : \; c_{\downarrow}^{(1)}(t) = 1$$

$$|\psi_b\rangle = |\uparrow\rangle : \; c_{\uparrow}^{(1)}(t) = -\frac{i}{\hbar} \int_0^t dt' \, e^{i\omega_0 t'} \, V_{ba} \sin \omega t'$$

$$= -\frac{i V_{ba}}{\hbar} \frac{1}{2i} \int_0^t dt' \left[e^{i(\omega_0+\omega)t'} - e^{i(\omega_0-\omega)t'} \right]$$

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

$\Downarrow$ FOR DRIVING FREQUENCIES

$$\omega \simeq \omega_0$$

$\uparrow$

CLOSE TO TRANSITION FREQ. ω_0

$$\omega_0 + \omega \gg |\omega_0 - \omega|$$

$$c_{\uparrow}^{(1)}(t) = +\frac{V_{\uparrow\downarrow}}{2i\hbar} \frac{e^{i(\omega_0-\omega)t} - 1}{(\omega_0 - \omega)}$$

$$= \frac{V_{\uparrow\downarrow}}{2i\hbar} \frac{e^{i(\omega_0-\omega)t/2}}{\omega_0 - \omega} \left[e^{i(\omega_0-\omega)t/2} - e^{-i(\omega_0-\omega)t/2} \right]$$

$$c_{\uparrow}^{(1)}(t) = \frac{V_{\uparrow\downarrow}}{\hbar} \frac{\sin\left[(\omega_0-\omega)t/2\right]}{(\omega_0-\omega)} e^{i(\omega_0-\omega)t/2}$$

↳ TRANSITION PROBABILITY $\downarrow \rightarrow \uparrow$ (SPIN FLIP)

$$\boxed{\begin{aligned} P_{\downarrow\rightarrow\uparrow}(t) &= \left| c_{\uparrow}^{(1)}(t) \right|^2 \\ &\simeq \frac{|V_{\uparrow\downarrow}|^2}{\hbar^2} \frac{\sin^2\left[(\omega_0-\omega)t/2\right]}{(\omega_0-\omega)^2} \end{aligned}}$$

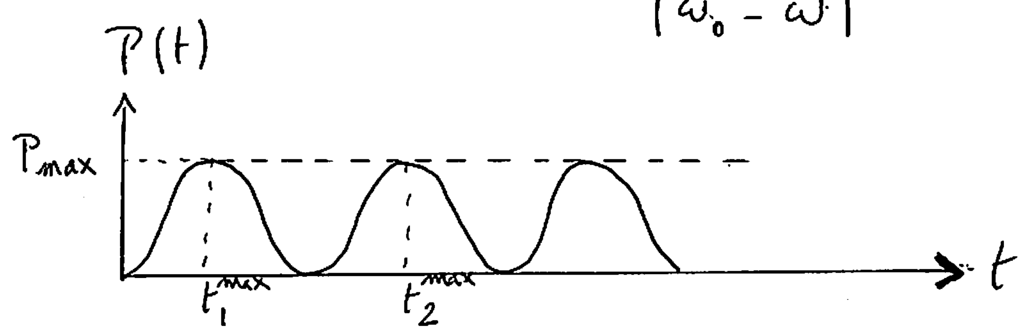
PROBABILITY OF SPIN FLIP AT TIME t

$P_{\downarrow\rightarrow\uparrow}(0) = 0$

$P_{\downarrow\rightarrow\uparrow}$ RISES TO MAX. $\dfrac{|V_{\uparrow\downarrow}|^2}{\hbar^2(\omega_0-\omega)^2} = \dfrac{(\mu_B B_1)^2}{\hbar^2(\omega_0-\omega)^2}$

$\hbar\omega_0 = 2\mu_B B_0$

AT TIMES $t_n^{max} = \dfrac{(2n+1)\pi}{|\omega_0-\omega|}$



↳ AT A TIME t

VARY ω

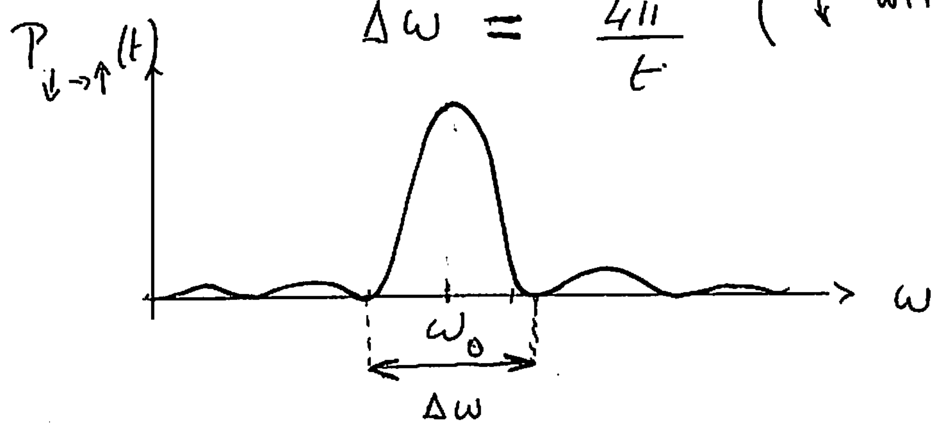
FOR $\omega \simeq \omega_0$

$$\sin^2\left[(\omega_0 - \omega)\, t/2\right] \simeq (\omega_0 - \omega)^2 \frac{t^2}{4}$$

$$P_{\downarrow\to\uparrow}(t) \simeq \left(\frac{|V_{\uparrow\downarrow}|\ t}{2\hbar}\right)^2 \quad \text{HEIGHT } (\nearrow \text{ WITH } t)$$

$$\text{WIDTH} \quad \frac{\Delta\omega\, t}{2} = (2\pi)$$

$$\Delta\omega = \frac{4\pi}{t} \quad (\downarrow \text{ WITH } t)$$



RESONANCE WHEN $\omega \to \omega_0$

CAVEAT : IF $P_{\downarrow\to\uparrow}(t) \nearrow$ AT SOME POINT P.T. BREAKS DOWN

$\downarrow$

EXACT SOLUTION $P_{\downarrow\to\uparrow}(t) \leq 1$ EVIDENTLY!

• EXACT SOLUTION : ROTATING WAVE METHOD

↳ $H' = \hat{V} \sin \omega t$

$$= \hat{V} \frac{1}{2i} \left(e^{i\omega t} - e^{-i\omega t} \right)$$

↳ RABI'S METHOD

$$c_b(t) = -\frac{V_{ba}}{2\hbar} \left\{ \underbrace{\frac{e^{i(\omega_0+\omega)t} - 1}{i(\omega_0+\omega)}}_{\text{FROM } e^{i\omega t} \text{ PART IN } H'} - \underbrace{\frac{e^{i(\omega_0-\omega)t} - 1}{i(\omega_0-\omega)}}_{\text{FROM } e^{-i\omega t} \text{ PART IN } H'} \right\}$$

FOR $\omega \simeq \omega_0$ KEEP ONLY 2° TERM

$$\boxed{H' = \hat{V} \left(\frac{i}{2} \right) e^{-i\omega t}}$$

ROTATING WAVE

↳ WITH THIS H', WE CAN SOLVE PROBLEM EXACTLY, WITHOUT USING PT

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

$$H'_{ba} = V_{ba} \frac{i}{2} e^{-i\omega t}$$

$$H'_{ab} = H'^{*}_{ba} = V^{*}_{ab} \left(-\frac{i}{2} \right) e^{+i\omega t}$$

↳ GENERAL SOLUTION FOR $H' = \hat{V}\left(\frac{i}{2}\right) e^{-i\omega t}$

$$\begin{cases} \dot{c}_a = -\frac{i}{\hbar} c_b \, e^{-i\omega_0 t} H'_{ab} \\ \dot{c}_b = -\frac{i}{\hbar} c_a \, e^{+i\omega_0 t} H'_{ba} \end{cases}$$

$$\Downarrow$$

$$\begin{cases} \dot{c}_a = -\frac{1}{2\hbar} V^*_{ab} \, e^{i(\omega-\omega_0)t} c_b \\ \dot{c}_b = +\frac{1}{2\hbar} V_{ba} \, e^{-i(\omega-\omega_0)t} c_a \end{cases}$$

$$\ddot{c}_b = \frac{1}{2\hbar} V_{ba} \, e^{-i(\omega-\omega_0)t} \left[-i(\omega-\omega_0) c_a + \dot{c}_a \right]$$

$$= -i(\omega-\omega_0)\dot{c}_b - \frac{1}{(2\hbar)^2} |V_{ab}|^2 c_b$$

$$\boxed{\ddot{c}_b + i(\omega-\omega_0)\dot{c}_b + \frac{1}{(2\hbar)^2}|V_{ab}|^2 c_b = 0}$$

TRY $\quad c_b \sim e^{i\lambda t}$

$$-\lambda^2 - (\omega-\omega_0)\lambda + \frac{1}{(2\hbar)^2}|V_{ab}|^2 = 0$$

$$\lambda^2 + (\omega - \omega_0)\lambda - \frac{1}{(2\hbar)^2}|V_{ab}|^2 = 0$$

$$\lambda = -\frac{(\omega - \omega_0)}{2} \pm \frac{1}{2}\sqrt{(\omega-\omega_0)^2 + \frac{|V_{ab}|^2}{\hbar^2}}$$

$$\boxed{\omega_R \equiv \frac{1}{2}\sqrt{(\omega-\omega_0)^2 + \frac{|V_{ab}|^2}{\hbar^2}}}$$

$\Uparrow$

RABI FLOPPING FREQUENCY

$$\therefore \quad c_b(t) = A\, e^{i\left[-\frac{(\omega-\omega_0)}{2} + \omega_R\right]t} + B\, e^{i\left[-\frac{(\omega-\omega_0)}{2} - \omega_R\right]t}$$

$$= e^{-i\frac{(\omega-\omega_0)}{2}t}\left[A\, e^{i\omega_R t} + B\, e^{-i\omega_R t}\right]$$

OR EQUIVALENTLY

$$c_b(t) = e^{-i\frac{(\omega-\omega_0)}{2}t}\left[C\cos\omega_R t + D\sin\omega_R t\right]$$

$$\rightsquigarrow \quad c_b(t=0) = 0 \quad \Rightarrow \quad C = 0$$

$$\| \quad c_b(t) = D\, e^{-i\frac{(\omega-\omega_0)}{2}t} \sin\omega_R t$$

$$\rightsquigarrow \quad c_a(t) = \frac{2\hbar}{V_{ba}} \dot{c}_b \, e^{+i(\omega-\omega_0)t}$$

$$= \frac{2\hbar}{V_{ba}} D \left[-\frac{i(\omega-\omega_0)}{2} \sin\omega_R t + \omega_R \cos\omega_R t \right] \cdot e^{\frac{i(\omega-\omega_0)t}{2}}$$

$$c_a(t=0) = 1 \quad \Rightarrow \quad \frac{2\hbar}{V_{ba}} D \, \omega_R = 1$$

$$D = \frac{V_{ba}}{2\hbar\omega_R}$$

$$\rightsquigarrow \quad \boxed{\begin{aligned} c_a(t) &= e^{\frac{i(\omega-\omega_0)t}{2}} \left[\cos\omega_R t - i \frac{(\omega-\omega_0)}{2\omega_R} \sin\omega_R t \right] \\ c_b(t) &= \frac{V_{ba}}{2\hbar\omega_R} e^{-\frac{i(\omega-\omega_0)t}{2}} \sin\omega_R t \end{aligned}}$$

THESE EXPRESSIONS ARE EXACT FOR $\omega \simeq \omega_0$

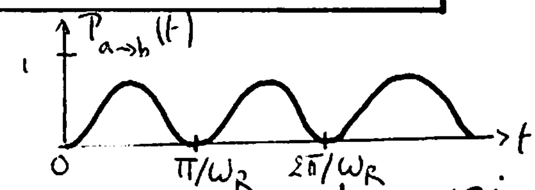
IN CONTRAST TO P.T. RESULTS

<u>CHECK</u> : $|c_a(t)|^2 + |c_b(t)|^2 = 1$ (EXACT !)

↳ PROBABILITY FOR TRANSITION $a \to b$

$$\boxed{P_{a\to b}(t) = |c_b(t)|^2 = \frac{|V_{ba}|^2}{(2\hbar\omega_R)^2} \cdot \sin^2 \omega_R t}$$

↳ EXACT RESULT $\omega \simeq \omega_0$



↳ RABI OSCILLATIONS

⇝ COMPARE WITH P.T. RESULT

$$P^{PT}_{a\to b}(t) = \frac{|V_{ba}|^2}{(\hbar(\omega-\omega_0))^2} \cdot \sin^2\left[\frac{(\omega-\omega_0)t}{2}\right]$$

PT RESULT IS OBTAINED FOR

$$|V_{ab}| \ll \hbar(\omega - \omega_0)$$

⇝ PT DOES NOT HOLD VERY CLOSE TO RESONANCE ($\omega = \omega_0$)

$$\Downarrow$$

$$\omega_R = \frac{1}{2}(\omega - \omega_0)$$

⇝ EXACT RESULT

MAX. FOR $\omega_R t = (2n+1)\frac{\pi}{2}$

$$t = \frac{(2n+1)\pi}{2\omega_R}$$

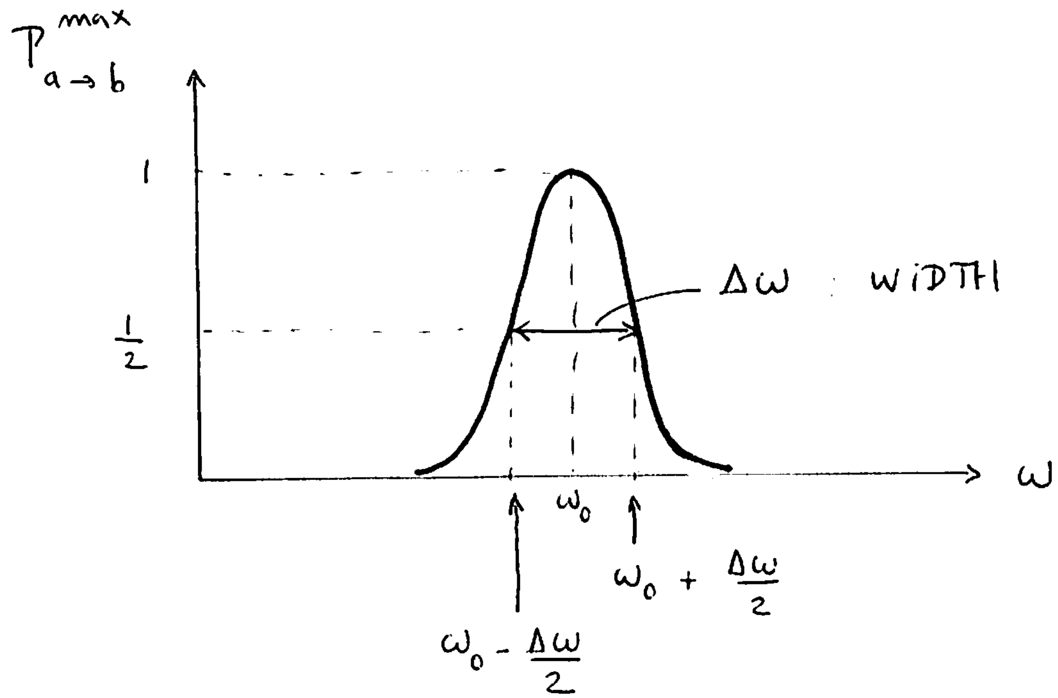
MAX PROBABILITY $P^{max}_{a\to b} = \dfrac{|V_{ba}|^2}{(2\hbar\omega_R)^2}$

WHEN $\omega = \omega_0 \Rightarrow \omega_R = \dfrac{|V_{ab}|}{2\hbar} \Rightarrow P^{max}_{a\to b} = 1$

$$P^{max}_{a \to b} = \frac{|V_{ba}|^2/\hbar^2}{(\omega-\omega_0)^2 + |V_{ba}|^2/\hbar^2}$$

$\downarrow$

RESONANCE FOR $\omega = \omega_0$

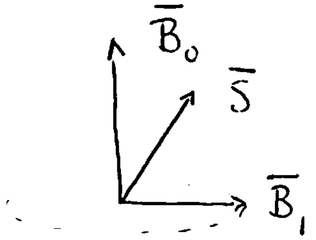


$$\frac{\Delta\omega}{2} = \frac{|V_{ba}|}{\hbar}$$

$\Delta\omega$ ALSO CALLED <u>F</u>ULL <u>W</u>IDTH AT <u>H</u>ALF <u>M</u>AXIMUM

FOR $\omega = \omega_0 \pm \frac{\Delta\omega}{2} \Rightarrow P^{max}_{a \to b} = \frac{1}{2}$

- <u>APPLICATION</u> : NUCLEAR MAGNETIC RESONANCE (NMR)



$$\omega_0 = \underset{\uparrow \text{ PROTON MASS}}{\frac{e}{2M_p}} \; \underset{\overset{\|}{5.59}}{g_p} \; B_0$$

FOR $B_0 = 1\,T \Rightarrow \frac{\omega_0}{2\pi} = 4.3 \; 10^7 \, Hz$

RESONANCE FREQUENCY OBTAINED FOR RF (RADIO FREQ.) B_1 FIELD