

# Part III Examples Class

## Advanced Quantum Physics

Easter 2009

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### Short questions

#### 1. Identical Particles

Explain why  ${}^7\text{Li}$  is a boson and  ${}^6\text{Li}$  a fermion.

#### 2. Lasers

Why is a two level system not suitable for use in a laser? Describe a suitable system.

#### 3. Spin-orbit interaction

Describe the form of the spin-orbit interaction and provide a simple account of its physical origin.

#### 4. Spectroscopic Terms and Hund's rules

Determine the possible Spectroscopic Terms for the following electronic configurations in an atom (a)  $2p^13p^1$  (b)  $2p^2$  (c)  $2p^5$ . For each case use Hund's rules to determine the ground state Term.

#### 5. Entanglement

Explain why the two qubits in the state  $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$  can be considered entangled. Describe a quantum gate circuit suitable for generating such a state.

#### 6. Landau levels

Using qualitative arguments explain why the resistance of a two-dimensional electron gas oscillates periodically with  $\frac{1}{B}$ , where  $B$  is the magnetic field perpendicular to the plane of the 2D gas.

## Long questions

### 7. Harmonic Oscillator, Ladder Operators; Perturbation Theory

A particle of mass  $m$  moves in a one-dimensional harmonic potential  $V(x) = \frac{1}{2}m\omega^2x^2$ . Define an operator  $\hat{A} = (2m\hbar\omega)^{-\frac{1}{2}}(\hat{p}_x + im\omega\hat{x})$ , where  $\hat{p}_x$  and  $\hat{x}$  are momentum and position operators for the particle.

- Show that  $\hat{A}\hat{A}^\dagger = \hat{H}/\hbar\omega - \frac{1}{2}$ ,  $\hat{A}^\dagger\hat{A} = \hat{H}/\hbar\omega + \frac{1}{2}$ ,  $[\hat{H}, \hat{A}] = \hbar\omega\hat{A}$  and  $[\hat{H}, \hat{A}^\dagger] = -\hbar\omega\hat{A}^\dagger$ , where  $\hat{H}$  is the Hamiltonian operator.
- Hence, show that the sequence of positive energy eigenvalues has the form  $(n + \frac{1}{2})\hbar\omega$ , where  $n$  is a positive integer or zero.
- A perturbing potential is superimposed of the form  $\lambda x^4$ . By expressing  $x$  in terms of the ladder operators, show that the shift in the energy levels to first order in  $\lambda$  is given by

$$\frac{3\hbar^2(2n^2 + 2n + 1)}{4m^2\omega^2}\lambda .$$

### 8. Variational Method

A particle of mass  $m$  moves in a one-dimensional potential  $\lambda x^4$ . Use the variational method to place the following upper bound on the ground state energy, taking a Gaussian as your trial function.

$$E_0 \leq \lambda^{\frac{1}{3}} \left( \frac{9\hbar^2}{16m} \right)^{\frac{2}{3}}$$

Compare with the exact result:

$$E_0 = 1.060\lambda^{\frac{1}{3}} \left( \frac{\hbar^2}{2m} \right)^{\frac{2}{3}}$$

You can use the standard integrals:

$$\int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} dx = \frac{1}{4\alpha} \sqrt{\frac{\pi}{2\alpha}} \quad ; \quad \int_{-\infty}^{\infty} x^4 e^{-2\alpha x^2} dx = \frac{3}{16\alpha^2} \sqrt{\frac{\pi}{2\alpha}}$$

## 9. LS Coupling; Zeeman effect

The yellow sodium D lines arise from transitions between the  ${}^2P_{\frac{1}{2}}$  and  ${}^2P_{\frac{3}{2}}$  excited states and the ground state  ${}^2S_{\frac{1}{2}}$ . Explain the notation used to specify the states and the assumptions about the Hamiltonian on which it is based.

Show that in a weak magnetic field  $B$  the  ${}^2P_{\frac{3}{2}}$  state will split into four energy levels with uniform spacing  $\frac{4}{3}\mu_B B$  and the  ${}^2S_{\frac{1}{2}}$  state into two energy levels with spacing  $2\mu_B B$ , where  $\mu_B$  is the Bohr Magneton. By considering terms in the Hamiltonian, explain how you would decide whether a particular magnetic field could be considered as weak.

The sodium D<sub>2</sub> line corresponds to the transition  ${}^2P_{\frac{3}{2}} \leftrightarrow {}^2S_{\frac{1}{2}}$ . If sodium atoms are excited in a discharge tube placed in a magnetic field  $B$ , how many D<sub>2</sub> emission lines will be observed if the discharge is viewed perpendicular to  $B$ ? What will be their states of polarization, and what will be their energies relative to that of the D<sub>2</sub> line in zero magnetic field?

*[Ans: 6 lines, with energy shifts  $\pm\frac{1}{3}\mu_B B$ ,  $\pm\mu_B B$ ,  $\pm\frac{5}{3}\mu_B B$ , with the last four plane polarized parallel to  $x$  or  $y$  and the first two plane polarized parallel to  $z$ .]*

When circularly polarised white light is passed through sodium vapour in a direction parallel to the weak magnetic field, just two absorption lines corresponding to the D<sub>2</sub> transition are observed; explain why this is so. Atoms so excited by circularly polarised light may decay back to the  ${}^2S_{\frac{1}{2}}$  state by fluorescence. Describe the energies and polarizations of the fluorescence radiation. What can you say about its directional properties?

*[Ans: Only the two  $\Delta m_J = +1$  transitions will be seen in absorption, i.e. those having energy shifts  $+\mu_B B$  and  $+\frac{5}{3}\mu_B B$ . In fluorescence, observe three lines; these two and that with energy shift  $-\frac{1}{3}\mu_B B$ .]*

*[The Landé  $g$ -factor is  $g = 1 + \frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}$ .]*

**Outline Solutions**  
**Part III Examples Class**  
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**1. Identical Particles**

${}^7\text{Li}$  has 3 protons, 4 neutrons and 3 electrons - a total of 10 fermions. If two  ${}^7\text{Li}$  atoms are able to exchange their constituent particles 10 exchanges will take place and the final overall wavefunction is equal to the initial one, hence  ${}^7\text{Li}$  is a composite boson. In contrast  ${}^6\text{Li}$  comprises 9 fermions, on exchange of all the constituent particles the final wavefunction is  $-1 \times$  the initial wavefunction, hence  ${}^6\text{Li}$  is a composite fermion.

**2. Lasers**

A two level system cannot attain a population inversion - where the upper level has a greater occupancy than the lower level. Population inversion is necessary for laser operation, this can take place with a three or more level system where the lower laser transition state rapidly decays to another level.

**3. Spin-orbit interaction**

The spin orbit interaction has the form  $E = -\gamma \mathbf{L} \cdot \mathbf{S}$ , the electron moving in the electric field of the nucleus experiences a magnetic field which has an energy of interaction with the magnetic moment of the electron.

**4. Spectroscopic Terms and Hund's rules**

Ordering of energy levels given by Hund's rules:

- (1) Combine the spins of the electrons to obtain possible values of total spin  $S$ . The largest permitted value of  $S$  lies lowest in energy.
- (2) For each value of  $S$ , find the possible values of total orbital angular momentum  $L$ . The largest value of  $L$  lies lowest in energy.
- (3) Couple the values of  $L$  and  $S$  to obtain the values of  $J$  (hence the name of the scheme). If the subshell is less than half full, the smallest value of  $J$  lies lowest; otherwise, the largest value of  $J$  lies lowest.

(a)  $2p^1 3p^1$  :  $S = 0, 1, L = 0, 1, 2$  giving  $^1S, ^3S, ^1P, ^3P, ^1D, ^3D$ . Combining  $S$  and  $L$  to give  $J$  gives  $^1S_0, ^3S_1, ^1P_1, ^3P_{0,1,2}, ^1D_2, ^3D_{1,2,3}$ .

Using Hund's rules we get  $^3D_1$  as the ground state.

(b)  $2p^2$  : Simple combination gives the same terms as in (a) but we now need to take into account symmetry since these are equivalent electrons. For  $S = 0$  the spin part of the wavefunction is antisymmetric so the spatial part must be symmetric and  $L = 0, 2$ . For  $S = 1$  the spin part of the wavefunction is symmetric and hence the spatial part antisymmetric and hence  $L = 1$ .

So the following terms from those given in (a) are allowed:

$^1S_0, ^3P_{0,1,2}, ^1D_2$ .

Using Hund's rules the  $^3P_0$  state lies lowest.

(c)  $2p^5$  : The configuration  $2p^5$  is equivalent to a single hole in a shell so  $L = 1$  and  $S = 1/2$ . Hence we have  $^2P_{1/2,3/2}$  of which  $J = 3/2$  lies lowest because the shell is more than half full.

## 5. Entanglement

In the state  $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$  there are strong correlations between the two qubits. If we measure the two qubits simultaneously then there is a probability of  $1/2$  that qubit 1 is in the state  $|0\rangle$  and qubit 2 is in the state  $|0\rangle$ , there is also a probability of  $1/2$  that qubit 1 is in the state  $|1\rangle$  and qubit 2 is in the state  $|1\rangle$ . However the probability that qubit 1 is in the state  $|0\rangle$  and qubit 2 is in the state  $|1\rangle$  is zero as is the probability that qubit 1 is in the state  $|1\rangle$  and qubit 2 is in the state  $|0\rangle$ .

The quantum gate arrangement consists of a Hadamard gate which feeds the control input of a CNOT gate - see slide 23.13 of the AQP course.

## 6. Landau levels

A full answer is given on slides 13.11-13.13 in the AQP course.

## 7. Harmonic Oscillator, Ladder Operators; Perturbation Theory

a)

$$\begin{aligned}
 \hat{A}\hat{A}^\dagger &= (2m\hbar\omega)^{-1} \left( \hat{p}_x^2 + m^2\omega^2\hat{x}^2 + im\omega[\hat{x}, \hat{p}_x] \right) \\
 &= \frac{1}{\hbar\omega} \left( \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 + \frac{1}{2}i\omega(i\hbar) \right) \\
 &= \hat{H}/\hbar\omega - \frac{1}{2}
 \end{aligned}$$

Likewise,  $\hat{A}^\dagger\hat{A} = \hat{H}/\hbar\omega + \frac{1}{2}$ , as above with the opposite sign on the commutator term.

The following useful results for commutators can easily be derived:

$$[\hat{p}_x^2, \hat{x}] = -2i\hbar\hat{p}_x \quad \text{and} \quad [\hat{x}^2, \hat{p}_x] = 2i\hbar\hat{x}$$

Using these, we have

$$\begin{aligned}
 [\hat{H}, \hat{A}] &= (2m\hbar\omega)^{-\frac{1}{2}} \left( [p_x^2/2m, im\omega\hat{x}] + [\frac{1}{2}m\omega^2\hat{x}^2, \hat{p}_x] \right) \\
 &= (2m\hbar\omega)^{-\frac{1}{2}} \left( -\frac{1}{2}i\omega \cdot 2i\hbar\hat{p}_x + \frac{1}{2}m\omega^2 \cdot 2i\hbar\hat{x} \right) \\
 &= \hbar\omega\hat{A}
 \end{aligned}$$

and similarly  $[\hat{H}, \hat{A}^\dagger] = -\hbar\omega\hat{A}^\dagger$ .

b) Suppose  $\psi_n$  is an eigenfunction of  $\hat{H}$ , i.e.  $\hat{H}\psi_n = E_n\psi_n$ . Then:

$$\begin{aligned}
 [\hat{H}, \hat{A}^\dagger]\psi_n &= -\hbar\omega\hat{A}^\dagger\psi_n \\
 \Rightarrow \hat{H}(\hat{A}^\dagger\psi_n) &= (E_n - \hbar\omega)\hat{A}^\dagger\psi_n
 \end{aligned}$$

Thus,  $\hat{A}^\dagger\psi_n$  is also an eigenstate of  $\hat{H}$  with eigenvalue  $E_n - \hbar\omega$ . Likewise,  $\hat{A}\psi_n$  is an eigenfunction with eigenvalue  $E_n + \hbar\omega$  – the operators  $\hat{A}$  and  $\hat{A}^\dagger$  act as raising and lowering operators. Consider the lowest energy level,  $\psi_0$ :

$$\hat{A}^\dagger\psi_0 = 0 \Rightarrow (\hat{A}\hat{A}^\dagger)\psi_0 = 0 = (\hat{H}/\hbar\omega - \frac{1}{2})\psi_0 \Rightarrow \hat{H}\psi_0 = \frac{1}{2}\hbar\omega\psi_0$$

and hence

$$E_n = (n + \frac{1}{2})\hbar\omega$$

since  $\psi_n$  is generated by acting  $n$  times with  $\hat{A}$ .

- c) Perturbation theory gives the energy shift as  $\Delta E_n = \langle n | \lambda x^4 | n \rangle$ . Write  $\hat{x}$  in terms of the ladder operators:

$$\hat{x} = (\hat{A} - \hat{A}^\dagger) \frac{(2m\hbar\omega)^{\frac{1}{2}}}{2im\omega}$$

Consider  $(\hat{A} - \hat{A}^\dagger)^4 |n\rangle$ . The only terms which are not orthogonal to  $\langle n|$  are those with two raising and two lowering operators, viz:

$$(\hat{A}^2 \hat{A}^{\dagger 2} + \hat{A} \hat{A}^\dagger \hat{A} \hat{A}^\dagger + \hat{A}^\dagger \hat{A}^2 \hat{A}^\dagger + \hat{A}^{\dagger 2} \hat{A}^2 + \hat{A}^\dagger \hat{A} \hat{A}^\dagger \hat{A} + \hat{A} \hat{A}^{\dagger 2} \hat{A}) |n\rangle$$

Now,  $\hat{A} |n\rangle = c_n |n+1\rangle$ , where we obtain  $c_n$  from the condition that both  $|n\rangle$  and  $|n+1\rangle$  are normalized:

$$|c_n|^2 = \langle n | \hat{A}^\dagger \hat{A} |n\rangle = n+1$$

using the result from part a). Likewise  $\hat{A}^\dagger |n\rangle = d_n |n-1\rangle$  where  $|d_n|^2 = n$ . Using these results, a little careful algebra gives:

$$(\hat{A} - \hat{A}^\dagger)^4 |n\rangle = n(n-1) + n^2 + n(n+1) + (n+1)(n+2) + (n+1)^2 + n(n+1) = 6n^2 + 6n + 3$$

Hence, we obtain

$$\Delta E_n = \frac{3\hbar^2(2n^2 + 2n + 1)}{4m^2\omega^2} \lambda$$

## 8. Variational Method

Gaussian trial function - first normalise it:

$$\phi = A e^{-\alpha x^2} = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha x^2}$$

Next evaluate  $\hat{H} |\phi\rangle$ :

$$\hat{H} |\phi\rangle = A \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \lambda x^4 \right] e^{-\alpha x^2} = A \left[ -\frac{\hbar^2}{2m} (4\alpha^2 x^2 - 2\alpha) + \lambda x^4 \right] e^{-\alpha x^2}$$

Using the standard integrals given,

$$\langle \phi | \hat{H} | \phi \rangle = \frac{\hbar^2 \alpha}{2m} + \frac{3\lambda}{16\alpha^2}$$

Minimizing w.r.t.  $\alpha$  gives:

$$\frac{\hbar^2}{2m} - \frac{3\lambda}{8\alpha^3} = 0 \quad \Rightarrow \quad \alpha = \left( \frac{3\lambda m}{4\hbar^2} \right)^{\frac{1}{3}}$$

and hence substituting back into the expectation value of  $\hat{H}$ :

$$E_0 \leq \lambda^{\frac{1}{3}} \left( \frac{9\hbar^2}{16m} \right)^{\frac{2}{3}}$$

which is within 2% of the exact result.

## 9. LS Coupling; Zeeman effect

The notation specifies the total angular momentum quantum numbers of the atom in the form  $^{2S+1}X_J$ , where  $X$  is a letter used to denote the orbital  $L$  quantum number in the usual way. This implicitly assumes that  $L$ ,  $S$  and  $J$  are all good quantum numbers, which is true in the *L-S coupling approximation*, i.e. when the spin-orbit interaction can be considered small compared to the residual non-central Coulomb repulsion between the electrons.

In a weak magnetic field, the magnetic interaction  $\mu_B(\hat{\mathbf{L}} + 2\hat{\mathbf{S}}) \cdot \mathbf{B}$  (assumed small compared to the spin-orbit term) is treated as a perturbation on the L-S coupled states. In this case, the energy shift is given by  $\Delta E = g\mu_B B m_J$ , where the Landé  $g$ -factor is  $g = \frac{4}{3}$  for the  $^2P_{\frac{3}{2}}$  state and  $g = 2$  for the  $^2S_{\frac{1}{2}}$  state. Hence, the  $^2P_{\frac{3}{2}}$  state will split into four energy levels with uniform spacing  $\frac{4}{3}\mu_B B$  and the  $^2S_{\frac{1}{2}}$  state into two energy levels with spacing  $2\mu_B B$ .

In a discharge tube, atoms will populate all of the  $m_J$  values of the  $^2P_{\frac{3}{2}}$  state. The electric dipole selection rules allow transitions with  $\Delta m_J = \pm 1, 0$  only. The  $\Delta m_J = 0$  transitions correspond to dipoles in the  $z$ -direction, and the  $\Delta m_J = \pm 1$  transitions to dipoles in the  $x$ - or  $y$ -directions. So the allowed decays from  $^2P_{\frac{3}{2}}$  to  $^2S_{\frac{1}{2}}$  are:

	$m_j$	$\Delta m_J$	$\Delta E$
a)	$+\frac{3}{2} \rightarrow +\frac{1}{2}$	-1	$+\mu_B B$
b)	$+\frac{1}{2} \rightarrow +\frac{1}{2}$	0	$-\frac{1}{3}\mu_B B$
c)	$+\frac{1}{2} \rightarrow -\frac{1}{2}$	-1	$+\frac{5}{3}\mu_B B$
d)	$-\frac{1}{2} \rightarrow +\frac{1}{2}$	+1	$-\frac{5}{3}\mu_B B$
e)	$-\frac{1}{2} \rightarrow -\frac{1}{2}$	0	$+\frac{1}{3}\mu_B B$
f)	$-\frac{3}{2} \rightarrow -\frac{1}{2}$	+1	$-\mu_B B$

Viewing perpendicular to the field in the  $y$ -direction, say, contributions from both  $x$ - and  $z$ -dipoles can be observed. Thus 6 lines will be seen, of which b) and d) are plane-polarized in the  $z$ -direction, and the other four plane-polarized parallel to  $x$ .

The circularly polarised light will induce  $\Delta m_J = +1$  transitions only (or alternatively  $\Delta m_J = -1$  with the other handedness of polarization). Only two absorption lines will be seen, corresponding to a) and c) in this case. Thus only the  $m_J = +\frac{3}{2}, +\frac{1}{2}$  substates of the  ${}^2P_{\frac{3}{2}}$  level will get excited. So, the only transitions seen in the fluorescence spectrum will be those starting from the  $m_J = +\frac{3}{2}, +\frac{1}{2}$  states, i.e. a), b) and c). Transitions a) and c) are both  $\Delta m_J = -1$ , associated with  $x - y$  dipoles; they will be circularly polarized when viewed along  $z$ , and plane polarized along  $x$  or  $y$  when viewed along  $y$  or  $x$  respectively. Transition b) has  $\Delta m_J = 0$ , associated with  $z$  dipoles; it will not be seen when viewed along  $z$ , and will be plane polarized along  $z$  when viewed in the  $x - y$  plane.