Problem Set #4

Problem 1

(a) The Hamiltonian for this system is

$$\hat{H} = -\hat{\vec{\mu}} \cdot \vec{B} = -\frac{g_N \mu_N}{2} B_0 \sigma_z \tag{1.1}$$

where μ is the nuclear magnetic moment of this nuclear spin. Note that nuclei have positive charge, hence the ground state, with magnetic moment parallel to the magnetic field, is spin up. The density matrix is therefore written as:

$$\hat{\rho} = \frac{N}{Z} e^{-\beta \hat{H}} = \frac{N}{Z} \begin{pmatrix} e^{\frac{\hbar}{2}\beta\omega_0} & 0 \\ 0 & e^{-\frac{\hbar}{2}\beta\omega_0} \end{pmatrix} \tag{1.2}$$

where $\beta = (k_B T)^{-1}$ is the thermodynamic beta, $\omega_0 = \frac{g_N \mu_N B_0}{\hbar}$ is the transition frequency, and

$$Z = \mathrm{tr}\left\{ e^{-\beta \hat{H}} \right\} = 2 \cosh \frac{\hbar \beta \omega_0}{2} \tag{1.3}$$

is the canonical partition function. The final density matrix we obtain is:

$$\hat{\rho} = \frac{N}{2} \operatorname{sech} \frac{\hbar \beta \omega_0}{2} \begin{pmatrix} e^{\frac{\hbar}{2}\beta\omega_0} & 0 \\ 0 & e^{-\frac{\hbar}{2}\beta\omega_0} \end{pmatrix} \tag{1.4}$$

1 point for assigning the spin up state to the ground state.
1 point for the correct density matrix. This includes substituting for E_1 and E_2 (Okay if this is done in a later part of the problem).

(b) Initial state is a steady state/commutes with system Hamiltonian, hence does not experience Larmor precession. A $\pi/2$ pulse along $\hat{x}$ sends $\uparrow_z$ to $\downarrow_y$, so the density matrix (in the rotating frame) is:

$$\hat{\rho} = \frac{N}{2} \begin{pmatrix} 1 & i \tanh \frac{\hbar\beta\omega_0}{2} \\ -i \tanh \frac{\hbar\beta\omega_0}{2} & 1 \end{pmatrix} \tag{1.5}$$

Alternatively the density matrix can be written in basis along y. Since the problem did not specify that the particle has a positive gyromagnetic ratio, dynamics with negative guromagnetic ratios are accepted, but the following parts have to match.
1 point for recognizing the correct effect of the $\pi/2$ pulse.
1 point for the correct density matrix.

(c) The magnetization can be found by taking the trace of the Pauli matrices with respect to the density operator.

$$\begin{aligned} M_z &= \mathrm{tr}\{\hat{\rho}\hat{\sigma_z}\} = 0 \\ M_x &= \mathrm{tr}\{\hat{\rho}\hat{\sigma_x}\} = 0 \\ M_y &= \mathrm{tr}\{\hat{\rho}\hat{\sigma_y}\} = -N \tanh \frac{\hbar\beta\omega_0}{2} \end{aligned} \tag{1.6}$$

These expectation values are constant in the interaction picture. To recover the time dependence we must transform back into the lab frame. This gives:

$$\begin{aligned} M_x(t) &= M_x(0)\cos\omega_0 t + M_y(0)\sin\omega_0 t \\ M_y(t) &= -M_x(0)\sin\omega_0 t + M_y(0)\cos\omega_0 t \end{aligned} \tag{1.7}$$

Note that the states are rotating clockwise. (counterclockwise if negative gyromagnetic ratio) Therefore, the magnetization is

$$\vec{M}(t) = -N\tanh\frac{\hbar\beta\omega_0}{2}\left(\sin\omega_0 t\hat{i} + \cos\omega_0 t\hat{j}\right) \tag{1.8}$$

1 point for reasonable work to find the magnetization vector.
1 point for the correct magnetization vectors.

(d) We need to find the number of hydrogen nuclei per volume. This is found by:

$$N = 2N_A M_W^{-1}\rho_W = 6.7\times 10^{22}\text{cm}^{-3} \tag{1.9}$$

Transition frequency is

$$\omega_0 = \frac{g_N\mu_N B_0}{\hbar} = 2.7\times 10^6 s^{-1} \tag{1.10}$$

Polarization is

$$\tanh\frac{\hbar\omega_0}{2k_B T} = 3.4\times 10^{-6} \tag{1.11}$$

$$\vec{M}\,(t) = 2N_A M_W^{-1}\rho_W\tanh\frac{g_N\mu_N B_0}{2k_B T}\left(\sin\omega_0 t\hat{i} + \cos\omega_0 t\hat{j}\right) = 2.3\times 10^{17}\text{cm}^{-3}\left(\sin\omega_0 t\hat{i} + \cos\omega_0 t\hat{j}\right) \tag{1.12}$$

1 point for involving correct constants.
1 point for correct answer.

(e) For 50% hyper-polarization,

$$\rho = N\begin{pmatrix} 3/4 & 0 \\ 0 & 1/4 \end{pmatrix} \tag{1.13}$$

$$\vec{M}(t) = \frac{N}{2}\left(\sin\omega_0 t\hat{i} + \cos\omega_0 t\hat{j}\right) \tag{1.14}$$

1 point for correct initial state.
1 point for correct answer.

Problem 2

$$\hat{H} = \frac{\mu_B}{\hbar}\hat{\vec{S}}\cdot\overleftrightarrow{g}\cdot\vec{B} = \frac{\mu_B}{\hbar}\left[\hat{S}_x(g_x(0)+\alpha_x\mathcal{E}\cos\omega t)B_x + \hat{S}_z(g_z(0)-\alpha_z\mathcal{E}\cos\omega t)B_z\right] \tag{2.1}$$

The time-independent H determines the spin quantization axis

$$\vec{\Omega}_0 = \frac{\mu_B}{\hbar}\left(g_x(0)B_x\hat{x} + g_z(0)B_z\hat{z}\right) \tag{2.2}$$

In order to have the maximal Rabi frequency, we just need to max the Rabi drive along the axis that perpendicular to $\vec{\Omega}_0$.

1 point for correct system Hamiltonian.

The Rabi drive field is

$$\vec{\Omega}_d = \frac{\mu_B}{\hbar}(B_x\alpha_x\hat{x} - B_z\alpha_z\hat{z})\mathcal{E}\cos\omega t \tag{2.3}$$

1 point for correct drive Hamiltonian.

Then, project the Rabi drive on the direction that perpendicular to $\vec{\Omega}_0$ to obtain the effective drive strength

$$\vec{\Omega}_d \cdot \vec{\Omega}_\perp = \frac{\mu_B\mathcal{E}B_xB_z}{\hbar}\frac{\alpha_x g_z(0) + \alpha_z g_x(0)}{\sqrt{g_x^2(0)B_x^2 + g_z^2(0)B_z^2}} \tag{2.4}$$

Let $B_x = \pm B_0\sin\theta$ and $B_z = \pm B_0\cos\theta$, then

$$\vec{\Omega}_d \cdot \vec{\Omega}_\perp = \pm\frac{\mu_B\mathcal{E}}{\hbar}\frac{[\alpha_x g_z(0) + \alpha_z g_x(0)]\cos\theta\sin\theta}{B_0\sqrt{g_x^2(0)\sin^2\theta + g_z^2(0)\cos^2\theta}} \tag{2.5}$$

1 point for evaluating effective drive strength.

The magnitude of such expression is maximized when $g_x^2(0)\sec^2\theta + g_z^2(0)\csc^2\theta$ is minimized, so we get the direction of B field to be

$$\theta = \pm\arctan\sqrt{\frac{g_z(0)}{g_x(0)}} \tag{2.6}$$

In vector form, the unit vector of the ideal direction is

$$\hat{B} = \pm\sqrt{\frac{g_z(0)}{g_x(0) + g_z(0)}}\hat{i} \pm \sqrt{\frac{g_x(0)}{g_x(0) + g_z(0)}}\hat{k} \tag{2.7}$$

1 point for correct answer.

Such direction might look weird on the first glance, but note that all α does is a constant factor in the magnitude (proportional to $|\vec{\alpha} \times \vec{g}_0|$), and when $\alpha_x = \alpha_z$, the strength of the drive is independent of direction, and is orthogonal to Ω_0.

Problem 3

(a)

$$\omega = \frac{1}{\hbar}\Delta E = \frac{3\hbar\pi^2}{2ma^2} + \frac{g\mu_B B_0}{\hbar} \tag{3.1}$$

1 point for correct transition energy, 1 point for evaluating transition frequency.

(b)

$$\langle 2\uparrow|\,\alpha\mathcal{E}\hat{p}_y\hat{\sigma}_z\,|1\downarrow\rangle = \frac{2\alpha\mathcal{E}}{a}\int_0^a \sin\frac{2\pi y}{a}(-i\hbar)\frac{\pi}{a}\cos\frac{\pi y}{a} = -\frac{8i\hbar\alpha\mathcal{E}}{3a} \tag{3.2}$$

Therefore the Hamiltonian in matrix form (with basis in the order of $|2\uparrow\rangle, |1\downarrow\rangle$) is

$$\hat{H}_d = \hbar\omega\frac{\hat{\sigma}_{z,l}}{2} + \frac{8\hbar\alpha\mathcal{E}(t)}{3a}\hat{\sigma}_{y,l} \tag{3.3}$$

If $\mathcal{E}(t) = \mathcal{E}\cos\omega t$, the Rabi frequency is

$$\Omega = \frac{8\alpha\mathcal{E}}{3a} \tag{3.4}$$

1 point for identifying the correct matrix element.
1 point for the correct Rabi frequency.

(c) In the interaction picture, the Block vector just rotates around the drive axis:

$$\vec{a}(t) = -\sin\Omega t\hat{i} - \cos\Omega t\hat{k} \tag{3.5}$$

$$\hat{\rho}(t) = \frac{1}{2}\left(\hat{I} + \vec{\sigma}_l \cdot \vec{a}(t)\right) = \frac{1}{2}\begin{pmatrix} 1-\cos\Omega t & -\sin\Omega t \\ -\sin\Omega t & 1+\cos\Omega t \end{pmatrix} \tag{3.6}$$

where σ_l denotes the logical Pauli operators.
1 point for correct approach to find the density matrix.
1 point for correct density matrix.

$$\mathrm{tr}\{\rho S_z\} = \frac{\hbar}{2}\vec{a}\cdot\hat{k} = -\frac{\hbar}{2}\cos\Omega t \tag{3.7}$$

(d)

$$\mathrm{tr}\{\rho S_x\} = \frac{\hbar}{2}\vec{a}\cdot\hat{i} = -\frac{\hbar}{2}\sin\Omega t \tag{3.8}$$

$$\mathrm{tr}\{\rho S_y\} = \frac{\hbar}{2}\vec{a}\cdot\hat{j} = 0 \tag{3.9}$$

Note that this solution was solved in the interaction picture. If you go to the lab frame then there will be additional time dependence.
1 point for setting up the expectation value as the trace (3 points total).
1 point for each correct spin expectation value (3 points total).

(e)

$$\langle 2\uparrow|\,\hat{y}\hat{\sigma}_y\,|1\downarrow\rangle = \frac{2}{a}\int_0^a \sin\frac{2\pi y}{a}y\cos\frac{\pi y}{a} = \frac{16ia}{9\pi^2} \tag{3.10}$$

Therefore,

$$\hat{y}\hat{\sigma}_y = -\frac{16a}{9\pi^2}\hat{\sigma}_{y,l} \tag{3.11}$$

Note that such operator does not make sense in interaction picture (what would y even means in interaction picture), although credit will still be granted.

$$\langle\hat{y}\hat{\sigma}_y\rangle = -\frac{16a}{9\pi^2}\left(\cos\omega t\,(0) + \sin\omega t\,(-\sin\Omega t)\right) = \frac{16a}{9\pi^2}\sin\omega t\sin\Omega t \tag{3.12}$$

This type of system is known as "ballistic spin resonance," see PRX 4, 011048 (2014).
1 point for setting up the expectation value as the trace.
1 point for correct expectation value.