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

↳ $c_a(t)$, $c_b(t)$?

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

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

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

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

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

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

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

$$\Downarrow$$

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

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

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

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

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

DEFINE :

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

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

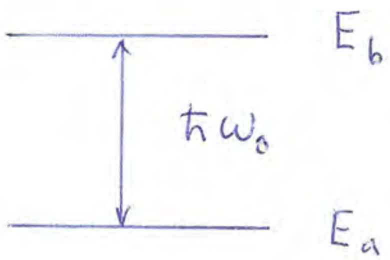
$$H'_{ba} = \left(H'_{ab}\right)^*$$

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

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

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

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

↓

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

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

↳ 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

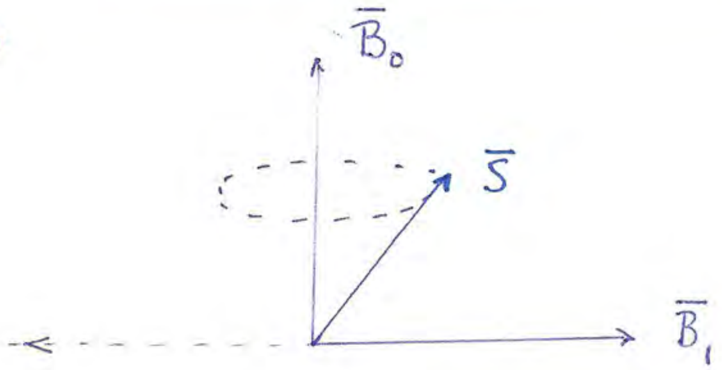
$$|c_a(t)|^2 + |c_b(t)|^2 = 1$$

↑ WILL BE APPROXIMATE TO THE GIVEN ORDER IN H'

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

SINUSOIDAL PERTURBATION

↳

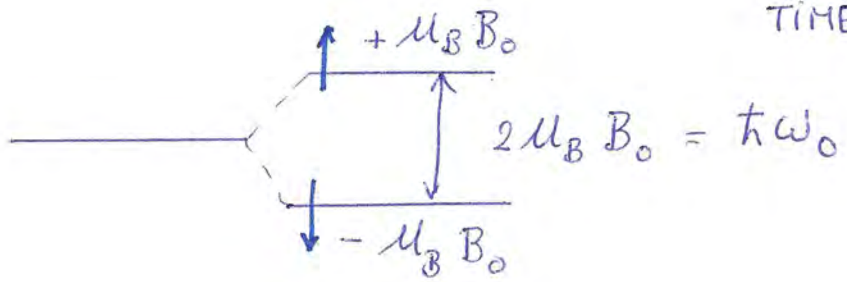


$$\overline{B} = B_0 \hat{e}_z + B_1 \sin \omega t \; \hat{e}_x$$

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

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

$\Uparrow$ TIME INDEPENDENT



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

FOR $\hat{V} = \mu_B B_1 \sigma_x$ $\qquad \langle \uparrow | \hat{V} | \uparrow \rangle = 0$

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

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

↳ 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

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

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

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

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

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

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

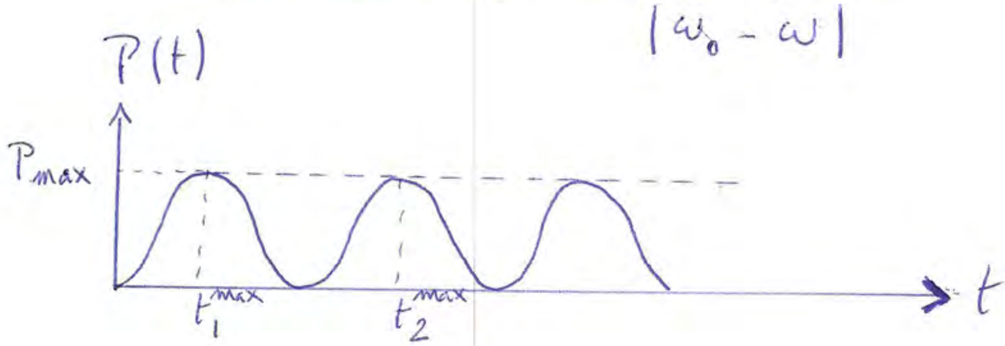
PROBABILITY OF SPIN FLIP AT TIME t

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

$P_{\downarrow\rightarrow\uparrow}$ 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

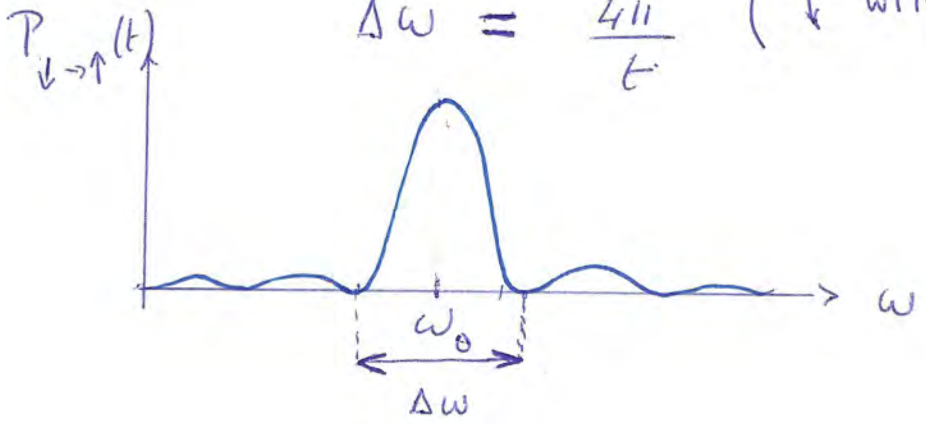
FOR $\omega \simeq \omega_0$

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

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

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

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



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 <u>EXACTLY</u>, <u>WITHOUT</u> 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 $\quad c_b \sim e^{i\lambda t}$

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

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

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

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

RABI FLOPPING FREQUENCY

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

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

OR EQUIVALENTLY

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

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

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

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

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

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

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

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

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

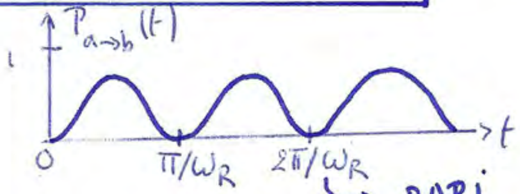
IN CONTRAST TO P.T. RESULTS

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

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

PT RESULT IS OBTAINED FOR

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

$$\Downarrow$$

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

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

⇝ EXACT RESULT

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

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

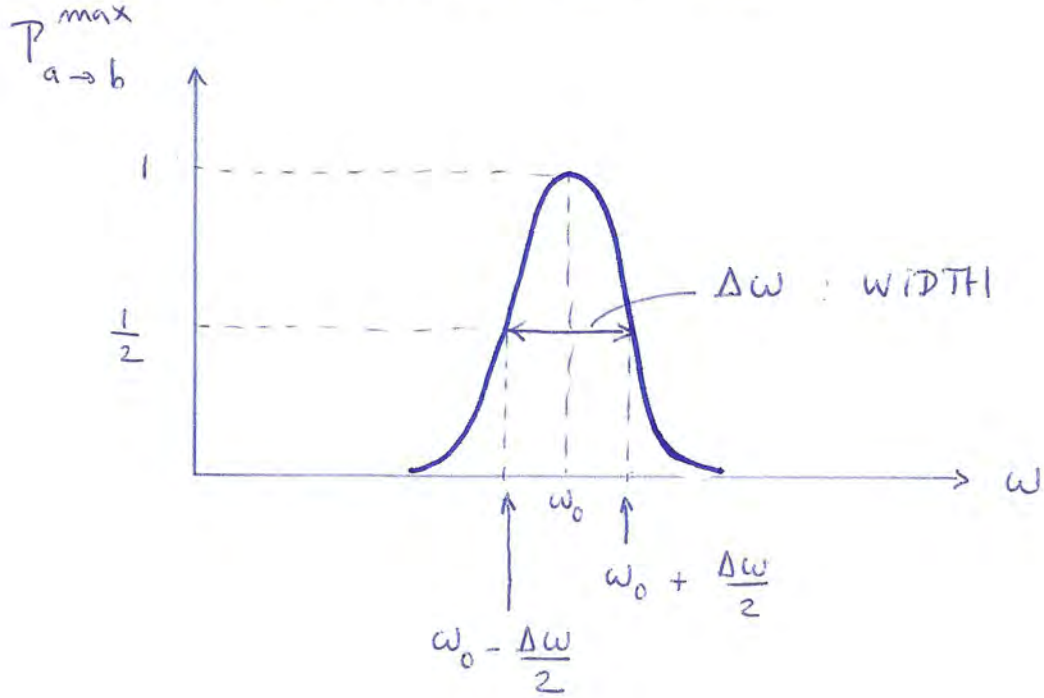
MAX PROBABILITY $P^{max}_{a\to b} = \dfrac{|V_{ba}|^2}{(2\hbar\omega_R)^2}$

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

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

$\downarrow$

RESONANCE FOR $\omega = \omega_0$

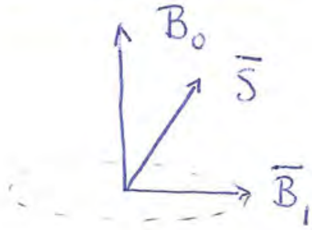


$$\frac{\Delta\omega}{2} = \frac{|V_{ba}|}{\hbar}$$

$\Delta\omega$ ALSO CALLED FULL WIDTH AT HALF MAXIMUM

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

- **APPLICATION** : NUCLEAR MAGNETIC RESONANCE (NMR)



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

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

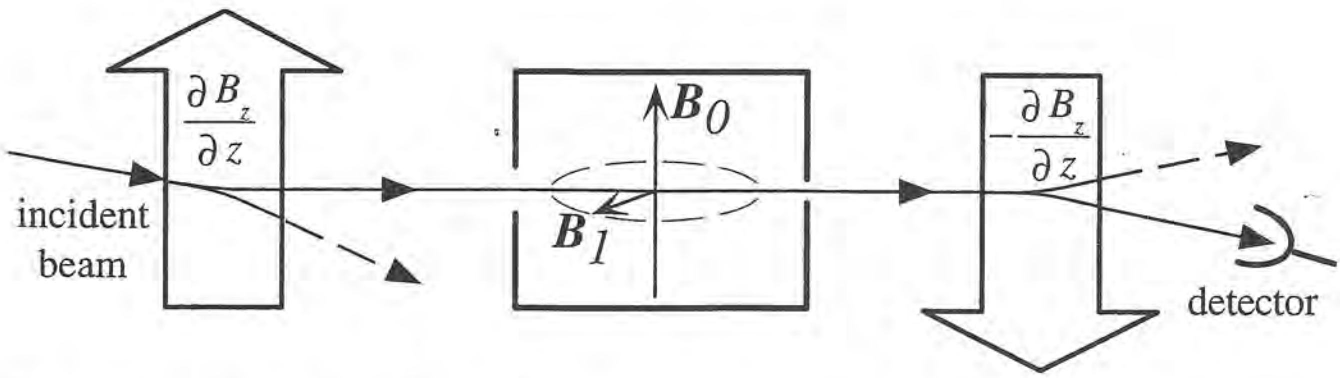


Fig. 12.3. Apparatus developed by Rabi for observing the magnetic resonance effect. In the absence of magnetic resonance, all particles emitted in the state $|+\rangle$ reach the detector. If the resonance occurs, the spins of the particles flip between the two magnets and the signal drops

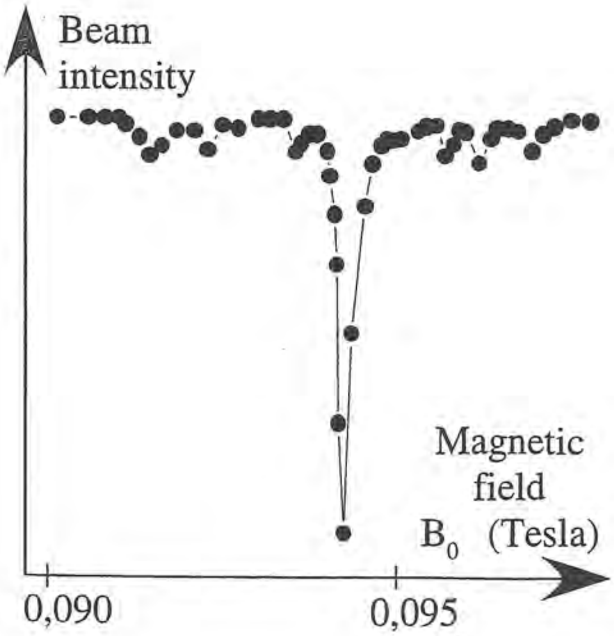


Fig. 12.4. Signal (obtained by Rabi) recorded on the detector of Fig. 12.3 with a beam of HD molecules, as a function of the field B_0 ($B_1 = 10^{-4}\,\mathrm{T}, \omega/2\pi = 4\,\mathrm{MHz}$)