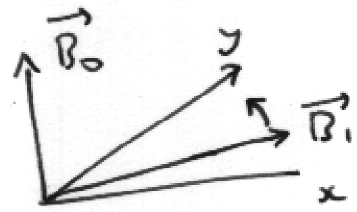
Lecture 16

Resonant perturbations

We start by considering the response of a spin-$\frac{1}{2}$ particle to an oscillating magnetic field.

The interesting case is to consider a constant field $\vec{B}_0$ superposed on a field of constant modulus but rotating with constant angular velocity ~~about~~ in the x-y plane:



Thus $\vec{B}_0 = B_0 \vec{e}_z$

$$\vec{B}_1 = B_1 (\vec{e}_x \cos\omega t + \vec{e}_y \sin\omega t)$$

Classically any object of angular momentum $\vec{J}$ and magnetic moment $\vec{m} = \gamma \vec{J}$ in a field $\vec{B}$ obeys:

$$\frac{d\vec{J}}{dt} = \vec{m} \times \vec{B}$$

Hence

$$\frac{d\vec{m}}{dt} = \gamma \vec{m} \times \vec{B}$$

Dotting this equation with $\vec{m}$ and $\vec{B}$ we get:

$$\frac{d}{dt}(\vec{m}^2) = 0 \qquad \text{and} \qquad \vec{B}\cdot\frac{d\vec{m}}{dt} = 0$$

Now if $\vec{B} = \vec{B}_0$ is constant then

$$\frac{d}{dt}(\vec{B}_0\cdot\vec{m}) = 0$$

which together with the first equation says that $\vec{m}$ rotates ("precesses") about $\vec{B}_0$ keeping a constant angle. This is "Larmor precession".

If we now add the rotating magnetic field $\vec{B}_1$ then the equation for the magnetic moment becomes

$$\frac{d\vec{m}}{dt} = \gamma\,\vec{m} \times (\vec{B}_0 + \vec{B}_1(t))$$

This is easier to understand if we work in a rotating frame XYZ where Z is identified with z while X, Y rotate with angular freq. ω in the (x,y) plane. Then

$$\vec{B}_1 = B_1\,\vec{e}_X$$

and also

$$\left(\frac{d\vec{m}}{dt}\right)_{rel} = \frac{d\vec{m}}{dt} - \omega\,\vec{e}_z \times \vec{m}$$

Hence:

$$\left(\frac{d\vec{m}}{dt}\right)_{rel} = \vec{m} \times (\gamma\vec{B}_0 + \gamma\vec{B}_1 + \omega\vec{e}_z)$$
$$= \vec{m} \times ((\gamma B_0 + \omega)\vec{e}_z + \gamma \hat{B}_1 \vec{e}_x)$$

Suppose at $t=0$ the spin is along the z-axis, and we apply a small field $\vec{B}_1$. Generically (as long as $\gamma B_0 + \omega \gg \gamma B_1$) the spin remains along the z-axis. However, at "resonance" when $\omega = -\gamma B_0$, the $\vec{e}_z$ term drops out. Now the spin precesses around the (rotating) X-axis – undergoing large deviations from its initial ~~posit~~ orientation.

Now consider the same phenomenon in quantum mechanics. A ~~two~~ spin-$\frac{1}{2}$ system can be represented by the operators

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and S_z has eigenvalues $m_s = \pm\frac{\hbar}{2}$, and eigenstates $\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

For future use we define $\omega_0 = -\gamma B_0$, $\omega_1 = -\gamma B_1$

So: $$\left(\frac{d\vec{m}}{dt}\right)_{rel} = \vec{m} \times ((\omega - \omega_0)\vec{e}_z - \omega_1 \vec{e}_x)$$

A generic state vector of this system is

$$\Psi(t) = \begin{pmatrix} a_+(t) \\ a_-(t) \end{pmatrix}$$

Now let the Hamiltonian be:

$$H(t) = -\vec{M} \cdot \vec{B}(t)$$

where $\vec{B}(t) = \vec{B}_0 + \vec{B}_1(t)$

The magnetic moment is proportional to the spin angular momentum, as we have seen above, so:

$$\vec{M} = \gamma \hat{\vec{S}} \quad \text{with } \hat{\vec{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z) \text{ as above.}$$

Also, $\gamma B_0 = -\omega_0$, $\gamma B_1 = -\omega_1$.

Thus $H(t) = \omega_0 \hat{S}_z + \omega_1(\cos\omega t\, \hat{S}_x + \sin\omega t\, \hat{S}_y)$

(we are neglecting the spatial degrees of freedom here, so $\vec{p}$ and $\vec{x}$ - dependent terms are ignored).

Using the representation of $\hat{\vec{S}}$, we get:

$$H = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix}$$

and the Schrödinger equation:

$$H\Psi = i\hbar \frac{d\Psi}{dt}$$

becomes:

$$i\frac{da_+(t)}{dt} = \tfrac{1}{2}\omega_0 a_+(t) + \tfrac{1}{2}\omega_1 e^{-i\omega t} a_-(t)$$

$$i\frac{da_-(t)}{dt} = \tfrac{1}{2}\omega_1 e^{i\omega t} a_+(t) - \tfrac{1}{2}\omega_0 a_-(t)$$

A simple change of variables:

$$b_\pm(t) = e^{\pm i\frac{\omega t}{2}} a_\pm(t)$$

converts the equation to:

$$i\frac{db_+}{dt} = -\tfrac{1}{2}(\omega-\omega_0)\, b_+ + \tfrac{1}{2}\omega_1 b_-$$

$$i\frac{db_-}{dt} = \tfrac{1}{2}\omega_1 b_+ + \tfrac{1}{2}(\omega-\omega_0)\, b_-$$

If we consider the wave function

$$\tilde{\Psi}(t) = \begin{pmatrix} b_+ \\ b_- \end{pmatrix} = \begin{pmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix}\begin{pmatrix} a_+ \\ a_- \end{pmatrix}$$

we see that it satisfies the Schrödinger eqn:

$$i\hbar\frac{d\tilde{\Psi}}{dt} = \tilde{H}\tilde{\Psi}$$

where $\tilde{H} = \frac{\hbar}{2}\begin{pmatrix} -(\omega-\omega_0) & \omega_1 \\ \omega_1 & \omega-\omega_0 \end{pmatrix}$

and now the Hamiltonian is time-independent!

[This is because

$$\begin{pmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix} = e^{i\frac{\omega t}{2}\sigma_3} = e^{i\omega t\frac{S_z}{\hbar}}$$

is the "rotation operator ~~for~~ in the spin-$\frac{1}{2}$ representation": in general $e^{i\theta\frac{\sigma_3}{2}}$ performs a rotation by an angle θ.]

Now that we have reduced the system to a simple Hamiltonian which is time-independent (like the classical problem in a rotating frame) we can state the problem we want to solve:

Suppose at time $t=0$ the system is in the state $\begin{pmatrix}1\\0\end{pmatrix}$. What is the probability $P_{+-}(t)$ of finding it in the state $\begin{pmatrix}0\\1\end{pmatrix}$ at time t?

For this we must construct the wave function $\psi(t)$ that is a linear combination of the two eigenvectors of $\tilde{H}$ and reduces to $\begin{pmatrix}1\\0\end{pmatrix}$ at $t=0$.

Next,

$$P_{+-} = \left| \left\langle \begin{pmatrix}0\\1\end{pmatrix} \middle| \psi(t) \right\rangle \right|^2 .$$

Diagonalising $\tilde{H}$, we find the (un-normalised) eigenvectors:

$$\begin{pmatrix} \omega_1 \\ \sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega \end{pmatrix}, \quad \begin{pmatrix} \omega_1 \\ -\sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega \end{pmatrix}$$

with eigenvalues $E_\pm = \pm\frac{\hbar}{2}\sqrt{\Delta\omega^2+\omega_1^2}$

Restoring their time dependence, the eigenvectors are:

$$\mathcal{N}_+ e^{-i\frac{E_+t}{\hbar}}\begin{pmatrix} \omega_1 \\ \sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega \end{pmatrix}, \quad \mathcal{N}_- e^{-i\frac{E_-t}{\hbar}}\begin{pmatrix} \omega_1 \\ -\sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega \end{pmatrix}$$

where
$$\mathcal{N}_+^2 = \omega_1^2 + (\Delta\omega^2+\omega_1^2) + \Delta\omega^2 + 2\Delta\omega\sqrt{\Delta\omega^2+\omega_1^2}$$
$$= 2\sqrt{\Delta\omega^2+\omega_1^2}\left(\sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega\right)$$
$$\mathcal{N}_-^2 = 2\sqrt{\Delta\omega^2+\omega_1^2}\left(\sqrt{\Delta\omega^2+\omega_1^2}-\Delta\omega\right)$$

Now construct a wave function

$$\Psi(t) = c_+\mathcal{N}_+ e^{-i\frac{E_+t}{\hbar}}\begin{pmatrix} \omega_1 \\ \sqrt{}+\Delta\omega \end{pmatrix} + c_-\mathcal{N}_- e^{-i\frac{E_-t}{\hbar}}\begin{pmatrix} \omega_1 \\ -\sqrt{}+\Delta\omega \end{pmatrix}$$

At $t=0$ the RHS should be $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, so

$$c_+\mathcal{N}_+\begin{pmatrix} \omega_1 \\ \sqrt{}+\Delta\omega \end{pmatrix} + c_-\mathcal{N}_-\begin{pmatrix} \omega_1 \\ -\sqrt{}+\Delta\omega \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Thus $c_+\mathcal{N}_+(\sqrt{}+\Delta\omega) + c_-\mathcal{N}_-(-\sqrt{}+\Delta\omega) = 0$

and $c_+\mathcal{N}_+\omega_1 + c_-\mathcal{N}_-\omega_1 = 1$

Thus, $(c_+N_+ - c_-N_-)\sqrt{} + (c_+N_+ + c_-N_-)\Delta\omega = 0$

$(c_+N_+ + c_-N_-)\omega_1 = 1$

So $c_+N_+ + c_-N_- = \frac{1}{\omega_1}$

$$c_+N_+ - c_-N_- = -\frac{\Delta\omega}{\omega_1\sqrt{}}$$

$$\Rightarrow \quad c_+N_+ = \frac{1}{2\omega_1}\left(1 - \frac{\Delta\omega}{\sqrt{\Delta\omega^2+\omega_1^2}}\right)$$

$$c_-N_- = \frac{1}{2\omega_1}\left(1 + \frac{\Delta\omega}{\sqrt{\Delta\omega^2+\omega_1^2}}\right)$$

So:

$$\psi(t) = \frac{1}{2\omega_1}\left(1 - \frac{\Delta\omega}{\sqrt{\Delta\omega^2+\omega_1^2}}\right)e^{-i\frac{E_+t}{\hbar}}\begin{pmatrix}\omega_1 \\ \sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega\end{pmatrix}$$

$$+ \frac{1}{2\omega_1}\left(1 + \frac{\Delta\omega}{\sqrt{\Delta\omega^2+\omega_1^2}}\right)e^{-i\frac{E_-t}{\hbar}}\begin{pmatrix}\omega_1 \\ -\sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega\end{pmatrix}$$

The amplitude of finding this in state $\begin{pmatrix}0\\1\end{pmatrix}$ is:

$$\left\langle \begin{smallmatrix}0\\1\end{smallmatrix} \middle| \psi(t)\right\rangle =$$

$$\frac{1}{2\omega_1}\left\{\left(1 - \frac{\Delta\omega}{\sqrt{\Delta\omega^2+\omega_1^2}}\right)e^{-i\frac{E_+t}{\hbar}}\left(\sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega\right)\right.$$

$$\left. + \left(1 + \frac{\Delta\omega}{\sqrt{\Delta\omega^2+\omega_1^2}}\right)e^{-i\frac{E_-t}{\hbar}}\left(-\sqrt{\Delta\omega^2+\omega_1^2}+\Delta\omega\right)\right\}$$

$$= \frac{1}{2\omega_1}\left\{e^{-iE_+t/\hbar}\frac{\omega_1^2}{\sqrt{\Delta\omega^2+\omega_1^2}} + e^{-i\frac{E_-t}{\hbar}} \cdot \frac{-\omega_1^2}{\sqrt{\Delta\omega^2+\omega_1^2}}\right\}$$

Since $E_- = -E_+$, this becomes:

$$\frac{-i\omega_1}{\sqrt{\Delta\omega^2+\omega_1^2}} \sin\frac{E_+ t}{\hbar} .$$

Hence $$\boxed{P_{+-} = \frac{\omega_1^2}{\Delta\omega^2+\omega_1^2} \sin^2\left(\tfrac{1}{2}\sqrt{\Delta\omega^2+\omega_1^2}\, t\right)}$$

This is known as <u>Rabi's formula</u>.

Now we again examine the limits considered earlier in the classical case. Let ω_1 be very small. For large $\Delta\omega \gg \omega_1$,

$$P_{+-} \sim \frac{\omega_1^2}{(\Delta\omega)^2} \sin^2\left(\tfrac{1}{2}\Delta\omega t\right) \ll 1$$

This varies sinusoidally but always remains very small because of the $\frac{\omega_1^2}{\Delta\omega^2}$ factor.

However when $\Delta\omega = 0$ the behaviour is totally different! Then,

$$P_{+-} \sim \sin^2\left(\tfrac{1}{2}\omega_1 t\right)$$

which becomes <u>unity</u> at time intervals

$$t = \frac{(2n+1)\pi}{\omega_1} .$$

Hence at resonance (only), a very weak rotating field is able to flip the spin from $\begin{pmatrix}1\\0\end{pmatrix}$ to $\begin{pmatrix}0\\1\end{pmatrix}$.

Note that the preceding calculation did not require perturbation theory! It is a special case of a more general approach to resonance, the "secular approximation".

Recall that in developing time-dependent perturbation theory, we had the equation

$$i\hbar \frac{db_m}{dt} = \lambda \sum_n e^{i\omega_{mn}t} W_{mn} b_n(t)$$

where $\Psi(t) = \sum_n b_n(t) e^{-iE_nt/\hbar} \psi_n(x)$

then we assumed all the $b_n(t)$ were close to their value at $t=0$:

$$b_n(t) = b_n^{(0)} + \lambda b_n^{(1)}(t) + \cdots$$

If we want to study a resonant perturbation over a long time, there is a better way to do things without assuming that

$$t \ll \frac{\hbar}{\lambda |W_{mk}|}$$

(which would not be justified).

What we do is to single out the states ψ_k, ψ_m (initial and final) for which we want to calculate P_{km}. For the corresponding $b_k(t)$ and $b_m(t)$ we make no perturbation expansion.

But for all the remaining b_n, $n \neq k, m$, we simply set them to zero.

The idea is that a resonant perturbation with $\omega \simeq \omega_{mk}$ will over a long time only couple ψ_k to ψ_m and not to any other ψ_n, $n \neq m, k$.

Hence we have:

$$i\hbar \frac{db_k}{dt} = \frac{\lambda}{2i} \sum_n \tilde{W}_{kn} \left(e^{i(\omega - \omega_{nk})t} - e^{-i(\omega + \omega_{nk})t} \right) b_n$$

$$\simeq \frac{\lambda}{2i} \left[\tilde{W}_{kk} \left(e^{i\omega t} - e^{-i\omega t} \right) b_k(t) + \tilde{W}_{km} \left(e^{i(\omega - \omega_{mk})t} - e^{-i(\omega + \omega_{mk})t} \right) \times b_m(t) \right]$$

and $$i\hbar \frac{db_m}{dt} \simeq \frac{\lambda}{2i} \left[\tilde{W}_{mk} \left(e^{i(\omega + \omega_{mk})t} - e^{-i(\omega - \omega_{mk})t} \right) b_k + \tilde{W}_{mm} \left(e^{i\omega t} - e^{-i\omega t} \right) b_m \right]$$

Thereby the system is effectively reduced to a two-state system.

Moreover when $\omega \simeq \omega_{mk}$ then the terms $e^{\pm i\omega t}$ or $e^{i(\omega + \omega_{mk})t}$ oscillate rapidly and their effect is "worked out" over time. So we simply drop them.

This leads to the much simpler system:

$$\frac{db_k}{dt} = \frac{-\lambda}{2\hbar} e^{i(\omega - \omega_{mk})t} \tilde{W}_{km} b_m(t)$$

$$\frac{db_m}{dt} = \frac{\lambda}{2\hbar} e^{-i(\omega-\omega_{mk})t} \tilde{W}_{mk} b_k(t)$$

We need to solve this system for $b_m(t)$,

then $P_{km}(t) = |b_m(t)|^2$.

This is easy to solve exactly at resonance:

with $\omega = \omega_{mk}$ we have:

$$\frac{db_k}{dt} = \frac{-\lambda}{2\hbar} \tilde{W}_{km} b_m(t)$$

$$\rightarrow \quad \frac{d^2 b_k}{dt^2} = \frac{-\lambda^2}{4\hbar^2} |\tilde{W}_{mk}|^2 b_k(t)$$

$$\Rightarrow \quad b_k(t) = A \cos \frac{\lambda|\tilde{W}_{mk}|}{2\hbar} t + B \sin \frac{\lambda|\tilde{W}_{mk}|}{2\hbar} t$$

Now impose $b_k(0) = 1$ which fixes $A = 1$.

~~Now~~ $\cancel{b_m(t) = A \sin \frac{\lambda|\tilde{W}_{mk}|t}{2\hbar} - B \cos \frac{\lambda|\tilde{W}_{mk}|}{2\hbar} t}$

~~But at $t=0$ the state is purely b_k, so $b_m(t=0) = 0$. This fixes $B=0$.~~

~~Hence~~

Next, $$b_m(t) = \frac{1}{\frac{\lambda}{2\hbar}\tilde{W}_{km}}\left(\frac{\lambda}{2\hbar}|\tilde{W}_{mk}| A \sin\frac{\lambda}{2\hbar}|W_{mk}|t - \frac{\lambda}{2\hbar}|\tilde{W}_{mk}| B \cos\lambda|W_{mk}|t\right)$$

At $t=0$ the state is pure b_k, with $b_m(t=0) = 0$. Hence $B=0$ and we get:

$$b_m(t) = \frac{|\tilde{W}_{mk}|}{\tilde{W}_{km}} \sin\frac{\lambda}{2\hbar}|\tilde{W}_{mk}|t$$

So $$P_{km}(t) = \sin^2\frac{\lambda}{2\hbar}|\tilde{W}_{mk}|t.$$

We clearly see the resonant behaviour.

It is more tedious to show that the general solution to the resonant equation is:

$$P_{km}(t) = \frac{\lambda^2|\tilde{W}_{mk}|^2}{\lambda^2|\tilde{W}_{mk}|^2 + \hbar^2(\omega-\omega_{mk})^2} \times \sin^2\left(\sqrt{\frac{\lambda^2|\tilde{W}_{mk}|^2}{\hbar^2} + (\omega-\omega_{mk})^2}\ \frac{t}{2}\right)$$

which is Rabi's formula in a general situation, with

$$\omega_1 \to \frac{\lambda|\tilde{W}_{mk}|}{\hbar}, \quad \Delta\omega \to \omega - \omega_{mk}$$