

SUMMER EXAMINATIONS 1999

B.Sc. (Honours) Experimental Physics: Paper 1

EP405: Quantum Mechanics

Prof. J. Enderby
Prof. R.M. Redfern
Dr. F.G. Anderson

Time Allowed: TWO hours

Answer THREE questions

Q.1 Define the angular momentum $\vec{\ell}$ in terms of \vec{r} and \vec{p} . Write down ℓ_z in terms of Cartesian coordinates and their derivatives.

Show that $[\ell_x, \ell_y] = i\hbar \ell_z$, and that $[\ell^2, \ell_z] = 0$.

Why do we express the angular wave functions in terms of eigenfunctions of ℓ^2 and ℓ_z instead of eigenfunctions of ℓ_x , ℓ_y , and ℓ_z ?

For the spherical harmonic Y_{2-1} what are $\ell^2 |Y_{2-1}\rangle$ and $\ell_z |Y_{2-1}\rangle$?

In the vector model of angular momentum, what is the length of $\vec{\ell}$? Can $\vec{\ell}$ be parallel to the z-axis? Explain. What is the expectation value of ℓ_x ? Describe the motion of $\vec{\ell}$.

Q.2 Show that, if two operators A and B commute, they share the same eigenfunctions for nondegenerate states.

Write down the Hamiltonian for a free particle. Show that each eigenfunction for the free particle has a definite momentum.

Let O_s be a symmetry operator, e.g. a rotation about a particular axis or a reflection through a particular plane, that leaves the potential $V(\vec{r})$ unchanged. What can be said about the symmetry of the eigenfunctions of the Hamiltonian? What conservation laws hold?

Consider a particle in the potential well defined by

$$V(x) = \begin{cases} 0 & x < -b \\ -V_0 & -b < x < +b \\ 0 & x > +b \end{cases}$$

What quality characterises the eigenfunctions of the Hamiltonian?

(continued overleaf)

Consider a hydrogen atom in a magnetic field parallel to the z-axis. What quantity is conserved? Explain.

Q.3 Describe the properties of the eigenvalues and eigenfunctions of a Hermitian matrix.

Consider a Hilbert (function) space. Describe how a function can be considered as a vector. How do we calculate the dot product between two vectors (functions) in Hilbert space?

Consider the Hamiltonian given by

$$H = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

within an orthonormal basis set of three states $\{|a\rangle, |b\rangle, |c\rangle\}$. Find the eigenfunctions and associated eigenvalues.

What is the matrix S such that $S^{-1} H S$ is a diagonal matrix?

What is the probability of finding the system in state $|b\rangle$ when the system is in the first excited state?

Q.4 Consider an electron in a 2D harmonic oscillator potential. The Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{k}{2}(x^2 + y^2).$$

The eigenfunctions are simple products of 1D oscillator states, one in the x direction and one in the y direction, $\psi = |m_x\rangle |n_y\rangle$. Draw a diagram of the first four energy levels giving the energy of each level ($\omega = \sqrt{k/m}$) and writing down each of the product states associated with that level.

We now turn on a steady magnetic field along the z axis (B_z). Write down the orbital Zeeman interaction Hamiltonian (H_z) describing the interaction between the electron's orbital motion and the applied magnetic field. Define all of your variables.

Calculate a general matrix element for this interaction

$$\langle a_x b_y | H_z | m_x n_y \rangle.$$

How are a_x^* and m_x , and b_y and n_y related?

Hint: $x = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (a^+ + a)$ and $p = i\left(\frac{\hbar m\omega}{2}\right)^{1/2} (a^+ - a)$.

Calculate the orbital Zeeman splittings within the first three energy levels.

Q.5 Consider the positive hydrogen molecule H_2^+ . We express the molecular orbitals in terms of linear combinations of atomic orbitals, in this case the atomic orbitals are an atomic s function on nucleus "a" $|s_a\rangle$ and an atomic s function on nucleus "b" $|s_b\rangle$. Write down the bonding molecular orbital (the bonding state) in terms of $|s_a\rangle$ and $|s_b\rangle$. Describe why this state gives rise to bonding between the two nuclei.

Write down the antibonding molecular orbital in terms of $|s_a\rangle$ and $|s_b\rangle$. Why doesn't this state give rise to bonding between the two nuclei?

What is an sp hybrid orbital? Show how this hybrid results in a directional bond.

Consider the ethylene molecule C_2H_4 shown below. Discuss the double bond between the carbon atoms in terms of sigma bonds and pi bonds. Why does this molecule remain planar?

