F61/62: Nuclear Magnetic Resonance

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Abstract

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1 Introduction

Nuclear magnetic resonance (or short: NMR) spectroscopy is

1.1 Basics of Nuclear Magnetic Resonance

For a given Nuclei, whose spin $\vec{J}$ is unequal to 0, one can calculate it's magnetic dipole moment.

$$\vec{\mu} = \hbar\gamma\vec{J} \tag{1}$$

Where γ is the gyromagnetic factor. In this experiment we will look at exclusively protons $\gamma_{proton} = 2.6752 \cdot 10^8 sec^{-1} Tesla^{-1}$.

The magnetization of N nuclei can be obtained, by summing over all nuclei per unit volume

$$\vec{M} = \frac{1}{V}\sum_{i=1}^{N}\mu_i \tag{2}$$

In an external magnetic field the magnetic dipoles will realign themselves parallel or antiparallel to the direction of the magnetic field. The occupation number of the 2 states $N_\pm$, parallel N_+ and antiparallel N_- , follow Dirac statistic, but they can be approximated with a Boltzmann distribution in this case

$$N_\pm = N_0 e^{-\frac{E_0 \pm \Delta E}{kT}} \tag{3}$$

with N_0 being a normalization factor. The parallel state is energetically favourable, hence $N_+ > N_-$.

If we insert (3) into (2) and use that $N = N_+ + N_-$ we can derive

$$\vec{M} = \frac{|\mu|N}{V}\sinh(\frac{|\mu|B}{kT})\vec{e_z} \tag{4}$$

You can expand (4) with the assumption of a weak field ($\mu B << kT$), and derive Curie's law where $M \sim \frac{\vec{B_0}}{T}$.

In general, the magnetization can have an arbitrary direction relative to the external field. It can be generated by applying a high frequency pulse ω_{HF} to the ground state. In the following we decompose it into the components $\vec{M}_\parallel$ parallel and $\vec{M}_\perp$ perpendicular to the external field.

The Magnetic dipole interacts with an external magnetic field $\vec{B_0}$

$$\Delta E = -\vec{\mu} \cdot \vec{B_0} \tag{5}$$

and as a result the general state of magnetization will dissipate it's excitation energy and reach the ground state asymptotically on a characteristic time scale.

The interaction results in a torque

$$\vec{\tau} = \vec{M} \times \vec{B_0} \tag{6}$$

and since $\vec{B_0}$ is parallel to $\vec{M}_\parallel$, the torque only acts on $\vec{M}_\perp$. Without a relaxation processes, the rate of change is given by

$$\frac{d\vec{M}_\perp}{dt} = -\gamma\vec{M}_\perp \times \vec{B_0} \tag{7}$$

This differential equation can be solved by an ansatz $\vec{M} = M_{\parallel}(cos(\omega_L t), sin(\omega_L t), 0)$ with ω_L being the Larmor frequency

$$\omega_L = \gamma B_0 \tag{8}$$

Consider the ground state magnetization $\vec{M}$ parallel to $\vec{B_0}$, pointing in the z-direction. A sinusoidal voltage of frequency ω_{HF} is applied on the along x.direction oriented coil, resulting in an induced magnetic field B_1 which longitudinally polarized along the x-direction. Then $\vec{M}$ precesses around the x-axis. During a time interval Δt the angle α of the precession is then

$$\alpha = \gamma B_1 \Delta t \tag{9}$$

If the time interval is chosen such that $\alpha = 90\,\deg$, then $\vec{M}$ is rotated into a perpendicular component $\vec{M_\perp}$ along the y-axis. Such a pulse is called a 90 deg pulse. Similarly we define 180 deg pulse which results in magnetization antiparallel to the static field $\vec{B_0}$.

1.2 Relaxation time

Now we want to consider the relaxation process, which can be described with the Bloch equations. Here we introduce the rotating fame of the transverse magnetization, where the transverse magnetization is constant, if no relaxation processes takes place. The Bloch equations assume that the time evolution is dominated by a restoring force which is proportional to the deflection from equilibrium

$$\frac{dM_\perp(t)}{dt} = -\frac{M_\perp(t)}{T_2} \tag{10}$$

$$\frac{dM_\parallel(t)}{dt} = -\frac{M_\parallel(t) - M_0}{T_1} \tag{11}$$

where T_2 is the spin-spin relaxation time, T_1 the spin-lattice relaxation time and M_0 the ground state magnetization.

In the laboratory system we can now write the equations (7) as

$$\frac{dM_\perp(t)}{dt} = -\frac{M_\perp(t)}{T_2} + \gamma(\vec{B} \times \vec{M})_\perp \tag{12}$$

$$\frac{dM_\parallel(t)}{dt} = -\frac{M_\parallel(t) - M_0}{T_1} + (\vec{B} \times \vec{M})_\parallel \tag{13}$$

1.2.1 Measuring Spin-spin relaxation T_2 with spin-echo method

$$M_\perp(t) = M_\perp^0 e^{-\frac{t}{T_{T_2}}} \tag{14}$$

$$M_\parallel(t) = M_0(1 - 2e^{-\frac{t}{T_{T_1}}}) \tag{15}$$

2 Layout of the experiment

The experiment is performed with Bruker minispec p20 in parts I and II, Bruker minispec mq7.5 in part III.

The electronic unit of Bruker minispec p20 can generate 2 pulses, i.e. Puls I, which should be set to 90deg pulse, and Puls II for 180deg pulse. Output signal can be set to be single or periodic with variable periodicity. 4 Buttons allow us to produce pulse sequence Puls I - Puls I, Puls II - Puls I, Puls I - Puls II, and Carr-Purcell sequence(Puls I - Puls II - Puls II - Puls II - ...).

The magnetic unit is connected to the p20 electronics by a cable, which transmits the high frequency pulses ω_{HF} generated by the electronics to the coil inside the magnet and, at the same time, transmits the signal induced in the coil back to the electronics. The coil signal ω_L is then mixed with the signal ω_{HF}. The mixing generate two signals, one with a frequency of the sum and one with the frequency of the difference, i.e. the working frequency (on the order of a few hundred Hertz). One use the working frequency for analysis. Note that ω_{HF} is fixed, whereas ω_L can be changed by turning the screw of the magnet.

The following picture shows an osizilloscope (up left), the electronic unit of p20 (down left) and the magnetic unit of p20 (right). The Bruker minispec mq7.5 is equipped with a permanent magnetic field of 0.17 T and a measurement frequency of 7.5 MHz. Signals are generated by the sensitive nuclei(hydrogen and fluorine) because of NMR and are detected by the minispec. The following picture shows a power supply(?) (left) and mq7.5 (right).

The experiment measurements, data acquisition and analysis of all 3 parts of this experiment was performed on two local computers in laboratory. The software we used was LabVIEW, a systems engineering software for applications that require test, measurement, and control hardware and access to data.