Problem sheet - HT tutorial 5

Self-assessed questions

Q1. The exchange principle for identical particles

(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?

[JW QM HT Q5.4]

Q2. Interactions between particles and exchange symmetry

Write down the potential energy as a function of particle positions for
(a) 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.
(b) 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?

[JW QM HT Q5.5]

Q3. Some practise with exchange symmetry and quantum states

Exchange symmetry quiz Which of the following are impossible? (and, as always, explain your reasoning)
(a) In the ground state of helium, both electrons have the spatial wavefunction $\psi(r,\theta,\phi)$.
(b) The potential energy of a pair of electrons in two potential wells centred at a and b (where $b \neq a$) is $V = C(a - x_1)^2 + C(b - x_2)^2$.
(c) A pair of electrons is in the state

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

(d) A pair of electrons is in the state

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

(e) A pair of electrons is in the state

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

(f) A group of three electrons is in the state

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

[JW QM HT Q5.6]

Main questions

Q1. The Zeeman effect

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.)

[JW QM HT Q4.4]

Q2. Helium atom: electron screening

(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_{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?

[JW QM HT Q5.1]

Q3. The variational principle

Given a system with a Hamiltonian H and eigenstates $|n\rangle$ labelled by an integer n with energies ε_n such that $\varepsilon_0 < \varepsilon_1 < \varepsilon_2 \cdots$, prove that for any normalized state $|\psi\rangle$ we have $\langle\psi|H|\psi\rangle \geq \varepsilon_0$. Use this fact to formulate the variational principle for a single parameter p family of states $|\psi(p)\rangle$.

Q4. Application of the variational principle

Variational method 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

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

Compare this with the calculation we did in the lectures. Which is better and why? [Here are some integrals:

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

[JW QM HT Q5.2]

Q5. Helium atom: ionization energy

(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. Using hydrogen-like wavefunctions for both electrons, the mean energy as a function of an effective nuclear charge Z is found to be

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

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.

[JW QM HT Q5.3]

Q6. Helium atom: structure of spectrum

Consider the helium atom in the approximation that the electron-electron repulsion is neglected. What is the ground state wave function for orthohelium where the electrons have a total spin $S = 1$ (triplet)? What is its degeneracy in this approximation? Why is this ground state higher in energy than that of parahelium where the electrons have a total spin $S = 0$ (singlet)?

Q7. Helium atom: splitting effects of electrons being indistinguishable

(**Singlet-triplet splitting**) 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).

[JW QM HT Q5.7]