



UNIVERSITY OF  
CAMBRIDGE

NST Part II Physics  
Michaelmas Term 2022  
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# ADVANCED QUANTUM PHYSICS

## Handout 9

- 
- ▶ Transitions
  - ▶ Time-dependent perturbation theory
  - ▶ Scattering

# *Transitions*

- So far, we have considered systems described by Hamiltonians  $H$  with no explicit time dependence
  - ⇒ if the system is initially in an energy eigenstate, it remains in that eigenstate at all times (stationary state)
- Now consider systems with an applied *time-dependent* perturbation :
$$\hat{H}(t) = \hat{H}_0 + \hat{H}'(t)$$
(e.g. an atom in a time-varying electromagnetic field)
  - the perturbation can induce ***transitions*** between eigenstates
- We first consider an unperturbed system with just two eigenstates; then consider the general case

# Transitions in Two-State Systems

- Consider an unperturbed system described by a Hamiltonian  $H_0$  with exactly two eigenstates, assumed to be known :

$$\hat{H}_0|\psi_1\rangle = E_1|\psi_1\rangle ; \quad \hat{H}_0|\psi_2\rangle = E_2|\psi_2\rangle$$

- Apply a *time-dependent* harmonic perturbation of driving frequency  $\omega$  :

$$\hat{H} = \hat{H}_0 + \hat{H}'(t) ; \quad \hat{H}'(t) = \hat{H}' \cos \omega t$$

- Without the perturbation  $H'(t)$ , the state of the system evolves as

$$|\psi(t)\rangle = c_1 e^{-i\omega_1 t} |\psi_1\rangle + c_2 e^{-i\omega_2 t} |\psi_2\rangle$$

where

$$E_1 \equiv \hbar\omega_1 ; \quad E_2 \equiv \hbar\omega_2$$

and where  $c_1$  and  $c_2$  are constants determined by the initial state of the system :

$$|\psi(0)\rangle = c_1 |\psi_1\rangle + c_2 |\psi_2\rangle$$

## Two-state transitions (2)

- This suggests that, when the perturbation  $H'(t)$  is switched on, we look for solutions where  $c_1$  and  $c_2$  can evolve with time :

$$|\psi(t)\rangle = c_1(t)e^{-i\omega_1 t}|\psi_1\rangle + c_2(t)e^{-i\omega_2 t}|\psi_2\rangle$$

- The state  $|\psi(t)\rangle$  must satisfy the time-dependent Schrödinger equation

$$(\hat{H}_0 + \hat{H}' \cos \omega t)|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle$$

Hence

$$\begin{aligned} (\hat{H}_0 + \hat{H}' \cos \omega t) [c_1(t)e^{-i\omega_1 t}|\psi_1\rangle + c_2(t)e^{-i\omega_2 t}|\psi_2\rangle] \\ = i\hbar \frac{\partial}{\partial t} [c_1(t)e^{-i\omega_1 t}|\psi_1\rangle + c_2(t)e^{-i\omega_2 t}|\psi_2\rangle] \end{aligned}$$

- Expanding out, and cancelling the  $H_0$  terms then gives

$$\begin{aligned} \hat{H}' \cos \omega t [c_1(t)e^{-i\omega_1 t}|\psi_1\rangle + c_2(t)e^{-i\omega_2 t}|\psi_2\rangle] & \\ = i\hbar \frac{dc_1(t)}{dt} e^{-i\omega_1 t}|\psi_1\rangle + i\hbar \frac{dc_2(t)}{dt} e^{-i\omega_2 t}|\psi_2\rangle & \end{aligned} \tag{9.4.1}$$

## Two-state transitions (3)

- Take the inner product of equation (9.4.1) with  $\langle \psi_1 |$  and  $\langle \psi_2 |$  in turn, and use

$$\langle \psi_1 | \psi_2 \rangle = 0$$

This gives a pair of coupled first-order differential equations for the time-dependent coefficients  $c_1(t)$  and  $c_2(t)$  :

$$\begin{aligned} [H'_{11}c_1(t)e^{-i\omega_1 t} + H'_{12}c_2(t)e^{-i\omega_2 t}] \cos \omega t &= i\hbar \frac{dc_1(t)}{dt} e^{-i\omega_1 t} \\ [H'_{21}c_1(t)e^{-i\omega_1 t} + H'_{22}c_2(t)e^{-i\omega_2 t}] \cos \omega t &= i\hbar \frac{dc_2(t)}{dt} e^{-i\omega_2 t} \end{aligned} \tag{9.5.1}$$

Here, the matrix elements of  $H'$  in the basis  $|\psi_1\rangle$ ,  $|\psi_2\rangle$  have been written as

$$H'_{11} \equiv \langle \psi_1 | \hat{H}' | \psi_1 \rangle , \quad H'_{22} \equiv \langle \psi_2 | \hat{H}' | \psi_2 \rangle$$

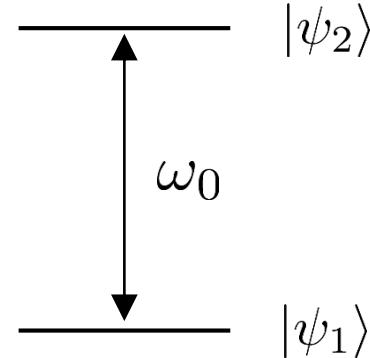
$$H'_{12} \equiv \langle \psi_1 | \hat{H}' | \psi_2 \rangle , \quad H'_{21} \equiv \langle \psi_2 | \hat{H}' | \psi_1 \rangle = (H'_{12})^*$$

## Two-state transitions (4)

- Now choose  $E_2 > E_1$ , and define the frequency difference  $\omega_0$  as

$$\boxed{\omega_0 \equiv \omega_2 - \omega_1}$$

$$(\omega_0 > 0)$$



- Setting  $\cos \omega t = \frac{1}{2} (e^{i\omega t} + e^{-i\omega t})$ , equations (9.5.1) can then be written as

$$i\hbar \frac{dc_1(t)}{dt} = \frac{H'_{11}}{2} c_1(t) [e^{i\omega t} + e^{-i\omega t}] + \frac{H'_{12}}{2} c_2(t) [e^{i(\omega-\omega_0)t} + e^{-i(\omega+\omega_0)t}]$$

$$i\hbar \frac{dc_2(t)}{dt} = \frac{H'_{22}}{2} c_2(t) [e^{i\omega t} + e^{-i\omega t}] + \frac{H'_{21}}{2} c_1(t) [e^{i(\omega+\omega_0)t} + e^{-i(\omega-\omega_0)t}]$$

Thus far, the analysis has been *exact* ...

# Resonant Transitions

- Suppose the driving frequency  $\omega$  is close to the frequency difference  $\omega_0$  :

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

The terms containing  $e^{\pm i\omega t}$ ,  $e^{\pm i(\omega+\omega_0)t}$  then oscillate rapidly compared to those containing  $e^{\pm i(\omega-\omega_0)t}$

- In the *rotating wave approximation* (RWA), the rapidly oscillating terms are neglected (they average to zero over even short time intervals), leaving

$$i\hbar \frac{dc_1(t)}{dt} = \frac{H'_{12}}{2} c_2(t) e^{i(\omega-\omega_0)t}; \quad i\hbar \frac{dc_2(t)}{dt} = \frac{H'_{21}}{2} c_1(t) e^{-i(\omega-\omega_0)t}$$

- Defining the (complex) constant  $\omega'$  by setting

$$H'_{12} = \langle \psi_1 | \hat{H}' | \psi_2 \rangle \equiv \hbar\omega'$$

(9.7.1)

these equations can be written

$$i \frac{dc_1(t)}{dt} = \frac{\omega'}{2} c_2(t) e^{i(\omega-\omega_0)t}; \quad i \frac{dc_2(t)}{dt} = \frac{(\omega')^*}{2} c_1(t) e^{-i(\omega-\omega_0)t}$$

(9.7.2)

## Resonant transitions (2)

- Eliminating  $c_1(t)$  gives a damped SHM equation for  $c_2(t)$  :

$$\frac{d^2c_2(t)}{dt^2} + i(\omega - \omega_0) \frac{dc_2(t)}{dt} + \frac{1}{4}|\omega'|^2 c_2(t) = 0 \quad (9.8.1)$$

- For the case  $\omega = \omega_0$ , where the driving frequency is precisely matched to the transition energy, the general solution to equation (9.8.1) is

$$c_2(t) = A \cos\left(\frac{1}{2}|\omega'|t\right) + B \sin\left(\frac{1}{2}|\omega'|t\right) \quad (9.8.2)$$

- We thus obtain *undamped oscillations* at the *Rabi frequency*,  $|\omega'|/2$  :

$$\boxed{\frac{|\omega'|}{2} = \frac{1}{2\hbar} \langle \psi_1 | \hat{H}' | \psi_2 \rangle}$$

[I. I. Rabi, Phys. Rev. 51 \(1937\) 652](#)

The Rabi frequency,  $|\omega'|/2$ , is determined by the coupling between the two unperturbed eigenstates induced by the perturbation  $H'$   
(weak coupling  $\Rightarrow$  low frequency transitions)

## Resonant transitions (3)

- Suppose the system is initially in the state  $|\psi_1\rangle$  at time  $t = 0$  :

$$c_1(0) = 1, \quad c_2(0) = 0$$

Then equation (9.8.2) gives  $A = 0$ , and hence

$$c_2(t) = B \sin\left(\frac{1}{2}|\omega'|t\right)$$

- Substituting into the rightmost of equations (9.7.2), with  $\omega = \omega_0$ , then gives  $c_1(t)$  as

$$c_1(t) = \frac{2i}{(\omega')^*} \frac{B|\omega'|}{2} \cos\left(\frac{1}{2}|\omega'|t\right)$$

- Setting  $t = 0$  in this equation then determines the coefficient  $B$  as

$$B = -i \frac{(\omega')^*}{|\omega'|}$$

- Hence, for  $\omega = \omega_0$  and  $c_1(0) = 1$ , we obtain the solution

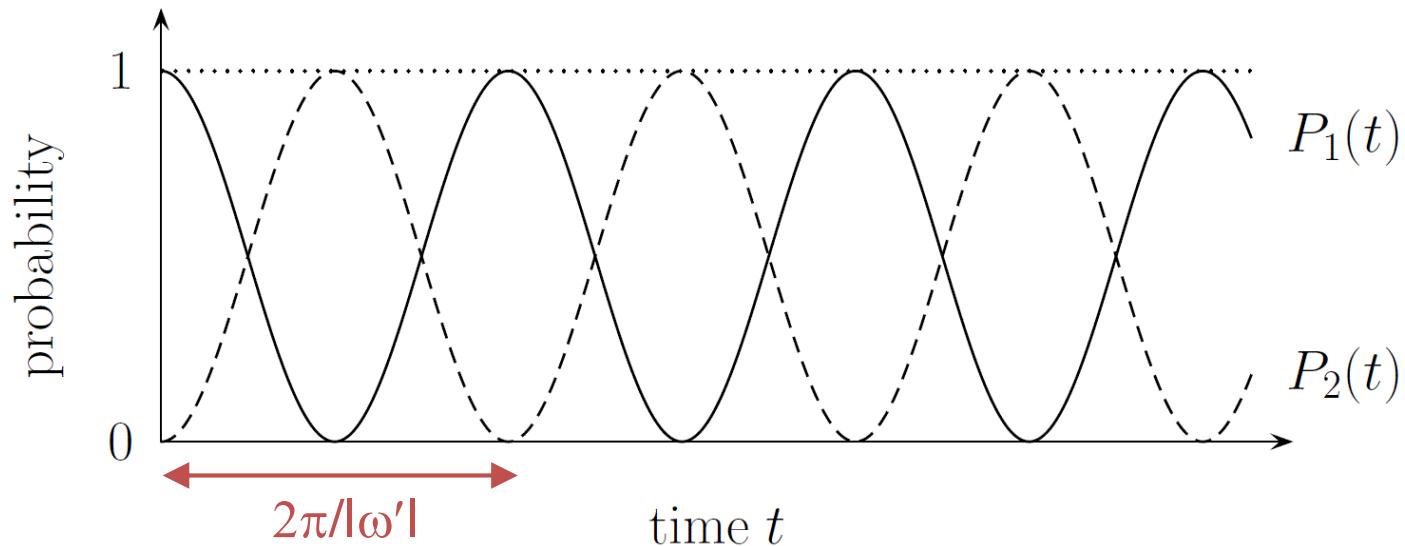
$$c_1(t) = \cos\left(\frac{1}{2}|\omega'|t\right), \quad c_2(t) = -i \frac{(\omega')^*}{|\omega'|} \sin\left(\frac{1}{2}|\omega'|t\right) \quad (9.9.1)$$

## Resonant transitions (4)

- The probabilities that the system is found in the state  $|\psi_1\rangle$ , or in the state  $|\psi_2\rangle$ , at time  $t$  are therefore given by

$$P_1(t) = |c_1(t)|^2 = \cos^2\left(\frac{1}{2}|\omega'|t\right), \quad P_2(t) = |c_2(t)|^2 = \sin^2\left(\frac{1}{2}|\omega'|t\right)$$

Thus, for a driving frequency  $\omega = \omega_0$ , the system oscillates between the states  $|\psi_1\rangle$  and  $|\psi_2\rangle$  at the Rabi frequency  $|\omega'|/2$  :



- $P_2(t)$  is the probability of a *transition* from the state  $|\psi_1\rangle$  at time  $t = 0$  to the state  $|\psi_2\rangle$  at time  $t > 0$

## Resonant transitions (5)

- For a general value of the driving frequency  $\omega$  close to  $\omega_0$ , try a solution to equation (9.8.1) of the form

$$c_2(t) = A e^{i\Omega t}$$

Solving the resulting quadratic equation for  $\Omega$  gives

$$\Omega = \frac{1}{2}(\omega - \omega_0) \pm \frac{1}{2}\sqrt{(\omega - \omega_0)^2 + |\omega'|^2}$$

- Hence the general solution for  $c_2(t)$  is now

$$c_2(t) = \exp\left[\frac{1}{2}i(\omega - \omega_0)t\right] \left[ A \exp\left(\frac{1}{2}i\omega_R t\right) + B \exp\left(-\frac{1}{2}i\omega_R t\right) \right]$$

where

$$\omega_R \equiv \sqrt{(\omega - \omega_0)^2 + |\omega'|^2}$$

- If the system is initially in the state  $|\psi_1\rangle$  at  $t = 0$ , we now have

$$c_1(0) = 1, \quad c_2(0) = 0 \quad \Rightarrow \quad A = -B$$

$$\Rightarrow \quad c_2(t) = 2iA \exp\left[\frac{1}{2}i(\omega - \omega_0)t\right] \sin\left(\frac{1}{2}\omega_R t\right)$$

(9.11.1)

## Resonant transitions (6)

- The coefficient  $c_1(t)$  can then be obtained by rearranging equation (9.7.2) as

$$c_1(t) = e^{i(\omega - \omega_0)t} \frac{2i}{(\omega')^*} \frac{dc_2(t)}{dt}$$

Substituting for  $c_2(t)$  from equation (9.11.1) then gives

$$c_1(t) = -\frac{2A}{(\omega')^*} \exp \left[ \frac{1}{2}i(\omega - \omega_0)t \right] \left[ \omega_R \cos \left( \frac{1}{2}\omega_R t \right) + i(\omega_0 - \omega) \sin \left( \frac{1}{2}\omega_R t \right) \right] \quad (9.12.1)$$

- The initial condition  $c_1(0) = 1$  determines the constant  $A$  as

$$A = -\frac{1}{2} \frac{(\omega')^*}{\omega_R} \quad (9.12.2)$$

Equation (9.11.1) then becomes

$$c_2(t) = -i \frac{(\omega')^*}{\omega_R} \exp \left[ \frac{1}{2}i(\omega - \omega_0)t \right] \sin \left( \frac{1}{2}\omega_R t \right)$$

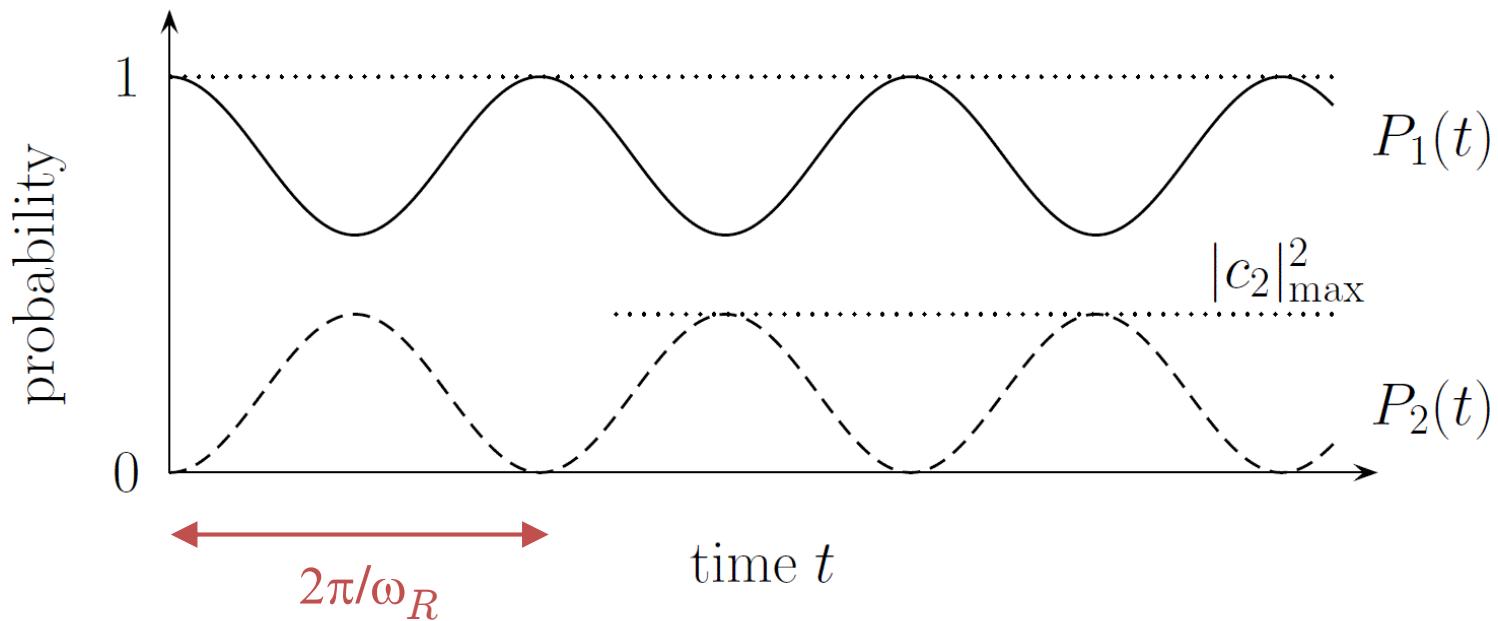
- Hence, for  $\omega \cong \omega_0$ , the probability of a transition to the state  $|\psi_2\rangle$  is

$$P_2(t) = |c_2(t)|^2 = \left( \frac{|\omega'|}{\omega_R} \right)^2 \sin^2 \left( \frac{1}{2}\omega_R t \right) \quad (9.12.3)$$

## Resonant transitions (7)

- From equation (9.12.3), the *maximum* transition probability is now

$$P_{\max}(1 \rightarrow 2) = |c_2|_{\max}^2 = \left( \frac{|\omega'|}{\omega_R} \right)^2 = \frac{|\omega'|^2}{(\omega - \omega_0)^2 + |\omega'|^2}$$



- Hence, if the driving frequency does not exactly match the difference in energy levels :
  - the transition probability is always less than unity
  - the oscillation frequency  $\omega_R$  is larger than  $\omega'$

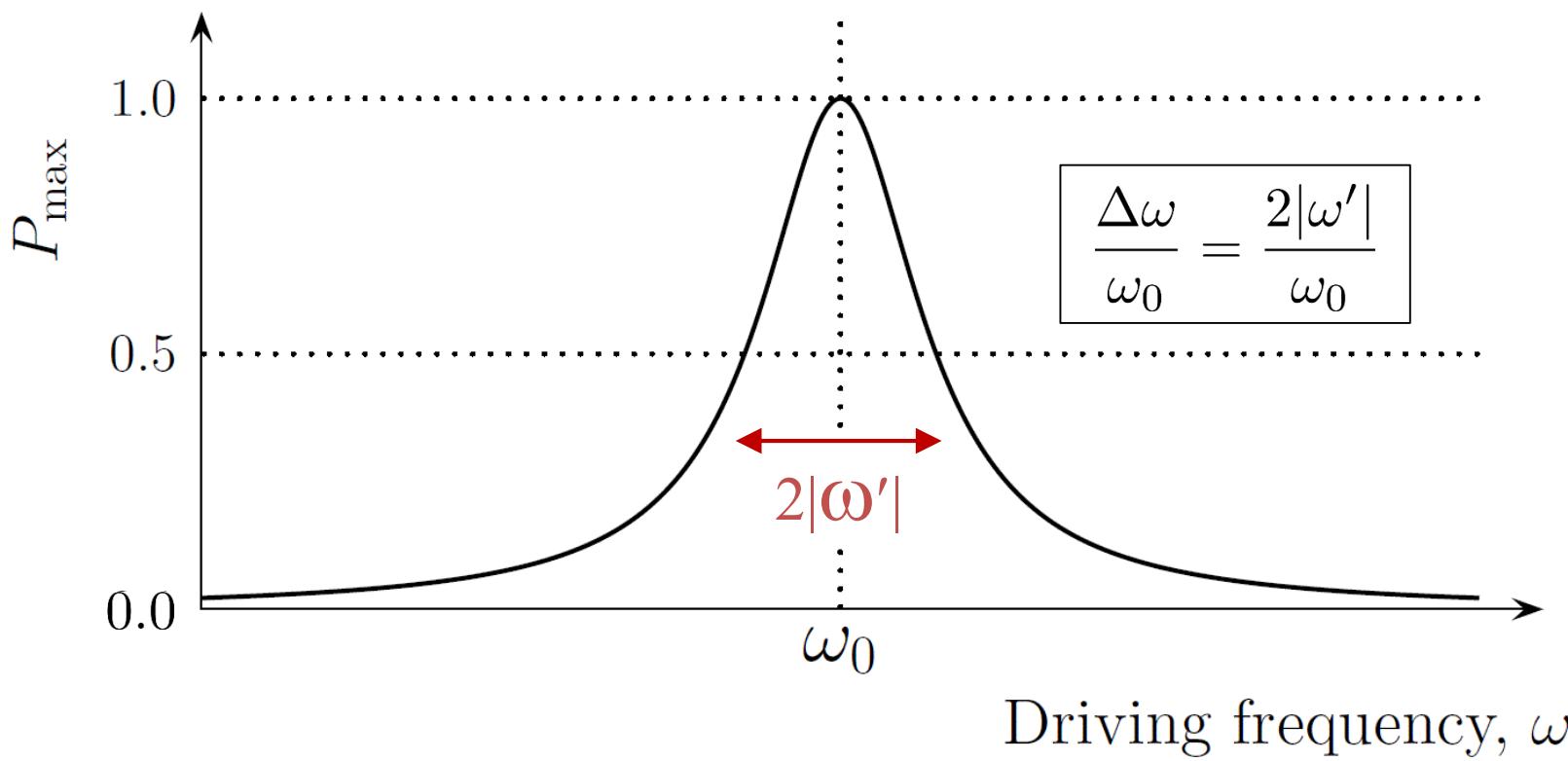
## Resonant transitions (8)

- Scanning the driving frequency  $\omega$  produces a *resonance* in the maximum transition probability

$$P_{\max}(\omega) = \frac{|\omega'|^2}{(\omega - \omega_0)^2 + |\omega'|^2}$$

(9.14.1)

- The (Lorentzian) resonance is centred on  $\omega = \omega_0$ , and has FWHM =  $2|\omega'|$ :



## Resonant transitions (9)

- For completeness, we should also check  $c_1(t)$  :

Substituting equation (9.12.2) into equation (9.12.1) gives  $c_1(t)$  as

$$c_1(t) = \frac{1}{\omega_R} \exp \left[ \frac{1}{2} i(\omega - \omega_0)t \right] \left[ \omega_R \cos \left( \frac{1}{2} \omega_R t \right) + i(\omega_0 - \omega) \sin \left( \frac{1}{2} \omega_R t \right) \right]$$

- The probability that the system is found in the original state  $|\Psi_1\rangle$  is then

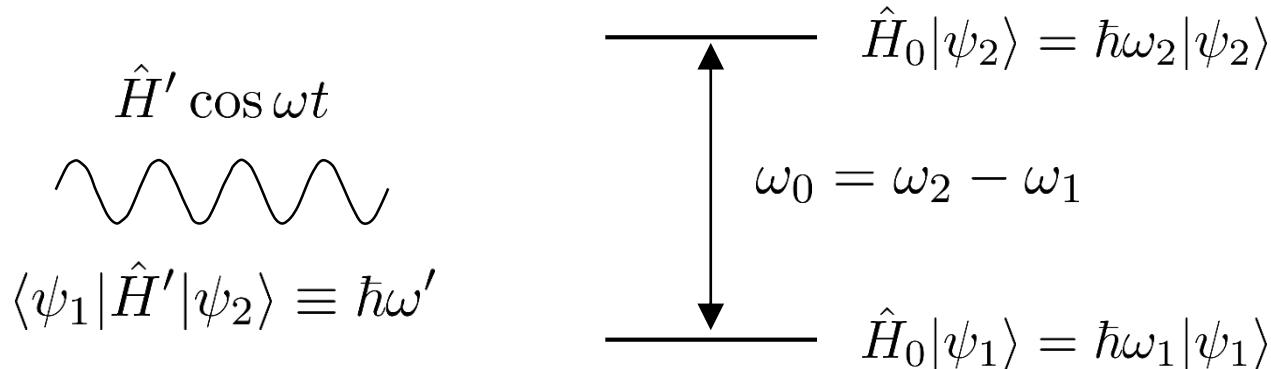
$$\begin{aligned} |c_1(t)|^2 &= \cos^2 \left( \frac{1}{2} \omega_R t \right) + \frac{(\omega_0 - \omega)^2}{\omega_R^2} \sin^2 \left( \frac{1}{2} \omega_R t \right) \\ &= 1 - \left( \frac{|\omega'|}{\omega_R} \right)^2 \sin^2 \left( \frac{1}{2} \omega_R t \right) \end{aligned}$$

- Hence, despite neglecting the rapidly oscillating terms, the probabilities still sum to unity :

$$|c_1(t)|^2 + |c_2(t)|^2 = 1$$

## Resonant transitions : Summary

- In summary, when a two-state system of separation  $\omega_0$  is driven by a perturbation of frequency  $\omega$  :



- For a driving frequency  $\omega$  close to the frequency gap  $\omega_0$  , we obtain  

*resonant transitions*
- The resonance is centred on  $\omega = \omega_0$ , and has a width determined by the coupling  $|\omega'|$  of the perturbation  $H'$  between the two states :

$$\frac{\Delta\omega}{\omega_0} = \frac{2|\omega'|}{\omega_0}$$

$|\omega'| \ll \omega_0 \Rightarrow \text{narrow resonance}$

## Resonant transitions : Examples

- The plots on the following slides show examples of the transition probabilities  $P_2(t)$  and  $P_{\max}(\omega)$  for the cases

- a)  $\omega_0 = 2\pi, \quad \omega' = (0.2)\pi \quad (|\omega'|/\omega_0 = 0.1) \quad \text{"wide"}$
- b)  $\omega_0 = 2\pi, \quad \omega' = (0.02)\pi \quad (|\omega'|/\omega_0 = 0.01) \quad \text{"narrow"}$

The driving frequencies  $\omega$  are chosen to be on, or close to, the peak of the resonance :

$$\begin{array}{lll}\omega = \omega_0 ; & \omega = \omega_0 \pm |\omega'| ; & \omega = \omega_0 \pm 2|\omega'| \\ (\omega_R = \omega') & (\omega_R = \sqrt{2}\omega') & (\omega_R = \sqrt{5}\omega')\end{array}$$

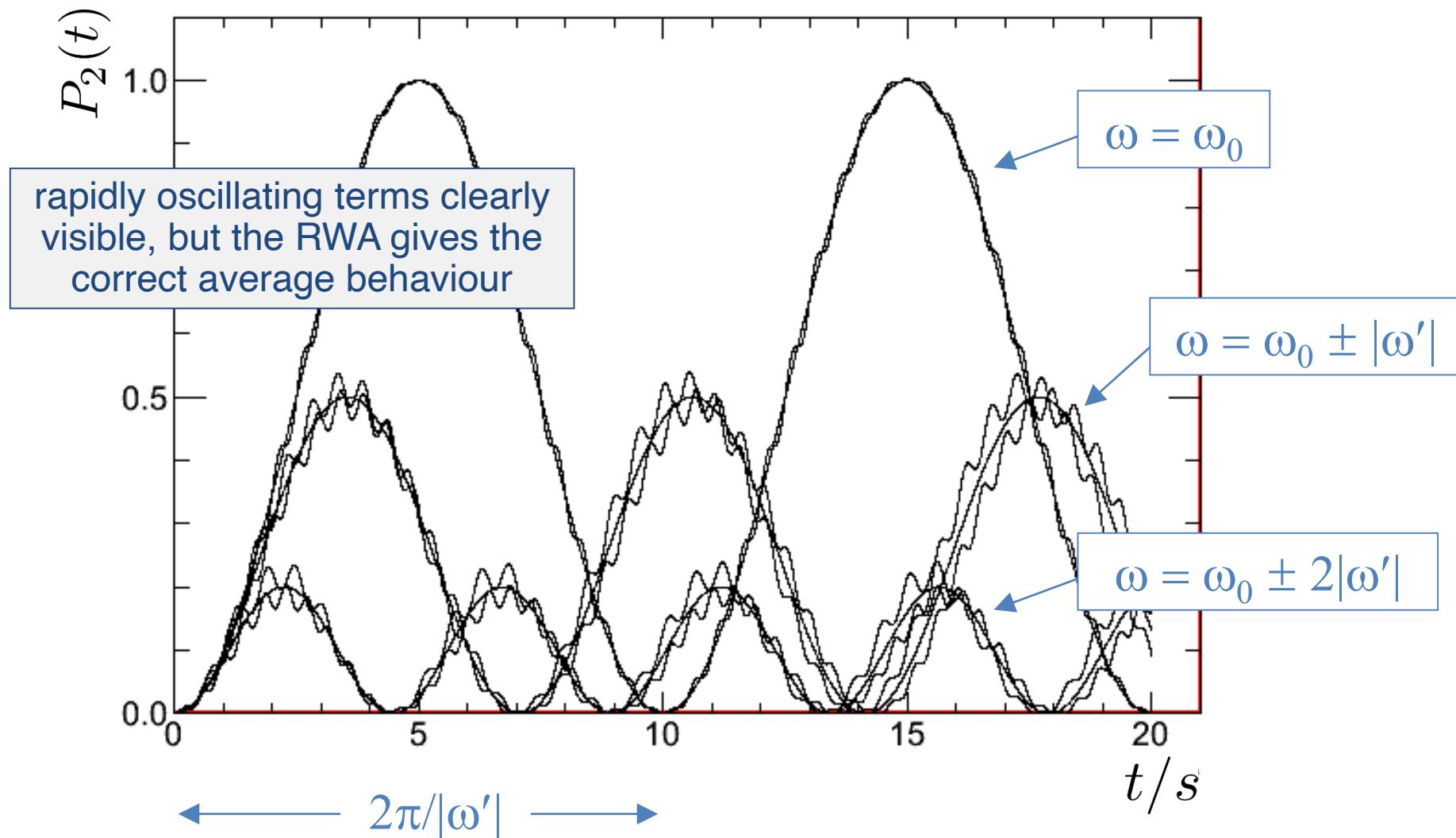
- In each case, we compare :

“exact” : obtained by numerical integration of the exact expressions on slide (9.6) (including any rapidly oscillating terms)

“RWA” : the predictions in the rotating wave approximation, from equations (9.12.3) and (9.14.1)  
(obtained by neglecting the rapidly oscillating terms)

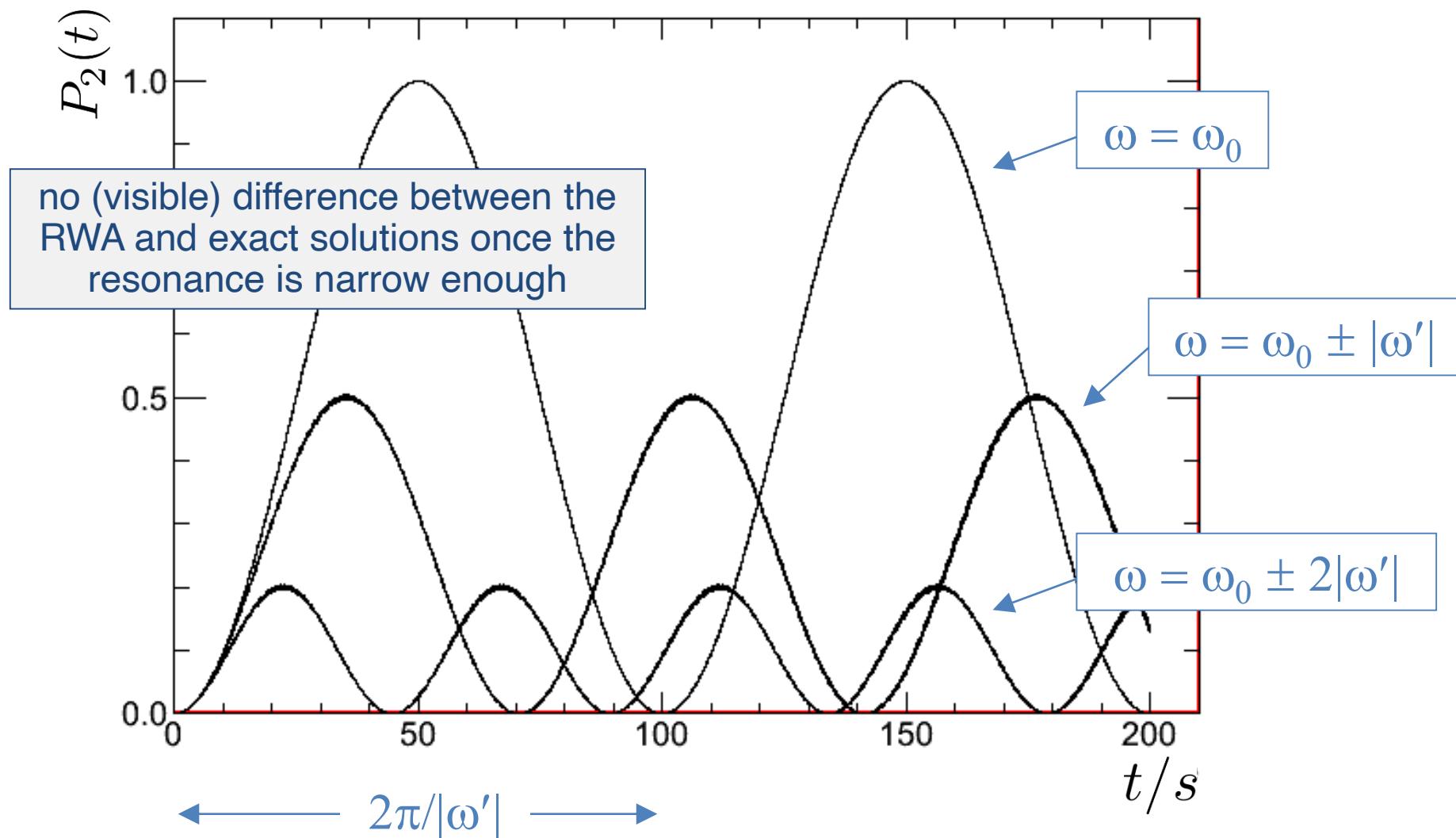
## Transition probability vs. time : “wide” resonance

$$\omega_0 = 2\pi, \quad \omega' = (0.2)\pi \quad (|\omega'|/\omega_0 = 0.1)$$



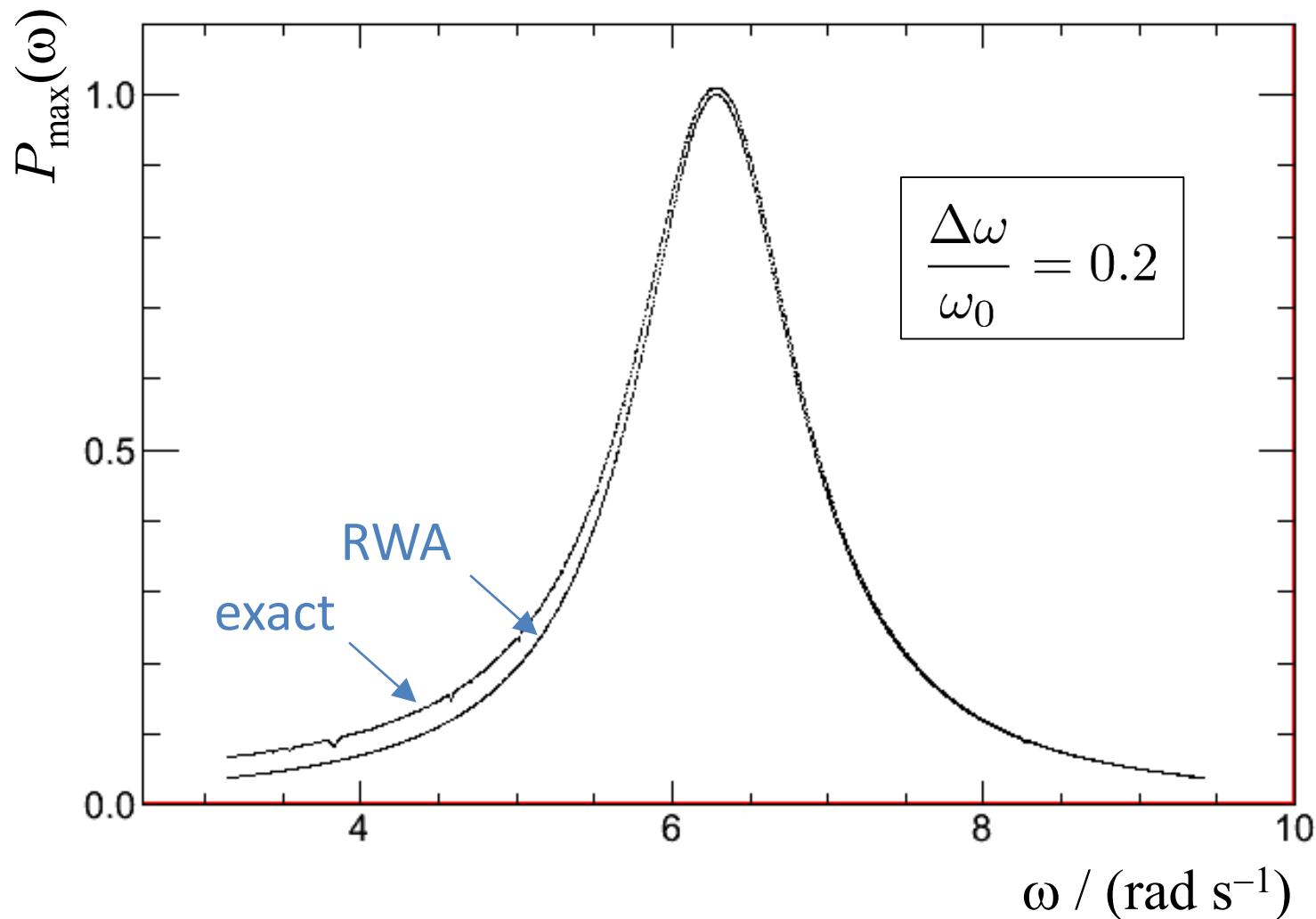
## Transition probability vs. time : “narrow” resonance

$$\omega_0 = 2\pi, \quad \omega' = (0.02)\pi \quad (|\omega'|/\omega_0 = 0.01)$$



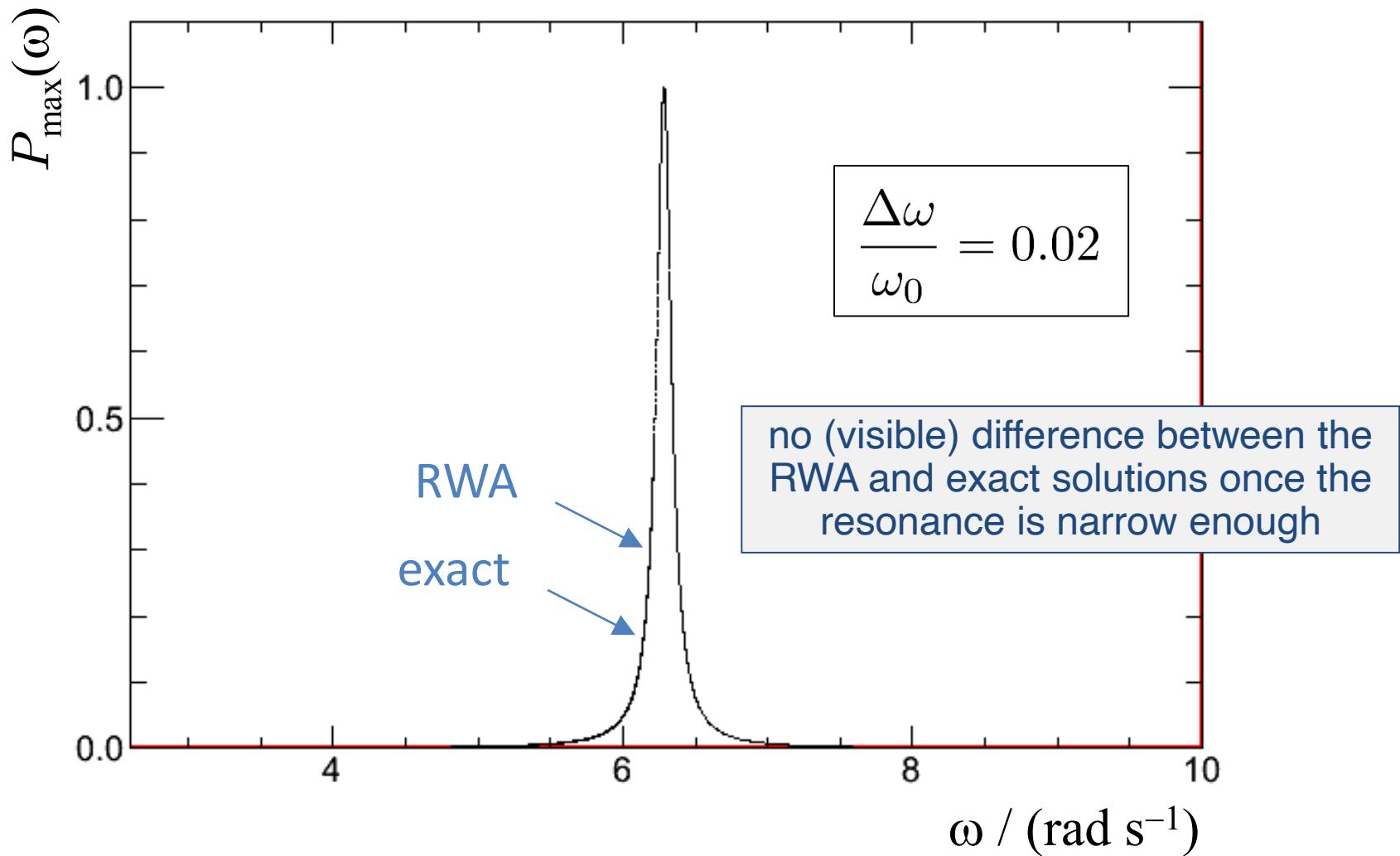
## Maximum probability vs. frequency : “wide” resonance

$$\omega_0 = 2\pi, \quad \omega' = (0.2)\pi \quad (|\omega'|/\omega_0 = 0.1)$$



## Maximum probability vs. frequency : “narrow” resonance

$$\omega_0 = 2\pi, \quad \omega' = (0.02)\pi \quad (|\omega'|/\omega_0 = 0.01)$$



# Spin Transitions

- Consider a spin-half particle with magnetic moment

$$\hat{\mu} = \gamma \hat{S}$$

at rest in a time-dependent magnetic field

$$\mathbf{B}(t) = (B_x \cos \omega t, 0, B_z) \quad (\omega, B_x, B_z > 0)$$

- The Hamiltonian

$$\hat{H}(t) = -\hat{\mu} \cdot \mathbf{B}(t) = -\gamma \hat{S} \cdot \mathbf{B}(t)$$

can be written as

$$\hat{H}(t) = \hat{H}_0 + \hat{H}' \cos \omega t$$

with

$$\hat{H}_0 = -\hat{\mu}_z B_z = -\gamma B_z \hat{S}_z , \quad \hat{H}' = -\hat{\mu}_x B_x = -\gamma B_x \hat{S}_x$$

- The time-independent component,  $H_0$ , has eigenstates

$$|\psi_1\rangle = |\uparrow\rangle ; \quad \hat{H}_0 |\uparrow\rangle = E_1 |\uparrow\rangle , \quad E_1 = -\frac{1}{2}\hbar\gamma B_z \equiv \hbar\omega_1$$
$$|\psi_2\rangle = |\downarrow\rangle ; \quad \hat{H}_0 |\downarrow\rangle = E_2 |\downarrow\rangle , \quad E_2 = +\frac{1}{2}\hbar\gamma B_z \equiv \hbar\omega_2$$

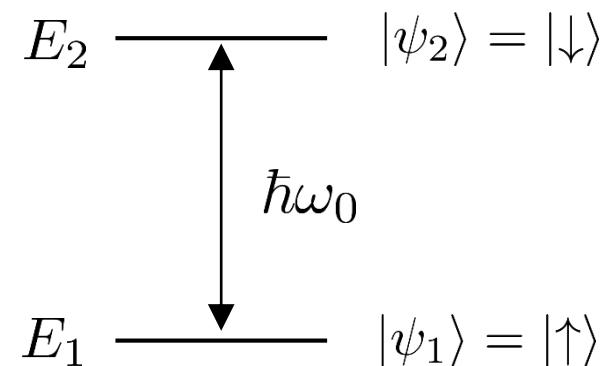
## Spin transitions (2)

- The energy gap between the two states is

$$\Delta E = E_2 - E_1 = \hbar\gamma B_z \equiv \hbar\omega_0$$

$$\Rightarrow \boxed{\omega_0 = \gamma B_z}$$

( if  $\gamma < 0$ , interchange  $|\uparrow\rangle$  and  $|\downarrow\rangle$  )



- The constant  $\omega'$  is defined as

$$\left. \begin{aligned} \hbar\omega' &= \langle \uparrow | \hat{H}' | \downarrow \rangle = -\gamma B_x \langle \uparrow | \hat{S}_x | \downarrow \rangle \\ \langle \uparrow | \hat{S}_x | \downarrow \rangle &= \frac{1}{2} \langle \uparrow | (\hat{S}_+ + \hat{S}_-) | \downarrow \rangle = \frac{1}{2} \hbar \end{aligned} \right\}$$

$$\Rightarrow \boxed{2\omega' = -\gamma B_x}$$

(so, in this case,  $\omega'$  is real)

- Resonant transitions occur for a driving frequency  $\omega = \omega_0$  :

$$\omega = \omega_0 = \gamma B_z$$

- We obtain a narrow resonance for  $B_x \ll B_z$  :

$$\frac{\Delta\omega}{\omega_0} = \frac{2|\omega'|}{\omega_0} = \frac{\gamma B_x}{\gamma B_z} = \frac{B_x}{B_z}$$

## Spin transitions (3)

- The spin state of the particle evolves with time as

$$|\psi(t)\rangle = c_1(t)e^{-i\omega_1 t}|\uparrow\rangle + c_2(t)e^{-i\omega_2 t}|\downarrow\rangle$$

Using

$$\langle \uparrow | \hat{S}_z | \uparrow \rangle = \frac{1}{2}\hbar, \quad \langle \downarrow | \hat{S}_z | \downarrow \rangle = -\frac{1}{2}\hbar, \quad \langle \uparrow | \hat{S}_z | \downarrow \rangle = \langle \downarrow | \hat{S}_z | \uparrow \rangle = 0$$

then shows that  $\langle S_z \rangle$  evolves as

$$\langle \hat{S}_z \rangle = \langle \psi(t) | \hat{S}_z | \psi(t) \rangle = \frac{\hbar}{2} [ |c_1(t)|^2 - |c_2(t)|^2] \quad (9.24.1)$$

- The ladder operators  $S_+ = S_x + iS_y$  and  $S_- = S_x - iS_y$  have matrix elements

$$\langle \uparrow | \hat{S}_+ | \downarrow \rangle = \langle \downarrow | \hat{S}_- | \uparrow \rangle = \hbar; \quad \langle \uparrow | \hat{S}_\pm | \uparrow \rangle = 0; \quad \langle \downarrow | \hat{S}_\pm | \downarrow \rangle = 0$$

$$\Rightarrow \begin{cases} \langle \psi(t) | \hat{S}_+ | \psi(t) \rangle &= \hbar c_1(t)^* c_2(t) e^{-i\omega_0 t} \\ \langle \psi(t) | \hat{S}_- | \psi(t) \rangle &= \hbar c_1(t) c_2(t)^* e^{+i\omega_0 t} \end{cases} \quad (\omega_0 = \omega_2 - \omega_1)$$

Hence  $\langle S_x \rangle$  and  $\langle S_y \rangle$  evolve as

$$\begin{aligned} \langle \hat{S}_x \rangle &= \langle \psi(t) | \hat{S}_x | \psi(t) \rangle = \hbar \operatorname{Re} [c_1(t)^* c_2(t) e^{-i\omega_0 t}] \\ \langle \hat{S}_y \rangle &= \langle \psi(t) | \hat{S}_y | \psi(t) \rangle = \hbar \operatorname{Im} [c_1(t) c_2(t)^* e^{+i\omega_0 t}] \end{aligned} \quad (9.24.2)$$

## Spin transitions (4)

- Suppose the driving frequency is exactly on resonance,  $\omega = \omega_0$ , and that the particle is initially in the “spin-up” state  $|\uparrow\rangle = |\Psi_1\rangle$  :

$$c_1(0) = 1 , \quad c_2(0) = 0$$

Equation (9.9.1) then gives

$$c_1(t) = \cos\left(\frac{1}{2}|\omega'|t\right) , \quad c_2(t) = i \sin\left(\frac{1}{2}|\omega'|t\right)$$

- Hence the three-vector of spin expectation values

$$\langle \hat{\mathbf{S}} \rangle = (\langle \hat{S}_x \rangle, \langle \hat{S}_y \rangle, \langle \hat{S}_z \rangle)$$

evolves with time according to equations (9.24.1) and (9.24.2) as

$$\langle \hat{\mathbf{S}} \rangle = \frac{1}{2}\hbar(\sin(\omega't)\sin(\omega_0t), \sin(\omega't)\cos(\omega_0t), \cos(\omega't))$$

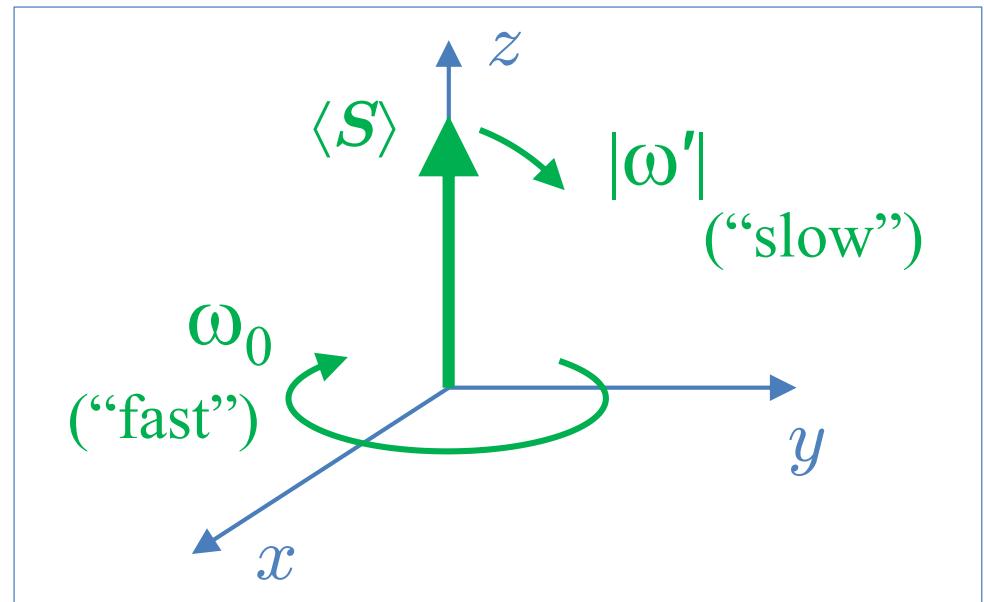
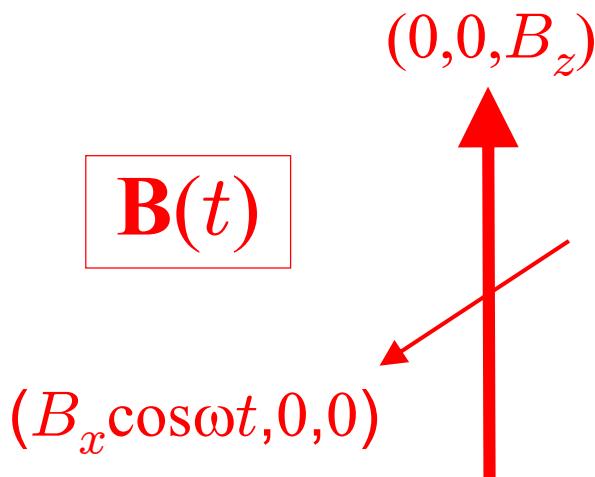
$$(\omega = \omega_0)$$

For  $t = 0$ , this gives the “spin-up” state  $|\uparrow\rangle$ , as expected :

$$\langle \hat{\mathbf{S}} \rangle_{(t=0)} = (0, 0, \frac{1}{2}\hbar)$$

## Spin transitions (5)

- The time evolution of  $\langle \hat{S} \rangle$  is a combination of :
  - precession about the  $z$  axis, with frequency  $\omega_0$
  - precession about a horizontal axis, with frequency  $|\omega'|$ , where this horizontal axis itself rotates about  $z$  with frequency  $\omega_0$



- In particular :

$$\omega' t = \pi \quad \Rightarrow \quad \langle \hat{\mathbf{S}} \rangle = (0, 0, -\frac{1}{2}\hbar)$$

$$\omega' t = \pi/2 \quad \Rightarrow \quad \langle \hat{\mathbf{S}} \rangle = \frac{1}{2}\hbar (\sin(\omega_0 t), \cos(\omega_0 t), 0)$$

## Spin transitions : 90° and 180° pulses

- Hence if we apply the oscillating field  $B_x$  for a time  $\Delta t$  such that

$$\omega' \Delta t = \pi ; \quad \Delta t = \frac{\pi}{\omega'} = \frac{2\pi}{\gamma B_x}$$

and then switch it off, leaving just the static field  $(0,0,B_z)$  :

- ⇒ the particle will undergo a “spin-flip” transition to the “spin-down” state  $|\downarrow\rangle$ , and then stay there

“180° pulse”

- If instead  $B_x$  is applied for a time  $\Delta t$  such that

$$\omega' \Delta t = \frac{\pi}{2} ; \quad \Delta t = \frac{\pi}{2\omega'} = \frac{\pi}{\gamma B_x}$$

- ⇒ the spin vector will rotate into the  $x$ - $y$  plane, and then stay in the  $x$ - $y$  plane, precessing around the  $z$  axis at frequency  $\omega_0 = \gamma B_z$

“90° pulse”

(Larmor precession in a static field : see slide 3.35)

## Spin transitions : towards applications

- For a *proton* in a  $B = 10$  T magnetic field,  
(a typical field strength used in *Nuclear Magnetic Resonance* (NMR))

the frequency gap between up and down spin states is

$$\nu_0 = \frac{\omega_0}{2\pi} = \frac{\gamma_p B_z}{2\pi} = \frac{g_p \mu_N B_z}{2\pi \hbar} = \frac{(5.586) \times (5.05 \times 10^{-27}) \times 10}{(6.626 \times 10^{-34})} = 426 \text{ MHz}$$

→ use *radio* frequencies (RF) to induce proton spin-flips

- For an *electron* in a  $B = 0.35$  T magnetic field,  
(a typical field strength used in *Electron Spin Resonance* (ESR))  
(a.k.a. *Electron Paramagnetic Resonance* (EPR))

$$\nu_0 = \frac{\omega_0}{2\pi} = \frac{\gamma_e B_z}{2\pi} = \frac{g_e \mu_B B_z}{2\pi \hbar} = \frac{2 \times (9.28 \times 10^{-24}) \times 0.35}{(6.626 \times 10^{-34})} \approx 9 \text{ GHz}$$

→ use *microwave* frequencies to induce electron spin-flips

# NMR / MRI / ESR (EPR)

- Spin transitions of (mainly) protons within molecules can be used to analyse the chemical composition of a sample
  - *Nuclear Magnetic Resonance* (NMR)
- In a given external magnetic field  $B_0$ , the transition frequency depends *slightly* on the chemical environment of the proton  
Known as the *chemical shift*, and parameterised in terms of the *shielding constant*  $\sigma$  defined as
$$B = B_0(1 - \sigma)$$
where  $B$  is the magnetic field at the position of the proton itself
- The resonant frequency inducing spin transitions then depends on the proton's environment as

$$\nu = \frac{\gamma B_0(1 - \sigma)}{2\pi}$$

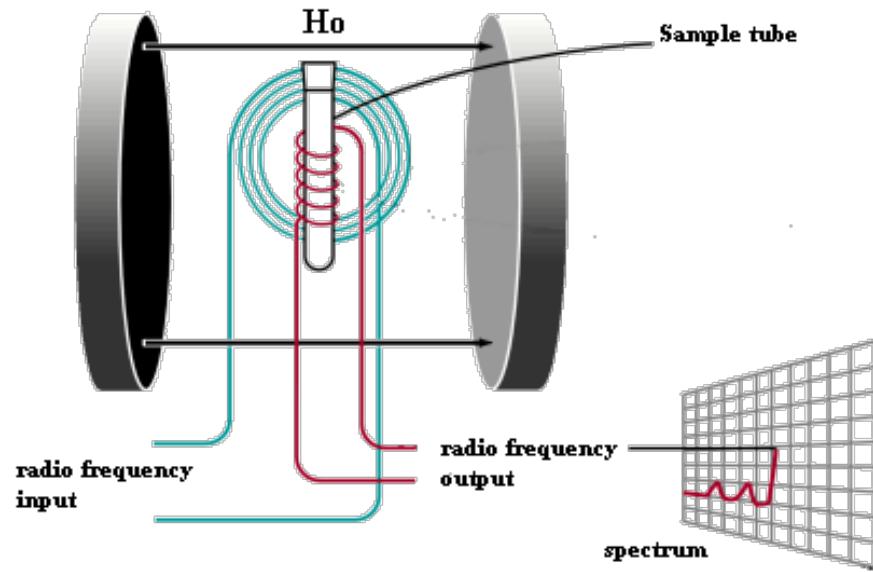
The typical effect is of order  $\delta = (\nu - \nu_0)/\nu_0 \sim \text{few ppm}$

## Spin transitions : NMR (2)

- In NMR, a sample is placed in a large, uniform, static magnetic field  $B_z$

This induces an energy level splitting between proton spin states which is slightly different for different chemical shifts

A small population difference between the split energy levels gives rise to a net magnetisation in the sample



- A coil surrounding the sample can apply a smaller, perpendicular, pulsed RF field  $B_x \cos \omega t$  ;  
this makes the net magnetisation precess about the  $z$  direction
- As it precesses, the magnetic field produced by the net magnetisation induces a radio signal in a second (output) coil surrounding the sample;  
Fourier analysis of the (complicated) induced RF output signal produces the NMR spectrum

## Spin transitions : NMR (3)

- At temperature  $T$ , in the large uniform field  $B_z$ , *slightly* fewer protons occupy the higher energy spin state :

$$N_2/N_1 = \exp(-\Delta E/k_B T)$$

e.g. for protons at  $T = 300$  K in a magnetic field  $B = 9.4$  T :

$$(\Delta N)/N \sim 3 \times 10^{-5}$$

Thus protons in the field  $B_z$  are, on average, slightly more “spin-up” than “spin-down”

- For the sample as a whole, this results in a *small net magnetisation* along the  $z$  axis,

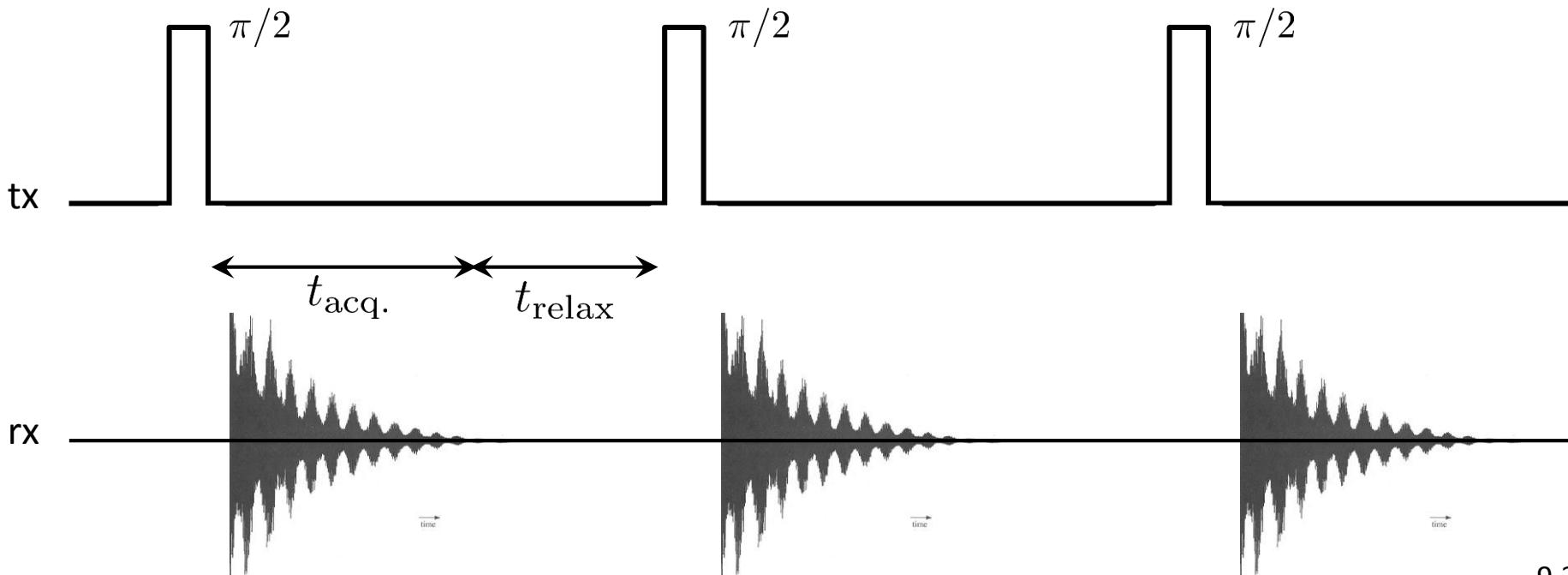
$$\langle \mathbf{M} \rangle = (0, 0, M)$$

Since  $\langle \mathbf{M} \rangle$  is small, its precession induces an inherently weak signal :

- need to use strong magnetic fields ( up to  $\sim 20$  T )
- preferably use nuclei with a relatively large magnetic moment and high natural abundance (protons,  $^{13}\text{C}$ ,  $^{19}\text{F}$ , ...)

## Spin transitions : NMR (4)

- In early NMR, the RF frequency  $\omega$  was scanned to sequentially excite (resonantly spin-flip) protons with different chemical shifts
- Today, *pulsed methods* are used to simultaneously excite a *range* of chemical shifts in a single shot, which is much less time consuming (at the price of extra processing: need to take the FT of the NMR signal)
- An example of a simple pulse/acquisition sequence :



## Spin transitions : NMR (5)

- Applying a  $90^\circ$  pulse at an (RF) frequency matching the proton spin-flip resonant frequency rotates the net magnetisation  $\langle \mathbf{M} \rangle$  into the  $x-y$  plane
  - $\langle \mathbf{M} \rangle$  then precesses rapidly about  $z$   
(at a slightly different frequency for each chemical shift)
  - $\langle \mathbf{M} \rangle$  can now be detected via its precessing magnetic field  
(e.g. via voltages induced in coils located in the  $x-y$  plane)

- While precessing about  $z$ , the net magnetisation  $\langle \mathbf{M} \rangle$  also slowly relaxes back towards equilibrium, with  $\langle \mathbf{M} \rangle$  aligned along  $+z$

This relaxation is due to complex interactions between the proton spins and the sample, and is relatively slow (typically milliseconds → seconds)

The oscillating induced signal therefore gradually decays with time

- The induced output signal contains a superposition of frequencies, one for each chemical shift in the sample

## Spin transitions : NMR (6)

- Fourier analysis of the output signal produces a frequency spectrum containing a narrow resonant peak for each chemical shift
- The process is repeated many times to obtain an acceptable signal to noise ratio
- An example of a state-of-the-art 900 MHz NMR spectrometer :

(Centre for Structural Biology, Vanderbilt University)

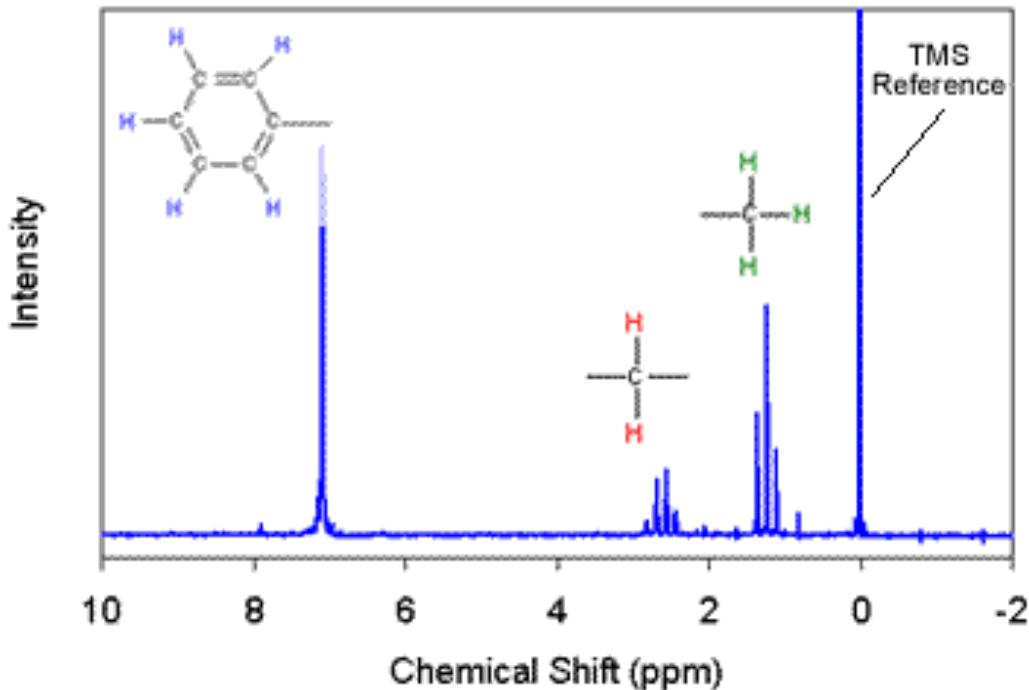
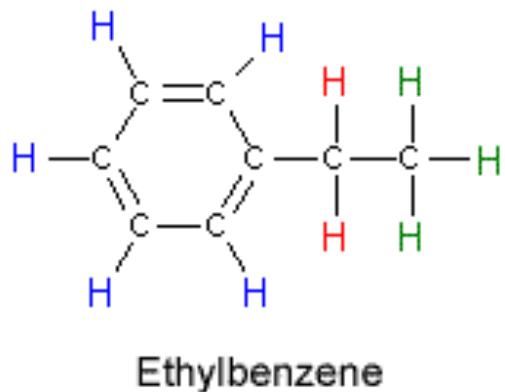
$$B = 21.2 \text{ T}$$

- determine the 3D structure of biological macromolecules



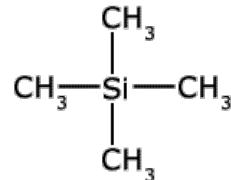
[structbio.vanderbilt.edu/nmr/](http://structbio.vanderbilt.edu/nmr/)

## NMR example : $^1\text{H}$ spectrum for ethylbenzene

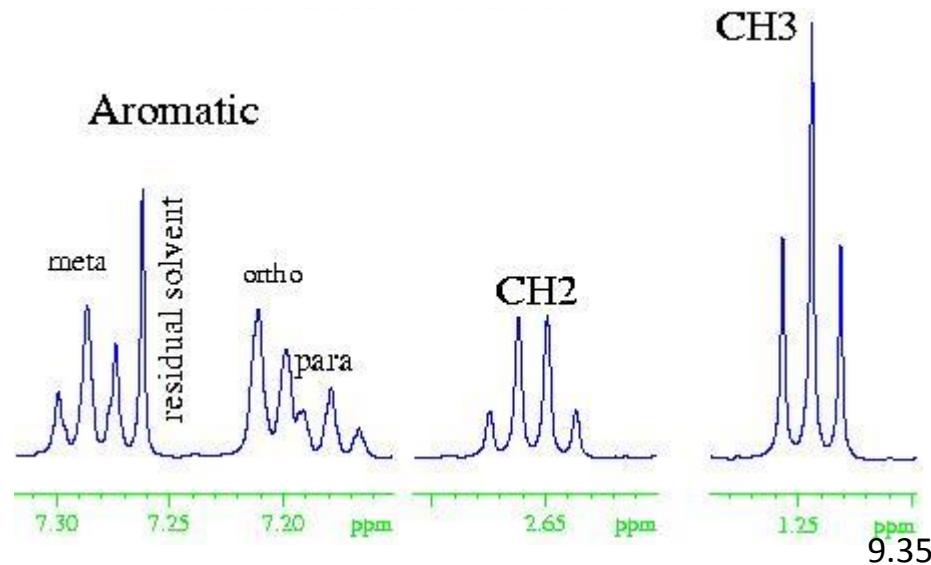


TMS = tetramethylsilane       $\text{Si}(\text{CH}_3)_4$

= the accepted standard  
for calibrating chemical  
shift in organic solvents

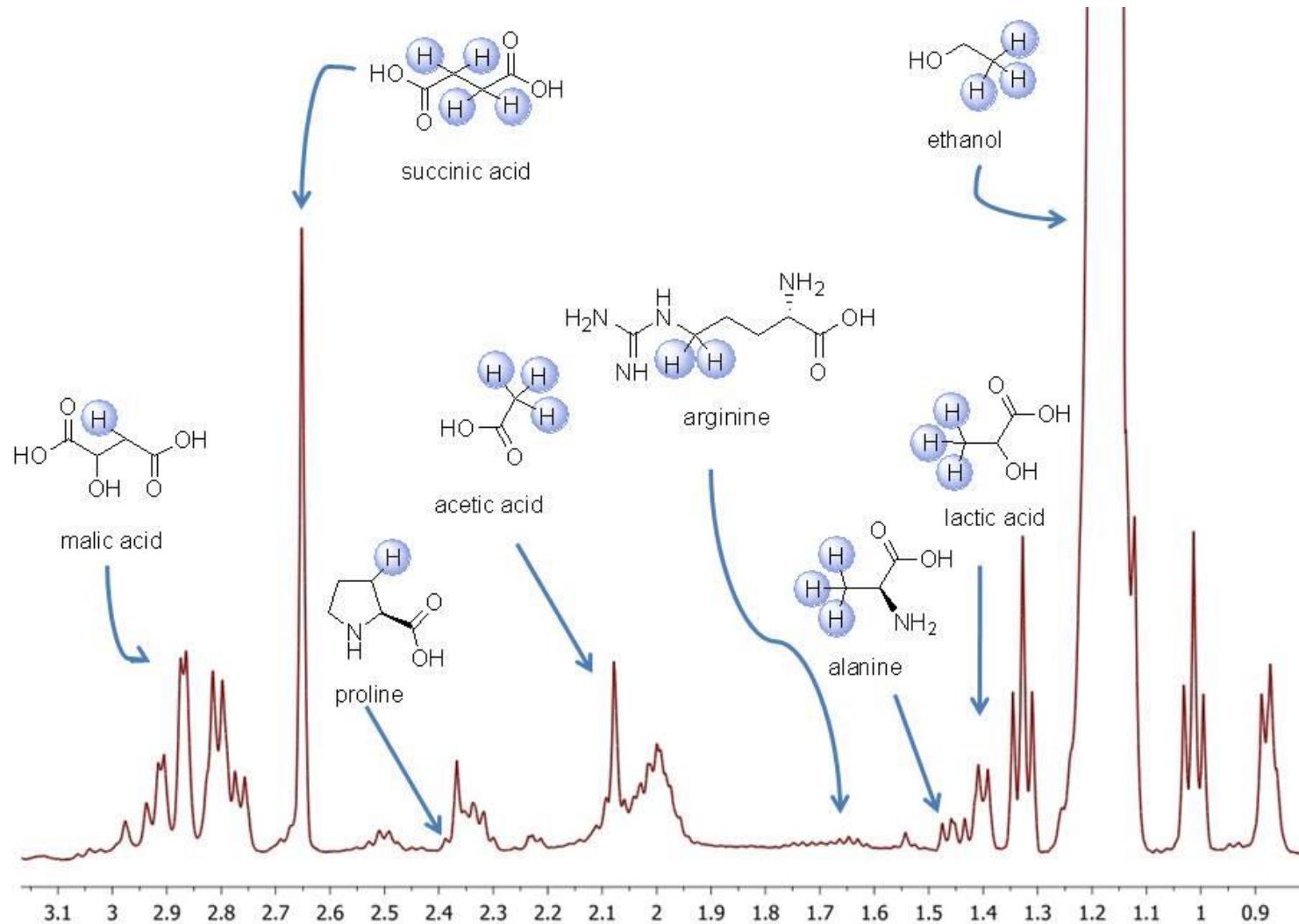


All twelve H atoms in TMS are  
equivalent; hence an NMR singlet



# NMR : a much more useful example

[www.unirioja.es/gsoe/NMR.htm](http://www.unirioja.es/gsoe/NMR.htm)



## Spin transitions : MRI

- NMR can be turned into an imaging technique :
    - *Magnetic Resonance Imaging (MRI)*
- Achieved by adding small, linear magnetic field gradients along  $x$ ,  $y$ ,  $z$
- ⇒ resonance occurs at different frequencies in different places
  - ⇒ can determine how many spins of particular types are in particular locations



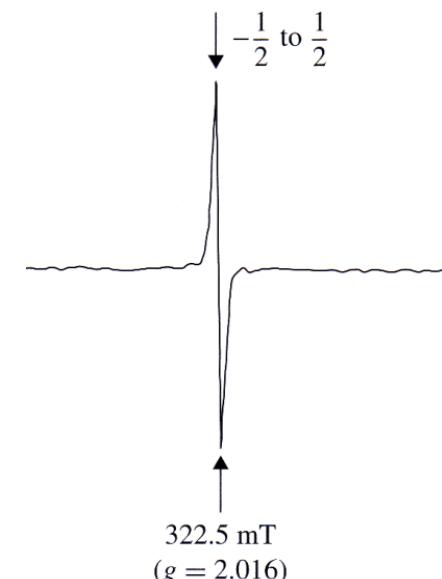
BMRI © J.Hornak

## Spin transitions : ESR

- Techniques analogous to NMR can be used to excite spin-transition resonances for *electrons* :
  - *Electron Spin (Paramagnetic) Resonance (ESR/EPR)*
- Useful for studying materials with unpaired electrons, for example metal complexes or organic radicals
- Involves higher resonant frequencies than for NMR (GHz rather than MHz) because the electron magnetic moment is relatively large (slide 3.62)

Typically a fixed frequency is used, and the magnetic field  $B_z$  is varied to sweep through the resonance

e.g. for a sample of  $\text{Fe}^{3+}$  ions with a  $B_x$  field oscillating at 9.10 GHz (in the  $\mu$ wave region)



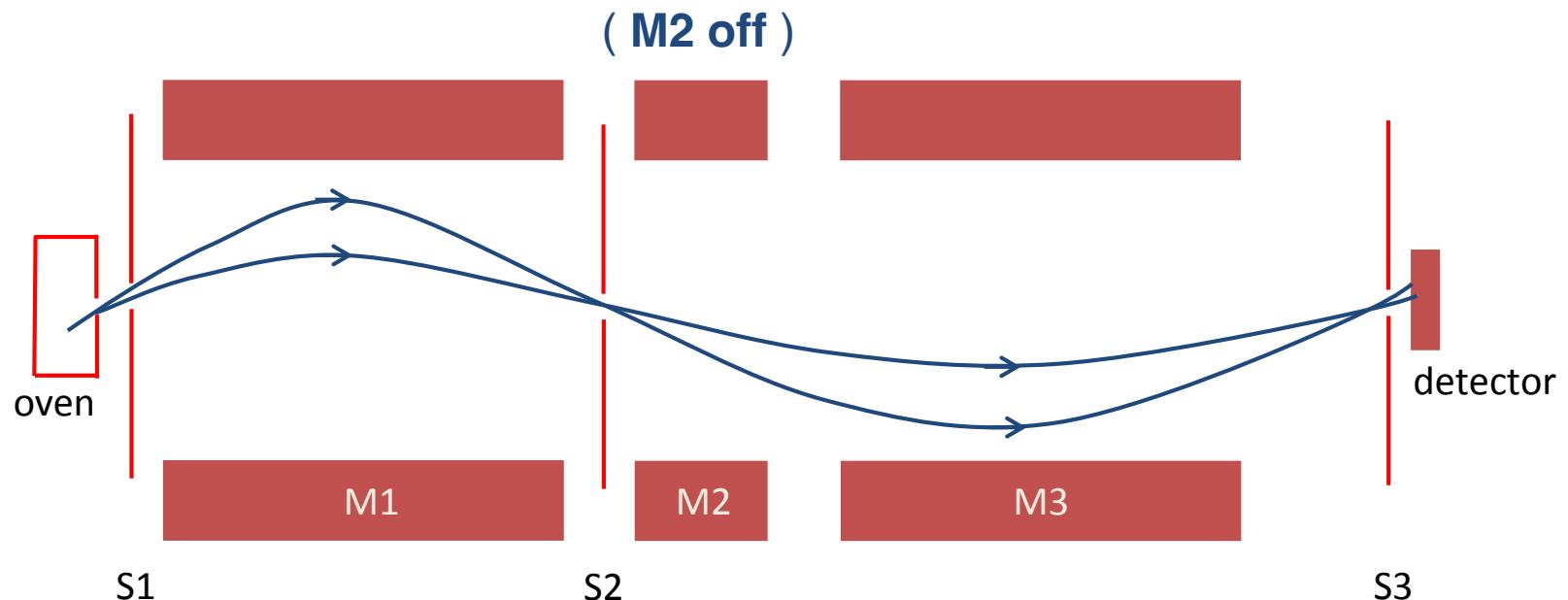
Usually (as here) it is the *derivative* of the signal that is recorded, rather than the signal itself

# Rabi Molecular Beam Experiment

- Spin transitions are at the heart of a technique pioneered by Rabi for the accurate measurement of the magnetic moments of protons, nuclei, ...  
(Columbia, NY, 1934-39) [I. I. Rabi et al., Phys. Rev. 55 \(1939\) 526](#)

→ molecular beam resonance or the magnetic resonance method

- Experimental layout, with transverse dimension greatly exaggerated :



## Rabi molecular beam experiment (2)

- Neutral atoms or molecules emerge from slit S1 with a spread of energies and directions, and in a mixture of different nuclear spin states  
(use atoms or molecules such that electrons have total  $L = S = 0$  )
- Magnets M1 and M3 are equal and opposite “Stern-Gerlachs” :
  - M1 and M3 produce large **B** fields (up to 1.2 T), with field gradients identical in magnitude (up to 10 T/cm) but opposite in direction

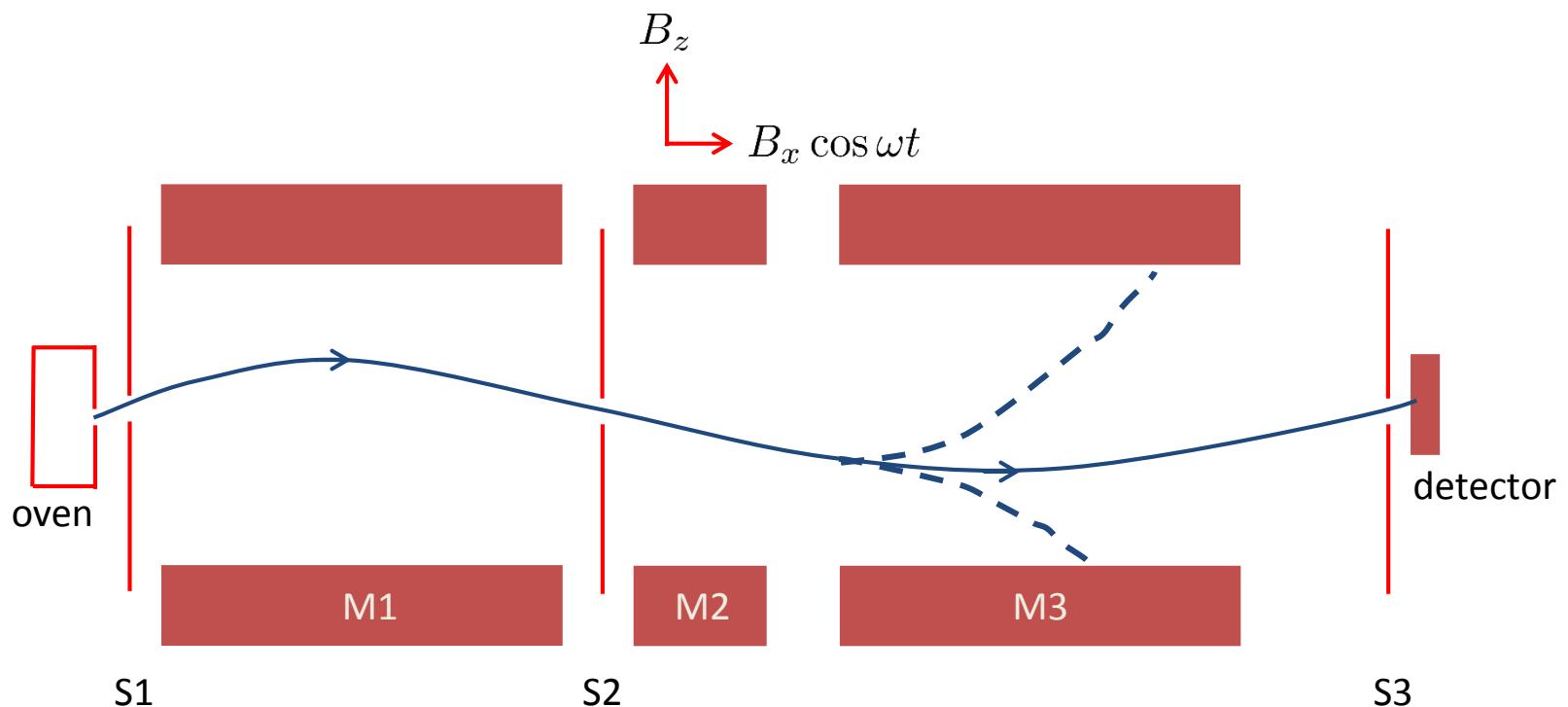
Since these fields are non-uniform, the trajectory followed by each atom depends on its spin state (as well as its initial energy and direction)
- Slit S2 only allows certain trajectories to pass through
  - for any given spin state, only certain combinations of initial energy and direction give a trajectory passing through S2
- With magnet **M2** turned **off**, trajectories passing through S2 are brought back together by M3, pass through slit S3, and are detected

## Rabi molecular beam experiment (2)

-- Now turn magnet **M2** on :

→ M2 applies a “large” static field in the  $z$  direction, and a “small” oscillating field in the  $x$  direction :

$$\mathbf{B}(t) = (B_x \cos \omega t, 0, B_z)$$



## Rabi molecular beam experiment (3)

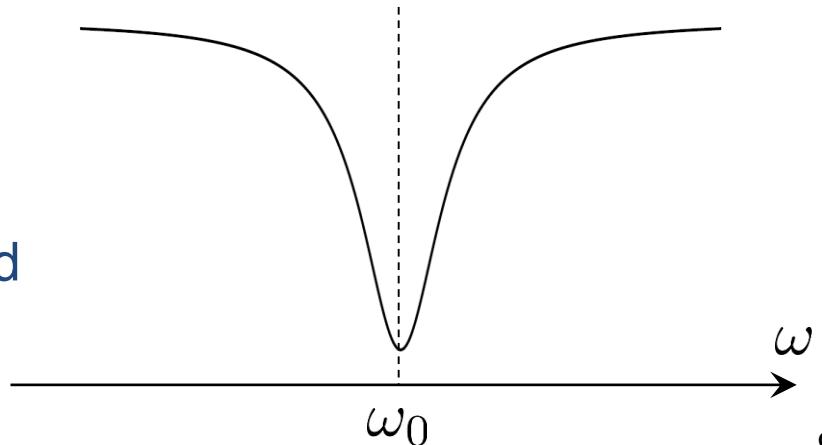
- The large field  $B_z$  induces a uniform energy spacing between spin states of different  $m_S$  given by (see slide 3.37)

$$\Delta E = \hbar\gamma B_z \equiv \hbar\omega_0 \quad \Rightarrow \quad \omega_0 = \gamma B_z \quad (9.42.1)$$

- When the frequency  $\omega$  of  $B_x$  is close to the frequency  $\omega_0$  :
  - spin transitions can occur, changing the spin state  $m_S$  of some of the atoms or molecules in the beam
  - these atoms or molecules will change to a different (dashed) trajectory through the (inhomogenous) magnetic field of M3
  - they will therefore not pass through S3, so will not be detected

Hence, at or near the frequency  $\omega_0$ , the detected intensity drops sharply

- a *resonant dip* in the transmitted intensity is observed



## Rabi molecular beam experiment (4)

- Suppose the frequency  $\omega$  of the M2 field  $B_x$  is scanned, and a resonant dip is observed at a frequency  $\omega = \omega_{\text{res}}$

The position of the resonance determines the frequency  $\omega_0$  corresponding to the energy spacing between spin states in the M2 field  $B_z$  :

$$\omega_0 = \omega_{\text{res}}$$

From equation (9.42.1), the observed resonant frequency  $\omega_{\text{res}}$  therefore determines the magnetic moment  $\mu$  (see slide 3.60) :

$$\gamma = \frac{\omega_{\text{res}}}{B_z} ; \quad \mu = \gamma s \hbar$$

- In practice, it may be more convenient to search for resonant dips in beam intensity by scanning the static field strength  $B_z$   
( rather than by scanning the frequency  $\omega$  of the oscillating field  $B_x$  )

## Rabi molecular beam experiment (5)

- For example, from a scan of  $B_z$ , with  $\omega$  kept fixed at 4 MHz :

$H_2$ ,  $D_2$ , HD molecules were used since the (much larger) electron magnetic moments cancel each other (since the  $e^-$  are in an overall S-state)

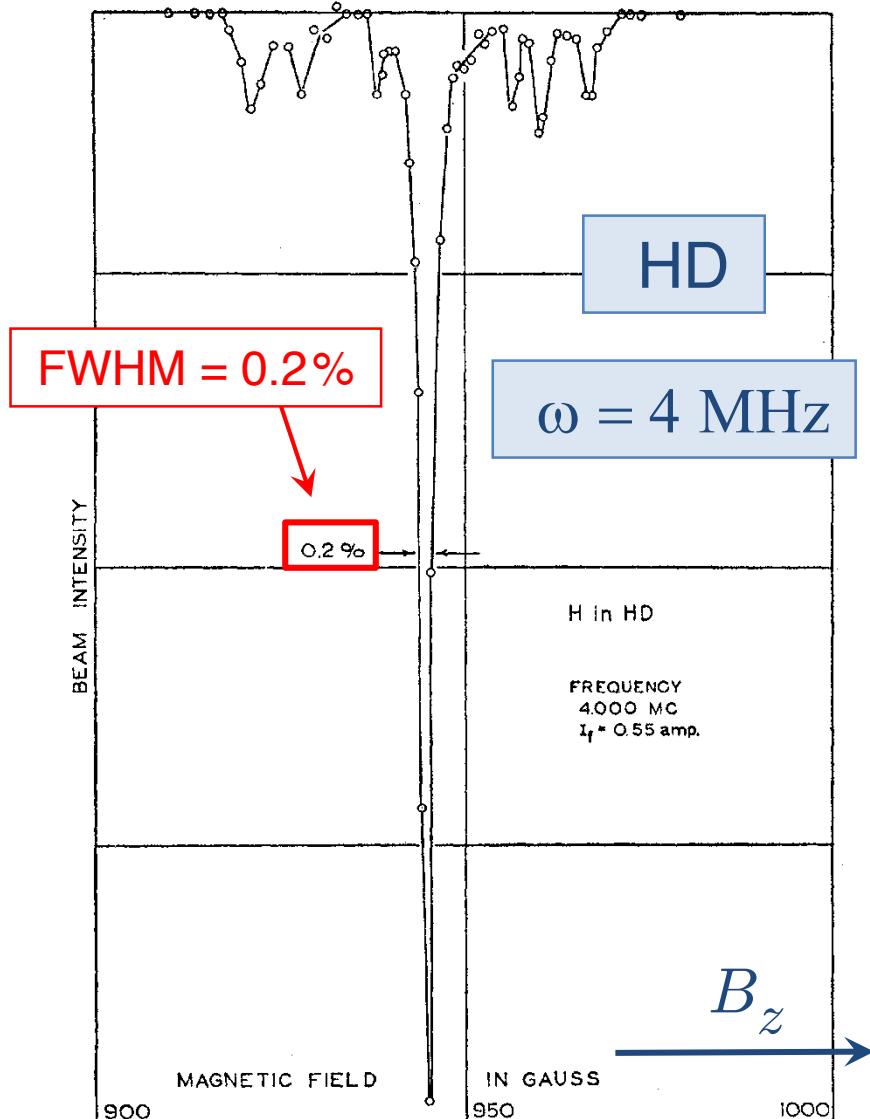
The HD resonance shown was also seen in  $H_2$ , but not in  $D_2$ , confirming it is due to a proton, not a deuteron

- The proton and deuteron magnetic moments were measured to be

$$\mu_p = (2.785 \pm 0.02) \mu_N$$

$$\mu_D = (0.855 \pm 0.006) \mu_N$$

[J. Kellogg et al., Phys. Rev. 56 \(1939\) 728](#)



# Time-Dependent Perturbation Theory

- Consider (still) a general *time-dependent* perturbation

$$\hat{H}(t) = \hat{H}_0 + \hat{H}'(t)$$

but now generalise to a system with any number of states (not just two)

Take the unperturbed eigenstates of  $H_0$  to be

$$\hat{H}_0|n\rangle = E_n|n\rangle ; \quad E_n \equiv \hbar\omega_n ; \quad \langle n|m\rangle = \delta_{nm}$$

- The time-dependent Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = [\hat{H}_0 + \hat{H}'(t)]|\psi(t)\rangle$$

- The state  $|\psi(t)\rangle$  can be expanded in terms of the eigenstates of  $H_0$  as

$$|\psi(t)\rangle = \sum_j c_j(t)e^{-i\omega_j t}|j\rangle$$

## Time dependent perturbation theory (2)

- Substituting into the Schrödinger equation gives

$$i\hbar \frac{\partial}{\partial t} \sum_j c_j(t) e^{-i\omega_j t} |j\rangle = [\hat{H}_0 + \hat{H}'(t)] \sum_j c_j(t) e^{-i\omega_j t} |j\rangle$$

- Expanding out the left-hand side, and cancelling the  $H_0$  terms gives

$$i\hbar \sum_j \frac{dc_j(t)}{dt} e^{-i\omega_j t} |j\rangle = \hat{H}'(t) \sum_j c_j(t) e^{-i\omega_j t} |j\rangle$$

- Taking the inner product with  $\langle k|$  then gives

$$i\hbar \frac{dc_k(t)}{dt} = \sum_j c_j(t) e^{i(\omega_k - \omega_j)t} H'_{kj}(t) \quad (9.47.1)$$

where the matrix elements of the perturbation  $H'(t)$  have been written as

$$H'_{kj}(t) \equiv \langle k | \hat{H}'(t) | j \rangle$$

- So far, this is all *exact*, and is a straightforward extension of the previous analysis of a two-state system

## Time dependent perturbation theory (3)

- Suppose the perturbation is small, and that the system is initially in the state  $|0\rangle$  :

$$c_0(0) = 1 ; \quad c_j(0) = 0 \quad (j \neq 0)$$

Then, in the RHS of equation (9.47.1), we can replace  $c_j(t)$  by  $c_j(0)$  to obtain the approximation

$$i\hbar \frac{dc_k(t)}{dt} = e^{i(\omega_k - \omega_0)t} H'_{k0}(t) \quad \left\{ \begin{array}{l} E_k \equiv \hbar\omega_k \\ E_0 \equiv \hbar\omega_0 \end{array} \right.$$

Hence, to leading-order,

$$c_k(t) = \frac{1}{i\hbar} \int_0^t e^{i(\omega_k - \omega_0)t'} H'_{k0}(t') dt' \quad (9.48.1)$$

- The probability that the system is in state  $|k\rangle$  at a time  $t > 0$ , i.e. the *transition probability* for  $|0\rangle \rightarrow |k\rangle$ , is then given by

$$P_{(0 \rightarrow k)}(t) = |c_k(t)|^2$$

- Higher order approximations can be obtained by iterating the above procedure if needed

## Fermi's Golden Rule

- Consider a (Hermitian) *monochromatic* perturbation of the form

$$\hat{H}'(t) = \hat{U}e^{-i\omega t} + \hat{U}^\dagger e^{i\omega t}$$

where  $U$  is a time-independent operator, not necessarily Hermitian, and where  $\omega$  is positive :

$$\omega > 0$$

- From equation (9.48.1), the leading-order amplitude for the transition  $|0\rangle \rightarrow |k\rangle$  is

$$\begin{aligned} c_k(t) &= \frac{1}{i\hbar} \int_0^t e^{i(\omega_k - \omega_0 - \omega)t'} U_{k0} dt' + \frac{1}{i\hbar} \int_0^t e^{i(\omega_k - \omega_0 + \omega)t'} U_{k0}^\dagger dt' \\ &= -\frac{1}{\hbar} U_{k0} \frac{e^{i(\omega_k - \omega_0 - \omega)t} - 1}{\omega_k - \omega_0 - \omega} - \frac{1}{\hbar} U_{k0}^\dagger \frac{e^{i(\omega_k - \omega_0 + \omega)t} - 1}{\omega_k - \omega_0 + \omega} \end{aligned} \quad (9.49.1)$$

where the matrix elements of  $U$  have been written for convenience as

$$U_{k0} \equiv \langle k | \hat{U} | 0 \rangle , \quad U_{k0}^\dagger \equiv \langle k | \hat{U}^\dagger | 0 \rangle$$

## Fermi's Golden Rule (2)

- Consider the first term on the right-hand side of equation (9.49.1) :

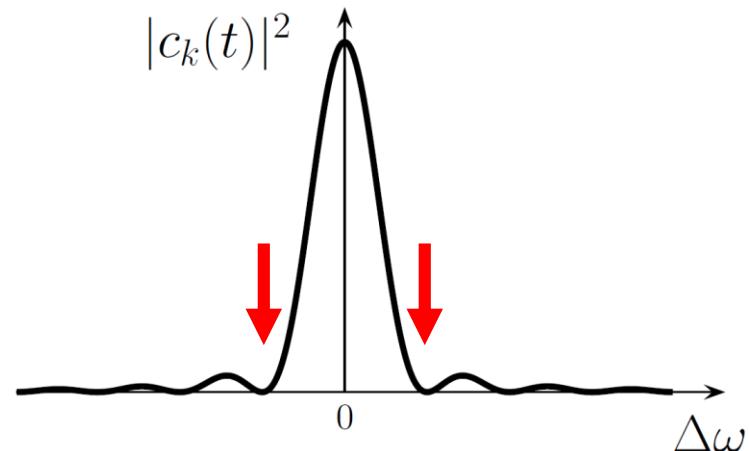
$$c_k(t) = -\frac{1}{\hbar} U_{k0} \frac{e^{i(\omega_k - \omega_0 - \omega)t} - 1}{\omega_k - \omega_0 - \omega}$$

- Using the identity  $|e^{i\alpha} - 1|^2 = 4 \sin^2(\alpha/2)$ , this term gives a transition probability

$$|c_k(t)|^2 = \frac{1}{\hbar^2} |U_{k0}|^2 \frac{\sin^2((\Delta\omega)t/2)}{(\Delta\omega/2)^2}$$

where

$$\Delta\omega \equiv (\omega_k - \omega_0 - \omega)$$



The dominant transitions are to higher energy states,  $\omega_k > \omega_0$ , with

$$\omega_k - \omega_0 \approx \omega$$

- The zeros on either side of the peak at  $\omega = \omega_k - \omega_0$  are located at

$$|\omega_k - \omega_0 - \omega| = 2\pi/t$$

i.e. the peak becomes narrower with time, its width decreasing as  $1/t$

## Fermi's Golden Rule (3)

- Eventually it becomes a  $\delta$ -function :

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

$$\lim_{t \rightarrow \infty} |c_k(t)|^2 = \frac{2\pi t}{\hbar^2} |U_{k0}|^2 \delta(\omega_k - \omega_0 - \omega)$$

- The transition *rate* to the state  $|k\rangle$  is then constant, and given by

$$\Gamma(0 \rightarrow k) \equiv \frac{|c_k(t)|^2}{t} = \frac{2\pi}{\hbar} |U_{k0}|^2 \delta(E_k - E_0 - \hbar\omega) \quad (9.51.1)$$

This is known as *Fermi's Golden Rule*

( but was first obtained by Dirac : [T. Visser, Am. J. Phys. 77 \(2009\) 487](#) )

- Thus, provided the driving frequency  $\omega$  is tuned appropriately, the perturbation  $\hat{H}'(t) = \hat{U}e^{-i\omega t}$  drives transitions to a higher energy state,

$$E_k = E_0 + \hbar\omega$$

at a rate proportional to  $|U_{k0}|^2 = |\langle k|\hat{U}|0\rangle|^2$

## Fermi's Golden Rule (3)

- Similarly, the perturbation  $\hat{H}'(t) = \hat{U}^\dagger e^{i\omega t}$ , responsible for the second term on the right-hand side of equation (9.49.1), drives transitions to a *lower* energy state

$$E_k = E_0 - \hbar\omega$$

with a transition rate given by

$$\Gamma(0 \rightarrow k) \equiv \frac{|c_k(t)|^2}{t} = \frac{2\pi}{\hbar} |U_{k0}^\dagger|^2 \delta(E_0 - E_k - \hbar\omega)$$

- For atomic transitions, the case  $E_k > E_0$  corresponds to *absorption*, while the case  $E_k < E_0$  corresponds to *emission*

## Fermi's Golden Rule (4)

- In many (most?) cases of interest (e.g. atomic transitions, scattering, ...), we need to consider transitions to a *continuum* of available final states

For example, consider a system where the density of available final states is specified via the function  $g(E_k)$  :

$$dN = g(E_k) dE_k$$

Then, for a perturbation  $\hat{H}'(t) = \hat{U}e^{-i\omega t}$ , the transition rate is obtained by integrating equation (9.51.1) over all possible final states :

$$\Gamma(0 \rightarrow k) = \frac{2\pi}{\hbar} \int_0^{\infty} |U_{k0}|^2 \delta(E_k - E_0 - \hbar\omega) g(E_k) dE_k$$

This gives the continuum version of Fermi's Golden Rule :

$$\boxed{\Gamma(0 \rightarrow k) = \frac{2\pi}{\hbar} |U_{k0}|^2 g(E_k)}$$

$$U_{k0} \equiv \langle k | \hat{U} | 0 \rangle$$

- This is the total transition rate to all available states of energy

$$E_k = E_0 + \hbar\omega$$

## Fermi's Golden Rule (5)

- Similarly, for a perturbation  $\hat{H}'(t) = \hat{U}^\dagger e^{i\omega t}$ , the total transition rate to all available states of energy

$$E_k = E_0 - \hbar\omega$$

is given by

$$\Gamma(0 \rightarrow k) = \frac{2\pi}{\hbar} |U_{k0}^\dagger|^2 g(E_k)$$

$$U_{k0}^\dagger \equiv \langle k | \hat{U}^\dagger | 0 \rangle$$

- We will use Fermi's Golden Rule to obtain transition rates for scattering processes and for atomic emission and absorption

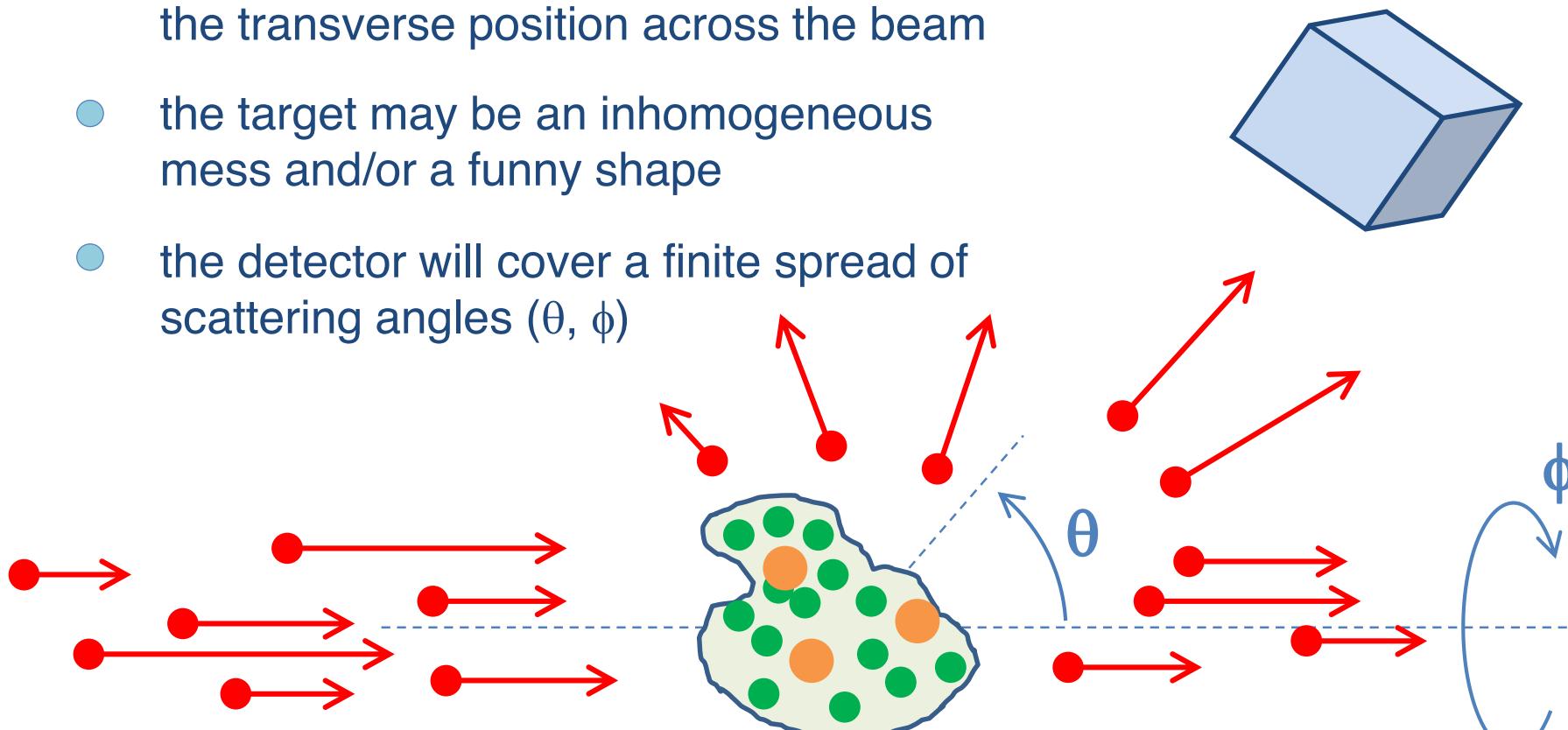
# Scattering

- Most of what we know about atomic, nuclear and particle physics has been discovered in scattering experiments
  - e.g. Rutherford's discovery of the nucleus, the discovery of subatomic particles (quarks etc.)
- In "low energy" physics, scattering phenomena provide the standard tools to explore solid state systems
  - neutron scattering, electron scattering, X-ray scattering, ...
- Here, will introduce the basic scattering formalism (*total and differential cross sections*) and treat scattering in the *Born Approximation* :
  - apply time-dependent perturbation theory (Fermi's Golden Rule) to the scattering of particles by a fixed potential

## A generic scattering experiment

- In a typical scattering experiment, we count the number of particles per second scattered into a detector :

- the incoming beam may contain a spread of particle energies
- the incoming particle flux will vary with the transverse position across the beam
- the target may be an inhomogeneous mess and/or a funny shape
- the detector will cover a finite spread of scattering angles ( $\theta, \phi$ )

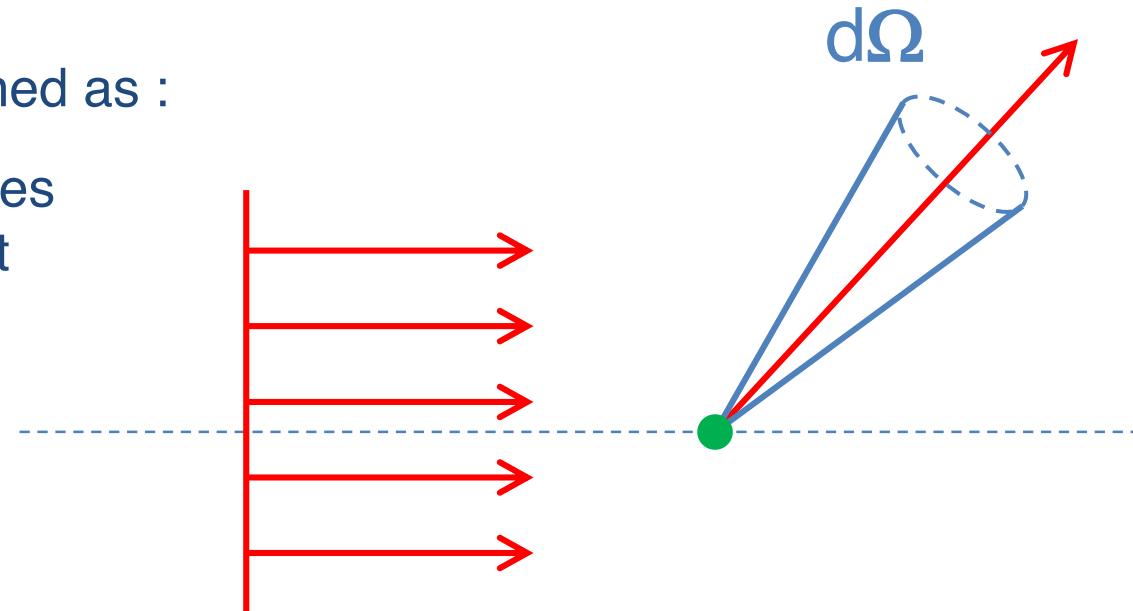


## The Differential Scattering Cross Section

- It is desirable, nay essential, to characterise the scattering process in a way which is independent of the experimental details :
  - consider a single target particle (“scattering centre”) of given type
  - illuminate the target particle with a mono-energetic beam of infinite transverse extent and uniform flux (i.e. a plane wave)
  - consider scattered particles which are directed into an infinitesimal element of solid angle  $d\Omega$  in the direction  $(\theta, \phi)$

The incident flux  $j$  is defined as :

$j = \# \text{ of incoming particles}$   
per unit time per unit  
transverse area



## The Differential Scattering Cross Section (2)

- The scattering rate as a function of angle is quantified by the *differential scattering cross section*, defined (*per target particle*) as

$$\frac{d\sigma}{d\Omega} \equiv \frac{\text{no. of particles scattered/unit time into } d\Omega}{\text{incident flux} \times d\Omega}$$

- The differential cross section  $d\sigma/d\Omega$  depends on :
  - the nature (electron, muon, ...) of the incoming and target particles
  - the beam energy
  - the scattering angles  $\theta$  and  $\phi$

It is *independent* of the details of the experimental setup (the target density and geometry, the beam intensity and profile, ...)

→ the scattering rate into a given detector can be found by integrating the differential cross section over all these details

- $d\sigma/d\Omega$  is often written in terms of the *scattering amplitude*  $f(\theta, \phi)$ , defined as

$$\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2$$

## The Total Scattering Cross Section

- The *total scattering cross section*  $\sigma$  characterises the scattering rate integrated over all angles, and is defined (*per target particle*) as

$$\sigma \equiv \frac{\text{total no. of particles scattered in any direction/unit time}}{\text{incident flux}}$$

- From the definitions of the total and differential cross sections, it follows that

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} \int_{-1}^{+1} \frac{d\sigma}{d\Omega} d\cos\theta d\phi$$

- The differential cross section  $d\sigma/d\Omega$  is, by definition, a ratio of two infinitesimal quantities, and is a function of the angles  $\theta$  and  $\phi$

The total cross section  $\sigma$  is a single quantity with dimensions of area  
( *not* a function of  $\theta$  and  $\phi$  which can be differentiated )

## Measurement of the Cross Section

- Consider a simple experiment in which a small, homogeneous target is illuminated by a wide, uniform, monoenergetic beam

Assume that the target is thin enough (e.g. a foil) that a given beam particle undergoes at most one scatter as it traverses the target

- Under these conditions, the total cross section  $\sigma$  is measured as

$$\sigma = \frac{N_{\text{scatt}}/T}{N_T \times (N_{\text{in}}/T/A)} = f_{\text{scatt}} \frac{A}{N_T} \quad (9.60.1)$$

where :

$A$  is the transverse area presented by the target to the incoming beam

$N_T$  is the total number of particles in the target

$N_{\text{in}}$  is the total number of beam particles incident on the target in time  $T$

$N_{\text{scatt}}$  is the total number of particles scattered (in any direction) in time  $T$

$f_{\text{scatt}} \equiv \frac{N_{\text{scatt}}}{N_{\text{in}}}$  is the fraction of scattered particles

## Measurement of the Cross Section (2)

- For a uniform foil of density  $\rho$  consisting of particles of mass  $m$ , the final factor in equation (9.60.1) is  $A/N_T = m/\rho$   
Thus the measured cross section depends only on the *nature* of the target, not its geometry
- Suppose that scattered particles are measured by a detector located in the direction  $(\theta, \phi)$ , and covering only a small region  $\Delta\Omega$  of solid angle

Then the differential cross section  $d\sigma/d\Omega$  for that direction is measured as

$$\frac{d\sigma}{d\Omega}(\theta, \phi) = \frac{N_{\text{scatt}}^{\Delta\Omega}/T}{N_T \times (N_{\text{in}}/T/A) \times \Delta\Omega} = \frac{N_{\text{scatt}}^{\Delta\Omega}}{N_{\text{in}}} \frac{A}{N_T} \frac{1}{\Delta\Omega}$$

where  $N_{\text{scatt}}^{\Delta\Omega}$  is the number of particles detected in time  $T$

- A widely used unit for cross sections is the *barn*, defined as

$$1 \text{ b} \equiv 10^{-28} \text{ m}^2$$

(cf: the cross sectional area of the proton  $\sim 10^{-30} \text{ m}^2$ )

## Interpretation of the Total Cross Section

- The total cross section  $\sigma$  has dimensions of area :
  - it can be thought of as the *effective transverse area*  $\sigma_{\text{eff}}$  presented by each scattering centre to the incoming beam
- To see this: for a target containing  $N_T$  particles, each having an effective transverse area  $\sigma_{\text{eff}}$ , the total *effective* area presented to the beam is

$$A_{\text{eff}} = N_T \sigma_{\text{eff}} \quad (9.62.1)$$

- If the *physical* transverse area presented by the target is  $A$ , then

$$f_{\text{scatt}} = \frac{A_{\text{eff}}}{A}$$

and equation (9.60.1) becomes

$$\sigma = \frac{A_{\text{eff}}}{A} \frac{A}{N_T} = \frac{A_{\text{eff}}}{N_T}$$

- Comparing with equation (9.62.1) above then immediately gives

$$\boxed{\sigma = \sigma_{\text{eff}}}$$

## Scattering in Classical Dynamics

- First consider *classical* scattering in a central potential  $V(r)$  :

- each incoming particle follows a well defined trajectory

There is a one-to-one correspondence between the scattering angle  $\theta$  and the impact parameter  $b$  :

$$b = b(\theta) \quad j$$

( usually, small  $b \Rightarrow$  large  $\theta$  )

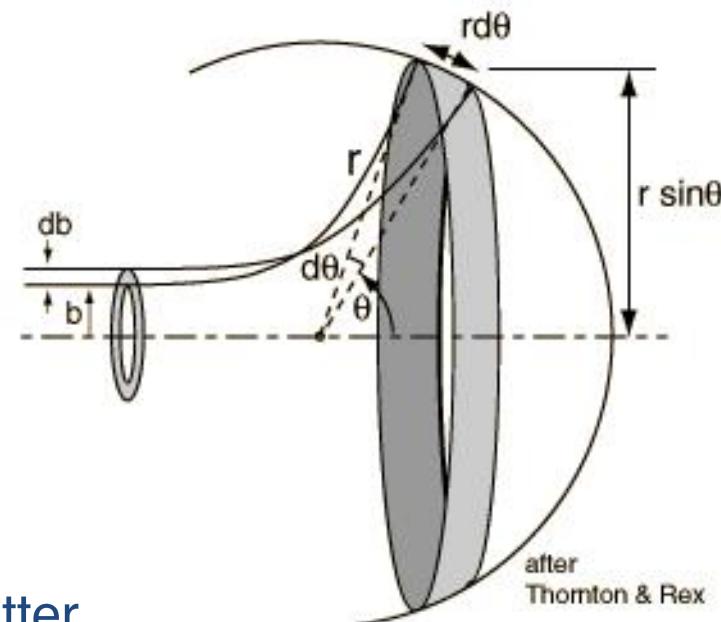
- Incoming particles between  $b$  and  $b + db$  scatter into outgoing angles between  $\theta$  and  $\theta + d\theta$  ; hence

$$\frac{d\sigma}{d\Omega} = \frac{j \times 2\pi b \, db}{j \times d\Omega} \quad (d\Omega = 2\pi d \cos \theta)$$

⇒

$$\boxed{\frac{d\sigma}{d\Omega} = b(\theta) \left| \frac{db(\theta)}{d \cos \theta} \right|}$$

( *classical* )

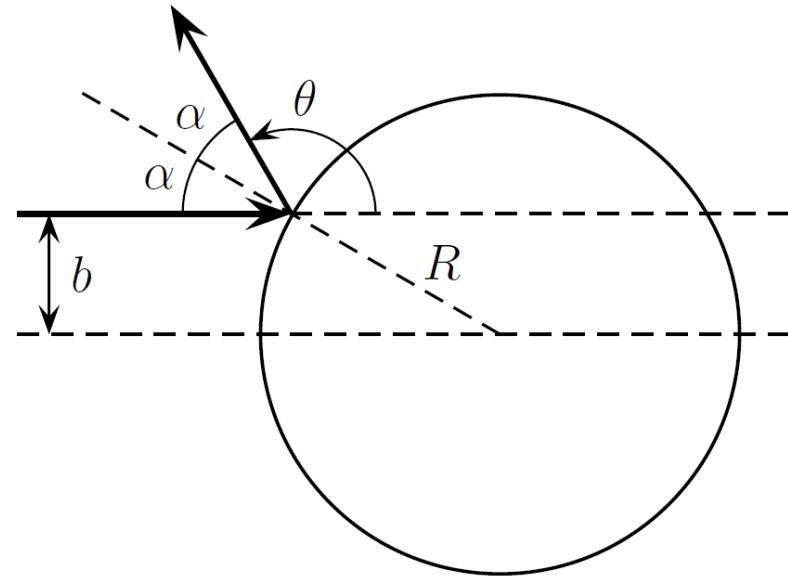


## Elastic Scattering from a Hard Sphere

- For example, consider classical *hard sphere elastic scattering* :

$$\begin{aligned} b(\theta) &= R \sin \alpha \\ &= R \sin \left( \frac{\pi - \theta}{2} \right) \\ &= R \cos(\theta/2) \end{aligned}$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = b(\theta) \left| \frac{db(\theta)}{d \cos \theta} \right| = \frac{1}{4} R^2$$



In this case, the differential cross section is independent of the scattering angle  $\theta$  (i.e. the scattering is isotropic)

- The total cross section,

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \frac{1}{4} R^2 \times 4\pi = \pi R^2$$

is equal to the *projected* (transverse) area of the sphere

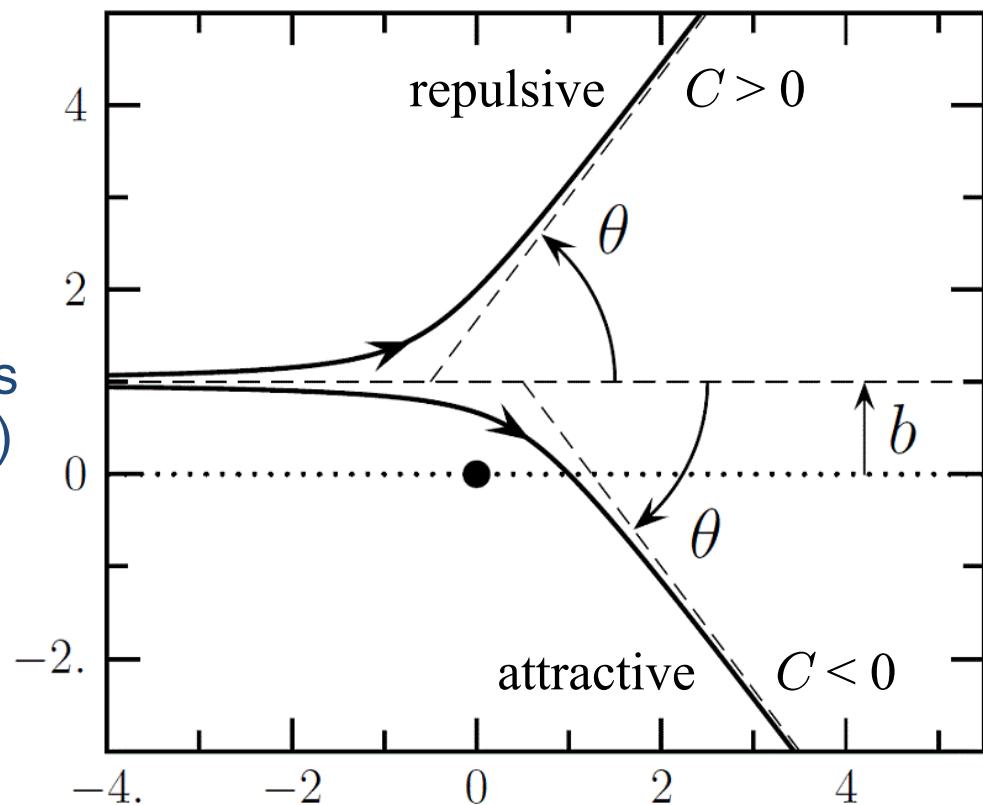
## Classical Coulomb Scattering

- For classical *Coulomb scattering*, the incoming particle follows a hyperbolic trajectory :

$$V(r) = \frac{C}{r} ; \quad C \equiv \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0}$$

The connection between impact parameter and scattering angle is the same for the repulsive ( $C > 0$ ) and attractive ( $C < 0$ ) cases :

$$b(\theta) = \frac{|C|}{2E} \cot \frac{\theta}{2}$$



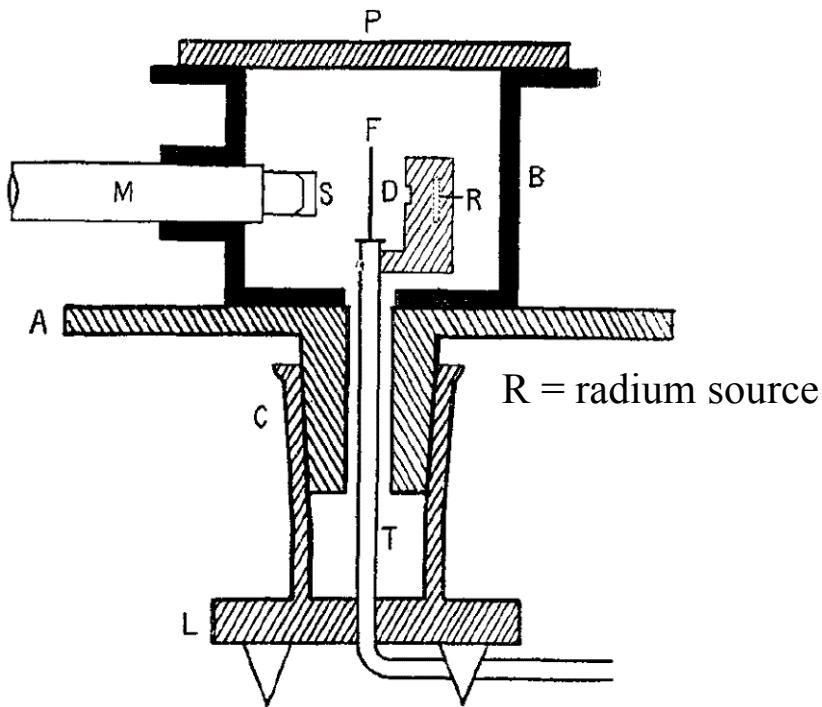
- This leads to the *Rutherford formula*

[E. Rutherford, Phil. Mag. 21 \(1911\) 669](#)

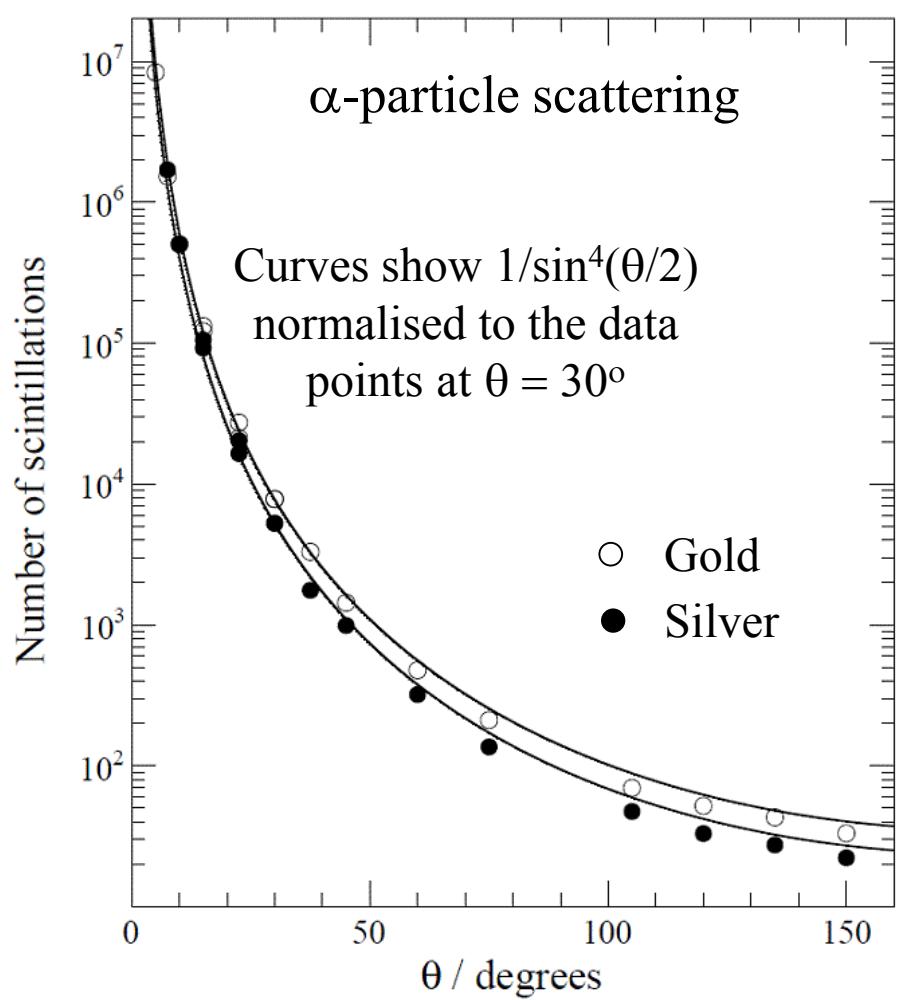
$$\frac{d\sigma}{d\Omega} = \frac{C^2}{16E^2} \frac{1}{\sin^4(\theta/2)}$$

## Classical Coulomb Scattering (2)

- Tested by Geiger and Marsden (1913) by scattering  $\alpha$ -particles from a gold or silver foil (F) :



Count scintillations on a rotatable ZnS screen (S) viewed by a microscope (M)



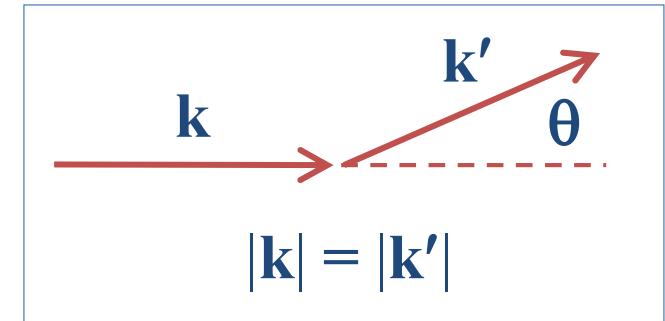
- Geiger and Marsden also tested the predicted  $(Z_1 Z_2/E)^2$  dependence

## Quantum Scattering

- Now consider a *quantum* description of scattering :
  - we no longer have a well-defined correspondence  $b(\theta)$  between impact parameter and scattering angle
  - scattering is inherently *probabilistic* in nature
- A full treatment of quantum scattering is a huge topic, and the appropriate approach depends on circumstances (relativistic or non-relativistic etc.)
  - (e.g. see TP2 for a more complete treatment)
- Here we limit ourselves to a consideration of “high energy” (but still non-relativistic) scattering from a fixed “small” potential  $V(\mathbf{r})$ 
  - the *Born approximation*
- The Born cross section will be obtained using Fermi’s Golden Rule in the zero frequency limit,  $\omega = 0$ 
  - ( in which case the perturbation  $H'(t)$  becomes the static potential  $V(\mathbf{r})$  )

# The Born Approximation

- Consider scattering from a fixed potential such that the potential energy  $V(\mathbf{r})$  is a small contribution to the overall Hamiltonian
  - applies mainly to the scattering of high energy particles
- In the initial state  $|\psi_i\rangle$  :
  - a free particle approaches from a large distance with three-momentum
$$\mathbf{p} = \hbar\mathbf{k}$$
- In the final state  $|\psi_f\rangle$  :
  - the scattered particle moves away with three-momentum
$$\mathbf{p}' = \hbar\mathbf{k}'$$
- Fermi's Golden Rule gives the transition rate as



$$\Gamma(i \rightarrow f) = \frac{2\pi}{\hbar} |\langle \psi_f | V(\mathbf{r}) | \psi_i \rangle|^2 g(E)$$

## The Born Approximation (2)

- In the limit  $\omega \rightarrow 0$  (where  $E' = E \pm \hbar\omega$ , slide 9.51) the incoming and outgoing energies must be equal (*elastic scattering*) :

$$E = \frac{|\mathbf{p}|^2}{2m} = \frac{|\mathbf{p}'|^2}{2m} ; \quad |\mathbf{k}| = |\mathbf{k}'|$$

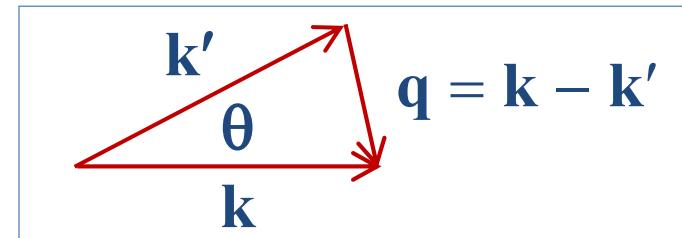
- We approximate the incoming and outgoing particles by plane waves :

$$\psi_i(\mathbf{r}, t) = \frac{1}{L^{3/2}} e^{i\mathbf{k} \cdot \mathbf{r} - iEt/\hbar} ; \quad \psi_f(\mathbf{r}, t) = \frac{1}{L^{3/2}} e^{i\mathbf{k}' \cdot \mathbf{r} - iEt/\hbar}$$

where we have chosen to normalise the wavefunctions to unity in a cube of arbitrary size  $L^3$

- The matrix element involved in Fermi's Golden Rule is then

$$\begin{aligned} \langle \psi_f | V(\mathbf{r}) | \psi_i \rangle &= \frac{1}{L^3} \int e^{-i\mathbf{k}' \cdot \mathbf{r}} V(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} d^3 \mathbf{r} \\ &= \frac{1}{L^3} \int V(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d^3 \mathbf{r} \end{aligned}$$



## The Born Approximation (3)

- Restricted to a solid angle  $d\Omega$ , the density of states  $g(E)$  available to the final state scattered particle is (see Appendix B of Handout 3)

$$g(E) = \frac{L^3 mk}{2\pi^2 \hbar^2} \times \frac{d\Omega}{4\pi} = \frac{L^3 mk}{8\pi^3 \hbar^2} d\Omega \quad (9.70.1)$$

The scattering rate into  $d\Omega$  in the direction  $(\theta, \phi)$  is then

$$\Gamma(i \rightarrow f) = \frac{2\pi}{\hbar} \left| \frac{1}{L^3} \int V(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d^3 r \right|^2 g(E) \quad (9.70.2)$$

The integral above is the Fourier transform of the potential energy  $V(\mathbf{r})$ , with respect to  $\hbar\mathbf{q}$ , the momentum transfer in the collision

- For an incoming plane wave,  $\psi(\mathbf{r}) = L^{-3/2} e^{i\mathbf{k} \cdot \mathbf{r}}$ , the flux is

$$\mathbf{j} = -\frac{i\hbar}{2m} [\psi(\mathbf{r})^* \nabla \psi(\mathbf{r}) - \psi(\mathbf{r}) \nabla \psi(\mathbf{r})^*] = \frac{\hbar\mathbf{k}}{mL^3}$$

The differential cross section is therefore given by

$$\frac{d\sigma}{d\Omega} \equiv \frac{\Gamma(i \rightarrow f)}{(\hbar k / mL^3) \times d\Omega} \quad (9.70.3)$$

## The Born Approximation (4)

- Substituting equations (9.70.1) and (9.70.2) into equation (9.70.3) then gives the cross section in the Born approximation as

$$\frac{d\sigma}{d\Omega} = \left( \frac{m}{2\pi\hbar^2} \right)^2 \left| \int V(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3\mathbf{r} \right|^2$$

(the arbitrary normalisation volume  $L^3$  has now cancelled)

- Thus, for non-relativistic scattering in the Born approximation, the scattering amplitude is given by

$$f(\theta, \phi) = \frac{m}{2\pi\hbar^2} \int V(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d^3\mathbf{r}$$

(see next term's Nuclear & Particles course for the *relativistic* version)

## The Born Approximation (5)

- For a given incoming beam momentum,  $p$ , and given scattering angle,  $\theta$ , the vectors  $\mathbf{k}$  and  $\mathbf{k}'$  take the form

$$\begin{aligned}\mathbf{k} &= (0, 0, k) , \quad \mathbf{k}' = (k \sin \theta, 0, k \cos \theta) \\ \Rightarrow \mathbf{q} &= \mathbf{k} - \mathbf{k}' = k(-\sin \theta, 0, 1 - \cos \theta) \\ \Rightarrow q &\equiv |\mathbf{q}| = |\mathbf{k} - \mathbf{k}'| = 2k \sin(\theta/2)\end{aligned}\quad (p = \hbar k)$$

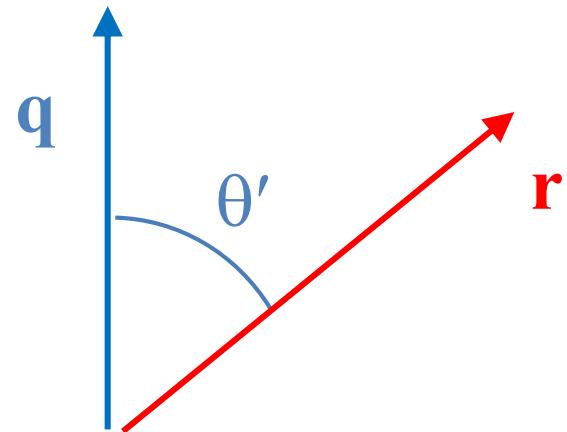
- To compute the FT of the potential  $V(\mathbf{r})$ , set up spherical polar coordinates defined relative to the vector  $\mathbf{q}$  :

(in the context of the FT integration, the vector  $\mathbf{q}$  is a constant, independent of the position vector  $\mathbf{r}$  )

Define  $\theta'$  to be the angle between the vectors  $\mathbf{q}$  and  $\mathbf{r}$  :

$$d^3\mathbf{r} = r^2 dr d\cos \theta' d\phi' = 2\pi r^2 dr d\cos \theta'$$

$$\mathbf{q} \cdot \mathbf{r} = qr \cos \theta'$$



## The Born Approximation (6)

- If the potential  $V$  is isotropic,  $V(\mathbf{r}) = V(r)$ , the FT integration becomes

$$\int V(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d^3\mathbf{r} = \int_0^\infty \int_{-1}^{+1} V(r) e^{iqr \cos \theta'} 2\pi r^2 dr d\cos \theta' \quad (q = |\mathbf{q}|)$$

- The integral over  $\cos \theta'$  can be carried out as (setting  $u \equiv \cos \theta'$ )

$$\int_{-1}^{+1} e^{iqru} du = \frac{2}{qr} \sin(qr)$$

- Hence, for an isotropic potential  $V(r)$ , the FT can be evaluated as

$$\boxed{\int V(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d^3\mathbf{r} = \frac{4\pi}{q} \int_0^\infty V(r) r \sin(qr) dr}$$

## Born Approximation : screened Coulomb potential

- For example, consider the scattering of particles of charges  $Z_1 e$  and  $Z_2 e$  via the (isotropic) *screened Coulomb potential* :

$$V(r) = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r} e^{-\lambda r}$$

- Then

$$\int V(\mathbf{r}) e^{i\mathbf{q} \cdot \mathbf{r}} d^3\mathbf{r} = \frac{4\pi}{q} \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0} \int_0^\infty e^{-\lambda r} \sin(qr) dr$$

where

$$q = |\mathbf{k} - \mathbf{k}'| = 2k \sin(\theta/2)$$

- The radial integral is  $\int_0^\infty e^{-\lambda r} \sin(qr) dr = \frac{q}{\lambda^2 + q^2}$

Hence the differential cross section for the screened Coulomb potential in the Born approximation is

$$\frac{d\sigma}{d\Omega} = \left( \frac{m}{2\pi\hbar^2} \right)^2 \left| \frac{Z_1 Z_2 e^2}{\epsilon_0} \frac{1}{4k^2 \sin^2(\theta/2) + \lambda^2} \right|^2$$

## Born Approximation : screened Coulomb potential (2)

- Taking the limit  $\lambda \rightarrow 0$ , we obtain the Rutherford cross section for scattering in a  $1/r$  potential :

$$V(r) = \frac{Z_1 Z_2 e^2}{4\pi\epsilon_0 r}$$

$$\boxed{\frac{d\sigma}{d\Omega} = \left( \frac{Z_1 Z_2 m e^2}{8\pi\epsilon_0 p^2 \sin^2(\theta/2)} \right)^2} \quad (p = \hbar k)$$

- The quantum cross section is therefore the same as the classical cross section (slide 9.65), for both an attractive and a repulsive  $1/r$  potential

This is a particular feature of the  $1/r$  potential (was Rutherford lucky?)

In general, the quantum and classical cross sections are different

e.g. for hard-sphere scattering (slide 9.64), the quantum cross section is *twice* the classical cross section :  $\sigma = 2\pi R^2$

- Examples Sheet : elastic scattering of non-relativistic electrons from hydrogen atoms at rest, in their ground state