Magnetic Resonance and External Fluctuation

The origin of a material's magnetic property is the magnetic moment from the angular momentum of its microscopic constituent such as electrons and the nuclei. For some material the tiny magnetic moments are aligned along a particular direction to produce a net magnetic field. In other words, the material has non-zero magnetization. For different kinds of material the tiny magnetic moments are randomly oriented, but when the material is put in an external magnetic field, the tiny magnetic moments rotate around the direction of the external magnetic field and in average the material develops a nonzero magnetization. If we turn off the external magnetic field the magnetization of the material may gradually decrease until it returns to its original value. It is due to the interaction between the magnetic moments, or their interaction with other microscopic degrees of freedom such as lattice vibration. This process is called the relaxation, which will be considered below using classical mechanics models.

Part A. Forced harmonic oscillator (3.6 pts)

We consider the problem of nuclear spin relaxation due to random fluctuation of other physical degrees of freedom such as lattice vibration or electron's magnetic dipole moments. In order to familiarize ourselves with a randomness in the solutions of a classical mechanics system, let us start with a forced harmonic oscillator of mass m and angular frequency ω_0. The energy of the oscillator changes because of the effect of a time-dependent external force.

$$m\frac{\mathrm{d}^2 q(t)}{\mathrm{d}t^2} + m\omega_0^2 q(t) = F(t) \tag{1}$$

where the external force is given by the following step-wise function.

$$F(t) = \begin{cases} 0, & t < 0 \\ +mf_0, & 0 \le t < T_0/2 \\ -mf_0, & T_0/2 \le t < T_0 \\ 0, & t \ge T_0 \end{cases}$$

Here $\omega_0 = 2\pi/T_0$ is the angular frequency of the oscillator $q(t)$. Suppose that the initial condition is given as $q(0) = A\sin\delta$, $\dot{q}(0) = A\omega_0\cos\delta$.

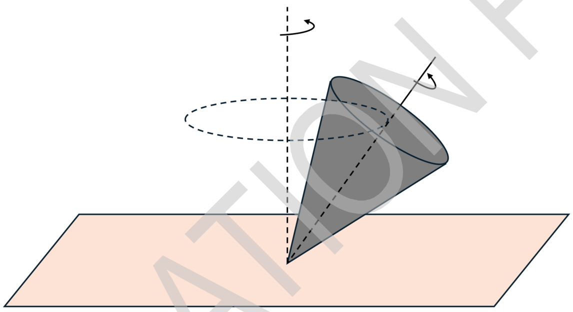
Before turning on the external force, energy is conserved and its value is $E_0 = \frac{m}{2}\omega_0^2 A^2$. Without losing generality we assume $-\pi \le \delta < \pi$.

A.1	Find the position q and the velocity $\dot{q} = \frac{\mathrm{d}q}{\mathrm{d}t}$ at $t = T_0$. Express them in terms of A, δ, f_0, ω_0.	1.2 pt

A.2	Consider the total mechanical energy $E(t) = \frac{m(\dot{q}^2+\omega_0^2 q^2)}{2}$. Calculate the difference of $E(t)$ between $t = T_0$ and $t = 0$, due to the effect of the external force $F(t)$. In other words, calculate $\Delta E \equiv E(t \ge T_0) - E(t \le 0)$ and express it in terms of A, δ, f_0, ω_0.	1.2 pt

A.3	Suppose that δ is a random variable with a uniform distribution in the range of $-\pi \leq \delta < \pi$. In other words, we have a large number of identical forced harmonic oscillators which all follow the same equation (1). Their initial conditions are given so that A is the same, but δ is chosen randomly from $-\pi \leq \delta < \pi$. Calculate the statistical average of the absorbed energy $\langle \Delta E \rangle$, and also the 2nd moment $\langle (\Delta E)^2 \rangle$.	1.2 pt

Part B: Precession of magnetic dipole moment and the use of rotating frame variables (6.4 pts)



The energy of a magnetic dipole moment under magnetic field $\vec{B}$ is given as

$E = -\vec{\mu} \cdot \vec{B} = -\gamma \vec{S} \cdot \vec{B}$

When we consider an infinitesimal rotation of the angular momentum $\vec{S}$and equate the energy difference with the product of torque ($\vec{\tau}$) and angular displacement, we obtain the equation for $\vec{S}$.

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

According to this equation, when $\vec{B}$ is constant the angular momentum $\vec{S}$ precesses around the direction of the magnetic field $\vec{B}$. This phenomenon is known as Larmor precession, and the frequency of the precession is given by $\gamma |\vec{B}|$ and in particular it is independent of the angle between $\vec{S}$ and $\vec{B}$.

Irradiation of circularly polarized light

Let us now consider turning on an oscillating magnetic field in xy-plane, in addition to a constant part along z-direction. The magnetic energy is then

$$E = -\omega_0 S_z - \omega_1 \cos(\omega_2 t) S_x - \omega_1 \sin(\omega_2 t) S_y \quad (2)$$

where ω_0, ω_1 are given by the relevant components of the magnetic field and γ, while ω_2 is the frequency of the oscillating magnetic field. We assume $\omega_0, \omega_1, \omega_2$ are all positive. The equations for $\vec{S}$ are

$$\dot{S}_x = +\omega_0 S_y - \omega_1 \sin(\omega_2 t) S_z$$
$$\dot{S}_y = -\omega_0 S_x + \omega_1 \cos(\omega_2 t) S_z$$
$$\dot{S}_z = -\omega_1 \cos(\omega_2 t) S_y + \omega_1 \sin(\omega_2 t) S_x$$

It is convenient to write these equations in terms of $S_\pm \equiv S_x \pm i S_y$. We have

$$\dot{S}_+ = -i\omega_0 S_+ + i\omega_1 e^{+i\omega_2 t} S_z$$
$$\dot{S}_- = +i\omega_0 S_- - i\omega_1 e^{-i\omega_2 t} S_z$$
$$\dot{S}_z = \frac{i\omega_1}{2}\left(e^{-i\omega_2 t} S_+ - e^{+i\omega_2 t} S_-\right)$$

For the next step, let us introduce spin in *rotating frame* using $S_\pm \equiv e^{\pm i\omega_2 t}\Sigma_\pm$, $S_z \equiv \Sigma_z$. One can show that the equations for $\Sigma_x \equiv \frac{1}{2}(\Sigma_+ + \Sigma_-)$, $\quad \Sigma_y \equiv \frac{i}{2}(\Sigma_- - \Sigma_+)$, and Σ_z can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{\Sigma} = \vec{M} \times \vec{\Sigma}$$

where $\vec{\Sigma} = (\Sigma_x, \Sigma_y, \Sigma_z)$ and $\vec{M} = (M_x, M_y, M_z)$.

B.1	Find the expressions for M_x, M_y, M_z in terms of $\omega_0, \omega_1, \omega_2$.	1.5 pt

The equations are simplified even further, if we consider a static rotation in xz-plane and define new variables $\Sigma_X, \Sigma_Y, \Sigma_Z$ as follows.

$$\Sigma_X = \cos\Theta\Sigma_x - \sin\Theta\Sigma_z$$
$$\Sigma_Y = \Sigma_y$$
$$\Sigma_Z = \sin\Theta\Sigma_x + \cos\Theta\Sigma_z$$

B.2	Derive the equations of motion for $\Sigma_X, \Sigma_Y, \Sigma_Z$ and express them using M_x, M_y, M_z and Θ.	0.9 pt

Then in terms of the new variables in doubly-rotating frame, the equations can be reduced to the following form,

$$\dot{\Sigma}_X = +\Omega\Sigma_Y$$
$$\dot{\Sigma}_Y = -\Omega\Sigma_X$$
$$\dot{\Sigma}_Z = 0$$

if Ω and $\tan\Theta$ are chosen appropriately.

B.3	By combining the answers of B.1 and B.2, find the expressions for Ω and $\tan\Theta$ in terms of $\omega_0, \omega_1, \omega_2$.	1.0 pt

Let us now consider a large number of spins with a statistical distribution of initial configurations: at $t = 0$, the average values satisfy $\langle S_x(0)\rangle = \langle S_y(0)\rangle = 0$ and $\langle S_z(0)\rangle > 0$. The spins all satisfy the same equation derived from Eq.(2).

B.4	Calculate $\langle S_z(t)\rangle$.	1.5 pt

B.5	If $\langle S_z(t)\rangle = 0$ at odd multiples of T_1 (i.e. $t = T_1, 3T_1, 5T_1, \cdots$) and $\langle S_z(t)\rangle > 0$ otherwise, what is the value of $\omega_1 T_1$?	1.5 pt