Answer ALL SIX questions from Section A and TWO questions from Section B

The numbers in square brackets in the right-hand margin indicate the provisional allocation of maximum marks per question section.

Section A

1. Show how an operator $\hat{A}$ may be represented by a matrix using a complete set of orthonormal basis states $|\psi_n\rangle$. **[4 marks]**

Outline briefly how a matrix representation of the Hamiltonian $\hat{H}$ of a quantum system can be used to solve the time-independent Schrödinger equation. **[4 marks]**

2. Two quantum state functions $|\psi\rangle$ and $|\chi\rangle$ are represented as follows using a basis or orthonormal states $|\phi_n\rangle$

$$|\psi\rangle = \sum_n c_n |\phi_n\rangle,$$

$$|\chi\rangle = \sum_n d_n |\phi_n\rangle$$

Evaluate $\langle\psi|\chi\rangle$ **[3 marks]**

Demonstrate the analogy with the scalar product of two Cartesian vectors **c**.**d** noting any differences and similarities. **[3 marks]**

3. If A and B are two observables, represented by operators $\hat{A}$ and $\hat{B}$, then the product of their uncertainties in a given normalised state $|\psi\rangle$ satisfies the inequality

$$\Delta A\,\Delta B \geq \frac{1}{2}\left|\left\langle\psi\,\middle|\,[\hat{A},\hat{B}]\,\middle|\,\psi\right\rangle\right|,$$

where $\Delta A = \langle(\hat{A} - \langle\hat{A}\rangle)^2\rangle$ and ΔB obeys a similar relation. Use this equation to derive the Heisenberg uncertainty principle for position and momentum of a particle in one dimension. You may assume their commutation relation. **[4 marks]**

A particle is in the ground-state of a quantum harmonic oscillator $\psi_0(x) = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2} \exp(-\alpha x^2/2)$. Evaluate Δx. **[4 marks]**

Note the standard integral

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{1}{2a}\left(\frac{\pi}{a}\right)^{1/2}.$$

4. An Hermitian operator $\hat{A}$ is defined by the relation $\langle\psi|\hat{A}|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*$ for arbitrary functions $|\phi\rangle$ and $|\psi\rangle$. If it has eigenvalues a_n and normalised eigenfunctions $|\phi_n\rangle$ show that its eigenvalues are real. **[3 marks]**

A general normalised state vector $|\psi\rangle$ is a linear superposition of the normalised eigenstates $|\phi_n\rangle$,

$$|\psi\rangle = \sum_n c_n|\phi_n\rangle.$$

Obtain the expectation value of $\hat{A}$ for the given state in terms of the c_n. Explain the physical significance of this quantity. **[3 marks]**

5. Outline the Stern-Gerlach experiment on a beam of silver atoms and its relevance for the understanding of quantum spin. **[6 marks]**

6. In quantum theory, particles can be either bosons or fermions. Explain the meaning of the terms "boson" and "fermion" by referring to spin as well as the symmetry properties of the wavefunction describing systems of more than one particle. Give examples of each type of particle. **[3 marks]**

State the Pauli exclusion principle for fermions, and show how it may be derived by considering the symmetry properties of a two-particle wavefunction. **[3 marks]**

Section B

7. The Hamiltonian of a one-dimensional quantum harmonic oscillator (angular frequency ω, mass of particle m) is expressed as:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2,$$

In the operator approach,we consider raising and lowering operators $\hat{a}_\pm$ defined in terms of the position and momentum operators $\hat{x}$ and $\hat{p}$ as:

$$\hat{a}_\pm = \frac{1}{\sqrt{2}}(\alpha\hat{x} \mp \frac{i}{\hbar\alpha}\hat{p}),$$

where $\alpha = \sqrt{\frac{m\omega}{\hbar}}$.

(a) Using, without proof, the commutation relation $[\hat{x}, \hat{p}] = i\hbar$ show that

$$[\hat{a}_-, \hat{a}_+] = 1$$

and that:

$$\hat{H} = \hbar\omega(\hat{N} + \frac{1}{2}),$$

where $\hat{N}$ is a Hermitian operator. Give $\hat{N}$ in terms of $\hat{a}_\pm$. **[8]**

(b) Using the relation $[\hat{H}, \hat{a}_\pm] = \hbar\omega\hat{a}_\pm$, show that if $|\phi_E\rangle$ is an eigenvector of $\hat{H}$ having eigenvalue E, then $\hat{a}_\pm|\phi_E\rangle$ is an eigenvector of $\hat{H}$ having eigenvalue $E \pm \hbar\omega$. **[5]**

(c) Express the operator $\hat{O} = i\hat{x}\hat{p}$ in terms of the raising and the lowering operators $\hat{a}_\pm$. **[5]**

Hence, or otherwise, represent $\hat{O}$ as a matrix, but truncated to a 4×4 matrix. **[4]**

(d) The harmonic oscillator is in a quantum state specified by the normalised state vector:

$$|\psi\rangle = \frac{i}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle.$$

where $|n\rangle$ denotes the n-th eigenstate. Using the matrix representation of $\hat{O}$ and $\hat{O}^2$, or otherwise,

1. calculate the expectation value of $\hat{O}$ in the state $|\psi\rangle$, **[5]**

2. obtain the matrix element $\langle 1|\hat{O}^2|1\rangle$. **[3]**

You may find the following relations useful:

$$\hat{a}_+|n\rangle = \sqrt{n+1}|n+1\rangle \quad ; \quad \hat{a}_-|n\rangle = \sqrt{n}|n-1\rangle.$$

8. A quantum state $|\Psi\rangle$ is represented by a complete set of orthonormal basis states

$$|\Psi\rangle = \sum_n c_n |\psi_n\rangle.$$

An alternative representation, using another orthonormal basis,

$$|\Psi\rangle = \sum_m d_m |\chi_m\rangle.$$

is sought.

(a) Show that a change of representation may be achieved using a matrix $\mathbf{S}$ of elements $S_{mn} = \langle \chi_m | \psi_n \rangle$, and a transformation between vectors,

$$\mathbf{d} = \mathbf{S}\ \mathbf{c},$$

explaining carefully your notation. **[5]**

(b) Noting that $\mathbf{c} = \mathbf{S}^\dagger\ \mathbf{d}$ and that $\mathbf{c}^\dagger = \mathbf{d}^\dagger \mathbf{S}$, specify the form of the elements of $\mathbf{S}^\dagger$ and show that $\mathbf{S}$ is unitary. **[4]**

(c) An Hermitian operator $\hat{\mathbf{A}}$ is represented, in the basis $|\chi_m\rangle$, as a matrix $\mathbf{A}_{\boldsymbol{\chi}}$. The corresponding expectation value, for state $|\psi\rangle$, may be written $\langle \hat{\mathbf{A}} \rangle = \mathbf{d}^\dagger \mathbf{A}_{\boldsymbol{\chi}} \mathbf{d}$. The operator could also be represented as another matrix, $\mathbf{A}_{\boldsymbol{\psi}}$ using the basis $|\psi_n\rangle$ where $\mathbf{A}_{\boldsymbol{\chi}} = \mathbf{S}\mathbf{A}_{\boldsymbol{\psi}}\mathbf{S}^{-1}$. Show that the expectation value of $\hat{\mathbf{A}}$ is independent of the representation. **[6]**

(d) The eigenvectors of the Pauli matrix $\boldsymbol{\sigma_y}$ have eigenvalues $+1$ and -1. We denote them as $|+\rangle$ and $|-\rangle$ respectively. They are given in terms of eigenstates of $\boldsymbol{\sigma_z}$ as follows:

$$\begin{aligned} |+\rangle &= \frac{1}{\sqrt{2}}|\alpha\rangle + \frac{i}{\sqrt{2}}|\beta\rangle, \\ |-\rangle &= \frac{1}{\sqrt{2}}|\alpha\rangle - \frac{i}{\sqrt{2}}|\beta\rangle. \end{aligned}$$

Obtain the transformation matrix $\mathbf{S}$ for the change in representation from the basis $|\alpha\rangle$, $|\beta\rangle$ to the basis $|\pm\rangle$. Give also $\mathbf{S^{-1}}$. **[6]**

(e) For the quantum state

$$|\Psi\rangle = \frac{i}{\sqrt{2}}|+\rangle + \frac{i}{\sqrt{2}}|-\rangle$$

The system corresponds to the Hamiltonian $\hat{H} = \boldsymbol{\sigma_z} + \mathbf{3}\boldsymbol{\sigma_y}$. Calculate $\langle \hat{H} \rangle$. **[6]**

(f) Represent the above Hamiltonian $\hat{H}$ in the $|\pm\rangle$ basis. **[3]**

Note the form of the Pauli spin matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

9. (a) Assuming the commutation relations $[J_x, J_y] = i\hbar J_z$ (and all cyclic permutations) show that the raising and lowering operators defined as $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$ satisfy

$$\hat{J}_+\hat{J}_- = \hat{J}^2 - \hat{J}_z^2 + \hbar J_z$$

and

$$\hat{J}_-\hat{J}_+ = \hat{J}^2 - \hat{J}_z^2 - \hbar J_z.$$

[6]

(b) Show also that $[\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm$. **[4]**

(c) Let $|j\,m\rangle$ denote the simultaneous eigenvectors of both $\hat{J}^2$ and $\hat{J}_z$, the corresponding eigenvalue equations being

$$\hat{J}^2|j\,m\rangle = \alpha|j\,m\rangle,$$
$$\hat{J}_z|j\,m\rangle = \beta|j\,m\rangle.$$

Hence show that the operation of $\hat{J}_+$ on the eigenvalue equation for $\hat{J}_z$ generates a series of eigenstates with eigenvalues equal to $\beta + n\hbar$ where n is an integer. **[5]**

(d) Explain, using physical arguments, why there must be maximal β_T and minimal β_B values of β. **[3]**

(e) By considering $\hat{J}_+\hat{J}_-|j\,m\rangle$ and $\hat{J}_-\hat{J}_+|j\,m\rangle$ it can be shown that

$$\alpha - \beta_T^2 - \hbar\beta_T = 0$$

and

$$\alpha - \beta_B^2 - \hbar\beta_B = 0.$$

Hence show that quantum angular momentum may take integer or half-integer values. **[4]**

(f) Two quantum particles have spin angular momenta $s_1 = 1/2$ and $s_2 = 1/2$. When not interacting they are associated with four single-particle basis states $|s_1 = 1/2,\, m_1 = \pm 1/2\rangle\ |s_2 = 1/2,\, m_2 = \pm 1/2\rangle$. They interact via a Hamiltonian

$$\hat{H} = A(S_{x1}S_{x2} + S_{y1}S_{y2}).$$

Express $\hat{H}$ in terms of the raising and lowering operators $S_{\pm 1}$, $S_{\pm 2}$. **[4]**

Hence represent the above Hamiltonian as a matrix. **[4]**

You may find useful the general formula for any angular momentum:

$$\hat{J}_\pm|j\,m_j\rangle = \hbar[j(j+1) - m_j(m_j \pm 1)]^{1/2}|j\,m_j \pm 1\rangle.$$

10. Give the Hamiltonian, in atomic units, for the electronic states of a neutral helium atom. **[3]**

Neglecting all effects of inter-electron repulsion and correlations, the electronic eigen-energies of the helium atom would correspond to those of two electrons in a hydrogenic atom,

$$E_{n_1,n_2} = -\frac{Z^2}{2n_1^2} - \frac{Z^2}{2n_2^2}$$

and are associated with eigenstates in product form,

$$\Psi(\mathbf{r_1}, \mathbf{r_2}) = \boldsymbol{\phi}_{\mathbf{n_1 l_1 m_1}}(\mathbf{r_1})\boldsymbol{\phi}_{\mathbf{n_2 l_2 m_2}}(\mathbf{r_2}),$$

where, in particular, a $1s$-type orbital, takes the form

$$\phi_{100}(\mathbf{r_i}) = \sqrt{\frac{Z^3}{\pi}} e^{-Zr_i}$$

where i denotes either 1 or 2.

Explain (without detailed mathematical derivations) how the above simplified model may be refined by considering the following:

(a) The use of first-order perturbation theory to estimate the ground state energy. **[6]**

(b) The variational principle and the role of the effective charge α. Explain the role of the relation $\left\langle \hat{H} \right\rangle = \alpha^2 - 2Z\alpha + 5\alpha/8$. **[6]**

(c) The application of the Pauli Principle to **both** the ground state and the singly-excited state with configuration $1s2s$. For the excited state discuss the form of the wavefunctions and account qualitatively for the difference in energies of the singlet and triplet states. **[6]**

(d) The atom is now singly-ionised to He^+, but is subjected to a weak external field of the form

$$\delta\hat{H} = \epsilon z + \beta r^2$$

Obtain the first-order perturbative correction to the energy of the ground state, justifying carefully your answer. **[9]**

You may find helpful the expression $\langle n|r^2|n\rangle = \frac{n^2}{2Z^2}\left[5n^2 + 1\right]$ valid for a hydrogenic atom of charge Z with principal quantum number n and $\ell = 0$.