PHYS 30101 APPLICATIONS OF QUANTUM PHYSICS EXAMPLES 5

These questions refer to Sections 3 (lecture 15) and 4 (lectures 16 to 18).

1. The lowest two states of an electron in a double quantum dot are described by the 2×2 matrix Hamiltonian

$$\widehat{H} = \frac{1}{2}\begin{pmatrix} \epsilon & -\Delta \\ -\Delta & -\epsilon \end{pmatrix},$$

where ϵ is the difference in potential energies between the two dots, and Δ the coupling between them (arising from tunnelling). The basis vectors

$$L = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad R = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

describe states where the electron is trapped on the left- and right-hand dot respectively.

   (a) Find the energy eigenvalues of this system.

   (b) Explain why, if $\Delta \ll \epsilon$, the energy eigenvectors are well approximated by L and R. Use first-order perturbation theory to show that their energies are $\pm\epsilon/2$ to first order in Δ.

   (c) Find the energy eigenvectors for the case $\epsilon = 0$. Use these to construct a general solution $\psi(t)$ to the TDSE in this case.

   (d) If the electron is initially located on the left-hand dot, $\psi(0) = L$, and $\epsilon = 0$, obtain the probability of finding it on the right-hand dot at a later time t.

2. The $3d$ ($n = 3$, $l = 2$) level in hydrogen is split by the spin-orbit interaction into two levels with an energy difference of 4.5×10^{-6} eV. State the values of the quantum number j for these levels, indicating which has the lower energy, and give their degeneracies.

   The spin-orbit interaction has the form

$$\widehat{H}_{so} = f(r)\widehat{\mathbf{L}} \cdot \widehat{\mathbf{S}}.$$

   Use the observed splitting to determine the radial matrix element

$$\mathcal{E}_{nl} = \langle f(r) \rangle \hbar^2$$

   for the $3d$ level. Show that the average energy of the set of $3d$ states is unchanged by this interaction.

3. The first excited levels of calcium have the outer electrons in a $(4s)^1\,(4p)^1$ configuration. Three of these are seen, with energies 1.87908 eV, 1.88555 eV and 1.89868 eV. Assuming that they are split by the spin-orbit interaction,

$$\widehat{H}_{so} = \frac{\mathcal{E}}{\hbar^2}\,\widehat{\mathbf{L}}\cdot\widehat{\mathbf{S}},$$

deduce the angular-momentum quantum numbers (L, S and J) of these levels. Compare the ratio of their splittings with the prediction of first-order perturbation theory.

4. Sketch the energy-level diagram for the $3d$ states of hydrogen in a weak magnetic field, indicating the quantum numbers of the levels. Calculate the magnetic splittings for a field of 10^{-2} T. [You may use the value for the Bohr magneton, $\mu_B = e\hbar/2m_e = 5.8\times10^{-5}$ eV/T.]

5. Find the Landé g-factors for the levels of calcium in question 3. Sketch a similar diagram for the splittings of these levels in a weak magnetic field. Estimate the size of the magnetic field for which the weak-field approximation breaks down.

6. The $n = 1$ level in the hydrogen atom corresponds just to the $1s_{1/2}$ level, which is doubly degenerate. The $n = 2$ level is composed of $2s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$ levels with their associated degeneracies of $2j + 1$. However, this level is split by fine-structure effects. Firstly, the spin-orbit splitting of the $2p_{1/2}$ and $2p_{3/2}$ levels and then relativistic effects conspire to place the $2s_{1/2}$ almost degenerate with the $2p_{1/2}$. For this question, take them as degenerate; but remember that there are sets of states there with different quantum numbers, otherwise you may get confused later!

   Draw a diagram of the fine structure of the $n = 1$ and $n = 2$ levels in atomic hydrogen, labelling levels carefully with quantum numbers.

   Calculate the weak-field Zeeman shifts for all the $n = 1$ and $n = 2$ states of hydrogen and develop your previous diagram to show how the fine structure splits due to the weak field.

   If you cannot recall what the words "selection rule" mean, or if you think you've never heard them before, read Section 9.4 in *Introduction to Quantum Mechanics* by A.C. Phillips before going any further, or ask someone to explain the concept to you.

   On your diagram of the weak-field hydrogen lines, mark all the electromagnetic transitions from the $n = 2$ states to those with $n = 1$ that are consistent with the $\Delta\ell = 1$, $\Delta m_j = 0, \pm1$ selection rule for electric dipole transitions. You should notice how the $2s_{1/2}$ states are left high and dry, with no transitions to $n = 1$ states.

Draw similar diagrams for the strong-field case, ignoring all fine structure effects. In this case, the electric selection rule is applied with $\Delta\ell = 1$, $\Delta m_\ell = 0, \pm 1$. Again the $2s$ states end up with no transitions out of them.

7. The orbital motion of an electron in a thin cylindrical quantum dot is governed by an electrostatic potential that is well approximated by a two-dimensional harmonic oscillator. It can be described by the Hamiltonian

$$\widehat{H}_{\rm orb} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}k\,(x^2+y^2),$$

where, for a thin enough dot, we may neglect any excitation in the z direction (see Section 2.2 in lecture 6). Show that the energy eigenvalues of the electron have the form

$$E_{\rm orb} = (N+1)\hbar\omega, \qquad \text{where } N = 0, 1, 2, \ldots,$$

and find the degeneracies of the first four levels.

After some heavy lifting with Hermite polynomials, it is possible to form linear combinations of the states in a given level that have definite values for L_z. The corresponding quantum number m_l can be shown to run over even numbers from $-N$ to $+N$ if N is even, and odd numbers from $-N$ to $+N$ if it is odd. Check that the degeneracies that you found above are consistent with this pattern.

As in a real atom, the electrostatic potential leads to a (small) spin-orbit interaction. If the dot is placed in a magnetic field B along its cylindrical axis, the full Hamiltonian for the electron is

$$\widehat{H} = \widehat{H}_{\rm orb} + \frac{\mathcal{E}_{\rm so}}{\hbar^2}\,\widehat{L}_z\widehat{S}_z + \frac{e}{2m}\left(\widehat{L}_z + 2\,\widehat{S}_z\right)B.$$

The states in the energy levels of the oscillator will be split by this depending on their quantum numbers m_l and m_s. Sketch, as functions of B, the energies of the states in the first two oscillator levels ($N = 0$ and 1).