

# Quantum and Atomic Physics: Questions

Prof Andrew Steane 2005

**Problem set 1.** Some general quantum knowledge; Hydrogen gross structure, wavefunctions, quantum numbers, spectrum, scaling.

## General familiarity

1. Give a rough sketch of the 10'th energy eigenfunction for a particle moving in one dimension in the triangular potential (i.e. V-shaped)  $V(x) = |x|$ . Get the following features right: the number of nodes, the overall symmetry, the behaviour at large  $|x|$ , the way the function exhibits kinetic energy.

2. Let  $\psi_n$  be a complete set of orthogonal, normalised wavefunctions. Prove that

$$\phi = \sum_n \psi_n \langle \psi_n | \phi \rangle$$

for any wavefunction  $\phi$ , and write down the corresponding result for  $|\phi\rangle$  in Dirac notation.

3. What is the operator for velocity, in non-relativistic quantum theory?

## Hydrogen

4. Write down the expression for the energy levels of hydrogen. Evaluate the ionization energy of hydrogen to 5 significant figures in electron volts, taking care to allow for the reduced mass of the electron. Calculate the wavelength of the transition from  $n = 4$  to  $n = 3$ .

5. Write down the definition of the fine structure constant  $\alpha$  in terms of  $e, \epsilon_0, \hbar$  and  $c$ . Evaluate  $\alpha$  and  $1/\alpha$  to 4 significant figures.

6. Write down an expression for the Bohr radius  $a_0$ , (a) in terms of  $e, \epsilon_0, \hbar, m$ ; (b) in terms of  $\alpha$  and other quantities.

7. Find the errors in the following, and suggest corrections:

- (a) The ground state of hydrogen is 2s.
- (b) The 2p–1p transition in hydrogen is ultraviolet.
- (c) The angular part of the wavefunction in hydrogen depends on  $n$  and  $l$ .

8. (a) Treating  $a_0$  as a parameter, write down the complete wavefunctions (including radial and angular parts) for the states 1s, 2s, and 2p (giving all three  $m_l$  possibilities in the last case). In each case draw neat graphs of the radial part of the wavefunction,  $R(r)$ , and also  $r^2|R(r)|^2$ . What is the significance of the latter? N.B. this question is not intended to test your mathematical abilities, but to produce familiarity with the wavefunctions. Look them up and copy them!

(b) How does  $R_{n,l}$  vary with  $r$  as  $r \rightarrow 0$ ? Draw on a single plot a ‘close-up’ of  $R_{n,l}$  in the region  $r < 10^{-15}$  m for the states 3s, 3p, 3d. What is the significance of this region?

9. Consider the probability density distributions for an electron in the 2p  $m_l = 0$  state and the 2p  $m_l = 1$  state, where  $m_l$  is the magnetic quantum number. Which distribution is shaped like an hour-glass, and which like a doughnut? Make an “artists impression” sketch of these 3-dimensional probability density distributions. How does the wavefunction (not the probability density) carry the information about the sign of  $m_l$  when  $m_l = 1$  or  $-1$ ?

10. We will sketch the radial part of the wavefunction for the  $n = 10, l = 9$  state of hydrogen. First consider

a. How many nodes has it got?

- b. How does it vary for small  $r$ ?  
 c. Now consider the radial effective potential

$$V_{\text{eff}} = \frac{l(l+1)\hbar^2}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}.$$

Solve  $V_{\text{eff}}(r) = E$  for  $r$ , where  $E$  is the total energy  $-E_1/n^2$ . Thus obtain the two places where the kinetic energy falls to zero for the  $n = 10, l = 9$  state. In between these two values of  $r$  is the classically allowed region. Outside the classically allowed region the wavefunction falls rapidly to zero. Bringing your results from (a), (b) and (c) together, sketch the radial part of the wavefunction.

11. Show that in the ground state of hydrogen,  $\langle r^n \rangle = (n+2)(a_0/2)\langle r^{n-1} \rangle$ . What is  $\langle r^0 \rangle$ ? Derive  $\langle r \rangle$  and  $\langle 1/r \rangle$  in terms of  $a_0$ . Hence find  $\langle V(r) \rangle$ , where  $V(r) = -e^2/4\pi\epsilon_0 r$ . Given the expression for the ground state energy, use this result to deduce the mean kinetic energy of the electron in the ground state and hence its r.m.s. speed  $v$ . Express  $v$  in terms of  $\alpha$  and the speed of light.

*This question is optional*

11a. Obtain the normalisation constant  $N$  in the ground state wavefunction  $\psi = N \exp(-r/a_0)$  without much further effort, as follows. First note that the results of question 10 can be obtained without needing to know  $N$ . Use the results of question (10) to obtain  $\langle 1/r^2 \rangle$  in the ground state. Then evaluate  $\langle 1/r^2 \rangle$  for the state  $\psi = N \exp(-r/a_0)$  by doing the easy integral. By equating this to the value you already have, deduce that  $N = (1/\pi a_0^3)^{1/2}$ .

## Scaling

12. How do the energy levels of hydrogen-like ions scale as a function of the nuclear charge  $Z$ ? The following wavelengths (as well as many others) are observed in emission from a plasma: 3.375 nm, 2.848 nm, 2.700 nm, 18.226 nm, 13.501 nm, 12.054 nm. Show that this spectrum is consistent with emission from a hydrogen-like ion, and identify the element. [Method: first make a reasonably accurate sketch of this spectrum on a frequency scale, then guess the identity of one or more of the transitions, then confirm your guess using your knowledge of the pattern to be expected, and hence deduce  $Z$ ].

13. A muon has mass 206 times the electronic mass and the same charge as an electron. The particle may be captured by an atom and the radiation which is emitted as the muon cascades through the energy levels can be measured.

- a. Assuming the muon-nucleus system can be treated as hydrogen-like, find the energy in MeV of the photon emitted as the muon goes from a state with principle quantum number 2 to the ground state in an atom of lead.  
 b. Is it reasonable to neglect the effect of the electrons in this calculation as a first approximation? (Consider the mean radius of the muon orbits). Do you think the influence of the nuclear charge has been accurately accounted for?

## Spectroscopy

14. Explain how the ionization potential may be derived from the emission spectrum of hydrogen. Outline a sensible way to analyse the experimental data in order to get a precise result.

15. Estimate how many lines of the Paschen series of hydrogen could be resolved by a good grating spectrometer whose grating had a width 10 cm. Would such an instrument also be useful for examining the Lyman series?

### Further questions

16. To what fractional precision has the Lamb shift of the ground state of hydrogen been measured? (A statement of the correct order of magnitude is acceptable). What motivates such measurements? [See introduction chapter in lecture notes for relevant information].

17. Which of the following are energy eigenstates for hydrogen (ignoring normalisation)? (N.B. The intention is that you answer this without operating on each wavefunction with the Hamiltonian. Rather, look up the energy eigenstate wavefunctions (radial and angular parts) and recognise them. If you are unsure in any given case, of course operating with the Hamiltonian will give an unambiguous answer, but that 'brute force' method is less insightful.)

- (a)  $e^{-r/a_0}$
- (b)  $re^{-r/2a_0}$
- (c)  $re^{-r/2a_0} \cos(\theta)$
- (d)  $e^{-r/a_0} \cos(\theta)$
- (e)  $re^{-r/2a_0} (\cos(\theta) + \sin(\theta)e^{i\phi})$
- (f)  $e^{-r/a_0} + (1 - r/2a_0)e^{-r/2a_0}$

Give any further remarks which occur to you as you think about this.

**Problem set 2.** perturbation theory; constants of the motion; fine structure: kinetic energy correction and spin-orbit interaction; scaling; isotope shift in hydrogen: nuclear volume and mass contribution.

### Some angular momentum general knowledge

1. The total angular momentum of a particle with orbital angular momentum  $\hat{\mathbf{I}}$  and spin angular momentum  $\hat{\mathbf{s}}$  is  $\hat{\mathbf{j}} = \hat{\mathbf{I}} + \hat{\mathbf{s}}$ . The eigenvalues of  $\hat{j}^2$ ,  $\hat{l}^2$  and  $\hat{s}^2$  are  $j(j+1)\hbar^2$ ,  $l(l+1)\hbar^2$  and  $s(s+1)\hbar^2$  respectively. State the possible values of  $j$  for the cases

- (a)  $l = 0$ , any  $s$
- (b)  $l = 1$ ,  $s = 1/2$
- (c)  $l = 1$ ,  $s = 1$
- (d)  $l = 1$ ,  $s = 3/2$

What is the general rule which tells you how many values of  $j$  to expect for arbitrary  $l$ ,  $s$ ? What basic information about the fine structure of hydrogen does all this tell us?

### Basic concepts of non-degenerate perturbation theory

2. Derive the expressions for the first order shift in energy, and change in the wavefunction, in non-degenerate perturbation theory.

3. This is a classic example of—and test of—perturbation theory. A particle of charge  $q$  and mass  $m$  is in a harmonic oscillator potential  $V = (1/2)m\omega^2x^2$ . A weak external electric field of magnitude  $f$  is applied along the  $x$  direction. This gives an electrostatic potential  $-fx$  and potential energy  $V_f = -qfx$ . Treating this as a small perturbation, calculate the shift in energy of all the states, as follows.

a. Write down the energy shift to be calculated,  $\delta E_n^{(1)}$ , in the form of a matrix element (don't do the integral yet), by quoting the standard result of first-order perturbation theory. (Call the energy eigenfunctions  $\psi_n^0$ .)

b. Now have a quick look at the overall form of the integral, and using your general knowledge of the quantum harmonic oscillator, deduce that the first order shift is zero for every  $n$ .

c. We will next work out the first order change in the wavefunctions (this will turn out to be non-zero). First write down the standard result, derived in question 1, involving a sum of matrix elements divided by energy differences.

d. We could in principle write out the integrals using the Hermite polynomials and Gaussian function, but that is hard work! Let's see if we can apply our knowledge of the harmonic oscillator. First, recall that the position  $x$  can be regarded as an operator, and written in terms of raising and lowering operators:

$$x = C(\hat{a} + \hat{a}^\dagger)$$

where  $C = (\hbar/2m\omega)^{1/2}$ . The raising and lowering operators have the effects

$$\begin{aligned}\hat{a}^\dagger \psi_n^0 &= \sqrt{n+1} \psi_{n+1}^0 \\ \hat{a} \psi_n^0 &= \sqrt{n} \psi_{n-1}^0\end{aligned}$$

Use these insights to evaluate the matrix element  $\langle \psi_n^0 | x | \psi_k^0 \rangle$  for arbitrary  $n$ ,  $k$  (you should find that there are two cases to consider).

e. Hence show that the first order change in state is

$$\delta \psi_n^{(1)} = \frac{qfC}{\hbar\omega} \left( (n+1)^{1/2} \psi_{n+1}^0 - n^{1/2} \psi_{n-1}^0 \right)$$

f. Write down the formula for the 2nd order energy shift, and use the result of part (e) to show it is  $\delta E_k^{(2)} = -q^2 f^2 / 2m\omega^2$ .

g. This is a nice test of perturbation theory, because the problem can be solved exactly by a simple insight. To get the general idea, plot a graph of  $V(x)$  and also of  $V(x) + V_f(x)$ . (For the purpose of this graph alone, choose  $m = \omega = q = f = 1$ ). The point is, the new potential energy is still exactly a quadratic, it is merely shifted over and down a bit. Therefore write  $V(x) + V_f(x) = A(x - x_0)^2 + B$  and find  $A$  and  $B$ . Use this to deduce the exact energy eigenvalues for this problem, and hence confirm your answers from parts (b) and (f).

### Fine structure and degenerate perturbation theory

4. Show that the first correction to the kinetic energy term in the Schrödinger equation, when one allows for special relativity in the case  $v \ll c$ , gives a perturbation

$$\delta H_m = -\frac{1}{2mc^2} (H^0 - V(r))^2.$$

Quoting the standard results of 1st order perturbation theory, show that for hydrogen the energy shift produced by this perturbation is

$$\delta E = -\frac{1}{2mc^2} \left( E_n^2 + 2E_n \frac{e^2}{4\pi\epsilon_0} \left\langle \frac{1}{r} \right\rangle + \left( \frac{e^2}{4\pi\epsilon_0} \right)^2 \left\langle \frac{1}{r^2} \right\rangle \right)$$

Obtain the shift of the ground state of hydrogen using your results from problem set 1, question 11. Express the result in terms of a suitable power of  $\alpha$  and other quantities. Evaluate the shift, in GHz.

5. a. Derive the expression for the spin-orbit interaction Hamiltonian in a one-electron atom or ion with nuclear charge  $Z$ . Use the simple method which leads to a factor of 2 error, and then put in the factor 1/2 correction due to Thomas precession, but don't spend time on the latter at this stage. b. What is the direction of the  $B$ -field experienced by the electron relative to its orbital angular momentum?

c. What is the direction of the intrinsic magnetic dipole of the electron relative to its spin angular momentum?

d. If the spin and orbital angular momentum vectors were described by classical mechanics, explain in qualitative terms how they would behave as a function of time.

6. Explain what a 'constant of the motion' is, and what is meant by a 'good quantum number'. Considering the fine structure (spin orbit coupling) of hydrogen in order to have a definite example, state the (relevant) constants of the motion and good quantum numbers. Give an example of one or more quantum numbers which are not good in this case.

7. With your expression from Q.5, use perturbation theory to derive the spin-orbit shift

$$\Delta E_{so} = \frac{g_s}{8} mc^2 Z^4 \alpha^4 \frac{1}{n^3} \left( \frac{j(j+1) - l(l+1) - s(s+1)}{l(l+1/2)(l+1)} \right)$$

You may quote the expression for  $\langle 1/r^3 \rangle$  from the lecture notes or another reference. The shift is of order  $Z^2 \alpha^2$  times the gross structure energy of the atom. What is the significance of this?

8. Find the splitting between the  $j = 3/2$  and the  $j = 1/2$  levels of the 2p configuration in hydrogen, in GHz. Estimate the size of the magnetic field experienced by the electron. Using the known  $n$ -dependence, find also the splitting of the 3p configuration. Draw a simple energy-level diagram showing all the  $n = 2$  and  $n = 3$  levels, labeling the levels with the appropriate quantum

numbers. Exaggerate the fine structure so that it is clearly indicated, but is to a consistent scale for both configurations. (You may ignore the Lamb shift).

9. Which quantum numbers are specified by the notation  $3^2D_{5/2}$ ? Give the names and the values which are indicated. How many degenerate quantum states are together included in the level  $3^2D_{5/2}$  of hydrogen?

10. (Optional) Show that the spin-orbit interaction, when small and therefore treatable as a perturbation, does not shift the ‘centre of gravity’ of the set of energy levels when it splits up a degenerate energy level into a group. The ‘centre of gravity’ of a set of energy levels is defined as the sum of  $g_i E_i$  where  $E_i$  are the energies and  $g_i$  the degeneracies, i.e. the number of quantum states in the level (e.g. the  $2j + 1$  states of different  $m_j$  for given  $j$ ). The case where  $s = 1/2$  as in hydrogen is fairly easy because you only have  $j = l \pm 1/2$  to consider, but if you wish you may like to prove the result for the more general case of any values of  $l$  and  $s$ .

11. Estimate the size of the fine structure of the 2p configuration in hydrogen-like sodium (i.e. sodium ions with all but the last electron removed). Why can’t we use perturbation theory to calculate the effect of the spin-orbit interaction in hydrogen-like uranium?

### Isotope shift

12. Calculate the difference between the ground state energy of hydrogen and deuterium owing to the different reduced mass. Calculate the isotope shift for the transition 2s–3p, in GHz (i.e. just calculate that part of the isotope shift which is caused by the difference in reduced mass).

13. Calculate by first-order perturbation theory the nuclear volume shift for a hydrogen isotope, using the model that all the nuclear charge is contained in a spherical shell of radius  $R$ . Compare your answer with the result described in the lecture notes where the nucleus is modeled (somewhat better) as a uniform sphere of charge. Taking  $R = 1$  fm, calculate the size of the shift and compare it to the mass shift calculated in question 12.

### Further points

14. (Optional—but it is easy and you might enjoy it). This is a trick which allows you to work out  $\langle 1/r \rangle$  for all the energy levels of hydrogen. Consider the quantity  $\langle \lambda/r \rangle$  where  $\lambda$  is small. We can interpret  $\langle \lambda/r \rangle$  as the first-order correction due to a perturbation  $\lambda/r$ . Now such a problem can be solved exactly: we just replace  $e^2/4\pi\epsilon_0$  by  $(e^2/4\pi\epsilon_0) - \lambda$ : explain why. Now  $e^2/4\pi\epsilon_0 = \alpha\hbar c$ , so we are replacing  $\alpha\hbar c$  by  $\alpha\hbar c - \lambda$ . Make this replacement in the formula  $-(1/2)\mu\alpha^2 c^2$  for the energy levels and hence show that the energy change to first order in  $\lambda$  is  $\lambda/a_0 n^2$ . Hence derive  $\langle 1/r \rangle$ .

15. (Optional) This confirms a point which has been assumed above, namely that the relativistic kinetic shift can be treated using the familiar states having quantum numbers  $n, l, m$ . Since we have degeneracy, we can’t take it for granted. Argue that the orbital angular momentum  $\hat{l}^2$  is a constant of the motion under both  $H^0$  and  $\delta H$ , as follows.

a. We already know  $[\hat{l}^2, H^0] = 0$  for any spherically symmetric problem, but in any case give a proof to make sure we know what we are doing. [Hint: work in spherical polar coordinates, and express the kinetic energy as an  $r$ -dependent part plus  $\hat{l}^2/2mr^2$ . If you actually carry out any differentiating, you have not taken the simplest route.]

b. Show that  $[\hat{l}^2, K] = 0$ , where  $\hat{K} = \hat{p}^2/2m$  is kinetic energy, e.g. by re-using part (a).

c. Our perturbation is proportional to kinetic energy squared. Use a general result for commutators of the form  $[A, B^2]$  to show that  $[\hat{l}^2, K] = 0$  implies  $[\hat{l}^2, K^2] = 0$ .

d. We have now proved both  $[\hat{l}^2, H^0] = 0$  and  $[\hat{l}^2, \delta H] = 0$  for our problem where  $H = H^0 + \delta H$ . What is the significance of these results to degenerate perturbation theory?

Quantum and Atomic Physics. Prof A. Steane. **Problem set 3.**

Zeeman effect; Helium gross structure; variational method; exchange symmetry

1. **Precession.** This question involves purely classical physics, it is included to make sure you understand the basic ideas of precession.

A toy gyroscope of mass  $m$  is placed on a table. One end of the axis of rotation rests on the table top, which supports the weight of the gyroscope and prevents it sliding across the table. The axis has length  $2d$  and makes an angle  $\theta$  with the vertical.

a. Show that the torque on the gyroscope which results from the normal reaction force and gravity is of magnitude  $T = dmgsin\theta$ , and show clearly its direction using a diagram.

b. Let  $\mathbf{L}$  be the angular momentum of the gyroscope. Show that the torque does not affect the vertical component of  $\mathbf{L}$ , and its effect of the horizontal component is such as to cause the gyroscope to precess about a vertical axis with frequency  $\omega = dmgs/L$ .

c. Now consider a (still classical) magnetic dipole in a magnetic field. Using the interaction energy  $-\boldsymbol{\mu} \cdot \mathbf{B}$ , show that the torque on the dipole is of magnitude  $\mu B \sin\theta$  where  $\theta$  is the angle between  $\boldsymbol{\mu}$  and  $\mathbf{B}$ , and also give its direction. Hence, using the results from (a) and (b), prove that the if  $\boldsymbol{\mu} = g\mu_B \mathbf{L}$ , where  $\mathbf{L}$  is the angular momentum with which the dipole moment is associated, then the dipole precesses about the magnetic field direction with precession frequency  $\omega_L = g\mu_B B/\hbar$ . (This is called the *Larmor precession frequency*).

d. Now consider a quantum treatment (so there is a bit of quantum mechanics in this question after all!) Choosing the  $z$  axis to be along the direction of  $\mathbf{B}$ , what do you expect for the behaviour of  $\langle \hat{\mathbf{L}} \rangle = \langle \hat{L}_x \rangle \mathbf{i} + \langle \hat{L}_y \rangle \mathbf{j} + \langle \hat{L}_z \rangle \mathbf{k}$ ?

(In case there is any uncertainty about the notation here: I am using  $\mathbf{i}, \mathbf{j}, \mathbf{k}$  simply as unit vectors along  $x, y, z$  directions.) No lengthy calculations are needed.

**Zeeman effect**

2. Explain what is meant by ‘weak’ and ‘strong’ magnetic fields in the context of the Zeeman effect. Give appropriate values of magnetic field for experiments on the  $1s-2p$  transition in hydrogen.

3. Explain which constants of the motion are relevant to the Zeeman effect.

4. The ground state  $g$  of the helium atom has zero angular momentum (both orbital and spin contributions are zero). The first excited state  $e$  (i.e. the lower level of the pair which together form the first excited configuration) has zero orbital angular momentum, and spin 1. Show that a weak applied magnetic field  $B$  will not change the ground state energy, and it will split the first excited state energy into three energy levels, and derive the splitting. Hence derive the effect on the observed radiation associated with transitions between  $e$  and  $g$ . (N.B. the transition between these two states is weak because it cannot occur by electric dipole radiation (to be discussed later), and its study is non-trivial because of the far-ultra-violet wavelength.)

**Helium atom; screening**

5. a. Account for the energies of configurations  $1s^2, 1s2s, 1s2p, 1s3s, 1s3p, 1s3d$  of helium in terms of a simple screening argument, as follows. All but the ground state configuration give a pair of terms (the singlet and the triplet); for present purposes just take the average energy of this pair. We will model the set as hydrogenic with an effective nuclear charge  $Z_{\text{eff}}(n, l)$ . Calculate  $Z_{\text{eff}}$  for all the configurations mentioned above, and notice the general pattern. Comment on how the dependence on both  $n$  and  $l$  can be understood by simple screening arguments. (To find the energy levels, look them up in a book. They are given in Woodgate and in Kuhn, for example, and in the Optics practical course).

b. Have we allowed for the energies of both electrons in these calculations? What are we taking

to be the situation corresponding to zero energy?

### Variational method

6. Apply the variational method to find an upper limit on the ground state of a particle in the potential  $V = \lambda x^4$ , using a Gaussian trial wavefunction  $\exp(-\alpha x^2/2)$  (and don't forget to normalize it!). You should find

$$E_0 \leq \frac{3}{8} \left( \frac{6\hbar^4 \lambda}{m^2} \right)^{1/3}$$

[Here are some integrals:

$$\int_{-\infty}^{\infty} x^n e^{-\alpha x^2} dx = \left( \frac{\pi}{\alpha} \right)^{1/2} \times \left\{ 1, \frac{1}{2\alpha}, \frac{3}{4\alpha^2} \right\} \text{ for } n = 0, 2, 4.]$$

7. a. If we make the (poor) approximation of ignoring the electron-electron repulsion altogether, what value (in eV) is obtained for the ionization potential of the ground state in helium? (Ionization is the case that one electron is removed.) How much additional energy would then be required to remove the second electron? Assuming these estimates have been made as precisely as reasonably possible without lengthy calculation, state the degree of precision of each of these two results (i.e. how close they may be expected to be to the true first and second ionization energies for helium.)

b. To do better, use the variational method as described in section 10.2 of the lecture notes. We use hydrogen-like wavefunctions for both electrons, scaled by an effective  $Z$ . The mean energy as a function of this parameter is found to be

$$E(Z) = -2E_R (4Z - Z^2 - 5Z/8).$$

Complete the variational procedure, and hence obtain an upper limit for the ground state energy, and a lower limit for the ionization energy of helium.

### Exchange Symmetry

8. a. State the Exchange Principle. Give the exchange symmetry requirement for (i) states of identical bosons and (ii) states of identical fermions. Derive the Pauli Exclusion Principle.  
 b. The Pauli Exclusion Principle specifies an important restriction on the possible states of identical fermions. Is there a restriction on the possible states of identical bosons, or are they unrestricted?

9. Write down the potential energy as a function of particle positions for

- The gravitational potential energy of two particles of the same mass, positioned somewhere in the vicinity of the earth and moon, but far from any other body.
- The electrostatic potential energy of the  $H_2$  molecule, which consists of two protons and two electrons.

Examine the exchange symmetry of the functions you have written down. They illustrate (if they are correct!) the fact that interaction energies do not depend on particle labelling.

c. Do these expressions depend on whether the particles are bosons or fermions?

10. Which of the following are impossible? (and, as always, explain your reasoning)

- In the ground state of helium, both electrons have the spatial wavefunction  $\psi(r, \theta, \phi)$ .
- The potential energy of a pair of electrons in two potential wells centred at  $a$  and  $b$  (where  $b \neq a$ ) is  $V = C(a - x_1)^2 + C(b - x_2)^2$ .
- A pair of electrons is in the state

$$\frac{1}{\sqrt{2}} (f(\mathbf{r}_1)g(\mathbf{r}_2) - g(\mathbf{r}_1)f(\mathbf{r}_2)) \otimes |\downarrow\rangle_1 \otimes |\uparrow\rangle_2$$

d. A pair of electrons is in the state

$$\frac{1}{\sqrt{2}} (f(\mathbf{r}_1)g(\mathbf{r}_2) \otimes |\uparrow\rangle_1 \otimes |\downarrow\rangle_2 - g(\mathbf{r}_1)f(\mathbf{r}_2) \otimes |\downarrow\rangle_1 \otimes |\uparrow\rangle_2)$$

e. A pair of electrons is in the state

$$\frac{1}{\sqrt{2}} (f(\mathbf{r}_1)g(\mathbf{r}_2) - g(\mathbf{r}_1)f(\mathbf{r}_2)) \otimes |\uparrow\rangle_1 \otimes |\uparrow\rangle_2$$

f. A group of three electrons is in the state

$$\frac{1}{\sqrt{2}} (f(\mathbf{r}_1)g(\mathbf{r}_2)h(\mathbf{r}_3) - f(\mathbf{r}_2)g(\mathbf{r}_3)h(\mathbf{r}_1) + f(\mathbf{r}_3)g(\mathbf{r}_1)h(\mathbf{r}_2)) \otimes |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \otimes |\uparrow\rangle_3$$

11. Fun with exchange operators. Let  $\mathcal{X}$  be the exchange operator. Prove that:

a.  $\mathcal{X}^2 = 1$

b.  $\mathcal{X}$  has eigenvalues  $\pm 1$ .

c. If  $\mathcal{X}Q\mathcal{X} = Q$  for operator  $Q$ , then  $[\mathcal{X}, Q] = 0$ .

d. If  $\mathcal{X}Q\mathcal{X} = W$ , then  $\mathcal{X}Q^2\mathcal{X} = W^2$ .

e. If  $[\mathcal{X}, H] = 0$  then non-degenerate eigenstates of  $H$  must also be eigenstates of  $\mathcal{X}$ .

f. If  $[\mathcal{X}, H] = 0$  then  $\langle + | H | - \rangle = 0$ , where

$$\mathcal{X} | + \rangle = | + \rangle, \quad \mathcal{X} | - \rangle = - | - \rangle$$

[Hint: if in doubt about operator manipulations, allow the operator product or sum to act on a state, and then if the result doesn't depend on the state, it must be a property of the operators themselves.]

12. More fun, and we will get to a nice result. Prove that

a.  $\mathcal{X}x_1\mathcal{X} = x_2$

b.  $\mathcal{X}\hat{p}_1\mathcal{X} = \hat{p}_2$  [Hint: do the differentiation, but think carefully. If in doubt, try the wavefunction  $ax_1^2 + bx_2^5$  just to get the hang of things.]

c.  $\mathcal{X}V(x_1, x_2)\mathcal{X} = V(x_2, x_1)$  [Hint: argue that  $V$  can always be expanded as a power series in powers of  $x_1$  and  $x_2$ , and just treat a general term  $x_1^n x_2^m$  from such a series.]

d.  $[\mathcal{X}, K] = 0$  where  $K = \hat{p}_1^2/2m + \hat{p}_2^2/2m$  is the combined kinetic energy of a pair of identical particles. [use part b. and 11.d. and 11.c.]

e. If  $V(x_1, x_2) = V(x_2, x_1)$  then  $[\mathcal{X}, H] = 0$ . [use parts c. and d. and 11.c.]

Since potential energy will never depend on particle labelling, (c.f. question 9) and using the extension of these results to include spin as well, the conclusion from part e. is that exchange symmetry is always a constant of the motion. Also, using 11.e., non-degenerate energy eigenstates of identical particles always have definite exchange symmetry (and you may like to show further that the degenerate energy eigenstates can always be combined in such a way as to ensure they have definite exchange symmetry).

13. (**Essential**) Explain carefully how the splitting between singlet and triplet states arises in helium. [A thorough argument including mathematical expressions as well as explanatory statements is needed.] Estimate the order of magnitude of the splitting (by considering the interaction which causes it).

14. Suppose there existed a particle called a hypertron which is in all respects like an electron, except it has a further property called 'hyperspin' which distinguishes it from an electron. Assume that we do not possess a means to detect the presence of hyperspin directly, and it does not contribute to the energy of interaction of hypertrons with everyday particles such as protons, electrons or photons. If some helium atoms contained one electron and one hypertron, how could they be told apart from helium atoms which contained two electrons? List as many features or experimental observations as you can.

15. A one-dimensional harmonic potential well has the form  $V(x) = (1/2)m\omega^2x^2$ . The lowest three energy eigenstates are  $g(x)$ ,  $f(x)$  and  $h(x)$  (to keep the notation uncluttered it will be convenient to use  $g, f, h$  rather than  $\psi_n(x)$ ). A convenient notation for fermionic spin states is  $\uparrow, \downarrow$  for  $|s = 1/2, m_s = \pm 1/2\rangle$  (spin half) and  $\uparrow\uparrow, \uparrow\downarrow, \downarrow\downarrow$  for  $|s = 3/2, m_s = 3/2 \cdots - 3/2\rangle$  (spin 3/2). Suppose three identical particles are in the well. Write down a possible form for the ground state, and hence deduce the ground state energy, when

- a. the particles each have spin zero
- b. the particles each have spin half
- c. the particles each have spin 3/2

(in all cases assume the particles do not interact with one another) [Hint: (b) and (c) require careful thought. Begin by listing some low-lying *single*-particle states having the form of a product “(spatial part)  $\otimes$  (spin part)”. Then use a determinant to help you write down a state which is antisymmetric w.r.t. exchange of any pair. For b. and c. the ground state of the 3-particle system is degenerate, so there is more than one correct answer.]

16. Imagine a situation in which there are 3 particles and only 3 states  $a, b, c$  available to them. Show that the total number of allowed, distinct configurations for this system is

- a. 27 if the particles are non-identical
- b. 10 if they are bosons
- c. 1 if they are fermions
- d. write down the state in the case of 3 fermions

17. Discuss under what conditions identical particles may be regarded as distinguishable. Make an order-of-magnitude estimate of the degree of approximation involved in treating as distinguishable the electrons in two hydrogen atoms separated by 1 nm (consider for example the impact on the energy levels).

Quantum and Atomic Physics. Prof A. Steane. **Problem set 4.**

Time-dependent perturbations; transitions; selection rules; magnetic resonance

**Basic concepts**

1. A particle is in the ground state of a simple box (infinite square potential well) of side  $L$ . Describe qualitatively the evolution of the system
  - a. If the length of the side of the box is suddenly doubled.
  - b. If the length of the side of the box is very slowly increased to  $2L$ .
  - c. What would be the result of an attempt to decrease the box's diameter suddenly to  $L/2$ ?
2. A harmonic oscillator starts in its ground state ( $n = 0$ ) at  $t = -\infty$ . A perturbation  $\delta H = -e\mathcal{E}x \exp(-t^2/\tau^2)$  is applied between  $t = -\infty$  and  $+\infty$ .
  - a. What is the probability that the oscillator makes a transition to the state  $n = 2$ ?
  - b. Show that the probability the oscillator makes a transition to the state  $n = 1$  is

$$P_{0 \rightarrow 1} = \frac{e^2 \mathcal{E}^2 \pi \tau^2}{2m\omega\hbar} e^{-\omega^2 \tau^2 / 2}$$

[there are two integrals to do here, one for the matrix element, and an integral over time. For the matrix element, you can either perform the integral in the  $x$  basis, or use raising/lowering operators.]

- c. Plot the dependence of  $P_{0 \rightarrow 1}$  on the timescale  $\tau$  of the perturbation, and comment on the behaviour in the limits  $\tau \rightarrow 0$  and  $\omega\tau \gg 1$ .

3. In the  $\beta$  decay  $\text{H}^3$  (1 proton + 2 neutrons in the nucleus)  $\rightarrow$  ( $\text{He}^3$ )<sup>+</sup> (2 protons + 1 neutron in the nucleus), the emitted electron has a kinetic energy of 16 keV. We will consider the effects on the motion of the atomic electron, i.e. the one orbiting the nucleus, which we assume is initially in the ground state of  $\text{H}^3$ .

- a. Show by a brief justification that the perturbation is sudden. What is the state of the atomic electron immediately after the perturbation (e.g. at a time around  $5 \times 10^{-17}$  s after the electron was emitted)?
  - b. Give the mean kinetic energy and mean potential energy of the atomic electron before and after the perturbation, expressing your results as multiples of the Rydberg energy (ignore the very slight change in reduced mass.) [Use your knowledge of hydrogen to avoid doing integrals]. Hence find the new mean energy.
  - c. Show that the probability for the electron to be left in the ground state of ( $\text{He}^3$ )<sup>+</sup> is  $2^3(2/3)^6 \simeq 0.7$ , and comment on how this result relates to the information you obtained in part (b). [Comment: the integral here is one you have done before, but to save time you might like to change variable to  $u = 3r/2$  to convert it exactly into a standard one for hydrogen, for which you then know the value].
  - d. Describe the main features of the subsequent behaviour of the ( $\text{He}^3$ )<sup>+</sup> ion when the electron is not left in the ground state.

**Atomic transitions, selection rules**

4. For a single atom, in the process called *electric dipole radiation*, what two physical entities are interacting together? Briefly discuss whether or not an isolated atom possesses an electric dipole moment.
5. This question illustrates the way selection rules can come about, by treating a system in a state of well-defined orbital angular momentum, such as the hydrogen atom when spin-orbit coupling is ignored. For such a system (i.e. one whose energy eigenfunctions have the form  $R(r)Y_{l,m_l}(\theta, \phi)$ ) find the electric dipole selection rules on  $m_l$ , by considering the components of the electric dipole

matrix element  $\langle er \rangle$  in the form of three integrals. [Hint: consider  $z$  and  $x \pm iy$ , expressing them in polars.]

6. State and derive the parity selection rule for electric dipole radiation.

### Magnetic resonance

7. A beam of hydrogen atoms is formed by effusion into vacuum from a small hole in an oven and a collimating aperture. A velocity-selector blocks all atoms except those in a narrow range of velocities centred around  $v$ . Let the  $x$  axis of a coordinate system be along the beam. The atomic beam passes through a region of large magnetic field gradient  $dB/dz$  (as in a Stern-Gerlach apparatus) perpendicular to  $x$ , followed by a region of constant uniform magnetic field 1 mT directed along  $z$ , followed by a third region like the first but with reversed field gradient. Atoms which emerge from the third magnet in the same direction they entered the first are detected.

- Briefly describe the motion of an atom in an arbitrary spin-state through this apparatus.
- A magnetic field  $B_a \cos(\omega t)$  directed along  $y$  and oscillating at angular frequency  $\omega$  with amplitude  $B_a \ll 1$  mT is applied in the second region (in addition to the constant uniform field there). This oscillating field can have a large effect on the atoms. Sketch rough graphs and describe in qualitative terms the detected signal as a function of  $\omega$  at fixed  $B_a$ , and as a function of  $B_a$  when  $\omega$  is tuned to resonance.
- Calculate the resonant frequency  $\omega_0$ .
- If the atomic beam is velocity-selected to have speed 800 m/s, and the length of the region where the oscillating magnetic field is applied is 10 cm, then what is the smallest value of  $B_a$  required to reduce the detected number of atoms to a minimum?

### Further optional questions

8. Let  $\psi(t)$  be the state of a system subject to a Hamiltonian  $H = H^0 + \delta H(t)$  where  $H^0$  is time-independent and has eigenfunctions  $\psi_n^0$ . The basic perturbation theory result, accurate to first order in  $\delta H$ , is

$$d_f(t) = \delta_{fi} - \frac{i}{\hbar} \int_0^t e^{i\omega_{fi}t'} \langle \psi_f^0 | \delta H(t') | \psi_i^0 \rangle dt'. \quad (1)$$

for the amplitude of the state  $\psi_f^0$  in  $\psi(t)$  when a system starts in the state  $\psi_i^0$  and is subject to perturbation  $\delta H(t)$  between times 0 and  $t$ . After first checking your notes, see if you can perform the derivation of this result without returning to them for help.

9. Here is an example of an electric dipole matrix element. It is for one of the Zeeman components of the 1s–2p transition in hydrogen, ignoring fine structure.

$$|\langle n = 2, l = 1, m = 0 | z | n = 1, l = 0, m = 0 \rangle|^2 = \frac{2^{15}}{3^{10}} a_0^2$$

Use the hydrogen wavefunctions to verify this result. [Use spherical polar coordinates. The radial integral can be looked up, or alternatively by a change of variable to  $u = 3r/4$  it can be converted into the same form as  $\langle r^2 \rangle$  for hydrogen ground state, for which you can use your previous study of such integrals in problem set 1.]