Answer THREE questions.

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

The following formulae may be used if required:

$$e^x = \sum_{j=0}^{\infty} \frac{x^j}{j!} \qquad \sin(x) = \sum_{j=0}^{\infty} (-1)^j \frac{x^{2j+1}}{(2j+1)!} \qquad \cos(x) = \sum_{j=0}^{\infty} (-1)^j \frac{x^{2j}}{(2j)!}$$

The Time-dependent Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

Spin-one matrix representation of spin operators

$$\hat{S}_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad \hat{S}_y = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix} \qquad \hat{S}_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

WKB Connection formulae

Right-hand barrier - with classical turning point at $x = a$:

$$\frac{2}{\sqrt{p(x)}} \cos\left(\int_x^a p(x')dx'/\hbar - \frac{\pi}{4} \right) \quad \leftarrow \quad \frac{1}{\sqrt{q(x)}} \exp\left[- \int_a^x q(x')dx'/\hbar \right]$$

$$-\frac{1}{\sqrt{p(x)}} \sin\left(\int_x^a p(x')dx'/\hbar - \frac{\pi}{4} \right) \quad \rightarrow \quad \frac{1}{\sqrt{q(x)}} \exp\left[+ \int_a^x q(x')dx'/\hbar \right]$$

Left-hand barrier - with classical turning point at $x = a$:

$$\frac{1}{\sqrt{q(x)}} \exp\left[- \int_x^a q(x')dx'/\hbar \right] \quad \rightarrow \quad \frac{2}{\sqrt{p(x)}} \cos\left(\int_a^x p(x')dx'/\hbar - \frac{\pi}{4} \right)$$

$$\frac{1}{\sqrt{q(x)}} \exp\left[+ \int_x^a q(x')dx'/\hbar \right] \quad \leftarrow \quad -\frac{1}{\sqrt{p(x)}} \sin\left(\int_a^x p(x')dx'/\hbar - \frac{\pi}{4} \right)$$

1. Using the ansatz $\psi(x) = A\exp[iS(x)/\hbar]$ the time-independent Schrödinger equation can be reduced to the equation:

$$\frac{-i\hbar}{2m}S''(x) + \frac{1}{2m}\left(S'(x)\right)^2 + V(x) - E = 0.$$

where $S'(x) = dS(x)/dx$, etc.

(a) By expanding $S(x)$ as a power series in $\hbar$ derive the following zeroth order and first order equations:

$$\frac{1}{2m}\left(S_0'(x)\right)^2 + V(x) - E = 0 \qquad\qquad \frac{-i}{2}S_0''(x) + S_1'(x)S_0'(x) = 0,$$

[3]

(b) Clearly stating the approximations made, and stating (without proof) the conditions under which they are valid, derive the WKB wavefunction in a classically allowed region where $V(x) < E$

$$\psi(x) = \frac{A}{\sqrt{p(x)}}\exp\left[i\int^x p(x')dx'/\hbar\right] + \frac{B}{\sqrt{p(x)}}\exp\left[-i\int^x p(x')dx'/\hbar\right],$$

where $p(x) = \sqrt{2m(E - V(x))}$. **[8]**

(c) Write down the form of a WKB wave-function in a classically forbidden region. **[1]**

(d) For a quantum well with smooth sides the WKB approximation leads to the following quantisation condition:

$$\int_{t_1}^{t_2} p(x')dx'/\hbar = \left(n + \frac{1}{2}\right)\pi\,,$$

where t_1 and t_2 are the positions of classical turning points and $n = 0, 1, 2, \ldots$ is a non-negative integer.

Consider a quantum well described by the potential $V(x) = V_0\sqrt{|x|/L}$ for $|x| < L$ and $V(x) = V_0$ for $|x| \geq L$. Given $mV_0L^2/(\pi^2\hbar^2) = 2$, and that $V_0 = 1$keV, calculate the number of bound states and the ground state energy.

You may use the integral

$$\int_0^1 (1 - \sqrt{y})^{1/2}dy = \frac{8}{15},$$

without proof. **[8]**

2. (a) A system subjected to a time-dependent perturbation is described by a Hamiltonian: $H = H_0 + \lambda V(t)$, where H_0 is solved, i.e. its eigenstates $|\phi_j\rangle$ and eigenenergies E_j are known, and $\lambda V(t)$ is a small time-dependent perturbation. We shall write the state of the system in the interaction picture, $|\psi_I(t)\rangle = \sum_j c_j(t)\,|\phi_j\rangle$. If $|\psi_I(t)\rangle = U_0(t)^\dagger\,|\psi_S(t)\rangle$ where $U_0(t) = \exp[-i(t/\hbar)H_0]$, show that the state of the system in the Schrödinger picture $|\psi_S(t)\rangle$ may be written:

$$|\psi_S(t)\rangle = \sum_j c_j(t) e^{-i\frac{E_j}{\hbar}t}\,|\phi_j\rangle\,.$$

[3]

(b) Using the notation A_S and A_I to denote observable A expressed in the Schrödinger and interaction pictures respectively, how must A_S and A_I be related to ensure that $\langle\psi_I(t)|\,A_I\,|\psi_I(t)\rangle = \langle\psi_S(t)|\,A_S\,|\psi_S(t)\rangle$? **[2]**

(c) How are A_S and A_I related in the special case that $[A_S, H_0] = 0$? **[1]**

(d) The coefficients $c_j(t)$ satisfy the equations of motion,

$$\dot{c}_j(t) = \frac{\lambda}{i\hbar}\sum_k c_k(t)\exp\left[i\omega_{jk}t\right]V_{jk}(t)\,,$$

Expanding $c_j(t)$ as a power series in λ, explain why the mth order terms in this expansion satisfy the following expressions:

$$\dot{c}_j^{(0)}(t) = 0 \qquad\qquad \dot{c}_j^{(m)}(t) = \frac{1}{i\hbar}\sum_k \exp[i\omega_{jk}t]V_{jk}(t)c_k^{(m-1)}(t)\,,$$

for $m = 1, 2, 3, \ldots$. **[2]**

(e) The states $|+1\rangle$, $|0\rangle$ and $|-1\rangle$, an orthonormal basis for a spin-one particle, are eigenstates of the z-spin operator $\hat{S}_z$ with eigenvalues $\hbar$, 0 and $-\hbar$. Consider a particle prepared in state $|+1\rangle$ at time $t = 0$. In an experiment, the particle is trapped and exposed to magnetic fields. Initially the Hamiltonian is $H_0 = \kappa\hat{S}_z$. At time $t = 0$ an additional magnetic field is introduced which is rotating in the x-y plane. This adds an extra term to the Hamiltonian $V = g(\cos(\omega t)\hat{S}_x + \sin(\omega t)\hat{S}_y)$ where $g \ll \kappa$.

Write down matrix representations of H_0 and V, simplifying them if appropriate. You may find the spin-one matrix representations in the rubric at the start of this paper helpful. **[3]**

(f) The particle's z-component of spin is measured at later time $t = \tau$. Show that (to first order) the probability that the particle's state is observed now to be $|0\rangle$ is

$$\underset{+1\to 0}{P}{}^{(1)} = \frac{|g|^2\tau^2}{2}\mathrm{sinc}^2\left(\frac{(\omega-\kappa)\tau}{2}\right)\,.$$

[7]

(g) Show that the first order transition probability from $|+1\rangle$ to $|-1\rangle$ is zero. Do you expect to see a non-zero probability to second order? Why? **[2]**

3. (a) Describe a physical scenario where it can be convenient to use the density matrix formalism. **[1]**

(b) In the density matrix formalism write down an example of a pure state, and an example of a mixed state. **[2]**

(c) A super-operator $S[\rho]$ is written in Kraus form

$$S[\rho] = \sum_j K_j \rho K_j^\dagger$$

where $\sum_j K_j^\dagger K_j = \mathbb{1}$. Given that ρ is a physical density operator, show that $\rho' = S[\rho]$ is Hermitian and that $\mathrm{Tr}[\rho'] = 1$. **[4]**

(d) An evolution equation (called a master equation) for an open quantum system can be written in the following Lindblad form

$$\frac{\partial \rho}{\partial t} = \frac{-i}{\hbar}[H_{\mathrm{eff}}\rho - \rho H_{\mathrm{eff}}^\dagger] + \sum_j L_j \rho L_j^\dagger$$

where $H_{\mathrm{eff}} = H_0 - (i\hbar/2)\sum_j L_j^\dagger L_j$. Explain the role of the operators H_0 and L_j in this equation. If all L_j operators are set to zero, what equation do we recover? **[3]**

(e) A three-level atom has energy levels $|1\rangle$ with energy $E_1 = 0$, and degenerate higher-lying energy levels $|2\rangle$ and $|3\rangle$ with energy $E_2 = E_3 = \hbar\omega$. The system undergoes spontaneous emission due to its interaction with its environment.
We describe the dynamics of the atom by a master equation in Lindblad form. Spontaneous emission from state $|2\rangle$ to state $|1\rangle$ is described by jump operator $\gamma_2|1\rangle\langle 2|$ and from state $|3\rangle$ to state $|1\rangle$ by jump operator $\gamma_3|1\rangle\langle 3|$. Spontaneous emission between states $|2\rangle$ and $|3\rangle$ is negligible. Identify H_0 and show that H_{eff} for this system has the form

$$H_{\mathrm{eff}} = \alpha\,|2\rangle\,\langle 2| + \beta\,|3\rangle\,\langle 3|$$

and identify α and β. Hence write down the Lindblad form master equation for this evolution. **[4]**

(f) The atom is prepared in the initial state $\rho(0) = (1/2)(|2\rangle\,\langle 2| + |3\rangle\,\langle 3|)$. Given that the state of the atom evolving in time will have the general form:

$$\rho(t) = \rho_1(t)\,|1\rangle\,\langle 1| + \rho_2(t)\,|2\rangle\,\langle 2| + \rho_3(t)\,|3\rangle\,\langle 3|$$

derive from the master equation evolution equations for $\rho_1(t)$, $\rho_2(t)$ and $\rho_3(t)$. Solve these evolution equations to find $\rho(t)$ given the initial conditions. **[6]**

4. (a) The evolution operator $U(t)$ transforms a state of a system at time 0, $|\psi(0)\rangle$ to the state of the system at time t, $|\psi(t)\rangle$, i.e. $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$. Show that for a time-independent Hamiltonian H, the evolution operator can be written:

$$U(t) = \exp\left[-i\frac{Ht}{\hbar}\right] .$$

You may assume the identity $\frac{\partial}{\partial t}\exp[At] = A\exp[At]$ for linear operator A. **[3]**

(b) In the following, the subscript H will be attached to operators and states in the Heisenberg picture, the subscript S will denote the Schrödinger picture. In the Heisenberg picture, time evolution is carried by operators, $\hat{O}_H(t) = U(t)^\dagger \hat{O}_S U(t)$. States are constant in time and represent initial conditions $|\psi_H\rangle = |\psi_S(0)\rangle$. Show that the expectation values of operators $\hat{O}$ at time t are equal in both pictures. **[2]**

(c) Given two observables, $\hat{A}$ and $\hat{B}$, which, in the Schrödinger picture, satisfy

$$[\hat{A}, \hat{B}] = \hat{C}$$

show that, the equivalent operators in the Heisenberg picture $\hat{A}_H(t)$, $\hat{B}_H(t)$ and $\hat{C}_H(t)$ satisfy

$$[\hat{A}_H(t), \hat{B}_H(t)] = \hat{C}_H(t).$$

[2]

(d) Show that, in the Heisenberg picture, observables $\hat{O}_H(t)$ satisfy the Heisenberg equation of motion

$$\frac{\partial}{\partial t}\hat{O}_H(t) = \frac{i}{\hbar}[H_H(t), \hat{O}_H(t)] .$$

[4]

(e) In the Heisenberg picture, the Hamiltonian for a one-dimensional free particle has the form:

$$H_H(t) = \frac{1}{2m}\hat{p}_H^2(t) .$$

Derive equations of motion for $\hat{x}_H(t)$ and $\hat{p}_H(t)$, and hence for expectation values $\langle\hat{x}\rangle(t)$ and $\langle\hat{p}\rangle(t)$. **[5]**

(f) Solve these equations of motion to compute $\langle\hat{x}\rangle(t)$ and $\langle\hat{p}\rangle(t)$ for a particle with initial conditions $\langle\hat{x}\rangle = 0$, $\langle\hat{p}\rangle = \kappa$. **[4]**

You may find the commutation relation $[\hat{x}, \hat{p}] = i\hbar\mathbb{1}$ and the identity $[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{A}$ useful.

5. (a) The states $|\phi_j\rangle$, for $j = 1$ to d, are vectors in a d-dimensional space. What conditions must the states satisfy to be an orthonormal basis for that space? **[2]**

(b) Let state vectors $|\phi_j\rangle$, where j is an integer from 1 to d, form an orthonormal basis. The following expression for the identity operator $\mathbb{1}$ is known as the closure relation, $\mathbb{1} = \sum_j |\phi_j\rangle\langle\phi_j|$. Verify this expression by showing that applying the operator $\sum_j |\phi_j\rangle\langle\phi_j|$ leaves a general state vector in this space invariant. **[3]**

(c) Prove that the eigenvalues of a Hermitian operator A are real. **[2]**

(d) Assuming without proof that the eigenvectors of a non-degenerate Hermitian operator A are orthogonal, prove that every such operator has the spectral decomposition

$$A = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j| \ .$$

[2]

(e) We can define a norm for a vector as $|| \, |\psi\rangle \, || = \sqrt{\langle\psi|\psi\rangle}$. Show that this norm satisfies the scaling property $||\lambda |\psi\rangle \, || = |\lambda| \, || \, |\psi\rangle \, ||$. **[3]**

(f) The Gram-Schmidt method is a procedure to compute a set of orthonormal states. Let $|\psi_j\rangle$ be a set of linearly independent vectors in an n-dimensional space, and let $|\phi_j\rangle$ be the set of orthonormal basis vectors output by the Gram-Schmidt process, where j spans from 1 to n. The process proceeds as follows:

i) Let

$$|\phi_1\rangle = \frac{|\psi_1\rangle}{|| \, |\psi_1\rangle \, ||} \, .$$

ii) For $m = 2$ to n let

$$|\phi_m\rangle = \frac{(\mathbb{1} - \sum_{j=1}^{m-1} |\phi_j\rangle\langle\phi_j|) \, |\psi_m\rangle}{||(\mathbb{1} - \sum_{j=1}^{m-1} |\phi_j\rangle\langle\phi_j|) \, |\psi_m\rangle \, ||} \, .$$

You are given the following information about states $|\alpha\rangle$, $|\beta\rangle$ and $|\gamma\rangle$, which are normalised vectors within a three-dimensional space.

$$\langle\alpha|\beta\rangle = \frac{1}{\sqrt{2}} \qquad \langle\alpha|\gamma\rangle = \frac{1}{\sqrt{3}} \qquad \langle\beta|\gamma\rangle = \sqrt{\frac{2}{3}}$$

Use the Gram-Schmidt process to identify an orthogonal basis for that space, expressing the vectors you find in terms of $|\alpha\rangle$, $|\beta\rangle$ and $|\gamma\rangle$. **[8]**

END OF PAPER