

# Final

## 1. Zeeman effect

(a) The sodium D-lines are the transitions of  $3 p_{3/2} \rightarrow 3 s_{1/2}$  (5890 Å) and  $3 p_{1/2} \rightarrow 3 s_{1/2}$  (5896 Å). The corresponding photon energies are 2.105 eV and 2.103 eV, respectively.

In a weak magnetic field, the  $3 p_{3/2}$  level splits into four levels with  $m_j = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$ , the  $3 p_{1/2}$  level into two levels with  $m_j = \frac{1}{2}, -\frac{1}{2}$ , and the  $3 s_{1/2}$  level into two levels with  $m_j = \frac{1}{2}, -\frac{1}{2}$ . Following Sakurai Eq. (5.3.32), the energy shifts are (in Gaussian units)

$$\Delta E_B = -\frac{e\hbar B}{2mc} m_j \left(1 \pm \frac{1}{2l+1}\right)$$

to give

$$\Delta E_B = -\frac{e\hbar B}{2mc} \frac{4}{3} m_j \text{ for } 3 p_{3/2},$$

$$\Delta E_B = -\frac{e\hbar B}{2mc} \frac{2}{3} m_j \text{ for } 3 p_{1/2},$$

$$\Delta E_B = -\frac{e\hbar B}{2mc} 2 m_j \text{ for } 3 s_{1/2}.$$

The Bohr magneton is  $\frac{e\hbar}{2mc} = -5.788 \cdot 10^{-5} \text{ eV/T}$ .

(b) Under the electric dipole transitions, we have the selection rules  $\Delta l = \pm 1$ , and  $\Delta m_j = 0, \pm 1$ . Therefore the allowed transitions,  $m_j' \rightarrow m_j$ , and corresponding photon energies are:

$3 p_{3/2} \rightarrow 3 s_{1/2}$

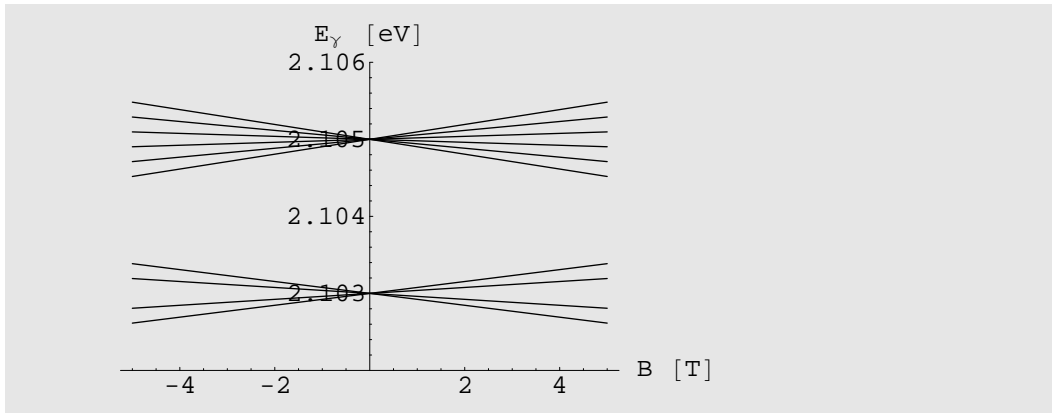
$$\begin{aligned} \frac{3}{2} \rightarrow \frac{1}{2} : E &= 2.105 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{3}{2} - 2 \frac{1}{2}\right) \text{ eV/T} = (2.105 + 5.788 \cdot 10^{-5} B/T) \text{ eV} \\ \frac{1}{2} \rightarrow \frac{1}{2} : E &= 2.105 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{1}{2} - 2 \frac{1}{2}\right) \text{ eV/T} = (2.105 - 1.929 \cdot 10^{-5} B/T) \text{ eV} \\ \frac{1}{2} \rightarrow -\frac{1}{2} : E &= 2.105 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{1}{2} - 2 \frac{-1}{2}\right) \text{ eV/T} = (2.105 + 9.647 \cdot 10^{-5} B/T) \text{ eV} \\ -\frac{1}{2} \rightarrow \frac{1}{2} : E &= 2.105 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{-1}{2} - 2 \frac{1}{2}\right) \text{ eV/T} = (2.105 - 9.647 \cdot 10^{-5} B/T) \text{ eV} \\ -\frac{1}{2} \rightarrow -\frac{1}{2} : E &= 2.105 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{-1}{2} - 2 \frac{-1}{2}\right) \text{ eV/T} = (2.105 + 1.929 \cdot 10^{-5} B/T) \text{ eV} \\ -\frac{3}{2} \rightarrow -\frac{1}{2} : E &= 2.105 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{-3}{2} - 2 \frac{-1}{2}\right) \text{ eV/T} = (2.105 - 5.788 \cdot 10^{-5} B/T) \text{ eV} \end{aligned}$$

$3 p_{1/2} \rightarrow 3 s_{1/2}$

$$\begin{aligned} \frac{1}{2} \rightarrow \frac{1}{2} : E &= 2.103 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{3}{2} - 2 \frac{1}{2}\right) \text{ eV/T} = (2.103 - 3.859 \cdot 10^{-5} B/T) \text{ eV} \\ \frac{1}{2} \rightarrow -\frac{1}{2} : E &= 2.103 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{3}{2} - 2 \frac{-1}{2}\right) \text{ eV/T} = (2.103 + 7.717 \cdot 10^{-5} B/T) \text{ eV} \\ -\frac{1}{2} \rightarrow \frac{1}{2} : E &= 2.103 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{3}{2} - 2 \frac{1}{2}\right) \text{ eV/T} = (2.103 - 7.717 \cdot 10^{-5} B/T) \text{ eV} \\ -\frac{1}{2} \rightarrow -\frac{1}{2} : E &= 2.103 \text{ eV} - \frac{e\hbar B}{2mc} \left(\frac{4}{3} \frac{3}{2} - 2 \frac{-1}{2}\right) \text{ eV/T} = (2.103 + 3.859 \cdot 10^{-5} B/T) \text{ eV}. \end{aligned}$$

The 5890 Å line splits into six equally spaced lines, while the 5896 Å splits into four lines with unequal spacings.

```
Plot[{2.105 + 5.788 10-5 B, 2.105 - 1.929 10-5 B, 2.105 + 9.647 10-5 B,
      2.105 - 9.647 10-5 B, 2.105 + 1.929 10-5 B, 2.105 - 5.788 10-5 B, 2.103 - 3.859 10-5 B,
      2.103 + 7.717 10-5 B, 2.103 - 7.717 10-5 B, 2.103 + 3.859 10-5 B},
     {B, -5, 5}, PlotRange -> {2.102, 2.106}, AxesLabel -> {"B [T]", "Eγ [eV]"}];
```



The fact that there are even number of lines with unequal splittings was called "anomalous Zeeman effect" because it could not be "explained" by semi-classical expectations without the spin.

By the way, for the magnetic field larger than a few Tesla, obviously the  $2 p_{1/2}$  and  $2 p_{3/2}$  states come close and hence the magnetic field cannot be treated "weak." Both Paschen-Back and Zeeman effects need to be considered simultaneously using the degenerate perturbation theory by diagonalizing the perturbation matrix as we discussed in the class. We will do this below in 4(c).

## 2. Dyson Series

(a) The Dyson series up to  $O(V^2)$  is

$$U_I(t) = 1 + \frac{-i}{\hbar} \int_0^t V_I(t') dt' + \left(\frac{-i}{\hbar}\right)^2 \int_0^t \int_0^{t'} V_I(t') V_I(t'') dt'' dt' + O(V^3).$$

We take its matrix element between the same states,

$$\langle i | U_I(t) | i \rangle = 1 + \frac{-i}{\hbar} \int_0^t \langle i | V_I(t') | i \rangle dt' + \left(\frac{-i}{\hbar}\right)^2 \int_0^t \int_0^{t'} \langle i | V_I(t') V_I(t'') | i \rangle dt'' dt' + O(V^3).$$

The second term is

$$\frac{-i}{\hbar} \int_0^t e^{iE_i t'/\hbar} V_{ii} e^{-iE_i t'/\hbar} dt' = \frac{-i}{\hbar} V_{ii} t,$$

which is identified with the term  $\frac{-i}{\hbar} \Delta_i^{(1)} t$  in Eq. (1). Therefore we reproduce the result from the time-independent perturbation theory

$$\Delta_i^{(1)} = V_{ii}.$$

The third term produces many interesting contributions. Inserting the complete set of intermediate states,

$$\begin{aligned} & \left(\frac{-i}{\hbar}\right)^2 \int_0^t \int_0^{t'} \langle i | V_I(t') V_I(t'') | i \rangle dt'' dt' \\ &= -\frac{1}{\hbar^2} \int_0^t \int_0^{t'} \sum_m \langle i | V_I(t') | m \rangle \langle m | V_I(t'') | i \rangle dt'' dt' \\ &= -\frac{1}{\hbar^2} \int_0^t \int_0^{t'} \sum_m V_{im} e^{-i(E_m - E_i)t'/\hbar} V_{mi} e^{i(E_i - E_m)t''/\hbar} dt'' dt' \\ &= -\frac{1}{\hbar^2} \int_0^t \int_0^{t'} (V_{ii} V_{ii} + \sum_{m \neq i} V_{im} e^{-i(E_m - E_i)t'/\hbar} V_{mi} e^{-i(E_i - E_m)t''/\hbar}) dt'' dt' \\ &= -\frac{1}{\hbar^2} \left( \frac{1}{2} V_{ii}^2 t^2 + \sum_{m \neq i} |V_{im}|^2 \int_0^t \int_0^{t'} e^{-i(E_m - E_i)(t' - t'')/\hbar} dt'' dt' \right) \\ &= -\frac{1}{\hbar^2} \left( \frac{1}{2} V_{ii}^2 t^2 + \sum_{m \neq i} |V_{im}|^2 \int_0^t \frac{1 - e^{-i(E_m - E_i)t'/\hbar}}{i(E_m - E_i)/\hbar} dt' \right) \\ &= -\frac{1}{\hbar^2} \left( \frac{1}{2} V_{ii}^2 t^2 + \sum_{m \neq i} |V_{im}|^2 \frac{1}{i(E_m - E_i)/\hbar} \left( t - \frac{e^{-i(E_m - E_i)t/\hbar} - 1}{-i(E_m - E_i)/\hbar} \right) \right) \\ &= -\frac{1}{2} \frac{1}{\hbar^2} V_{ii}^2 t^2 + \sum_{m \neq i} |V_{im}|^2 \frac{1}{E_i - E_m} \left( \frac{-i}{\hbar} t + \frac{e^{-i(E_m - E_i)t/\hbar} - 1}{E_i - E_m} \right) \\ &= -\frac{1}{2} \frac{1}{\hbar^2} V_{ii}^2 t^2 + \frac{-i}{\hbar} \left( \sum_{m \neq i} \frac{|V_{im}|^2}{E_i - E_m} t \right) + \left( \sum_{m \neq i} \frac{|V_{im}|^2}{(E_i - E_m)^2} e^{-i(E_m - E_i)t/\hbar} \right) \\ & \quad - \left( \sum_{m \neq i} \frac{|V_{im}|^2}{(E_i - E_m)^2} \right). \end{aligned}$$

The first term is  $\frac{1}{2!} \left(\frac{-i}{\hbar} \Delta_i^{(1)} t\right)^2$ , while the second term is  $\frac{-i}{\hbar} \Delta_i^{(2)} t$  with

$$\Delta_i^{(2)} = \sum_{m \neq i} \frac{|V_{im}|^2}{E_i - E_m}.$$

The last term is a part of the wave function renormalization factor

$$Z_i = 1 - \sum_{m \neq i} \frac{|V_{im}|^2}{(E_i - E_m)^2}.$$

Finally, the third term is the time–evolution of the state  $m$  mixed to the state  $i$  due to the perturbation by  $\frac{V_{im}}{E_i - E_m}$ . For  $t \rightarrow \infty$ , this term oscillates rapidly and can be dropped; however it is there for a finite  $t$ .

**N.B.:** Just in case you are wondering why this works, here is the reason (not a part of the exam).

Using the notation of the time–independent perturbation theory, our initial and the final states are the unperturbed  $|i^{(0)}\rangle$ . It can be expanded in the true Hamiltonian eigenstates as

$$|i^{(0)}\rangle = \sum_m |m\rangle \langle m | i^{(0)}\rangle = |i\rangle \langle i | i^{(0)}\rangle + \sum_{m \neq i} |m\rangle \langle m | i^{(0)}\rangle.$$

The wave function renormalization factor is  $Z_i = |\langle i | i^{(0)}\rangle|^2$ , and hence (with a proper phase convention)

$$|i^{(0)}\rangle = Z_i^{1/2} |i\rangle + \sum_{m \neq i} |m\rangle \langle m | i^{(0)}\rangle.$$

The time–evolution operator in the interaction picture is  $U_I(t) = e^{iH_0 t/\hbar} U(t)$  (Eq. (5.6.9) in Sakurai with  $t_0 = 0$ ), so

$$\begin{aligned} \langle i^{(0)} | U_I(t) | i^{(0)}\rangle &= \langle i^{(0)} | e^{iH_0 t/\hbar} U(t) | i^{(0)}\rangle = e^{iE_i^{(0)} t/\hbar} \langle i^{(0)} | U(t) | i^{(0)}\rangle \\ &= e^{iE_i^{(0)} t/\hbar} (Z_i \langle i | U(t) | i\rangle + \sum_{m \neq i} \langle m | U(t) | m\rangle |\langle m | i^{(0)}\rangle|^2) \\ &= Z_i e^{-i(E_i - E_i^{(0)}) t/\hbar} + \sum_{m \neq i} e^{-i(E_m - E_i^{(0)}) t/\hbar} |\langle m | i^{(0)}\rangle|^2. \end{aligned}$$

If you expand this expression up to  $O(V^2)$ , you recover precisely the result obtained above. This technique and that below are somehow not discussed in any textbooks I know. If you find one, let me know.

(b) Following the same steps as above,

$$\begin{aligned} &\left(\frac{-i}{\hbar}\right)^2 \int_0^t \int_0^{t'} \langle i | V_I(t') V_I(t'') | i\rangle dt'' dt' \\ &= -\frac{1}{\hbar^2} \int_0^t \int_0^{t'} \sum_m \langle i | V_I(t') | m\rangle \langle m | V_I(t'') | i\rangle dt'' dt' \\ &= -\frac{1}{\hbar^2} \int_0^t \int_0^{t'} \sum_m V_{im} \cos \omega t' e^{-i(E_m - E_i) t'/\hbar} V_{mi} \cos \omega t'' e^{-i(E_i - E_m) t''/\hbar} dt'' dt' \\ &= -\frac{1}{\hbar^2} \int_0^t \int_0^{t'} (V_{ii}^2 \cos \omega t' \cos \omega t'' \\ &\quad + \sum_{m \neq i} V_{im} \cos \omega t' e^{-i(E_m - E_i) t'/\hbar} V_{mi} \cos \omega t'' e^{-i(E_i - E_m) t''/\hbar}) dt'' dt'. \end{aligned}$$

Because we are interested in the term that grows as  $t$ , we can drop all the other terms. Namely, the integrand of the first term oscillates rapidly for large  $t$  and  $t'$ , and we drop it. The second term is

$$\begin{aligned} &-\frac{1}{\hbar^2} \sum_{m \neq i} V_{im} V_{mi} \int_0^t \int_0^{t'} \cos \omega t' e^{-i(E_m - E_i) t'/\hbar} \\ &\quad \times \frac{1}{2} (e^{-i(E_i - E_m + \hbar \omega) t''/\hbar} + e^{-i(E_i - E_m - \hbar \omega) t''/\hbar}) dt'' dt' \\ &= -\frac{1}{\hbar^2} \sum_{m \neq i} V_{im} V_{mi} \int_0^t \cos \omega t' e^{-i(E_m - E_i) t'/\hbar} \\ &\quad \times \frac{1}{2} \left( \frac{e^{-i(E_i - E_m + \hbar \omega) t'/\hbar} - 1}{-i(E_i - E_m + \hbar \omega)/\hbar} + \frac{e^{-i(E_i - E_m - \hbar \omega) t'/\hbar} - 1}{-i(E_i - E_m - \hbar \omega)/\hbar} \right) dt' \\ &= -\frac{1}{\hbar^2} \sum_{m \neq i} V_{im} V_{mi} \int_0^t \cos \omega t' \frac{1}{2} \left( \frac{e^{-i\omega t'} - e^{-i(E_m - E_i) t'/\hbar}}{-i(E_i - E_m + \hbar \omega)/\hbar} + \frac{e^{i\omega t'} - e^{-i(E_m - E_i) t'/\hbar}}{-i(E_i - E_m - \hbar \omega)/\hbar} \right) dt'. \end{aligned}$$

The terms with  $e^{-i(E_m - E_i) t'/\hbar}$  oscillate rapidly and can be dropped. Then,

$$= -\frac{1}{\hbar^2} \sum_{m \neq i} V_{im} V_{mi} \int_0^t \frac{1}{4} (e^{i\omega t'} + e^{-i\omega t'}) \left( \frac{e^{-i\omega t'}}{-i(E_i - E_m + \hbar \omega)/\hbar} + \frac{e^{i\omega t'}}{-i(E_i - E_m - \hbar \omega)/\hbar} \right) dt'.$$

Only the terms without the oscillatory factors give  $O(t)$  contributions,

$$\begin{aligned} &= \frac{-i}{\hbar} \sum_{m \neq i} V_{im} V_{mi} \frac{1}{4} \left( \frac{1}{E_i - E_m + \hbar \omega} + \frac{1}{E_i - E_m - \hbar \omega} \right) t \\ &= \frac{-i}{\hbar} \sum_{m \neq i} V_{im} V_{mi} \frac{1}{4} \frac{2(E_i - E_m)}{(E_i - E_m + \hbar \omega)(E_i - E_m - \hbar \omega)} t \\ &= \frac{-i}{\hbar} \frac{1}{2} \sum_{m \neq i} \frac{|V_{mi}|^2 (E_i - E_m)}{(E_i - E_m)^2 - (\hbar \omega)^2} t \end{aligned}$$

Therefore,

$$\Delta_i^{(2)} = \frac{1}{2} \sum_{m \neq i} \frac{|V_{mi}|^2 (E_i - E_m)}{(E_i - E_m)^2 - (\hbar \omega)^2}.$$

The expression does not go back to that in the time-independent perturbation theory in the limit  $\omega \rightarrow 0$ . This is because the quantity is the time average of the oscillating function  $\langle \cos^2 \omega t \rangle = \frac{1}{2}$ .

(c) In this case, the perturbation is  $V = e E_0 z \cos(kx - \omega t)$ , hence

$$\Delta_i^{(2)} = \frac{1}{2} e^2 E_0^2 \sum_{m \neq i} \frac{|z_{mi}|^2 (E_i - E_m)}{(E_i - E_m)^2 - (\hbar \omega)^2}.$$

Here, we used the electric dipole approximation and set  $kx = 0$ .

This energy shift should be compared to the energy of the electromagnetic wave

$$\int d^3x \frac{1}{2} (E_0 \cos(kx - \omega t))^2 = \int d^3x \frac{1}{4} E_0^2,$$

where the time average  $\langle \cos^2 \omega t \rangle = \frac{1}{2}$  is taken. Therefore, it corrects the Lagrangian density as

$$\frac{1}{4} E_0^2 \rightarrow \frac{1}{4} E_0^2 \left( 1 - \frac{N}{V} 2 e^2 \sum_{m \neq i} \frac{|z_{mi}|^2 (E_i - E_m)}{(E_i - E_m)^2 - (\hbar \omega)^2} \right),$$

where  $\frac{N}{V}$  is the number density of hydrogen atoms, so the polarizability is

$$\alpha = 2 e^2 E_0^2 \sum_{m \neq i} \frac{|z_{mi}|^2 (E_m - E_i)}{(E_i - E_m)^2 - (\hbar \omega)^2}$$

which agrees with the static case when  $\omega \rightarrow 0$ .

(d) With the polarizability and the number density  $N/V$ ,

$$n(\omega) = \left( 1 + \frac{N}{V} \alpha \right)^{1/2} = 1 + \frac{N}{V} 2 e^2 E_0^2 \sum_{m \neq i} \frac{|z_{mi}|^2 (E_m - E_i)}{(E_i - E_m)^2 - (\hbar \omega)^2}.$$

Clearly the denominator is smaller for larger  $\hbar \omega < |E_i - E_m|$ , and so the index of refraction increases as wavelength decreases. This leads to the prediction that ...

... red is at the top and violet at the bottom in a rainbow, which obviously explains our experience. See, e.g.,

<http://accept.la.asu.edu/PiN/mod/light/opticsnature/rainbows.html>

Now you can proudly tell your parents that you fully understand the rainbow from the first principle.

### 3. Uranium $\alpha$ -decay

We compute the integral

$$\begin{aligned}
 v &= \frac{2(z-2)q^2}{r}; \quad tp = \frac{2(z-2)q^2}{E0}; \\
 \text{Tint}[r_] &= \text{Integrate}[\sqrt{2m(v-E0)}, r] \\
 &= \sqrt{2} \left( r \sqrt{m \left( -E0 + \frac{2q^2(-2+z)}{r} \right)} - \right. \\
 &\quad \left. \frac{2q^2 \sqrt{r} \sqrt{m \left( -E0 + \frac{2q^2(-2+z)}{r} \right)}}{\sqrt{E0} \sqrt{4q^2 + E0r - 2q^2z}} (-2+z) \text{Log} \left[ \frac{2\sqrt{E0} \sqrt{r} + 2\sqrt{4q^2 + E0r - 2q^2z}}{\sqrt{E0} \sqrt{4q^2 + E0r - 2q^2z}} \right] \right)
 \end{aligned}$$

to give the turning points and probabilities

```

ergtomev = 624150.97;
constants = {m -> 3727.37917 / (2.99792458 * 1010)2,
             ħ -> 6.58211915 * 10-22, z -> 92, a -> 5 * 10-13, q -> 4.802 * 10-10 * sqrt(ergtomev)};
energies = {1, 3, 10, 30};
T = Exp[-(2/h) (Tint[b] - Tint[a])];
(tp /. E0 -> energies /. constants) * .01
(T /. b -> tp - $MachineEpsilon) /. E0 -> energies /. constants // Re

```

```
{2.59064 * 10-13, 8.63545 * 10-14, 2.59064 * 10-14, 8.63545 * 10-15}
```

```
{4.08218 * 10-128, 6.29166 * 10-63, 3.4855 * 10-23, 0.000152428}
```

*Mathematica note:*

We know that the WKB integral blows up at the classical turning point  $b$ , so this must be handled numerically. In the computation above we take  $b \rightarrow b - \epsilon$ , where  $\epsilon$  is the '\$MachineEpsilon', or the upper bound of positive numbers  $\delta$  for which  $1.0 + \delta = 1.0$  on one's computer.

## 4. Paschen–Back Effect

Because we consider states with  $J_z = \frac{3}{2} \hbar$  and  $\frac{1}{2} \hbar$ , we need to look at

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle = |1, 1\rangle \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle,$$

such that

$$\begin{aligned} \left| \frac{3}{2}, \frac{1}{2} \right\rangle &= \frac{1}{\sqrt{3}} J_- \left| \frac{3}{2}, \frac{3}{2} \right\rangle = \frac{1}{\sqrt{3}} J_- |1, 1\rangle \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle \\ &\Rightarrow \sqrt{\frac{2}{3}} |1, 0\rangle \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle + \frac{1}{\sqrt{3}} |1, 1\rangle \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle. \end{aligned}$$

It is easy to find the orthogonal linear combination,

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle = -\frac{1}{\sqrt{3}} |1, 0\rangle \otimes \left| \frac{1}{2}, \frac{1}{2} \right\rangle + \sqrt{\frac{2}{3}} |1, 1\rangle \otimes \left| \frac{1}{2}, -\frac{1}{2} \right\rangle.$$

(a) When  $V_1 \gg V_2$ , we first diagonalize  $V_1$  with the eigenvalues given by states of definite  $j$ ,

$$\vec{L} \cdot \vec{S} = \hbar^2 \frac{1}{2} (j(j+1) - l(l+1) - s(s+1)) = \hbar^2 \frac{1}{2} (j(j+1) - 2 - \frac{3}{4})$$

which is

$$\hbar^2 \frac{1}{2} \left( \frac{3}{2} \frac{5}{2} - 2 - \frac{3}{4} \right) = \hbar^2 \frac{1}{2} \text{ for } j = \frac{3}{2},$$

$$\hbar^2 \frac{1}{2} \left( \frac{1}{2} \frac{3}{2} - 2 - \frac{3}{4} \right) = -\hbar^2 \text{ for } j = \frac{1}{2}.$$

Therefore, the energy shifts due to the first order in  $V_1$  are

$$\Delta_1^{(1)} = \frac{\hbar^2}{2m^2 c^2} \left\langle \frac{e^2}{r^3} \right\rangle \frac{1}{2} = \frac{\hbar^4}{96 a^4 c^2 m^3} \text{ for } j = \frac{3}{2},$$

$$\Delta_1^{(1)} = -\frac{\hbar^2}{2m^2 c^2} \left\langle \frac{e^2}{r^3} \right\rangle = -\frac{\hbar^4}{48 a^4 c^2 m^3} \text{ for } j = \frac{1}{2}$$

using the expectation values calculated in HW #11. Further shifts due to the first order in  $V_2$  are

$$\Delta_2^{(1)} = -\frac{e \hbar B}{2 m c} \left( 1 + g \frac{1}{2} \right) = -\frac{e \hbar B}{m c} \text{ for } j = \frac{3}{2}, m_j = \frac{3}{2},$$

$$\begin{aligned} \Delta_2^{(1)} &= -\frac{e \hbar B}{2 m c} \left( \frac{2}{3} \left( 0 + g \frac{1}{2} \right) + \frac{1}{3} \left( 1 + g \frac{-1}{2} \right) \right) = -\frac{e \hbar B}{2 m c} \left( \frac{1}{3} + g \frac{1}{6} \right) \\ &= -\frac{e \hbar B}{3 m c} \text{ for } j = \frac{3}{2}, m_j = \frac{1}{2}, \end{aligned}$$

$$\begin{aligned} \Delta_2^{(1)} &= -\frac{e \hbar B}{2 m c} \left( \frac{1}{3} \left( 0 + g \frac{1}{2} \right) + \frac{2}{3} \left( 1 + g \frac{-1}{2} \right) \right) = -\frac{e \hbar B}{2 m c} \left( \frac{2}{3} - g \frac{1}{6} \right) \\ &= -\frac{e \hbar B}{6 m c} \text{ for } j = \frac{1}{2}, m_j = \frac{1}{2}. \end{aligned}$$

Therefore the total shifts are

$$\Delta^{(1)} = \frac{\hbar^4}{96 a^4 c^2 m^3} - \frac{e \hbar B}{m c} \text{ for } j = \frac{3}{2}, m_j = \frac{3}{2},$$

$$\Delta^{(1)} = \frac{\hbar^4}{96 a^4 c^2 m^3} - \frac{e \hbar B}{3 m c} \text{ for } j = \frac{3}{2}, m_j = \frac{1}{2},$$

$$\Delta^{(1)} = -\frac{\hbar^4}{48 a^4 c^2 m^3} - \frac{e \hbar B}{6 m c} \text{ for } j = \frac{1}{2}, m_j = \frac{1}{2}.$$

(b) When  $V_1 \gg V_2$ , we first diagonalize  $V_1$  with the eigenvalues given by states of definite  $m_l$  and  $m_s$ ,

$$\Delta_2^{(1)} = -\frac{e \hbar B}{2 m c} (m_l + g m_s) = -\frac{e \hbar B}{2 m c} \left(1 + g \frac{1}{2}\right) = -\frac{e \hbar B}{m c} \text{ for } m_l = 1, m_s = \frac{1}{2},$$

$$\Delta_2^{(1)} = -\frac{e \hbar B}{2 m c} (m_l + g m_s) = -\frac{e \hbar B}{2 m c} \left(1 + g \left(-\frac{1}{2}\right)\right) = 0 \text{ for } m_l = 1, m_s = -\frac{1}{2},$$

$$\Delta_2^{(1)} = -\frac{e \hbar B}{2 m c} (m_l + g m_s) = -\frac{e \hbar B}{2 m c} \left(0 + g \frac{1}{2}\right) = -\frac{e \hbar B}{2 m c} \text{ for } m_l = 0, m_s = \frac{1}{2}.$$

The expectation values of the spin orbit term is obtained using

$\langle \vec{L} \cdot \vec{S} \rangle = \hbar^2 m_l m_s$ . Therefore,

$$\Delta_1^{(1)} = \frac{\hbar^2}{2 m^2 c^2} \left\langle \frac{e^2}{r^3} \right\rangle \cdot 1 \cdot \frac{1}{2} = \frac{\hbar^4}{96 a^4 c^2 m^3} \text{ for } m_l = 1, m_s = \frac{1}{2},$$

$$\Delta_1^{(1)} = \frac{\hbar^2}{2 m^2 c^2} \left\langle \frac{e^2}{r^3} \right\rangle \cdot 1 \cdot \left(-\frac{1}{2}\right) = -\frac{\hbar^4}{96 a^4 c^2 m^3} \text{ for } m_l = 1, m_s = -\frac{1}{2},$$

$$\Delta_1^{(1)} = \frac{\hbar^2}{2 m^2 c^2} \left\langle \frac{e^2}{r^3} \right\rangle \cdot 0 \cdot \frac{1}{2} = 0 \text{ for } m_l = 0, m_s = \frac{1}{2}.$$

So the total shifts are

$$\Delta^{(1)} = \frac{\hbar^4}{96 a^4 c^2 m^3} - \frac{e \hbar B}{m c} \text{ for } m_l = 1, m_s = \frac{1}{2},$$

$$\Delta^{(1)} = -\frac{\hbar^4}{96 a^4 c^2 m^3} \text{ for } m_l = 1, m_s = -\frac{1}{2},$$

$$\Delta^{(1)} = -\frac{e \hbar B}{2 m c} \text{ for } m_l = 0, m_s = \frac{1}{2}.$$

(c) For the  $J_z = \frac{3}{2} \hbar$  state, both  $V_1$  and  $V_2$  are already diagonal to the extent that we ignore mixing with states other than  $2p$ . Indeed, the answers from (a) and (b) were the same, which is the full answer

$$\Delta^{(1)} = \frac{\hbar^4}{96 a^4 c^2 m^3} - \frac{e \hbar B}{m c} \text{ for } m_j = \frac{3}{2}.$$

For the  $J_z = \frac{1}{2} \hbar$ , there are two states that mix. We have to diagonalize the matrix in the spirit of degenerate perturbation theory. Using the  $(j, m_j)$  basis, the spin-orbit term is diagonal,

$$\begin{pmatrix} \frac{\hbar^4}{96 a^4 c^2 m^3} & 0 \\ 0 & -\frac{\hbar^4}{48 a^4 c^2 m^3} \end{pmatrix}$$

while the magnetic moment term is not,



$$\begin{aligned}
& -\frac{e\hbar B}{2mc} \times \\
& \begin{pmatrix} \frac{2}{3} \left(0 + g \frac{1}{2}\right) + \frac{1}{3} \left(1 + g \frac{-1}{2}\right) & \sqrt{\frac{2}{3}} \left(-\frac{1}{\sqrt{3}}\right) \left(0 + g \frac{1}{2}\right) \\ & + \frac{1}{\sqrt{3}} \sqrt{\frac{2}{3}} \left(1 + g \left(-\frac{1}{2}\right)\right) \\ \sqrt{\frac{2}{3}} \left(-\frac{1}{\sqrt{3}}\right) \left(0 + g \frac{1}{2}\right) & \\ + \frac{1}{\sqrt{3}} \sqrt{\frac{2}{3}} \left(1 + g \left(-\frac{1}{2}\right)\right) & \frac{1}{3} \left(0 + g \frac{1}{2}\right) + 2 \left(1 + g \left(-\frac{1}{2}\right)\right) \end{pmatrix} \\
& = -\frac{e\hbar B}{2mc} \begin{pmatrix} \frac{2}{3} & -\frac{\sqrt{2}}{3} \\ -\frac{\sqrt{2}}{3} & \frac{1}{3} \end{pmatrix}.
\end{aligned}$$

Therefore, we need to diagonalize the matrix

$$\begin{pmatrix} \frac{\hbar^4}{96 a^4 c^2 m^3} - \frac{e\hbar B}{3mc} & \frac{e\hbar B}{3\sqrt{2} mc} \\ \frac{e\hbar B}{3\sqrt{2} mc} & -\frac{g\hbar^4}{48 a^4 c^2 m^3} - \frac{e\hbar B}{6mc} \end{pmatrix};$$

$$\text{eigen} = \text{Eigenvalues} \left[ \left\{ \left\{ \frac{\hbar^4}{96 a^4 c^2 m^3} - \frac{e\hbar B}{3mc}, \frac{e\hbar B}{3\sqrt{2} mc} \right\}, \left\{ \frac{e\hbar B}{3\sqrt{2} mc}, -\frac{\hbar^4}{48 a^4 c^2 m^3} - \frac{e\hbar B}{6mc} \right\} \right\} \right]$$

$$\begin{aligned}
& \left\{ \frac{1}{192 a^8 c^4 m^6} \left( -\hbar^4 a^4 c^2 m^3 - 48 \hbar a^8 B c^3 e m^5 - \right. \right. \\
& \quad \left. \left. \sqrt{3} \sqrt{3} \hbar^8 a^8 c^4 m^6 - 32 \hbar^5 a^{12} B c^5 e m^8 + 768 \hbar^2 a^{16} B^2 c^6 e^2 m^{10} \right) \right\}, \\
& \left. \frac{1}{192 a^8 c^4 m^6} \left( -\hbar^4 a^4 c^2 m^3 - 48 \hbar a^8 B c^3 e m^5 + \right. \right. \\
& \quad \left. \left. \sqrt{3} \sqrt{3} \hbar^8 a^8 c^4 m^6 - 32 \hbar^5 a^{12} B c^5 e m^8 + 768 \hbar^2 a^{16} B^2 c^6 e^2 m^{10} \right) \right\}
\end{aligned}$$

$$\rightarrow \Delta^{(1)} = -\frac{\hbar^4}{192 a^4 c^2 m^3} - \frac{e\hbar B}{4mc} \mp \frac{1}{64\sqrt{3}} \sqrt{3 \left( \frac{\hbar^4}{a^4 c^2 m^3} \right)^2 - 64 \left( \frac{\hbar^4}{a^4 c^2 m^3} \right) \left( \frac{e\hbar B}{2mc} \right) + 3072 \left( \frac{e\hbar B}{2mc} \right)^2}$$

for  $m_j = \frac{1}{2}$ .

To verify that the eigenvalues are consistent with the results in (a), we expand them to the first order in  $B$ ,

**Simplify[PowerExpand[Series[eigen, {B, 0, 1}]]]**

$$\left\{ -\frac{\hbar^4}{48 (a^4 c^2 m^3)} - \frac{(\hbar e) B}{6 (c m)} + O[B]^2, \frac{\hbar^4}{96 a^4 c^2 m^3} - \frac{(\hbar e) B}{3 (c m)} + O[B]^2 \right\}$$

To verify that the eigenvalues are consistent with the results in (b), we expand them to the zeroth order in  $B^{-1}$ ,

**Simplify[PowerExpand[Series[eigen, {B, ∞, 0}]]]**

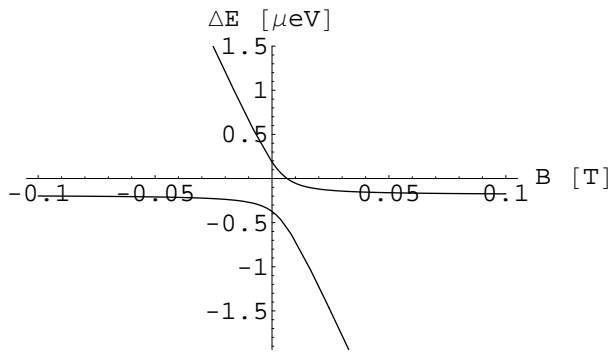
$$\left\{ -\frac{\hbar e}{2 (c m) B} + O\left[\frac{1}{B}\right]^1, -\frac{\hbar^4}{96 (a^4 c^2 m^3)} + O\left[\frac{1}{B}\right]^1 \right\}$$

Both of them work out. Now we plot the eigenvalues as a function of the magnetic field. The Bohr magneton is  $\frac{e\hbar}{2mc} = 5.788 \times 10^{-5}$  eV /T, while  $\frac{\hbar^4}{a^4 c^2 m^3} = 1.789 \times 10^{-5}$  eV. Therefore the two-by-two matrix is

$$\text{eigennum} = \text{Eigenvalues}\left[\left\{\left\{\frac{1.789 \cdot 10^{-5}}{96} - \frac{2}{3} \cdot 5.788 \cdot 10^{-5} B, \frac{\sqrt{2}}{3} \cdot 5.788 \cdot 10^{-5} B\right\}, \left\{\frac{\sqrt{2}}{3} \cdot 5.788 \cdot 10^{-5} B, -\frac{1.789 \cdot 10^{-5}}{48} - \frac{1}{3} \cdot 5.788 \cdot 10^{-5} B\right\}\right\}\right]$$

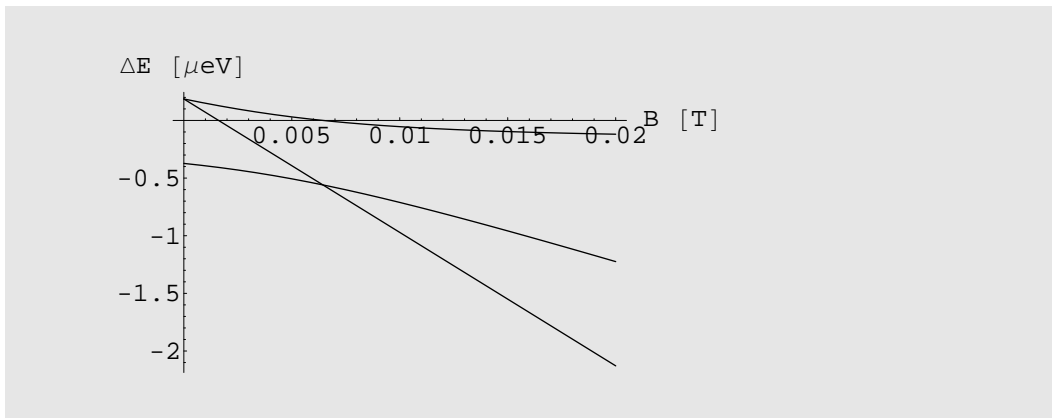
$$\left\{\frac{1}{2} \left(-1.86354 \times 10^{-7} - 0.00005788 B - 0.00005788 \sqrt{0.0000932961 - 0.00643933 B + 1. B^2}\right), \frac{1}{2} \left(-1.86354 \times 10^{-7} - 0.00005788 B + 0.00005788 \sqrt{0.0000932961 - 0.00643933 B + 1. B^2}\right)\right\}$$

```
Plot[{eigennum[[1]] * 10^6, eigennum[[2]] * 10^6},
      {B, -0.1, 0.1}, AxesLabel -> {"B [T]", "ΔE [μeV]"}];
```



The plot clearly interpolates the two limits (a) and (b), and respects the no level-crossing theorem. Adding the  $m_j = \frac{3}{2}$  state and zooming in a bit,

```
mixp = Plot[{eigennum[[1]] * 10^6, eigennum[[2]] * 10^6}, {B, 0, 0.02},
            AxesLabel -> {"B [T]", "ΔE [μeV]"}, DisplayFunction -> Identity];
purep = Plot[ $\left(\frac{1.789 \cdot 10^{-5}}{96} - 2 * 5.788 \cdot 10^{-5} B\right) * 10^6$ , {B, 0, 0.02}, DisplayFunction -> Identity];
Show[mixp, purep, DisplayFunction -> $DisplayFunction];
```



we clearly see the transition from the regime near  $B = 0$ , where the spin-orbit coupling is dominant and  $2 p_{1/2}$  is depressed, to the regime at large  $B$ , where  $J_z$  is dominant.