

Atomic Physics 8.421 Spring 2018 (Prof. M. Zwierlein)
Midterm Quiz

Note: Often, later parts of a problem can be answered even if you miss the answer of an earlier part.

1) Energies and length scales in the Hydrogen atom (4 points)

- a. (2 p.) The Rydberg energy is $E_R = \frac{m_e e^4}{2\hbar^2}$, where m_e is the electron mass. What are the energy levels (ignoring spin) of positronium where the proton of the hydrogen atom is replaced by a positron?
- b. (2 p.) Use the Rydberg energy and the assumptions of the Bohr model to derive the expression for the Bohr radius of the hydrogen atom a_0 and of positronium a_+ .

2) Atoms in DC electric fields (12 points)

- a. (2 p.) Write down the perturbation Hamiltonian V for the DC Stark effect in an atom.
- b. (2 p.) In second order perturbation theory, the energy shift is $\sum_m \frac{|\langle m | V | n \rangle|^2}{E_n - E_m}$, where the sum is over all states $m \neq n$. Using a., give the dc Stark shift for the ground state of an atom (still in terms of a sum over certain matrix elements). Explain the sign (in few words).
- c. (4 p.) What are the induced dipole moment and the polarizability of the atom?
- d. (2 p.) By approximating the excited levels to be at the same effective energy \bar{E}_m , and taking the electric field to be along z , relate the polarizability of the ground state $|0\rangle$ to $\langle 0 | z^2 | 0 \rangle$.
- e. (2 p.) Given $\langle 0 | z^2 | 0 \rangle = a_0^2$, and taking $\bar{E}_m \approx 0$, obtain an estimate for the ground state polarizability of hydrogen in terms of powers of the Bohr radius a_0 and a numerical prefactor.

3) Driving a two-level system (14 points)

The Hamiltonian for a two-level system (i.e. a pseudo-spin) of energy splitting $\hbar\omega_0$ in the presence of a drive at frequency ω and time-dependent Rabi frequency $\omega_R(t)$ is, in the lab frame basis $\{|g\rangle_{\text{lab}}, |e\rangle_{\text{lab}}\}$ of ground and excited state:

$$H = \frac{\hbar}{2} \begin{pmatrix} -\omega_0 & \omega_R(t)e^{i\omega t} \\ \omega_R(t)e^{-i\omega t} & \omega_0 \end{pmatrix}$$

The system is initially in the ground state $|g\rangle_{\text{lab}}$. The excitation is switched on at $t = 0$.

- a. (4 p.) Write down the transformation to a new Hamiltonian in the frame rotating with frequency ω about the pseudo-spin z -axis, and find that new Hamiltonian.
- b. (4 p.) We now assume resonance $\omega = \omega_0$. Write down Schrödinger's equation for the components $c(t)$ and $d(t)$ of the wave function $|\Psi(t)\rangle = c(t)|g\rangle_{\text{rot}} + d(t)|e\rangle_{\text{rot}}$ (here, $\{|g\rangle_{\text{rot}}, |e\rangle_{\text{rot}}\}$

is the basis in the rotating frame).

c. (4 p.) Assuming weak excitation, i.e. $c(t) \approx 1$, calculate the amplitude $d(t)$ to find the system in the excited state at time t , in terms of the time-dependent function $\omega_R(t)$.

d. (2 p.) Setting $\omega_R(t) = \alpha t$, calculate the probability $|d(t)|^2$ to find the system in the excited state after time t .

4) Hyperfine structure of a diatomic molecule (20 pts.)

A diatomic molecule in its singlet ground state (total spin quantum number $S = 0$) experiences a hyperfine interaction due to the two nuclear spins \vec{I}_1 and \vec{I}_2 . Let $I_1 = 1/2$ and $I_2 = 3/2$. We will first place ourselves in the rotational ground state.

a. (5 p.) The interaction between nuclear spins is $H = ah\vec{I}_1 \cdot \vec{I}_2$. Introducing the total nuclear spin $\vec{I} = \vec{I}_1 + \vec{I}_2$, find the eigenenergies and their degeneracies. Show that the “center of mass” of all states obeys a sum rule.

b. (3 p.) In an applied magnetic field, the nuclear spins experience a Zeeman interaction $H_Z = -g_1\mu_N\vec{I}_1 \cdot \vec{B} - g_2\mu_N\vec{I}_2 \cdot \vec{B}$, where the g_i are the nuclear g -factors (each on the order of unity), and μ_N is the nuclear magneton. Write down the condition for being in the high-field regime. In this regime, write down the eigenenergies, treating the hyperfine interaction as a perturbation.

c. (4 p.) At low fields, the Zeeman interaction is a perturbation, the dominant energy term being the hyperfine interaction calculated in a). The Zeeman interaction can be approximated by $E_Z \approx -g_I m_I \mu_N B$. Find the g_I -factor for the total nuclear spin quantum number I , by considering the projection of each nuclear spin onto the total spin. Check that your result is reasonable in the limit of $g_1 = 0$ and $g_2 = 0$ and in the case of “stretched” states.

d. (4 p.) Specializing to the case $g_1 = 10$ (i.e. large) and $g_2 = 1$ (i.e. small), make a clear qualitative sketch of the energy levels as a function of magnetic field, from zero field to the high field regime.

e. (4 p.) The diatomic molecule has rotational energy $B\vec{J}^2$ giving rise to rotational levels described by the rotational angular momentum \vec{J} , and associated quantum numbers $J = 0, 1, 2, \dots$ and $M_J = -J, \dots, J$.

- i. Which rotational levels could potentially be affected by an electric quadrupole interaction?
- ii. Which of the nuclei could potentially feature an electric quadrupole moment?

iii. The electric quadrupole interaction is $H_Q = hbC(C+1)$ with $C = \vec{I}_N \cdot \vec{J}$, where \vec{I}_N stands for the nuclear moment(s) found in ii. Introducing the total angular momentum $\vec{F} = \vec{I}_N + \vec{J}$, find the eigenenergies of H_Q . (Thus we assume zero magnetic field and neglect the weak interaction between nuclear spins from a.).

Midterm Spring 2018

1) Energies and length scales in the Hydrogen Atom

$$E_R = \frac{m_e e^4}{2 \hbar^2}$$

a) positronium: effective mass $\mu = \frac{m_e}{2}$

$$\Rightarrow E_n = -\frac{m_e e^4}{4 \hbar^2} \frac{1}{n^2}$$

b) Since $V = -\frac{e^2}{r}$

$$\begin{aligned} \text{we have } E_0 &= \langle V \rangle + \langle T \rangle \\ &= \langle V \rangle - \frac{1}{2} \langle V \rangle \\ &= \frac{1}{2} \langle V \rangle = \frac{1}{2} e^2 \langle \frac{1}{r} \rangle \end{aligned}$$

$$\Rightarrow \langle \frac{1}{r} \rangle = \frac{m_e e^2}{\hbar^2} = \frac{1}{\alpha_0} \Rightarrow \alpha_0 = \frac{\hbar^2}{m_e e^2}$$

For positronium, replace $m_e \rightarrow \mu = \frac{1}{2} m_e$; $\alpha_0 = \frac{2 \hbar^2}{m_e e^2}$.

2) Atoms in DC electric fields

a. $V = -\vec{d} \cdot \vec{\mathcal{E}} = +e\vec{r} \cdot \vec{\mathcal{E}}$

b. $\Delta E = - \sum_m \frac{|K_m | e \vec{r} \cdot \vec{\mathcal{E}} |_0|^2}{E_m - E_0}$

$$= - e^2 \mathcal{E}^2 \sum_m \frac{|K_m | z |_0|^2}{E_m - E_0}$$

< 0 as ground state gets repelled from all excited states

c. $d = - \frac{\partial E}{\partial \mathcal{E}} = 2e^2 \mathcal{E} \sum_m \frac{|K_m | z |_0|^2}{E_m - E_0}$

$$\alpha = \frac{\partial d}{\partial \mathcal{E}} = 2e^2 \sum_m \frac{|K_m | z |_0|^2}{E_m - E_0}$$

d. all $E_m \rightarrow \bar{E}_m$

$$\Rightarrow \alpha = 2 \frac{e^2}{\bar{E}_m - E_0} \sum_m |K_m | z |_0|^2$$

$$= 2 \frac{e^2}{\bar{E}_m - E_0} \underbrace{\langle 0 | z \sum_m |K_m | z |_0 \rangle}_{= 1} = 1$$

$$= 2 \frac{e^2}{\bar{E}_m - E_0} \langle 0 | z^2 | 0 \rangle$$

e. $\bar{E}_m \sim 0; E_0 = - \frac{e^2}{2a_0}$

$$\Rightarrow \alpha = \frac{4e^2}{e^2} a_0 \langle 0 | z^2 | 0 \rangle = 4 a_0^3$$

3) Driving a two-level system

$$H = \frac{\hbar}{2} \begin{pmatrix} -\omega_0 & \omega_R(t) e^{i\omega t} \\ \omega_R(t) e^{-i\omega t} & \omega_0 \end{pmatrix}$$

a. Derivation (not required):

$$\text{Transform state } |\psi(t)\rangle = T(t) |\tilde{\psi}(t)\rangle$$

lab frame \uparrow rotating frame

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

$$= i\hbar \left(\frac{d}{dt} T(t) \right) |\tilde{\psi}(t)\rangle + T(t) i\hbar \frac{d}{dt} |\tilde{\psi}(t)\rangle$$

$$\Rightarrow i\hbar \frac{d}{dt} |\tilde{\psi}(t)\rangle = \left(T^+ H T - i\hbar T^+ \left(\frac{d}{dt} T \right) \right) |\tilde{\psi}(t)\rangle$$

$$= \tilde{H} |\tilde{\psi}(t)\rangle$$

$$\Rightarrow \tilde{H} = T^+ H T - i\hbar T^+ \left(\frac{d}{dt} T \right)$$

For going into the rotating frame, use

$$T = e^{i\omega t S_z} = e^{i\frac{\omega t}{2} \sigma_z}$$

$$T^\dagger \sigma_z T = \sigma_z \quad \text{since } T \text{ commutes with } \sigma_z.$$

$$T = \begin{pmatrix} e^{i\frac{\omega t}{2}} & 0 \\ 0 & e^{-i\frac{\omega t}{2}} \end{pmatrix}$$

$$H_1 = \frac{\hbar \omega_R (I)}{2} \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix}$$

$$\begin{aligned} T^\dagger H_1 T &= \frac{\hbar \omega_R}{2} \left(\begin{pmatrix} e^{-i\frac{\omega t}{2}} & 0 \\ 0 & e^{i\frac{\omega t}{2}} \end{pmatrix} \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \begin{pmatrix} e^{i\frac{\omega t}{2}} & 0 \\ 0 & e^{-i\frac{\omega t}{2}} \end{pmatrix} \right) \\ &= \frac{\hbar \omega_R}{2} \left(\begin{pmatrix} e^{-i\frac{\omega t}{2}} & 0 \\ 0 & e^{i\frac{\omega t}{2}} \end{pmatrix} \begin{pmatrix} 0 & e^{i\frac{\omega t}{2}} \\ e^{-i\frac{\omega t}{2}} & 0 \end{pmatrix} \right) \\ &= \frac{\hbar \omega_R}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar \omega_R}{2} \sigma_x \end{aligned}$$

$$-i\hbar T^\dagger \frac{d}{dt} T = \frac{\hbar \omega}{2} \sigma_z$$

$$\Rightarrow \tilde{H} = \frac{\hbar}{2} \begin{pmatrix} 0 & \omega_R \\ \omega_R & 0 \end{pmatrix}$$

$$3) b) \omega = \omega_0$$

$$\tilde{H} = \frac{\hbar}{2} \begin{pmatrix} 0 & \omega_R(t) \\ \omega_R(t) & 0 \end{pmatrix}$$

$$\begin{aligned} i\hbar \frac{d}{dt} |\tilde{\psi}(t)\rangle &= i\hbar (\dot{c} |g\rangle_{rot} + \dot{d} |e\rangle_{rot}) \\ &= \tilde{H} |\tilde{\psi}(t)\rangle = \frac{\hbar}{2} \omega_R(t) (d |g\rangle_{rot} + c |e\rangle_{rot}) \end{aligned}$$

$$\Rightarrow i\hbar \dot{c} = \frac{\hbar \omega_R}{2} d$$

$$i\hbar \dot{d} = \frac{\hbar \omega_R}{2} c$$

c)
$$\boxed{d = -i \frac{1}{2} \int_0^t dt' \omega_R(t')}$$

$$d) d(t) = -i \frac{1}{2} \int_0^t dt' \omega t'$$

$$= -i \frac{1}{2} \omega \frac{t^2}{2}$$

$$= -i \frac{1}{4} \omega t^2$$

$$\boxed{|d(t)|^2 = \frac{1}{16} \omega^2 t^4}$$

4) Hyperfine structure of a diatomic molecule

a. $H = \alpha h \vec{I}_1 \cdot \vec{I}_2$

$$= \alpha h \frac{1}{2} (\vec{I}^2 - \vec{I}_1^2 - \vec{I}_2^2)$$

$$= \alpha h \frac{1}{2} (I(I+1) - \frac{3}{4} - \frac{15}{4})$$

$$= \alpha h \frac{1}{2} (I(I+1) - \frac{9}{2})$$

$$I=1: \quad \alpha h \frac{1}{2} (2 - \frac{9}{2}) = \alpha h \frac{1}{2} (-\frac{5}{2}) = -\frac{5}{4} \alpha h$$

degeneracy $2I+1 = 3$

$$I=2: \quad \alpha h \frac{1}{2} (6 - \frac{9}{2}) = \alpha h \frac{1}{2} (\frac{3}{2}) = +\frac{3}{4} \alpha h$$

degeneracy $2I+1 = 5$

sum rule: $-\frac{5}{4} \alpha h \cdot 3 + \frac{3}{4} \alpha h \cdot 5 = \underline{\underline{0}}$ correct.

b. High field: $\mu_N \cdot B \gg \alpha h$

Eigenenergies: $E = -g_1 \mu_N m_{I_1} B - g_2 \mu_N m_{I_2} B + \alpha h m_{I_1} m_{I_2}$

$$c. E_2 = -g_I m_I \mu_r B$$

$$g_I = g_1 \frac{\vec{I}_1 \cdot \vec{I}}{I^2} + g_2 \frac{\vec{I}_2 \cdot \vec{I}}{I^2}$$

$$\vec{I}_1 \cdot \vec{I} = \vec{I}_1 \cdot (\vec{I}_1 + \vec{I}_2) = \vec{I}_1^2 + \frac{1}{2} (\vec{I}^2 - \vec{I}_1^2 - \vec{I}_2^2)$$

$$= \frac{1}{2} (I(I+1) + \vec{I}_1^2 - \vec{I}_2^2)$$

$$= \frac{1}{2} (I(I+1) + \frac{3}{4} - \frac{15}{4})$$

$$= \frac{1}{2} (I(I+1) - 3)$$

$$\vec{I}_2 \cdot \vec{I} = \frac{1}{2} (I(I+1) + 3)$$

$$\Rightarrow g_I = (g_1 + g_2) \cdot \frac{1}{2} + \frac{3}{2} (g_2 - g_1) \frac{1}{I(I+1)}$$

check: $g_1 = 0$, stretched state $I = 2, m_I = 2$

\Rightarrow expect the full magnetic moment of spin 2

$$\text{which is } g_2 \mu_r I_2 = \frac{3}{2} g_2 \mu_r.$$

The magnetic moment is $g_I \mu_r I = 2g_I \mu_r$.

$$\Rightarrow \text{Expect } g_I = \frac{3}{4} g_2.$$

$$\begin{aligned} \text{Formula gives } g_I &= g_2 \left(\frac{1}{2} + \frac{3}{2} \frac{1}{I(I+1)} \right) \\ &= g_2 \left(\frac{1}{2} + \frac{3}{2} \frac{1}{6} \right) \\ &= \frac{3}{4} g_2 \quad \Rightarrow \text{check} \end{aligned}$$

For $g_2 = 0$, stretched state $I=2, m_I=2$

\Rightarrow expect magnetic moment $g_1 \mu_N I_1 = \frac{1}{2} g_1 \mu_N$

The magnetic moment is $g_I \mu_N I = 2 g_I \mu_N$

\Rightarrow expect $g_I = \frac{1}{4} g_1$.

Formula gives
$$g_I = g_1 \left(\frac{1}{2} - \frac{3}{2} \cdot \frac{1}{I(I+1)} \right)$$
$$= g_1 \left(\frac{1}{2} - \frac{3}{2} \cdot \frac{1}{6} \right)$$
$$= g_1 \cdot \frac{1}{4} \Rightarrow \text{check.}$$

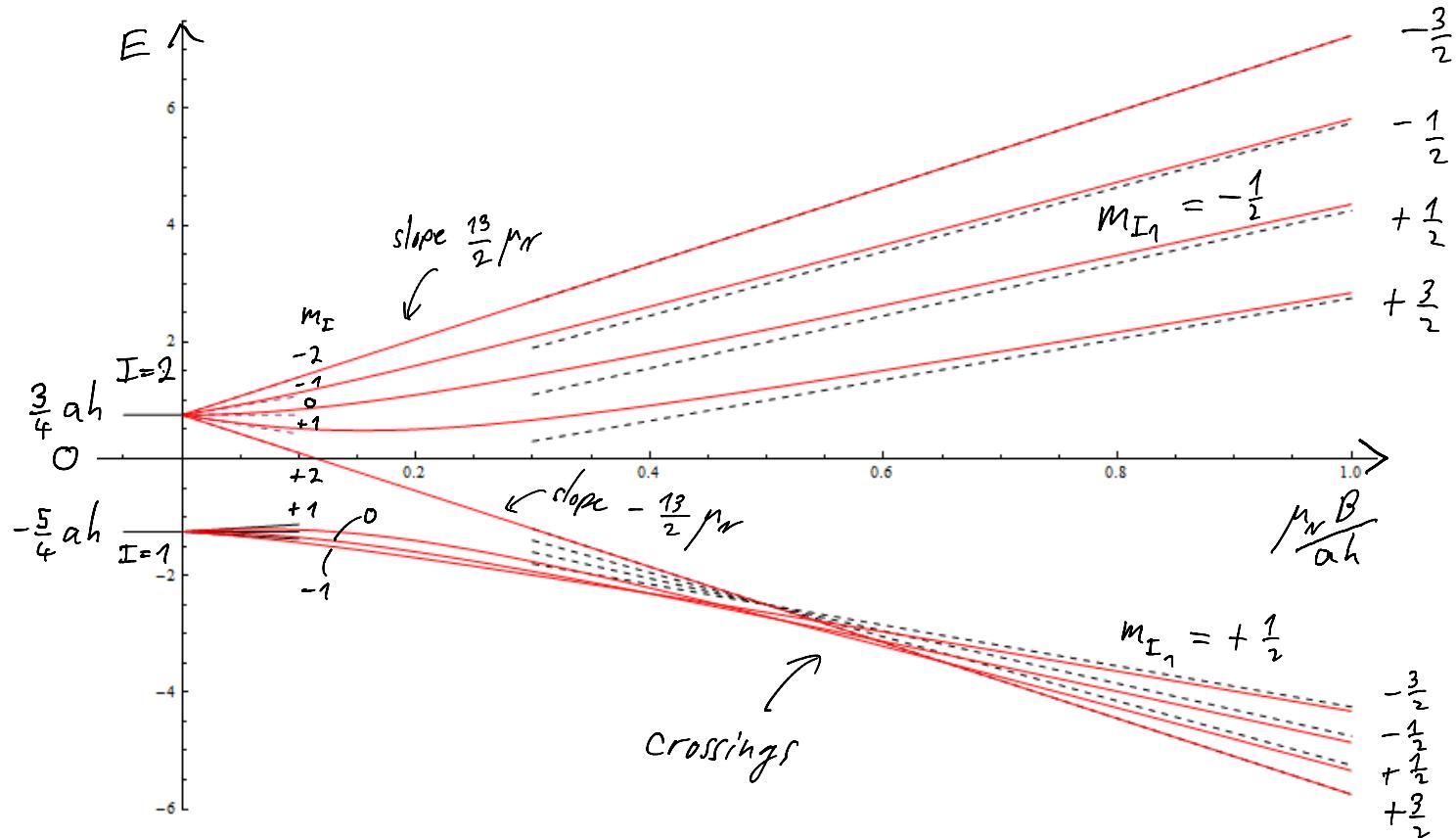
Generally, in the stretched state $I=2, m_I=2$

magnetic moment $(g_1 I_1 + g_2 I_2) \mu_N$
$$= g_I I \mu_N = 2 g_I \mu_N$$

\Rightarrow expect $g_I = \frac{1}{2} (g_1 \frac{1}{2} + g_2 \frac{3}{2})$

and that's what our formula gives.

d) red: full solution; black dashed: low & high field regimes $m_{I_2} =$



$$g_{I=2} = \frac{1}{2}(g_1 + g_2) + \frac{3}{2}(g_2 - g_1) \frac{1}{I(I+1)}$$

$$= \frac{11}{2} - \frac{27}{2} \frac{1}{2 \cdot 3} = \frac{13}{4}$$

$$g_{I=1} = \frac{11}{2} - \frac{27}{2} \frac{1}{1 \cdot 2} = -\frac{5}{4}$$

(or get $g_{I=2}$ from slope of shaded state

$$g_{I=2} \cdot 2 = g_1 \cdot \frac{1}{2} + g_2 \cdot \frac{3}{2} = \frac{10}{2} + \frac{3}{2} = \frac{13}{2}$$

$$\Rightarrow g_{I=2} = \frac{13}{4}$$

e) i. only $J \geq 1$ can be sensitive to a electric quadrupole interaction, as only these states can have an electric field gradient (potential energy curvature) at the origin

ii. Only $I_2 = \frac{3}{2}$ can have an electric quadrupole, since we need $J \geq 1$.

iii. Introduce $\bar{F} = \bar{I}_2 + \bar{J}$

$$\text{Then } C = \frac{1}{2} (\bar{F}^2 - \bar{I}_2^2 - \bar{J}^2)$$

$$= \frac{1}{2} (F(F+1) - I_2(I_2+1) - J(J+1))$$

\Rightarrow eigenenergies $E_Q = h\hbar C(C+1)$
with this C .

F takes on values $J + \frac{3}{2}$

$$J + \frac{1}{2}$$

$$J - \frac{1}{2}$$

$$J - \frac{3}{2} \quad (\text{if } J > 1)$$