Maths of Waves and Fields 23/24

1. a) A particle of mass m is moving in two dimensions in a potential $V(\mathbf{r})$. Write down the time-independent Schrödinger equation of the particle. Explain any symbols you have used.

[4 marks]

b) i) Write down the definition of the momentum operator \hat{p}_x in one dimension. Show that the function

$$\psi(x) = e^{i\alpha x},$$

with constant α , is an eigenfunction of \hat{p}_x . Determine the eigenvalue of $\psi(x)$.

 A particle is moving in one-dimensional free space and is described by a spatial function

$$\phi(x) = \cos(\beta x),$$

where β is a constant. What are the possible outcomes of a measurement of the particle's momentum and what are their probabilities?

[5 marks]

c) Two operators, Â and Â, can act on wavefunctions Ψ. Define the commutator of the two operators and explain what the expression [Â, Â]Ψ represents. Show that the commutator of the position and momentum operators in one dimension is given by

$$[\hat{x}, \hat{p}_x] = i\hbar$$
.

What is the implication of this result for measurements of these quantities?

[6 marks]

Complex Variables and Vector Spaces 23/24

b) State whether each of the following operators is unitary, Hermitian, both or neither.

(i)
$$\mathbf{L} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$
, (ii) $\mathbf{O} = \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}$.

[4 marks]

c) An operator \hat{A} is said to be anti-Hermitian if $\hat{A}^{\dagger} = -\hat{A}$. From the definition of the adjoint, show that the eigenvalues of \hat{A} are pure imaginary.

[6 marks]

- 2. All vector spaces may be assumed to be finite dimensional for this question.
 - a) i) Show that the trace of a linear operator is basis invariant.

[4 marks]

ii) A Hermitian operator \hat{A} on a finite dimensional vector space has eigenvalues λ_j and normalised eigenvectors $|\lambda_j\rangle$. Show that the trace of \hat{A} is given by

$$\operatorname{Tr}(\hat{A}) = \sum_{j} \lambda_{j}.$$

[3 marks]

iii) Consider an operator that scales one component of a given orthonormal basis by a real number, while leaving all other components unchanged. Can we be sure this operator is Hermitian? Justify your answer.

[4 marks]

b) Consider the vector space \mathbb{R}^2 which has orthonormal basis vectors $\{|x\rangle, |y\rangle\}$. A Hermitian operator ρ can be written as

$$\rho = \frac{3}{8}(|x\rangle\!\langle x| + |y\rangle\!\langle y|) + \frac{1}{8}(|x\rangle\!\langle y| + |x\rangle\!\langle y|).$$

- i) Write the matrix representation of ρ with respect to the $\{|x\rangle, |y\rangle\}$ basis vectors. [2 marks]
- ii) Find the eigenvalues and normalised eigenvectors of $\rho.$

[7 marks]

iii) Hence or otherwise calculate

$$S(\rho) = -\operatorname{Tr}(\rho \log_2 \rho).$$

[5 marks]

Applications of Quantum Mechanics 23/24

b) Using Pauli spin matrices, verify that the following relation holds between the spin operators \widehat{S}_x , \widehat{S}_y and \widehat{S}_z :

$$[\widehat{S}_x, \widehat{S}_y] = i\hbar \widehat{S}_z.$$

[5 marks]

a) i) An electron is in a spin state described by

$$\chi_0 = \frac{1}{\sqrt{5}} (2\alpha_z - \beta_z).$$

If a measurement is made of the z component of the electron's spin, what are the possible values that might be measured and with what probabilities?

[2 marks]

ii) Express χ_0 in the basis of α_x and β_x . Describe how the outcomes would be different if the measurement were applied to the x component of the spin.

[6 marks]

iii) The electron experiences a constant magnetic field of strength B along the z axis. At time t = 0, the spin state is given by χ_0 . Find an expression for its spin state $\chi(t)$ at any later time t.

[5 marks]

iv) Find the probability for the electron to be observed in the state α_y at a later time t.

[6 marks]

b) Consider a two-electron system described by the Hamiltonian

$$\widehat{H} = \lambda \widehat{\mathbf{S}}_1 \cdot \widehat{\mathbf{S}}_2,$$

where λ is a constant. Calculate the expectation values of the energy for the resulting spin-singlet and spin-triplet states.

[6 marks]

Mathematical Fundamentals of Quantum Mechanics

1. a) A Hermitian operator has eigenstates |a_i⟩ with eigenvalues a_i. The corresponding physical quantity is measured for a system in the state |ψ⟩, which is not an eigenstate of Â. State the possible results of the measurement, and their probabilities. Use these to show that the average result of the measurement is given by the expectation value ⟨ψ|Â|ψ⟩.

[5 marks]

b) A particle mass of m is in a state $|\psi\rangle$ and moves in the xy plane subject to the potential $V(x,y)=\beta x$, where β is a positive constant. Use Ehrenfest's theorem to find expressions for the rates of change of the expectation values of the components of its momentum, $\langle \widehat{p}_x \rangle$ and $\langle \widehat{p}_y \rangle$. Comment briefly on what your answer shows about the motion of this particle.

[6 marks]

d) A spin- $\frac{1}{2}$ particle is in the spin-up state along a strong magnetic field in the z direction. A small magnetic field B_y is added along the y axis. Find the resulting first-order shift in the energy of the particle.

[3 marks]

3. a) A particle moves in the potential

$$V(x) = \begin{cases} \infty & \text{for } x < 0 \\ \beta x & \text{for } x > 0 \,, \end{cases}$$

where β is a positive constant.

i) Explain why

$$\psi(x) = x \exp\left(-\frac{x}{2a}\right)$$

is a suitable trial wave function to use for a variational approximation to the ground state of this particle. Also, give a physical explanation why the expectation value of the energy of this state should have a minimum as a function of the parameter a.

[6 marks]

ii) Use the trial function in part (i) with a as a variational parameter to obtain an upper bound on the ground-state energy E_0 .

[11 marks]

b) A particle with mass m and energy E=0 is incident on a barrier with the form

$$V(x) = \begin{cases} -V_0 & \text{for } x < 0 \\ V_0 - \beta x & \text{for } x > 0 \end{cases},$$

where V_0 and β are positive constants. Sketch this potential, indicating the classically forbidden region. Use the WKB approximation to find the dependence of the tunnelling factor on V_0 and β .

[8 marks]

4.i) Write down an expression for the first-order shifts in energy of the non-degenerate states of a system subject to a small perturbing Hamiltonian $\lambda \hat{H}^{(1)}$, explaining all of your notation. Why can this expression not always be used for states that are degenerate in the absence of the perturbation? When is it still valid for such states?

[6 marks]

ii) The energy eigenstates of a symmetric two-dimensional harmonic oscillator can be labelled by their excitation quantum numbers in a Cartesian basis, $|n_x, n_y\rangle$, with energies $\hbar\omega(n_x+n_y+1)$.

This oscillator is subject to a perturbation of strength λ , with $0 < \lambda \ll 1$, such that the Hamiltonian is

$$\widehat{H} = \frac{1}{2m}(\widehat{p}_x^2 + \widehat{p}_y^2) + \frac{m\omega^2}{2} \Big(\widehat{x}^2 + \widehat{y}^2 + 4\lambda \widehat{x}\,\widehat{y}\Big),$$

where \hat{p}_x and \hat{p}_y are components of the momentum operator. For the ground state, find the first-order shift in the energy. Which excited state(s) of the unperturbed Hamiltonian will contribute to the second-order shift in the ground-state energy?

[7 marks]

 In the absence of the perturbation, the second excited level is triply degenerate. Show that in the following basis for the subspace of degenerate states,

$$\{|2,0\rangle, |1,1\rangle, |0,2\rangle\},\$$

the perturbation has the form

$$\sqrt{2}\,\hbar\omega\lambda\left(\begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{array}\right).$$

Hence verify that the energy of one state in this subspace has no shift to first order in λ . Find this state. Find also the first-order energy shifts of the other two states.

[12 marks]

Introduction to Quantum Mechanics 22/23

b) A particle is in the following mixed state

$$\Psi(x,t) = \frac{1}{\sqrt{5}}\Psi_1(x,t) + \frac{2}{\sqrt{5}}\Psi_2(x,t),$$

where $\Psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar}$ are stationary states.

What are the possible outcomes of a measurement of the particle's energy?

Determine the expectation value of the energy of the particle.

[4 marks]

d) State the definition of the Hermitian conjugate, \hat{A}^{\dagger} , of an operator \hat{A} , and the definition of a Hermitian operator.

Show that the momentum operator \hat{p}_x is a Hermitian operator.

[7 marks]

2. a) Consider a 1D simple quantum harmonic oscillator of classical angular frequency ω . Draw on one sketch, the potential energy function, energy levels, and wavefunctions of the three lowest energy states.

[8 marks]

c) Now consider a 1D oscillator consisting of a mass on a spring that can be extended elastically, but not compressed, corresponding to a potential energy function:

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2 & \text{if } x > 0, \\ \infty & \text{if } x \le 0. \end{cases}$$

Write down the full set of energy eigenvalues of this oscillator and sketch the eigenfunction of its ground state. Find the first excitation energy (i.e. the difference between the energies of the ground state and first excited state). Briefly state the reasoning behind your results.

[6 marks]

Complex Variables and Vector Spaces 22/23

1. a) An operator \hat{A} is termed anti-hermitian if it satisfies $\hat{A}^{\dagger} = -\hat{A}$. Show that the eigenvalues of an anti-hermitian operator \hat{A} are pure imaginary.

[6 marks]

2. A two-dimensional complex vector space has an orthonormal-basis $|0\rangle$ and $|1\rangle$. The Pauli operators on this space are defined as

$$\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0|, \quad \hat{\sigma}_y = -i|0\rangle\langle 1| + i|1\rangle\langle 0|, \quad \text{and} \quad \hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1|.$$

a) Write down the matrix representation of all three Pauli operators with respect to the $\{|0\rangle, |1\rangle\}$ basis.

[3 marks]

- b) Find the eigenvalues and corresponding normalised eigenvectors for $\hat{\sigma}_y.$ [5 marks]
- c) A rotation operator in this two-dimensional vector space can be defined as

$$\hat{R}(\theta) = \exp(-i\theta\hat{\sigma}_y),$$

where θ is a real constant. Find the spectral representation of $\hat{R}(\theta)$, and show that it is unitary for all values of θ .

[4 marks]

d) Show that the rotation operator in part (c) has the matrix representation,

$$\mathbf{R}(\theta) = \left(\begin{array}{cc} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{array} \right),$$

with respect to the $\{|0\rangle, |1\rangle\}$ basis.

[7 marks]

e) Consider the operator,

$$\hat{\rho} = \beta \hat{\sigma}_x + \gamma \hat{\sigma}_z,$$

where β and γ are real constants. Show that the rotation operator $\hat{R}(\theta)$ diagonalises $\hat{\rho}$ when

$$\theta = -\frac{1}{2}\arctan\left(\frac{\beta}{\gamma}\right).$$

Applications of Quantum Mechanics 22/23

c) The spin of an electron is described by the spinor

$$\chi = A \begin{pmatrix} 1 \\ i \end{pmatrix}.$$

i) Determine the value of the normalisation constant A. If a measurement is made of S_x , what are the possible outcomes and their associated probabilities?

[4 marks]

ii) Calculate the expectation value of a measurement of S_y .

[3 marks]

d) An electron is confined within a cuboidal quantum dot of sides of length a, 2a and 2a. Write down an expression for the energy levels of the system.

[4 marks]

2. a) A particle of mass m is located in a harmonic oscillator potential, $V(x) = \frac{1}{2}m\omega^2x^2$. At time t = 0, the particle is described by the normalised wave function

$$\psi(x,0) = a_0\phi_0(x) + a_1\phi_1(x) + a_2\phi_2(x),$$

where ϕ_n are the eigenfunctions of the harmonic oscillator and a_n are complex constants.

- i) What are the possible results of a measurement of the energy of this system?
 [2 marks
- ii) Write down an expression for $\psi(x,t)$, describing this particle at an arbitrary time t in terms of the harmonic oscillator eigenfunctions $\phi_n(x)$.

[6 marks]

iii) Using the result from (ii), show that the time evolution of the expectation value of position, $\langle x(t) \rangle$, can be written as $A\cos(\omega t) + B\sin(\omega t)$, where A and B are constants. Note that you are not required to derive A and B explicitly.

[8 marks]

You may use the equality,

$$\int_{-\infty}^{\infty} \phi_n(x) x \phi_k(x) dx = \sqrt{\frac{\hbar}{m\omega}} \left[\sqrt{\frac{k+1}{2}} \delta_{n,k+1} + \sqrt{\frac{k}{2}} \delta_{n,k-1} \right].$$

b) Consider the oscillator potential in (a) with the following perturbation:

$$V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^6 + \mu x^7,$$

where λ and μ are constants.

i) Using perturbation theory, estimate the ground-state energy.

[7 marks]

ii) Under what circumstances would your answer be a good approximation? [2 marks]

You may use the normalised ground-state eigenfunction of a harmonic oscillator,

$$\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{m\omega}{2\hbar}x^2\right],$$

and the standard integral,

$$\int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = \frac{1 \times 3 \times 5 \times \dots \times (2n-1)}{2^n} \sqrt{\frac{\pi}{\alpha^{2n+1}}}$$

- 3. a) Ladder operators for a spin- $\frac{1}{2}$ system are defined as $\hat{S}_{\pm} = \hat{S}_x \pm i\hat{S}_y$.
 - i) Expressing \widehat{S}_x and \widehat{S}_y in terms of the ladder operators, show that $\langle \widehat{S}_x \rangle$ and $\langle \widehat{S}_y \rangle$ are both zero for a system in the eigenstate β_z .

[5 marks]

ii) For the same system, find $\langle \widehat{S}_{x}^{2} \rangle$ and $\langle \widehat{S}_{y}^{2} \rangle$ and hence show that,

$$\Delta S_x \Delta S_y = \frac{1}{4} \hbar^2$$
,

where
$$\Delta S_i = \sqrt{\langle \hat{S}_i^2 \rangle - \langle \hat{S}_i \rangle^2}$$
 with $i = \{x, y\}$.

5 marks

b) Consider two spin-¹/₂ particles interacting with one another and with an external magnetic field B, directed along the z-axis. The Hamiltonian is given by

$$\hat{H} = -g\mu_B \left(\hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2\right) \cdot \mathbf{B} + \lambda \hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2,$$

where g is the g factor and λ is a positive constant.

i) For the case of very strong magnetic fields, µ_B|B| ≫ λ, where the mutual interaction of the two particles can be neglected, write down expressions for the the eigenvalues and eigenvectors of Ĥ.

[6 marks]

ii) Similarly, for the case of very weak magnetic fields, $\mu_B|\mathbf{B}| \ll \lambda$, write down expressions for the the eigenvalues and eigenvectors of \hat{H} .

[6 marks]

iii) Draw schematic diagrams for the energy levels in (i) and (ii), and discuss the degeneracy of energy levels in each case.

[3 marks]

4. An essential component of a quantum computer is the controlled-NOT gate. Acting on two Qbits, it flips the state of the second Qbit if the first has the value 1 and leaves the second unchanged if the first has the value 0. If the spins of two electrons are used to encode the Qbits, the effect of the gate can be represented by the operator \(\hat{C} \) with the properties:

$$\widehat{C}\alpha_z(1)\alpha_z(2) = \alpha_z(1)\beta_z(2),$$

 $\widehat{C}\alpha_z(1)\beta_z(2) = \alpha_z(1)\alpha_z(2),$
 $\widehat{C}\beta_z(1)\alpha_z(2) = \beta_z(1)\alpha_z(2),$
 $\widehat{C}\beta_z(1)\beta_z(2) = \beta_z(1)\beta_z(2).$

a) Consider the initial state where electron 1 is spin-up along the x-axis, and electron 2 is spin-up along the z-axis:

$$\alpha_x(1)\alpha_z(2)$$
.

Show that \hat{C} acts on this state to produce an entangled state.

[7 marks]

Show that when both electrons are initially spin-up along the x-axis,

$$\alpha_x(1)\alpha_x(2)$$
,

 \hat{C} produces an unentangled state.

[8 marks]

c) Find the effect of the gate on the other three states where both electrons have spins either up or down along the x-axis:

$$\alpha_x(1)\beta_x(2)$$
, $\beta_x(1)\alpha_x(2)$, $\beta_x(1)\beta_x(2)$.

[6 marks]

d) Hence, show that for these states, the gate acts as if the spin of electron 2 is the control Qbit, flipping the spin of the first Qbit if the second has the value 0. Hint: Any sign change of the states under \(\hat{C} \) is irrelevant.

[4 marks]

Mathematical Fundamentals of Quantum Mechanics 22/23

 a) In the basis of its energy eigenstates, the Hamiltonian of a two-state system is represented by

$$\widehat{H} \longrightarrow \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}.$$

If the system is in the normalised state

$$|\psi\rangle \longrightarrow \frac{1}{2} \left(\frac{1}{\sqrt{3}i} \right),$$

evaluate the expectation value $\langle \psi | \hat{H} | \psi \rangle$. Show that your answer is consistent with the probability postulate of quantum mechanics (the "Born rule").

[5 marks]

c) What is the WKB condition for the bound-state energies of a one-dimensional potential well with one infinite side? Define all your terms. What are the conditions for its validity?

[5 marks]

e) A two-state Qbit has orthogonal states |0⟩ and |1⟩. Which of the following states of two Qbits are entangled? Give brief justifications for your answers.

$$\begin{split} |A\rangle &= \sqrt{\frac{1}{2}} \Big(|0\rangle \otimes |0\rangle - |1\rangle \otimes |0\rangle \Big), \\ |B\rangle &= \frac{5}{13} |0\rangle \otimes |0\rangle - \frac{12}{13} |1\rangle \otimes |1\rangle, \\ |C\rangle &= \frac{1}{2} \Big(|0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle - |1\rangle \otimes |1\rangle \Big), \\ |D\rangle &= \sqrt{\frac{1}{10}} \Big(|0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle - 2|1\rangle \otimes |0\rangle - 2|1\rangle \otimes |1\rangle \Big). \end{split}$$

[5 marks]

2. i) The propagator (time-evolution operator) $\widehat{U}(t,t_0)$ for some quantum system acts on the state of the system at time t_0 , $|\psi(t_0)\rangle$, to give the subsequent state of the system, $|\psi(t)\rangle$, at some later time t. Starting from the time-dependent Schrödinger equation for a system with a Hamiltonian \widehat{H} that does not depend on time, show that the propagator can be expressed in the form

$$\widehat{U}(t,t_0) = \exp\left(-\frac{\mathrm{i}}{\hbar}\widehat{H}(t-t_0)\right).$$

[6 marks]

ii) In an orthonormal basis, the Hamiltonian of a certain two-state system is represented by

$$\widehat{H} \longrightarrow \frac{\hbar \gamma}{5} \begin{pmatrix} 4 & 3 \\ 3 & -4 \end{pmatrix},$$

where γ is a real constant. Without finding the eigenvectors, obtain the representation of the propagator $\widehat{U}(t,0)$ in the same basis. Hence find the subsequent state vector if the initial state of the system is:

(a)
$$|u\rangle \longrightarrow \begin{pmatrix} 1\\0 \end{pmatrix}$$
, (b) $|v\rangle \longrightarrow \frac{1}{\sqrt{10}} \begin{pmatrix} 1\\-3 \end{pmatrix}$.

[10 marks]

iii) From your answers to part (ii), deduce the representations of the eigenstates of \widehat{H} , and the corresponding eigenvalues.

[4 marks]

iv) This Hamiltonian can describe a stationary electron in a magnetic field of strength B, with the matrix in part (ii) being its representation in the basis of eigenstates of \widehat{S}_z . Relate γ to B, and give the direction of the magnetic field. Describe the motion of the electron spin if it is initially in the state $|u\rangle$.

[5 marks]

- 3. i) A system is governed by a Hamiltonian \widehat{H} . For a given normalised trial wave function ψ , show that the expectation value of the Hamiltonian in this state is an upper bound on the true ground-state energy of the system. Explain under what circumstances an upper bound can be found for the energy of an excited state, giving an example. [8 marks]
 - ii) A particle of mass m moves in a one-dimensional potential

$$V(x) = \frac{1}{2}m\omega^2 x^2 + \lambda \mathrm{e}^{-\beta x^2},$$

where λ and β are real constants. Select an appropriate harmonic oscillator eigenstate from the formula sheet as a trial wave function, replacing the oscillator length x_0 with the variational parameter σ . Show that for a given σ , a variational upper bound on the energy of the ground state is

$$E_b(\sigma) = \frac{1}{4} \left(\frac{\hbar^2}{m\sigma^2} + m\omega^2 \sigma^2 \right) + \frac{\lambda}{\sqrt{\sigma^2 \beta + 1}}.$$

[Hint: It may help to use the fact that the momentum operator \hat{p} is Hermitian.] [11 marks]

iii) If $|\lambda|$ is small, the value of σ which minimises this bound can be written, to first order in λ , as $\sigma_m = x_0 + \alpha \lambda$, where x_0 is the oscillator length for the potential with $\lambda = 0$, and α is some combination of the other parameters of the problem. Without finding α , show that, to the same order in λ , the corresponding variational bound is

$$E_b = \frac{1}{2}\hbar\omega + \frac{\lambda}{\sqrt{x_0^2\beta + 1}},$$

and relate this result to first-order perturbation theory.

[6 marks]

4. i) A particle of mass m moves in a one-dimensional harmonic potential

$$V(x) = \frac{1}{2}m\omega^2 x^2.$$

Use the definitions of the operators \hat{a} and \hat{a}^{\dagger} given in the formula sheet to write the Hamiltonian in terms of these operators, and show that $[\hat{H}, \hat{a}] = -\hbar \omega \hat{a}$.

[6 marks]

ii) The ket $|n\rangle$ denotes an eigenstate of the Hamiltonian with energy $E_n=(n+\frac{1}{2})\hbar\omega$. Use the results of part (i) to show that, for n>0, $\hat{a}|n\rangle=\sqrt{n}\,|n-1\rangle$.

[6 marks]

iii) Consider a "coherent state" $|\lambda\rangle$ defined by

$$|\lambda\rangle = A \sum_{n=0}^{\infty} \frac{\lambda^n}{\sqrt{n!}} |n\rangle,$$

where λ is a complex number and A is a normalisation constant. Show that $|\lambda\rangle$ is an eigenstate of \hat{a} and find the corresponding eigenvalue.

[5 marks]

iv) Find the normalisation constant A for the state $|\lambda\rangle$. Defining the number operator $\hat{n} = \hat{a}^{\dagger}\hat{a}$, show that the uncertainty in the number of quanta is given by

$$(\Delta n)^2 = \langle \widehat{n} \rangle.$$

[8 marks]

Introduction to Quantum Mechanics 21/22

- a) i) The normalized wavefunction of a particle moving in one dimension is Ψ. Consider an operator associated with a physical measurement, A.
 Write down the definition of the expectation value of Â.
 Briefly describe the physical meaning of this value and how it is related to the outcomes of particular measurements of A.
 [5 marks]
 - ii) Write down the definition of the Hermitian conjugate, \hat{A}^{\dagger} , of the operator \hat{A} . Show that this definition results in the relation $(\hat{A}\hat{B})^{\dagger} = \hat{B}^{\dagger}\hat{A}^{\dagger}$.

- 2. a) Consider a 1D simple quantum harmonic oscillator of classical angular frequency ω .
 - i) Draw on one sketch, the potential energy function, energy levels, and wavefunctions of the three lowest energy states.
 [8 marks]
 - ii) Calculate the value of the zero-point energy of the oscillator if its classical angular frequency is $2.0 \times 10^{13} \, \mathrm{s}^{-1}$. [2 marks]
 - iii) If the particle in the quantum harmonic oscillator is charged, transitions between energy levels can involve the absorption or emission of a single photon. Explain how the frequency of this photon is related to the classical frequency of the oscillator.
 [3 marks]
 - iv) In a carbon monoxide (CO) molecule, the effective spring constant of the covalent bond has a value of $1860\,\mathrm{N\,m^{-1}}$. Estimate the first excitation energy for vibrational motion of a CO molecule. You may take the atomic masses of carbon and oxygen to be 12.0 and 16.0 respectively.

3. a) For a particle of mass m moving in one dimension, write down the definition of the momentum operator \hat{p}_x and derive the kinetic energy operator \hat{T} .

The particle is moving in a region of free space with a wavefunction

$$\psi(x) = A\cos kx$$
,

where A and k are constants. Show that $\psi(x)$ is not an eigenfunction of \hat{p}_x but is an eigenfunction of \hat{T} .

What are the possible outcomes of a measurement of the particle's momentum?

[9 marks]

Complex Variables and Vector Spaces 21/22

4. An operator \hat{S} acts on a two-dimensional complex vector space. With respect to a particular orthonormal basis, it is represented by the matrix

$$\mathbf{S} = \frac{1}{5} \begin{pmatrix} 4 & 3 \\ 3 & -4 \end{pmatrix}.$$

A second operator $\widehat{R}(\alpha)$ is defined by

$$\widehat{R}(\alpha) = \exp(i\alpha\widehat{S}),$$

where α is a real parameter.

a) Show that \hat{S} is both Hermitian and unitary.

[3 marks]

b) Show that the eigenvalues of \widehat{S} are ± 1 and find its normalized eigenvectors, working in the basis used to define **S**.

[8 marks]

c) Find \widehat{S}^2 and hence show that $\widehat{R}(\alpha)$ can be expressed in the form

$$\widehat{R}(\alpha) = \cos \alpha \,\widehat{I} + i \sin \alpha \,\widehat{S} \,,$$

where \widehat{I} is the identity operator. Show also that $\widehat{R}(\alpha)$ is unitary for all α .

9 marks

d) Find the eigenvalues and eigenvectors of $\widehat{R}(\alpha)$. [You should not need to solve another matrix eigenvalue equation for this.] Verify that the eigenvalues and eigenvectors have the properties expected for a unitary operator.

[5 marks]

Applications of Quantum Mechanics 21/22

1. a) A system is composed of two different particles with quantum numbers j₁ = 7/2 and j₂ = 3/2 describing their angular momenta. What are the allowed values of the quantum numbers J and M_J associated with the total angular momentum of the whole system?

[4 marks]

b) State whether the following states of two particles are entangled or separable:

$$\psi(1,2) = \frac{1}{\sqrt{2}} \left[\alpha_z(1)\beta_z(2) - \beta_z(1)\beta_z(2) \right],$$

and

$$\phi(1,2) = \frac{1}{\sqrt{2}} \left[\alpha_z(1)\beta_z(2) - \beta_z(1)\alpha_z(2) \right].$$

Give your reasoning.

[4 marks]

c) A quantum dot is defined by the potential:

$$V(x,y,z) = \frac{1}{2}k\big(4x^2 + 4y^2 + z^2\big).$$

i) Give an expression for the energy levels of a particle of mass m placed in the dot, giving a brief justification for your answer.

[4 marks]

d) An electron sits in a magnetic field B that points in the +z-direction. At t=0, the electron is in the state

$$\gamma = \frac{1}{\sqrt{3}} \begin{pmatrix} i\sqrt{2} \\ 1 \end{pmatrix}.$$

Write down the state of the electron at time t, and hence find $\langle \widehat{S}_x \rangle$ as a function of time.

[5 marks]

a) A particle of mass m is located in a perturbed harmonic potential:

$$V(x) = \frac{1}{2}m\omega^2 x^2 + V_0 \exp(-\lambda x^2)$$
, with $V_0 > 0$ and $\lambda > 0$.

 Use perturbation theory to find the ground state energy to first order in V₀.
 You may use the normalised ground-state eigenfunction of a one-dimensional harmonic oscillator,

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{m\omega}{2\hbar}x^2\right],$$

and the standard integral $\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$.

[6 marks]

- ii) Under what circumstances would your answer be a good approximation?

 [4 marks]
- b) The probability that a particle with mass m and energy E tunnels through a one-dimensional potential barrier V(x) can be approximated by:

$$T\sim \exp\left[-2\int_a^b\sqrt{\frac{2m}{\hbar^2}\big(V(x)-E\big)}\ dx\right].$$

i) Without performing a detailed derivation, explain how this formula arises and describe the circumstances under which it is valid. What do the limits a and b of the integral correspond to?

[4 marks]

ii) A particle of mass m is incident on a parabolic barrier of the form $V(x) = V_0 - \alpha x^2$, where V_0 and α are constants. The incident energy E is less than V_0 , the maximum value of the potential. Find the values of a and b in this case.

[4 marks]

iii) Show that an estimate for the tunnelling probability is given by:

$$T \sim \exp \left[-\pi (V_0 - E) \sqrt{\frac{2m}{\alpha \hbar^2}}\right].$$

You may use the standard integral:

$$\int_{-1}^{+1} \sqrt{1 - z^2} \, dz = \frac{\pi}{2}.$$

[7 marks]

a) Using the Pauli spin matrices, verify that:

$$\hat{S}_{+}\beta_{z} = \hbar\alpha_{z}$$
 and $\hat{S}_{-}\alpha_{z} = \hbar\beta_{z}$,

where $\hat{S}_{\pm} = \hat{S}_x \pm i \hat{S}_y$ are the ladder operators for a spin- $\frac{1}{2}$ system.

What are the results for the operations $\hat{S}_{+}\alpha_{z}$ and $\hat{S}_{-}\beta_{z}$?

[6 marks]

b) What is the largest value of the z-component of the total spin of two spin-½ particles?

Write down a product of spinors that describes this state.

[2 marks]

c) For the combined system, the lowering operator is defined as $\widehat{S}_{-} = \widehat{S}_{-}^{(1)} + \widehat{S}_{-}^{(2)}$, where superscripts refer to the two different particles.

By considering successive operations of \widehat{S}_{-} on your spinor product, show that there are in total three magnetic substates. What is the quantum number of the total spin for these states?

[7 marks]

d) Classify the three states you have found as separable or entangled.

[3 marks]

e) An electron and positron can form a bound system called positronium, similar to an electron and a proton in the hydrogen atom, where the lowest states have no orbital angular momentum. The degeneracy of the levels formed by different couplings of intrinsic spin \$\hat{\mathbf{S}} = \hat{\mathbf{S}}^{(1)} + \hat{\mathbf{S}}^{(2)}\$ is lifted by a spin-dependent interaction of the form:

$$\widehat{H} = \gamma \ \widehat{\mathbf{S}}^{(1)} \cdot \widehat{\mathbf{S}}^{(2)},$$

where γ is a constant. Find the separation in energy of the lowest singlet and triplet states.

[7 marks]

Mathematical Fundamentals of Quantum Mechanics 21/22

1. a) A 1D harmonic oscillator is in the state

$$|\psi\rangle = N\Big(|0\rangle + 2|1\rangle + 3i|2\rangle\Big),$$

where $|n\rangle$ denote the energy eigenstates, and N is a normalisation constant. Find the expectation value of the energy.

[5 marks]

b) The Hamiltonian for a certain spin- $\frac{1}{2}$ particle has the form

$$\widehat{H} \longrightarrow \mu B \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

in the S_z basis. Use Ehrenfest's theorem to find $\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle \hat{S}_z \rangle$. Comment on what your result shows about the time dependence of the particle's spin.

[6 marks]

c) Evaluate the matrix element $\langle 1|\hat{x}^3|0\rangle$ where $|n\rangle$ are eigenstates of the harmonic oscillator.

[5 marks]

e) A particle of mass m is in the ground state in an infinite square well with walls at x=0 and a. It is subject to a perturbing potential $V(x)=\lambda\,\delta(x-a/2)$, where $\delta(x)$ is the Dirac δ -function and λ is a constant. Find its energy to first order in λ .

5 marks

 $^{2}.$ i) A system has angular momentum quantum number j = 1. Write down the 3×3 matrix representing \hat{J}_z in its own eigenbasis. Find the matrix representing \hat{J}_+ in the same basis, and hence write down J_{-} and show that

$$\widehat{J}_x \xrightarrow{J_z} \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \widehat{J}_y \xrightarrow{J_z} \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

[6 marks]

- ii) Write down the eigenvalues of J_x and J_y for this system. Verify that $(1,0,-1)^{\top}$ is an eigenvector of \widehat{J}_x in the J_z basis, and that $(1,0,1)^{\top}$ is an eigenvector of \widehat{J}_y , stating the corresponding eigenvalues. Find all the normalised eigenvectors of \widehat{J}_y . [8 marks]
- iii) A particle with angular momentum j=1 is prepared in the state with $J_z=+\hbar$. It passes first through a Stern-Gerlach apparatus that measures J_v .
 - a) Find the probabilities of getting each of the possible values of J_{ν} .
 - b) The particle then passes through a second apparatus which measures J_x . Given that the first measurement yielded $J_y = 0$, find the probability of getting $J_x = 0$.

[4 marks]

 Now suppose that, between the first and second measurements, the particle experiences a constant magnetic field B in the z-direction. The particle has a magnetic moment μ . Write down an expression for the propagator U(t,0) in the J_z basis. Given that the first measurement yielded $J_y = 0$, find the new probability of getting $J_x = 0$ as a function of the time between the measurements.

[7 marks]

3. a) The Hamiltonian for the electron in a hydrogen atom is

$$\widehat{H} = \frac{\widehat{\mathbf{p}}^2}{2m} - \frac{\alpha \hbar c}{\widehat{r}}.$$

Use the normalised ground state of the 3D oscillator,

$$\psi(\mathbf{r}) = (\pi x_0^2)^{-3/4} \exp(-r^2/2x_0^2),$$

as a trial wave function for this system.

Show that the expectation value of the energy in this state is

$$\langle \widehat{H} \rangle = \frac{3\hbar^2}{4mx_0^2} - \frac{2\alpha\hbar c}{\sqrt{\pi} \ x_0}.$$

[Hint: Rewrite the kinetic term in a symmetric form before you express it in the position representation.]

[8 marks]

ii) Find the best upper bound on the ground state energy for this trial function, and compare your result with the exact energy, $-\alpha^2 mc^2/2$.

[6 marks]

b) Use the WKB approximation to find the dominant energy dependence of the tunnelling probability through a quadratic barrier,

$$V(x) = V_0 - Kx^2,$$

for a particle with mass m and energy E, where $E \ll V_0$. [You may use the following integral,

$$\int \sqrt{a^2 - x^2} \, dx = \frac{1}{2} x \sqrt{a^2 - x^2} + \frac{1}{2} a^2 \arcsin(x/a) + \text{const.}$$

[11 marks]

Introduction to Quantum Mechanics 20/21

1. A quantum harmonic oscillator in three dimensions is defined by the Hamiltonian

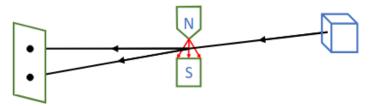
$$\widehat{H} = \frac{-\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{1}{2} k \left(x^2 + y^2 + z^2 \right) .$$

a) Describe how the method of separation of variables can be used to find the eigenfunctions and eigenvalues of this Hamiltonian.

Write down the energy eigenvalues in terms of three quantum numbers n_x , n_y , n_z . Calculate the degeneracy of the nth excited energy level.

[7 marks]

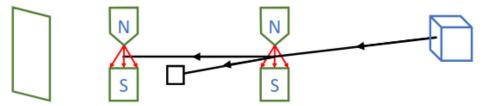
- 2. a) Silver atoms have a non-zero magnetic moment.
 - i) In the Stern-Gerlach experiment, a beam of silver atoms travelling in the y direction is passed through a non-uniform magnetic field that points in the z direction, as shown in the diagram.



Explain why two spots are observed on the screen. Contrast this with what would have been expected in classical physics.

[5 marks]

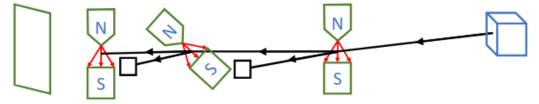
ii) One of the two beams coming out of the magnet is blocked and the other is fed into a second magnet oriented in the same way as the first, as shown in this diagram.



Give an explanation of what is observed on the screen this time.

[5 marks]

iii) In a new configuration, three magnets are set up: the first in the z direction and one of the beams coming from it is blocked; the second in the x direction and again one of the beams coming from it is blocked; and the third in the z direction, as shown in this diagram.



Give an explanation of what is observed on the screen this time.

[5 marks]

Complex Variables and Vector Spaces 20/21

- 3. a) A Hermitian operator ρ acts on vectors in the N-dimensional complex vector space C^N. The operator has eigenvalues {ρ_i} and orthonormal eigenvectors {|e_i⟩}. Write down the spectral representation of ρ̂. By considering its action on a general vector |v⟩ ∈ C^N, verify that the expression you have written down is equivalent to ρ̂.
 [6 marks]
 - b) The state of polarisation of a beam of light may be represented by a matrix

$$\boldsymbol{\rho} = \frac{1}{2} \begin{pmatrix} 1+q & u-iv \\ u+iv & 1-q \end{pmatrix},$$

where (q, u, v) are real parameters that satisfy $0 < q^2 + u^2 + v^2 \le 1$.

i) Show that the eigenvalues of ρ are $(1 \pm p)/2$, where $p^2 = q^2 + u^2 + v^2$. Find the corresponding eigenvectors. You do not need to normalise your vectors.

[10 marks]

- ii) Verify that the eigenvalues and eigenvectors found in part (i) have any properties that you would expect on general grounds, given the form of the matrix ρ .

 [5 marks]
- iii) For the special case $q^2 + u^2 + v^2 = 1$, use the spectral representation to explain why ρ can be written in the form

$$\boldsymbol{\rho} = \begin{pmatrix} a\,\overline{a} & a\,\overline{b} \\ b\,\overline{a} & b\,\overline{b} \end{pmatrix},$$

where a and b are the components of a unit vector. No detailed calculation is required.

[4 marks]

1. a) The eigenfunctions of a particle in an infinite square well between x = 0 and x = a are

$$\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right),\,$$

where the quantum number n = 1, 2, 3...

Explain why the eigenfunction has units of $length^{-1/2}$. Using the form of the eigenfunctions, deduce the eigenvalues explaining clearly how you reach your answer.

[6 marks]

b) A particle moving in the infinite square well is subject to an additional perturbation given by:

$$V_1 = V_0 \left(x - \frac{a}{2} \right)^2,$$

where V_0 is a constant.

- i) Sketch the potential, clearly annotating your diagram with relevant quantities. [2 marks]
- ii) Calculate the first-order change in the energy of a state with quantum number n and explain the circumstances in which your answer would give a good estimate of the shift in energy.

[9 marks]

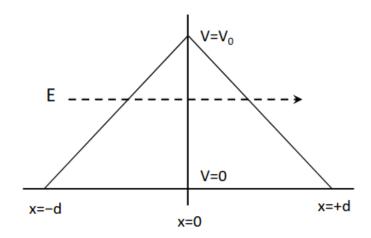
You may use the following standard integrals:

$$\int z \sin^2 z \, dz = \frac{z^2}{4} - \frac{z}{4} \sin 2z - \frac{1}{8} \cos 2z + C$$

$$\int z^2 \sin^2 z \, dz = \frac{z^3}{6} + \left(\frac{1}{8} - \frac{z^2}{4}\right) \sin 2z - \frac{1}{2} z \cos 2z + K,$$

where C and K are constants of integration.

2. A particle with energy E is incident on a triangular potential barrier. As shown in the diagram below, E is less than the height of the barrier V_0 .



a) i) Write down a function V(x) that describes the barrier.

[4 marks]

ii) If the limits of the classically forbidden region are x=-a and x=+a, find an expression for a in terms of quantities defined on the diagram.

[2 marks]

iii) Show that an estimate of the tunnelling probability through the barrier is given by:

$$T \approx \exp\left(-\frac{8}{3}\frac{d}{V_0}\sqrt{\frac{2m\left(V_0 - E\right)^3}{\hbar^2}}\right).$$

Under what circumstances would you expect this to be a good estimate?

[10 marks]

3. The eigenvectors of \widehat{S}_x and \widehat{S}_y are given by:

$$\alpha_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix}$$
 and $\beta_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix}$

$$\alpha_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$$
 and $\beta_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$.

a) Verify that α_y and β_y are eigenvectors of \widehat{S}_y and determine their eigenvalues.

[3 marks]

- b) An electron sits in a uniform magnetic field of strength B in the x direction.
 - i) What is the Hamiltonian associated with the electron spin? Write down a general solution $\chi(t)$ of the time-dependent Schrödinger equation.

[4 marks]

ii) If the electron is initially in a state $\chi(0) = \alpha_z$, find an expression for the time taken for the state to evolve from α_z to $-i\beta_z$. Explain what effect the factor -i has on measurements of spin observables.

[7 marks]

c) i) Two operators are defined as $\widehat{A} = \widehat{S}_z + i\widehat{S}_x$ and $\widehat{B} = \widehat{S}_z - i\widehat{S}_x$. Evaluate the results of operating on α_y and β_y with \widehat{A} and \widehat{B} . Comment on the effect of the two operators on the eigenvectors.

[6 marks]

ii) Use your results for Part c(i) to find the expectation value $\langle \widehat{S}_z \rangle$ for the state $\frac{1}{\sqrt{5}} [2\alpha_y - \beta_y]$.

[5 marks]

Mathematical Fundamentals of Quantum Mechanics 20/21

i) Two orthogonal axes are specified by the unit vectors

$$\mathbf{e}'_x = \cos\phi \,\mathbf{e}_x + \sin\phi \,\mathbf{e}_y, \qquad \mathbf{e}'_y = -\sin\phi \,\mathbf{e}_x + \cos\phi \,\mathbf{e}_y.$$

Show that the matrix representations of the corresponding operators, $\widehat{S}_{x'}$ and $\widehat{S}_{y'}$, for a spin- $\frac{1}{2}$ particle are, in the usual basis of S_z eigenstates:

$$S_{x'} = \frac{\hbar}{2} \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}, \qquad S_{y'} = \frac{\hbar}{2} \begin{pmatrix} 0 & -ie^{-i\phi} \\ ie^{i\phi} & 0 \end{pmatrix}.$$

[5 marks]

ii) Write down the eigenvalues of $\widehat{S}_{x'}$. Show that its eigenstates are given by

$$|x'+\rangle \xrightarrow{z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\phi} \end{pmatrix}, \qquad |x'-\rangle \xrightarrow{z} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{i\phi} \end{pmatrix}.$$

[6 marks]

iii) A measurement is made of S_x , giving $+\frac{\hbar}{2}$. Immediately afterwards, a measurement is made of $S_{x'}$. What is the probability of it giving $+\frac{\hbar}{2}$? Immediately after getting $S_{x'} = +\frac{\hbar}{2}$, another measurement is made of S_x . What is the probability of it giving $+\frac{\hbar}{2}$?

[4 marks]

iv) An electron is subject to a magnetic field in the x' direction, $\mathbf{B} = B \mathbf{e}'_x$. The electron is initially spin-down in the z direction. Find an expression for its state at subsequent times. Calculate the expectation value of \widehat{S}_z as a function of time. Without calculating $\langle \widehat{S}_{x'} \rangle$ and $\langle \widehat{S}_{y'} \rangle$, describe the motion of the system.

[10 marks]

- 2. A particle moves in two dimensions and is confined to a square box by a potential that is infinite outside the region 0 < x < a and 0 < y < a. In most of the box, the potential vanishes, except in one quarter of the box, 0 < x < a/2 and 0 < y < a/2, where the potential has the constant value V_0 .
 - i) For the case $V_0 = 0$, write down the energies and wave functions for the three eigenstates with lowest energies.

[3 marks]

Treating V₀ as a perturbation, find the shift in the ground-state energy to first order in V₀.

[5 marks]

iii) Explain briefly why the energies of the first two excited states cannot be calculated in a similar way. For these states, calculate the four matrix elements of the perturbing Hamiltonian, and hence find the energy shifts to first order in V_0 .

[12 marks]

iv) Deduce the wave functions corresponding to the states you found in part (iii) and comment on their symmetries.

[5 marks]

You may use the following integrals:

$$\int_0^{a/2} \sin^2(n\pi x/a) \, \mathrm{d}x = \frac{a}{4} \quad \text{for all integer } n \neq 0,$$

$$\int_0^{a/2} \sin(\pi x/a) \sin(n\pi x/a) \, \mathrm{d}x = \begin{cases} \frac{an}{\pi (n^2 - 1)} (-1)^{n/2 + 1} & \text{for even integer } n \\ 0 & \text{for odd integer } n \neq \pm 1 \end{cases}$$

3. The Hamiltonian for a two-dimensional system has the form of a modified harmonic oscillator:

$$\widehat{H} = \frac{1}{2m} \left(\widehat{p}_x^2 + \widehat{p}_y^2 \right) + \frac{1}{2} m\omega^2 \left(\widehat{x}^2 + \widehat{y}^2 \right) + \omega \left(\widehat{x} \, \widehat{p}_y - \widehat{y} \, \widehat{p}_x \right).$$

i) By expressing the coordinates and momenta in terms of raising and lowering operators, \hat{a}_x , \hat{a}_x^{\dagger} , \hat{a}_y , and \hat{a}_y^{\dagger} , show that the Hamiltonian can be written in the form

$$\widehat{H}=\hbar\omega\Big(\widehat{a}_{x}^{\dagger}\widehat{a}_{x}+\widehat{a}_{y}^{\dagger}\widehat{a}_{y}+1+\mathrm{i}\left(\widehat{a}_{y}^{\dagger}\widehat{a}_{x}-\widehat{a}_{x}^{\dagger}\widehat{a}_{y}\right)\Big).$$

[12 marks]

ii) New raising and lowering operators can be defined by

$$\widehat{A} = \frac{1}{\sqrt{2}} (\widehat{a}_x - i \, \widehat{a}_y), \qquad \widehat{B} = \frac{1}{\sqrt{2}} (\widehat{a}_x + i \, \widehat{a}_y),$$

$$\widehat{A}^{\dagger} = \frac{1}{\sqrt{2}} (\widehat{a}_x^{\dagger} + i \, \widehat{a}_y^{\dagger}), \qquad \widehat{B}^{\dagger} = \frac{1}{\sqrt{2}} (\widehat{a}_x^{\dagger} - i \, \widehat{a}_y^{\dagger}).$$

Verify that these satisfy the usual commutation rules,

$$\left[\widehat{A},\widehat{A}^{\dagger}\right]=1, \qquad \left[\widehat{A},\widehat{B}^{\dagger}\right]=0.$$

[5 marks]

iii) Verify that the Hamiltonian

$$\hat{H} = 2\hbar\omega \left(\widehat{A}^{\dagger} \widehat{A} + \frac{1}{2} \right)$$

is equivalent to the one given in part (i). Use this to write down the energy eigenvalues of this system. What can you say about the degeneracy of each level? [In addition to the commutation rules in part (ii), you may assume that $[\widehat{B}, \widehat{B}^{\dagger}] = 1$.] [8 marks]