PHY662, Spring 2004
Outline for Thurs. Jan. 29, 2004
Magnetic resonance: NMR, MRI

29th January 2004

1 Miscellaneous

1. New homework version.
2. Spins and direction.

2 Magnetic resonance

Here, we will follow the outline of the calculation given in Baym.

The key result is this:

> If you put a spin in a constant magnetic field, there is a well-defined precession rate $\omega_0 = \gamma|\vec{B}_o|$. If you in addition apply an oscillatory magnetic field of strength B_1 of frequency ω that is near to ω_0, the up/down amplitudes will strongly oscillate. The frequency of this oscillation in the amplitudes is $\omega_1 = \gamma B_1/2$. The amplitude is maximal when $\omega = \omega_0$ (resonance). As the energy of the spin depends on its orientation, this change in amplitude means that the spin is absorbing or radiating electromagnetic energy.

The calculation we will follow will be slightly simplified compared with Baym's discussion by a slightly different (impractical) choice for the oscillatory external magnetic field. The choice will be $\vec{B}_1 = \frac{B_1}{2}\cos(\omega t)\hat{x} - \frac{B_1}{2}\sin(\omega t)\hat{y}$ (the more realistic calculation uses only one of these components, i.e., $\vec{B}_1$ is linearly polarized in real life; the factor of $\frac{1}{2}$ makes the results agree with the linear polarized case $\vec{B}_1 = B_1\cos(\omega t)$). Let the static magnetic field be given by $\vec{B}_0 = B_o\hat{z}$. The spin Hamiltonian is then

$$\mathcal{H} = -\gamma\vec{S}\cdot\vec{B} = -\gamma[B_0 S_z + \frac{B_1}{2}S_x\cos(\omega t) - \frac{B_1}{2}S_y\sin(\omega t)]\,.$$

The primary time dependence comes from B_0 and we are working in the $\hat{z}$-basis, so it is reasonable to remove the time independence of the precession in the static field by rewriting the wave function (spinor) $|\psi\rangle$ as a product of the primary time dependence and a "slow" part, $|\psi'(t)\rangle$:

$$|\psi(t)\rangle = e^{i\omega t\sigma_z/2}|\psi'(t)\rangle \, .$$

The Schrodinger equation $i\hbar\frac{\partial}{\partial t}|\psi\rangle = \mathcal{H}|\psi\rangle$ is then (since $S_z = \frac{\hbar}{2}\sigma_z$, etc. and setting$\omega_1 = \gamma B_1/2$):

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}e^{i\omega t\sigma_z/2}|\psi'(t)\rangle &= [-\gamma B_0 S_z - \gamma\frac{B_1}{2}S_x\cos(\omega t) + \gamma\frac{B_1}{2}S_y\sin(\omega t)]e^{i\omega t\sigma_z/2}|\psi'(t)\rangle \\ &= \hbar[-\frac{1}{2}\omega_0\sigma_z - \frac{\omega_1}{2}\sigma_x\cos(\omega t) + \frac{\omega_1}{2}\sigma_y\sin(\omega t)]e^{i\omega t\sigma_z/2}|\psi'(t)\rangle \end{aligned}$$

Since $\frac{\partial}{\partial t}e^{i\omega t\sigma_z/2}|\psi'\rangle = \frac{i}{2}\omega\sigma_z e^{i\omega t\sigma_z/2}|\psi' > + e^{i\omega t\sigma_z/2}\frac{\partial}{\partial t}|\psi' >$, multiplying both sides by $e^{-i\omega t\sigma_z}$ and cancelling out the $\hbar$'s gives the equation

$$-\frac{\omega}{2}\sigma_z|\psi'\rangle + i\frac{\partial}{\partial t}|\psi'\rangle = -\frac{1}{2}\omega_0\sigma_z|\psi' > + e^{-i\omega t\sigma_z/2}[\frac{\omega_1}{2}\sigma_x\cos(\omega t) - \frac{\omega_1}{2}\sigma_y\sin(\omega t)]e^{i\omega t\sigma_z}|\psi'(t)\rangle \, .$$

Now, σ_z *anticommutes* with σ_x and σ_y. So $\sigma_z\sigma_x = -\sigma_x\sigma_z$. But

$$\sigma_z^2\sigma_x = -\sigma_z\sigma_x\sigma_z = \sigma_x\sigma_z^2 \, .$$

This means that odd powers of σ_z anticommute with σ_x while even powers commute. A similar demonstration holds for σ_y. Using the expansion for the exponential, this means that

$$e^{-i\omega t\sigma_z/2}\sigma_x = \sigma_x e^{i\omega t\sigma_z/2} \, ,$$

giving

$$\begin{aligned} i\frac{\partial}{\partial t}|\psi'\rangle &= \left\{\frac{\omega-\omega_0}{2}\sigma_z - \frac{\omega_1}{2}\left[\sigma_x\cos(\omega t) - \sigma_y\sin(\omega t)\right]e^{i\omega t\sigma_z}\right\}|\psi'\rangle \\ &= \left\{\frac{\omega-\omega_0}{2}\sigma_z - \frac{\omega_1}{2}\left[\sigma_x\cos(\omega t) - \sigma_y\sin(\omega t)\right]\left[\cos(\omega t) + i\sin(\omega t)\sigma_z\right]\right\}|\psi'\rangle \\ &= \left\{\frac{\omega-\omega_0}{2}\sigma_z - \frac{\omega_1}{2}\begin{bmatrix} 0 & \cos(\omega t) + i\sin(\omega t) \\ \cos(\omega t) - i\sin(\omega t) & 0 \end{bmatrix}\begin{bmatrix} e^{i\omega t} & 0 \\ 0 & e^{-i\omega t} \end{bmatrix}\right\}|\psi'\rangle \\ &= \left\{\frac{\omega-\omega_0}{2}\sigma_z - \frac{\omega_1}{2}\begin{bmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{bmatrix}\begin{bmatrix} e^{i\omega t} & 0 \\ 0 & e^{-i\omega t} \end{bmatrix}\right\}|\psi'\rangle \\ &= \left\{\frac{\omega-\omega_0}{2}\sigma_z - \frac{\omega_1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right\}|\psi'\rangle \\ &= \left(\frac{\omega-\omega_0}{2}\sigma_z - \frac{\omega_1}{2}\sigma_x\right)|\psi'\rangle \, . \end{aligned}$$

As the operator $\Omega = (\omega - \omega_0)\sigma_z - \omega_1\sigma_x$ is independent of time, the solution to this equation for $|\psi'\rangle$ is

$$\begin{aligned} |\psi'(t)\rangle &= e^{-it\vec{\Omega}/2}|\psi'(0)\rangle \\ &= e^{-it\Omega t\hat{\Omega}/2}|\psi'(0)\rangle \, , \end{aligned}$$

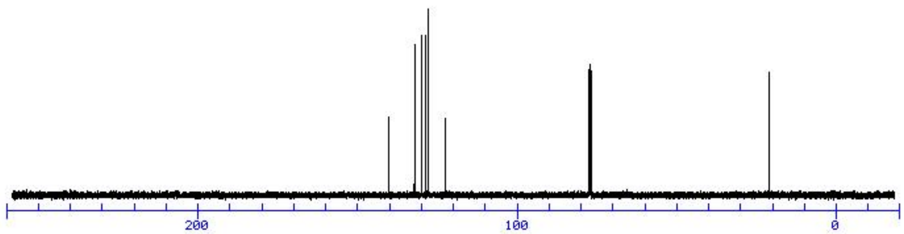


Figure 1: NMR spectrum. A plot of intensity of signal vs. frequency for C_7H_7Br from http://www.chem.ucla.edu/cgi-bin/webspectra.cgi?Problem=bp15&Type=C.

where $\Omega = \left[(\omega-\omega_0)^2+\omega_1^2\right]^{1/2}$ and $\hat{\Omega} = \vec{\Omega}/\Omega$. Substituting back in for the real spinor gives

$$|\psi(t)\rangle = e^{i\omega t\sigma_z/2}e^{-i\Omega t\hat{\Omega}/2}|\psi(0)\rangle \, .$$

This expression can be used to calculate the ampltitudes for the spinor, given that the particle is in a static magnetic field and a small oscillating one.

For example, suppose $|\psi(0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\omega = \omega_0$. Then $\hat{\Omega} = -\omega_1\sigma_x$ is just proportional to the "spin-flip" operator $\sigma_x = \frac{1}{\hbar}(S_+ + S_-)$. Up spins are turned down and down spins are turned up. The operator $e^{-\Omega t\hat{\Omega}/2}$ just rotates the spinor by an angle $\Omega t = \omega_1 t$ in this case. This "spin flipping" leads to an oscillation in the populations of the up and down spins, with the probability of switching between the two states becoming unity at time $\pi\omega_1^{-1}$. If the oscillating field has this duration, it is called a "π-pulse". (The $e^{i\omega t\sigma_z/2}$ in front gives a relative phase to the up/down amplitudes, *after* this spin flip has been applied and can be ignored for calculating the relative probabilities of up/down, but not other probabilities.)

$\Rightarrow$*Go back and note where there are changes for* $\vec{B}_1 = B_1\cos(\omega t)$. Use example of $\dot{a} = [\sin(\omega t) - 1]a$, with $\omega \gg 1$, noting that $\int_0^{2\pi/\omega} dt\, \sin(\omega t)t = \frac{2\pi}{\omega^2}$.

3 NMR, MRI

NMR: Consider the H-atom, which is *essentially* a proton, immersed in a relatively strong (few Tesla) magnetic field. Expose the atom to a $\frac{\pi}{2}$-pulse. Then $\langle\vec{\mu}\rangle$ rotates at frequency γB_0. This rotating magnetic dipole *radiates energy*. With enough radiating protons, you can pick up a signal. Note that this signal is low energy, radio frequency (RF). This radiation provides the basis of a method to detect atoms and the effects of their chemical environment (homework problem #3, set #3). People can even reconstruct the structure of proteins!

MRI: One gets chemical information, in a somewhat different fashion, but more importantly, one can get the spatial location of different types of tissue, where the characteristics of the relaxation of the radiation varies.

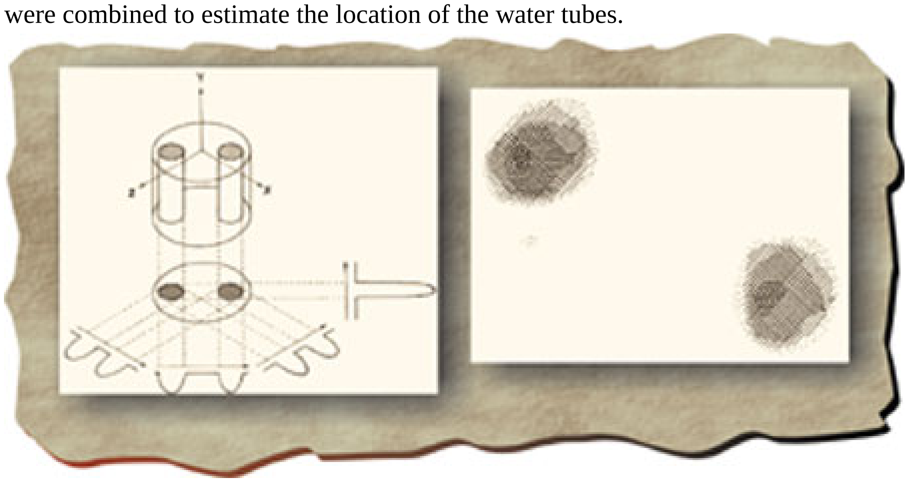
The tricky part is how to encode spatial information in the radio signal that the MRI machine receives.

3.1 MRI - One dimension (1D) - frequency encoding

The signal (picked up in a detection coil) from the excited protons has a frequency that depends on B_0. By making B_0 depend on, say, the x-position, after applying a $\frac{\pi}{2}$-pulse, one gets a signal composed of different frequencies, with the magnitude of the signal at a particular frequency dependent on the magnitude of excited protons at a given location. The spatial information is encoded in the frequency. Something like

$$S(t) \sim \int d\omega\, S(\omega) \sim \int d\omega\, n(x)\,,$$

where S is the signal in time or frequency space and $n(x)$ is the total density in the plane defined by x. Here is an early MRI image from 1973 that helped win a Nobel prize in 2003. Paul Lauterbur used an NMR machine with controllable linear field gradients to measure the density of water along four directions. These four projections were combined to estimate the location of the water tubes.



[From Physics Today, December 2003 - excerpted from *Nature*, 1973].

3.2 MRI - Slice selection

Before applying the gradient in the $\hat{x}$-direction, you can select a *slice* to excite. This can be done by applying a $\hat{z}$-gradient in the magnetic field so that B_0 depends on z. Then the resonance condition $\omega = \omega_0$ is satisfied only near a selected z. The $\frac{\pi}{2}$-pulse only excites a *2D layer* of protons.

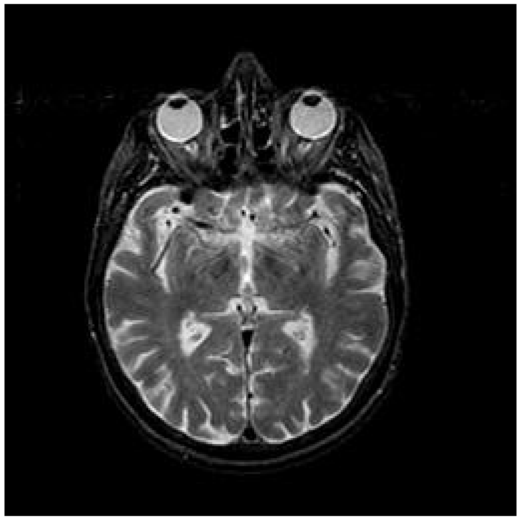


Figure 2: MRI image of a brain from The Whole Brain Atalas at www.med.harvard.edu. The image is a T_2-image, which plots, in space, how quickly the phase (xy-coherence) decays after a $\frac{\pi}{2}$-pulse.

3.3 MRI - 3D imaging

Here slice selection with a $\hat{z}$-gradient and $\frac{\pi}{2}$-pulse is followed by "phase encoding" and then frequency encoding. After many $\frac{\pi}{2}$-pulses and applied field gradients, one reconstructs the characteristics of volume elements in space. I won't describe phase encoding (one applies a gradient in a third direction, briefly, to rotate the spins in the xy plane in a spatially dependent fashion, which leads to phase differences in the radiation). Then there are lots of other tricks, like spin echo, etc., that get rather clever, but quite technical. The results are incredibly impressive, though, and allow for real-time imaging of beating hearts and flowing chemical activity, as well as the usual static 3D pictures.