Physics 8.421 Spring 2008 Solution set for assignment #3
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1. **Energy shifts in hydrogen due to the size of the proton**

   (a) Since the charge density is everywhere finite, the field $\vec{E}$ is continuous, while the spherical symmetry of the problem gives $\vec{E} = E_r\hat{r}$. Invoking Gauss' law $\oint \vec{E}\cdot d\vec{S} = 4\pi Q_{\text{enc}}$ (cgs units) for a spherical surface of radius r around the origin gives:

$$4\pi r^2 E_r = 4\pi \begin{cases} \frac{4}{3}\pi r^3 \rho_0 & (r < a) \\ \frac{4}{3}\pi a^3 \rho_0 & (r > a) \end{cases}$$

$$E_r = \frac{4}{3}\pi a \rho_0 \begin{cases} \frac{r}{a} & (r < a) \\ \frac{a^2}{r^2} & (r > a) \end{cases}$$

   Then,

$$\boxed{\phi(r) = -\int_\infty^r E_{r'}dr' = \frac{4}{3}\pi a^2 \rho_0 \begin{cases} \frac{1}{2}\left(3 - \left(\frac{r}{a}\right)^2\right) & (r < a) \\ \frac{a}{r} & (r > a) \end{cases}}$$

   (b) The total charge of the proton is e, so that

$$\rho_0 = \frac{e}{\frac{4}{3}\pi a^3}$$

   The potential for the electron is thus

$$U = -e\phi = -\frac{e^2}{a}\begin{cases} \frac{1}{2}\left(3 - \left(\frac{r}{a}\right)^2\right) & (r < a) \\ \frac{a}{r} & (r > a) \end{cases}$$

   The effect of the finite size of the proton is the deviation of the potential from the point source case, $U = -e^2/r$.

$$\Delta U = \begin{cases} -\frac{e^2}{2a}\left(3 - \left(\frac{r}{a}\right)^2 - \frac{2a}{r}\right) & (r < a) \\ 0 & (r > a) \end{cases}$$

   Working in first order perturbation theory, the energy shift of the $1S$ state, ΔU_{1S}, is given as

$$\Delta U_{1S} = \langle \psi_{1S}|\Delta U|\psi_{1S}\rangle = \int \Delta U |\psi_{1S}(\vec{r})|^2 d\vec{r}$$

   Since the proton radius a is very much less than the Bohr radius a_0, $\psi_{1S}(\vec{r}) \sim \psi_{1S}(0)$ in the region where ΔU is non-zero.

$$\Delta U_{1S} = \frac{1}{\pi a_0^3}\int_{r<a} \Delta U d\vec{r} = \frac{4}{5}\frac{e^2}{2a_0}\left(\frac{a}{a_0}\right)^2$$
$$= \frac{4}{5}13.606 \text{ eV}\left(\frac{0.9 \text{ fm}}{53 \text{ pm}}\right)^2 = 3.14 \times 10^{-9} \text{ eV} = \boxed{759 \text{ kHz}}$$

(c) Since the probability density at the origin scales as n^{-3}, $\Delta U_{2S} = \Delta U_{1S}/8$ and the shift of the $1S - 2S$ transition frequency is

$$\Delta U_{1S-2S} = \left(1 - \frac{1}{8}\right) \Delta U_{1S} = 664 \text{ kHz}$$

Since $\Delta U_{1S-2S} \propto a^2$,

$$\frac{\delta\left(\Delta U_{1S-2S}\right)}{\Delta U_{1S-2S}} = 2\frac{\delta a}{a}$$

$$\delta\left(\Delta U_{1S-2S}\right) \sim 2\frac{0.01}{0.9} 664 \text{ kHz} = \boxed{15 \text{ kHz}}$$

The frequency of the $1S - 2S$ transition is

$$3/4 \times 13.606 \text{ eV} = 10.2 \text{ eV} = 2.5 \times 10^{15} \text{ Hz}$$

Therefore, this requires $\boxed{6 \times 10^{-12}}$ relative frequency accuracy.

2. **Atoms in magnetic fields: the Breit-Rabi formula**

(a) Using $I_\pm = I_x \pm iI_y$ and $J_\pm = J_x \pm iJ_y$, we can rewrite the Hamiltonian as

$$H = \frac{ah}{\hbar^2}\left(\frac{I_+J_- + I_-J_+}{2} + I_zJ_z\right) + \left(g_J\frac{J_z}{\hbar} - g_I\frac{I_z}{\hbar}\right)\mu_0 B_z$$

This manifestly commutes with F_z (note that the action of each term leaves $m_I + m_J$ unchanged). Since $[H, F_z] = 0$, m_F is a good quantum number; i.e. states of different m_F are not mixed. Therefore, it is legitimate to solve the problem within a subspace of fixed $m_F = m$.
When $J = 1/2$, this subspace is spanned by $\{|m_I = m - \frac{1}{2}, m_J = \frac{1}{2}\rangle, |m_I = m + \frac{1}{2}, m_J = -\frac{1}{2}\rangle\}$. If we describe the Hamiltonian in this basis, it is expressed as the following 2×2 matrix.

$$\begin{pmatrix} ah\left(m-\frac{1}{2}\right)\frac{1}{2} + \left(\frac{g_J}{2} - g_I\left(m-\frac{1}{2}\right)\right)\mu_0 B_z & \frac{ah}{2}\sqrt{I\left(I+1\right) - \left(m+\frac{1}{2}\right)\left(m-\frac{1}{2}\right)}\sqrt{\frac{1}{2}\frac{3}{2}+\frac{1}{2}\frac{1}{2}} \\ \frac{ah}{2}\sqrt{I\left(I+1\right) - \left(m-\frac{1}{2}\right)\left(m+\frac{1}{2}\right)}\sqrt{\frac{1}{2}\frac{3}{2}+\frac{1}{2}\frac{1}{2}} & ah\left(m+\frac{1}{2}\right)\left(-\frac{1}{2}\right) + \left(-\frac{g_J}{2} - g_I\left(m+\frac{1}{2}\right)\right)\mu_0 B_z \end{pmatrix}$$

Introducing $x = (g_I + g_J)\,\mu_0 B_z / ahF^+$ with $F^+ = I + 1/2$, this can be simplified to

$$-\frac{ah}{4} - g_I m \mu_0 B_z + \frac{ah}{2}\begin{pmatrix} m + F^+x & \sqrt{F^{+2} - m^2} \\ \sqrt{F^{+2} - m^2} & -m - F^+x \end{pmatrix}$$

The eigenvalues of the matrix in the last term are

$$\lambda = \pm F^+\sqrt{1 + \frac{2mx}{F^+} + x^2}$$

So the eigenenergies are

$$E_m^\pm = -\frac{ah}{4} - mg_I\mu_0 B_z \pm \frac{ahF^+}{2}\sqrt{1+\frac{2mx}{F^+}+x^2} \tag{1}$$

This analysis does not cover the stretched states $m = \pm F^+$ where $m_I = \pm I$, $m_J = \pm 1/2$ and the sign is the same in both. These states are actually much simpler to deal with, since they have no near-degenerate partner to mix with: the energy is just the expectation value of the Hamiltonian in the state. The result is

$$E_{\pm F^+} = -\frac{ah}{4} \mp F^+ g_I\mu_0 B_z + \frac{ahF^+}{2}(1 \pm x)$$

so that equation 1 with the positive sign in front of the radical is valid also for the stretched states.

It is worth noting that the two states with the same m have different energy shifts. Also, we can check that the "center of mass" is zero, i.e. that the average shift over all the states vanishes.

$$\begin{aligned}
\sum_{-F^++1}^{F^+-1} E_m^+ + E_m^- &= -\frac{ah}{4} \times 2 \times (2F^+ - 1) = -ahF^+ + \frac{ah}{2} \\
E_{+F^+} &= -\frac{ah}{4} - F^+ g_I\mu_0 B_z + \frac{ahF^+}{2}(1+x) \\
E_{-F^+} &= -\frac{ah}{4} + F^+ g_I\mu_0 B_z + \frac{ahF^+}{2}(1-x) \\
E_{+F^+} + E_{-F^+} &= -\frac{ah}{2} + ahF^+
\end{aligned}$$

(b) $I = 3/2$ gives $F^+ = 2$.

$$\begin{aligned}
\frac{E_m^\pm}{2ah} &= -\frac{1}{8} - \frac{g_I}{g_I+g_J}mx \pm \frac{1}{2}\sqrt{1+mx+x^2} \\
\frac{E_2}{2ah} &= -\frac{1}{8} - \frac{g_I}{g_I+g_J}2x + \frac{1}{2}(1+x) \\
\frac{E_{-2}}{2ah} &= -\frac{1}{8} - \frac{g_I}{g_I+g_J}(-2)x + \frac{1}{2}(1-x)
\end{aligned}$$

These energy levels are shown in figure (1). There are 8 lines in the figure, but it is not possible to resolve them at the scale of the figure. Let us consider specific ranges of x values.

Since $g_I/g_J \ll 10^{-3}$, we can take $x \sim g_J\mu_0 B_z/2ah$. Thus x is a good measure of the ratio of the effect of the hyperfine Hamiltonian to that of the Zeeman Hamiltonian caused by the electron spin. In other words, x represents the degree of coupling between $|m_I = m - \frac{1}{2}, m_J = \frac{1}{2}\rangle$ and $|m_I = m + \frac{1}{2}, m_J = -\frac{1}{2}\rangle$ in the $\{m_F = m\}$ subspace.

i. $x \ll 1$, figure (2)
Here the levels are mainly determined by the hyperfine interaction term and the Zeeman term lifts its degeneracy. Levels split proportional to the g-factors, which you will calculate later on.

ii. $x \sim 1$, figure (2)
Both terms compete and show interesting phenomena like field-independent transitions, which is the topic of the next few questions.

iii. $x > 1$, figures (3-1) and (3-2)
Now the Hamiltonian starts to look like

$$H \sim m_J g_J \mu_0 m_J B_z + ahm_J m_I$$

So the electron spin dominates the spectrum ($g_J \mu_0 m_J B_z$), but its degeneracy is lifted by ($ahm_J m_I$).

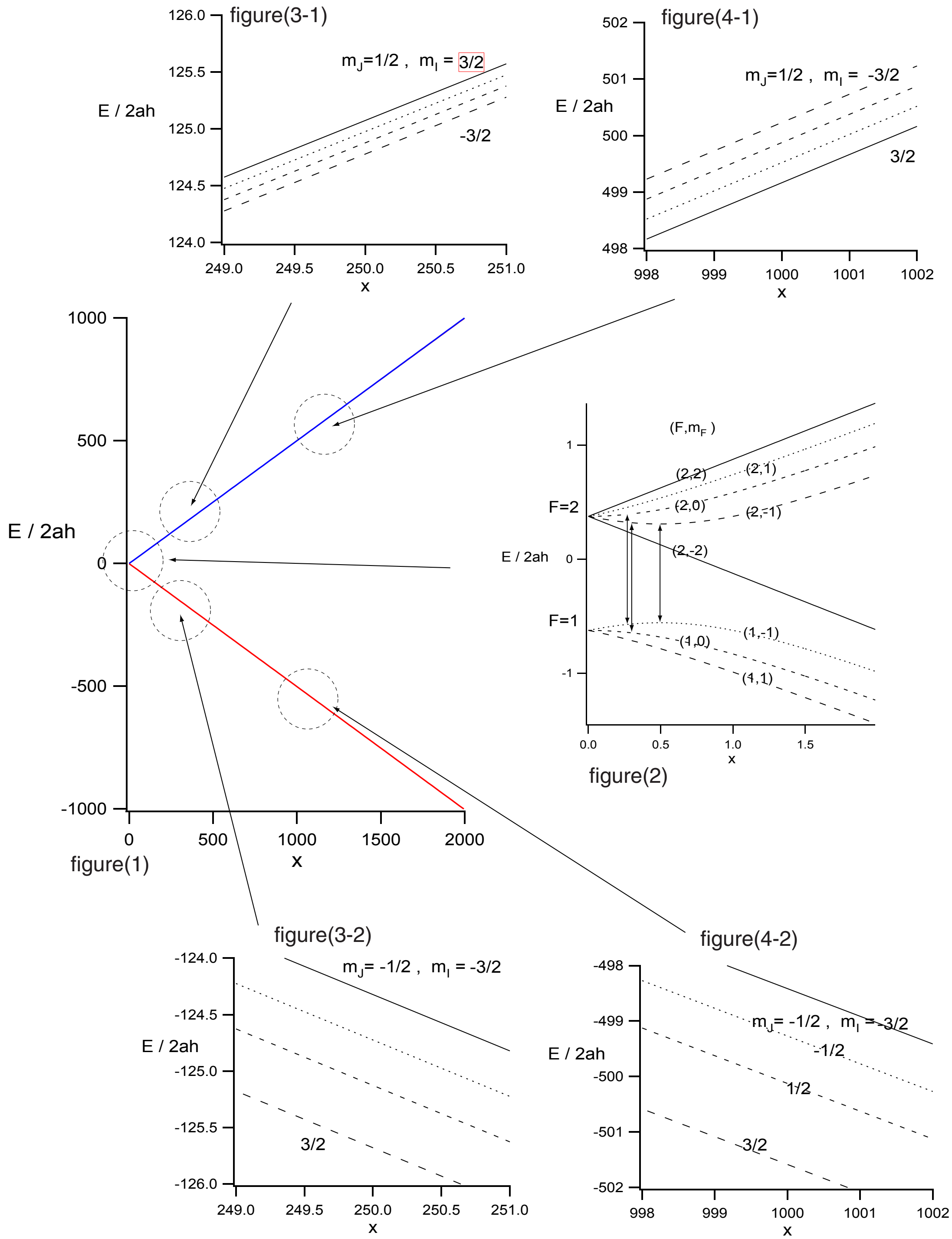
iv. $x > g_J/g_I$, figures (4-1) and (4-2)
Now even the nuclear magnetic moment's Zeeman energy is larger than the hyperfine interaction, and the Hamiltonian becomes

$$H \sim g_J \mu_0 m_J B_z - g_I \mu_0 m_I B_z$$

In other words, the energy cost of anti-aligning the nuclear magnetic moment to the field can overpower the energy reduction of aligning the nuclear and electron magnetic moments. So although the electron spin still dominates the spectrum, the way the degeneracy lifted is different than in the previous case. For example, $|m_J = 1/2, m_I = 3/2\rangle$ has the highest energy of all the eight levels in figure (3). This is no longer true if $x \gg g_J/g_I$; then $|m_J = 1/2, m_I = -3/2\rangle$ has the highest energy. The order of the four $m_J = 1/2$ lines are reversed.

(c) As magnetic field is increased from zero, the energy of $|F = 2, m_F = 0\rangle$ does not initially vary (since $m = 0$) and then starts to increase as mixing with $|F = 1, m_F = 0\rangle$ becomes important. The energy of $|F = 0, m_F = -1\rangle$ first goes up and then decreases. So the energy difference of those two levels first decreases, goes through a *minimum* (at $x \sim 0.3$), and then starts to increase. If the frequency of the transition is measured at the field corresponding to this minimum, the change of the transition frequency with magnetic field fluctuations is of order $\Delta E = O((\Delta x)^2)$ instead of $O(\Delta x)$. This is called a "first order field independent transition". From figure (b), we can find four of those transitions at low ($x \ll 1$) field.

$$\begin{array}{rl} |1,0\rangle \leftrightarrow |2,0\rangle & x \approx 0 \\ |1,-1\rangle \leftrightarrow |2,-1\rangle & x \approx 1/2 \\ |1,0\rangle \leftrightarrow |2,-1\rangle & x \approx 2-\sqrt{3} \\ |1,-1\rangle \leftrightarrow |2,0\rangle & x \approx 2-\sqrt{3} \end{array}$$


figure(3-1)
E / 2ah
m_J=1/2 , m_I = 3/2
-3/2
x
figure(4-1)
m_J=1/2 , m_I = -3/2
3/2
figure(1)
figure(2)
(F,m_F)
(2,2)
(2,1)
(2,0)
(2,-1)
(2,-2)
F=2
F=1
(1,-1)
(1,0)
(1,1)
figure(3-2)
m_J= -1/2 , m_I = -3/2
figure(4-2)
m_J= -1/2 , m_I = -3/2
-1/2
1/2
-3/2

(d) For a state to be magnetically trappable, its energy must be an *increasing* function of magnetic field, so that it will be confined in a local minimum of the field. Of the four transitions found in the preceding exercise, only $\boxed{|1,-1\rangle \leftrightarrow |2,0\rangle}$ is between states both of which are trappable *at the field for which the transition is first-order field-insensitive.*

(e) Using $F^+ = I + 1/2 = 2$ and $\mu_0 B_z / ahF^+ = x/(g_I + g_J)$:

$$\frac{E_1^+ - E_{-1}^-}{2ah} = -2\frac{g_I}{g_I + g_J}x + \frac{1}{2}\left(\sqrt{1+x+x^2} + \sqrt{1-x+x^2}\right)$$

$$\frac{\partial}{\partial x}\left(\frac{E_1^+ - E_{-1}^-}{2ah}\right) = -2\frac{g_I}{g_I + g_J} + \frac{1}{4}\left(\frac{1+2x}{\sqrt{1+x+x^2}} - \frac{1-2x}{\sqrt{1-x+x^2}}\right)$$

We seek the field for which this derivative vanishes. Now the solution we are looking for will be for small x. We can see this either by noting that $x = 0$ is a solution if we neglect the first term that accounts for the nuclear magnetic moment (it is a small correction since $g_I/g_J \sim 5 \times 10^{-4}$), or by considering that $x = 1 \Leftrightarrow B_z = ahF^+/\mu_0(g_I + g_J) = 2.44\ \mathrm{kG}$, which is a very large field by the standards of an atomic physics laboratory. We therefore make a small-x expansion:

$$\frac{E_1^+ - E_{-1}^-}{2ah} = -2\frac{g_I}{g_I + g_J}x + 1 + \frac{3}{8}x^2 + O(x^3)$$

$$\frac{\partial}{\partial x}\left(\frac{E_1^+ - E_{-1}^-}{2ah}\right) = -2\frac{g_I}{g_I + g_J} + \frac{3}{4}x + O(x^2)$$

This vanishes for $x = 8g_I/3(g_I + g_J) = 1.325 \times 10^{-3}$, so the field at which the transition is first-order field-insensitive is $\boxed{B_z = 3.23\ \mathrm{G}}$.

(f) At zero field, the inhomogeneous width is given by

$$\begin{aligned}\Delta\left(\frac{E_1^+ - E_{-1}^-}{h}\right) &= \left|\frac{\partial}{\partial x}\left(\frac{E_1^+ - E_{-1}^-}{h}\right)_{x=0}\right|\Delta x \\ &= 2a \times 2\frac{g_I}{g_I + g_J}\Delta x \\ &\approx 6.835\ \mathrm{GHz} \times 10^{-3}\frac{30\ \mathrm{mG}}{2.44\ \mathrm{kG}} \approx \boxed{84\ \mathrm{Hz}}\end{aligned}$$

While near the field-independent point it is given by

$$\begin{aligned}\Delta\left(\frac{E_1^+ - E_{-1}^-}{h}\right) &= \left|\frac{1}{2}\frac{\partial^2}{\partial x^2}\left(\frac{E_1^+ - E_{-1}^-}{h}\right)_{x=1.325\times 10^{-3}}\right|(\Delta x)^2 \\ &= 2a \times \frac{1}{2}\frac{3}{4}(\Delta x)^2 \\ &\approx 6.835\ \mathrm{GHz} \times \frac{3}{8}\left(\frac{30\ \mathrm{mG}}{2.44\ \mathrm{kG}}\right)^2 \approx \boxed{0.4\ \mathrm{Hz}}\end{aligned}$$

A modest adjustment of the bias field can thus narrow up the microwave transition by two orders of magnitude or, more realistically, reveal the next-largest line-broadening mechanism.

3. **Atomic g factors**
As derived in the class, the general formula for the Landé g factor is

$$g = \left(1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}\right)\left(\frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)}\right)$$

By plugging in numbers, we obtain

$$\begin{aligned} {}^2P_{1/2} &: \begin{cases} -1/6 & F=1 \\ 1/6 & F=2 \end{cases} \\ {}^2P_{3/2} &: 2/3 \quad F=1,2,3 \\ {}^2S_{1/2} &: \begin{cases} -1/2 & F=1 \\ 1/2 & F=2 \end{cases} \end{aligned}$$

The formula gives $g = 2/3$ for ${}^2P_{3/2}, F = 0$ but this is meaningless since the $F = 0$ state has no magnetic moment.

For the stretched states the formula is unnecessary: all the angular momenta are then aligned with each other and their magnetic moments just add. Thus for ${}^2S_{1/2}, F = 2$ we have a total magnetic dipole μ_0 from the electron spin and a total angular momentum $F = 2$, so the g factor is $1/2$; while for ${}^2P_{3/2}, F = 3$ we have a total magnetic dipole $2\mu_0$ (one each from electron spin and orbital angular momentum) and a total angular momentum $F = 3$ for a g factor of $2/3$.