**Physik IV** FS 2009
**Blatt 10** Abgabe: 08.05.09, 10:15

### 1. Kohärenz, Relaxation und Resonanz eines Elektronspins*

Es sei ein äusseres Magnetfeld von 1 T in der $\hat{z}$-Richtung angelegt.

a) Schreibe die Blochsche Gleichung für den Elektronenspin auf und schreibe sie in Komponenten aus, unter Verwendung von $x = x(t) = \langle \hat{s}_x \rangle$, $y = y(t) = \langle \hat{s}_y \rangle$ und $z = z(t) = \langle \hat{s}_z \rangle$, und löse die Differentialgleichung mit der Anfangsbedingung von Blatt 9:

$$|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \quad (1)$$

b) Nun wollen wir eine phänomenologische Wechselwirkung des Elektronspins mit der Umgebung einführen indem wir eine endliche Spin-Relaxationszeit $T_1 < \infty$ annehmen.

i) Was ist der Zeitbereich möglicher Kohärenzzeiten $T_2$?

ii) Was ist die Bedeutung der Kohärenzzeit $T_2$ (im Gegensatz zu $T_1$)?

iii) Wir nehmen nun an, dass ein thermodynamisches Gleichgewicht vorherrscht und dass die Wahrscheinlichkeit, dass der Spin im Grundzustand ist 90% ist. Bei welcher Temperatur ist das erfüllt?

iv) Schreibe nun wieder die Blochschen Gleichungen auf unter der Annahme, dass für $t \to \infty$ das in iii) erwähnte Gleichgewicht erreicht wird, aber unter Berücksichtigung einer allgemeinen Relaxationszeit $T_1$ und einer allgemeinen Kohärenzzeit $T_2$. Schreibe die Blochschen Gleichungen in Komponenten aus und löse die gekoppelte Differentialgleichung, wieder mit obiger Anfangsbedingung. Wie unterscheidet sich nun die Spin Dynamik für $T_1 = T_2 = \infty$ und $T_1 < \infty$, $T_2 < \infty$?

c) Es sei immer noch ein äusseres Magnetfeld von 1 T in der $\hat{z}$-Richtung angelegt. Wie koennte man Elektron Spin Resonanz erreichen? Beschreibe dazu i) die Richtung und ii) die Frequenz des zusätzlich anzulegenden Magnetfeldes. Was ist die Rabifrequenz und wodurch ist sie bestimmt?

**2.** For this exercise and the next one, consider the case of a non-uniform magnetic field. Here, each spin feels a slightly different value of $B_0$ and thus precesses at a slightly different frequency. In this case, it will be useful for us to consider the net magnetization as the sum of the individual magnetic moments of each proton.

$$\vec{M} = \sum_{i=1}^{N} \vec{\mu}_i \quad (2)$$

where each magnetic moment $\vec{\mu}_i$ is a classical vactor of constant magnitude $e\hbar/2Mc$, obeying the precession equation

$$\dot{\vec{\mu}}_i = \gamma \vec{\mu}_i \times \vec{B}_i \tag{3}$$

Now model the magnetic field at each proton as

$$\vec{B}_i = (B_0 + b_i)\hat{\mathbf{k}} \tag{4}$$

where $B_0$ is the average field value and the individual variations $b_i$ have a mean of zero. In the rotating reference frame the precession equations then become

$$\dot{\vec{\mu}}_i = \gamma \vec{\mu}_i \times (b_i \mathbf{k_r}) \tag{5}$$

Let us consider a system in thermal equilibrium for times $t < 0$ with $\vec{M} = M_0\hat{\mathbf{k}}$. Let's apply a 90° pulse at $t = 0$ with rotation being about $\hat{i}_r$ in the rotating reference frame. Just after the pulse the magnetic moment of each proton becomes, in this rotating frame

$$\vec{\mu}_i(0) = \frac{e\hbar}{2Mc}\hat{j}_r \tag{6}$$

and hence the magnetization is $\hat{M}(0) = M_0\hat{j}_r$.

Solve the precession equations for the individual moments $\vec{\mu}_i$ in the rotating frame for times $t \ll T_1$, then evaluate the sum to get the net magnetization $\vec{M}(t)$. Show that this net magnetization decays due to dephasing with a characteristic timescale

$$\frac{1}{T_2^*} = \gamma\sqrt{< b_i^2 >} \tag{7}$$

Hint: what you will get here is a sum of phases of the form

$$\sum_{n=1}^{N} e^{i\Phi_n} \tag{8}$$

To evaluate this sum, expand each phase as a series, then sum each order in $\Phi$ separately.

$$\sum_{n=1}^{N} e^{i\Phi_n} = \sum_{n=1}^{N}\{1 + i\Phi_n + \frac{1}{2}(i\Phi_n)^2 + ...\} = N + \sum_{n=1}^{N} i\Phi_n + \frac{1}{2}\sum_{n=1}^{N}(i\Phi_n)^2 + ... \tag{9}$$

The series you wind up with will have an (approximate) exponential representation with a characteristic decay time equal to $T_2^*$.

**3.** Now apply a 180° pulse at a much later time $t = \tau$ when the initial free-induction-decay signal has long since died away, i.e. $\tau > T_2$. Show that the magnetization will return to its full initial value at time $t = 2\tau$, then decays again with the same time constant $T_2^*$. This phenomenon is known as spin echo. Hint: Replace the x-y-plane in the rotating frame with the real and imaginary axes of the complex plane, write the vector $\vec{\mu}_i$ as a complex number and express the precession equation in this complex notation. Remember that the 180° pulse essentially rotates all of the spins around the x-axis, in the rotating reference frame, and this will be particularly easy to represent if the complex plane is used to represent the x-y-plane. This is the starting point for a lot of NMR dephasing analysis and is widely used in the NMR literature.

If there are several uncorrelated mechanisms that cause the variation in $\vec{B}_i$, then the dephasing rates for each just add to give a total dephasing rate $T_2^*$

$$\frac{1}{T_2^*} = \frac{1}{T_2^A} + \frac{1}{T_2^B} + ... \tag{10}$$

Some examples of sources of nonuniformity are

1. Inhomogeneities in the field of the permanent magnet used to supply the field $\vec{B}$, and

2. Interactions between individual spins

If you were doing research you would probably want to look at the interactions between the spins and be uninterested in the inhomogeneities of the magnet. Because the inhomogeneities in the magnet do not change with time, any dephasing they cause can be recovered using this spin-echo technique. The spin-spin interactions, however, change over time, and the dephasing they cause cannot be recovered by spin-echo.

We then may expect the net magnetization to decay immediately following the initial 90° pulse as

$$M(t) \sim M(0)e^{-(t/T_2^*)^2} \tag{11}$$

This initial decay is known as the free-induction-decay, or FID. Spin-spin interactions and other effects should keep the spin echo signal from returning to its full initial height $M(0)$ and the height of the spin echo should decay as well with a time constant of $T_2 \gg T_2^*$.

This provides us with a way of seperating the irreversible dephasing time $T_2$ from the total dephasing time $T_2^*$. Because $T_2$ is intrinsic to the sample and $T_2^*$ depends on your apparatus, it is usually $T_2$ that you are interested in.