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:

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

Schrödinger's Equation

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

Pauli operators

$$\sigma_z |\uparrow\rangle = |\uparrow\rangle \qquad \sigma_z |\downarrow\rangle = -|\downarrow\rangle \qquad \sigma_x |\uparrow\rangle = |\downarrow\rangle \qquad \sigma_x |\downarrow\rangle = |\uparrow\rangle \qquad \sigma_y |\uparrow\rangle = i |\downarrow\rangle \qquad \sigma_y |\downarrow\rangle = -i |\uparrow\rangle$$

where $|\uparrow\rangle$, $|\downarrow\rangle$ are orthonormal basis states for the two-dimensional spin-half state space.

Matrix Representation of the Pauli operators

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

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. (a) Give an example of a physical scenario where it would be convenient to work in the density matrix formalism. **[1]**

(b) What is the density operator for a pure state with state vector representation $|\psi\rangle$? **[1]**

(c) In the density matrix representation, the expectation value of an operator A with respect to state ρ is given by the following expression:

$$\langle A\rangle = \mathrm{Tr}[A\rho]\,.$$

Show that, for a pure state with state vector $|\psi\rangle$, this expression reduces to $\langle A\rangle = \langle\psi|\,A\,|\psi\rangle$. **[3]**

(d) To be a valid physical density operator, ρ must be Hermitian, have trace equal to 1, and have solely non-negative eigenvalues. A general 2×2 complex valued matrix can be written,

$$M = \begin{bmatrix} a & b \\ c & d \end{bmatrix}\,, \tag{1}$$

where a, b, c and d are complex numbers. What conditions must a, b, c and d satisfy to ensure that i) M is Hermitian and ii) M has trace equal to 1. **[4]**

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

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

where the Kraus operators K_i must satisfy $\sum_j K_j^\dagger K_j = \mathbb{1}$.
Given that ρ is a physical density operator, show that i) $\rho' = S[\rho]$ is Hermitian and that ii) $\mathrm{Tr}[\rho'] = 1$. **[4]**

(f) A spin-half particle is held in a trap. The particle's initial state is ρ_0. The trap is known to undergo fluctuations in its magnetic field, which cause the particle's state to evolve under a super-operator with the following Kraus operators:

$$K_1 = \frac{1}{2}\mathbb{1} \qquad K_2 = \frac{1}{2}\sigma_x \qquad K_3 = \frac{1}{2}\sigma_y \qquad K_4 = \lambda\sigma_z\,, \tag{2}$$

where λ is a real number.

i. What value must λ take for these to be valid Kraus operators? **[2]**

ii. Show that regardless of the input state ρ_0, the particle will evolve under the action of this super-operator to the state

$$\rho_1 = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

[5]

2. (a) Describe two applications of the WKB approximation and outline the conditions which must be satisfied for it to be a good approximation. **[3]**

(b) In the WKB approximation, a wave-function in the classically allowed region, $V(x) < E$, has the form

$$\psi(x) = \frac{A}{\sqrt{p(x)}} \exp\left[i \int^x p(x')dx'/\hbar\right] + \frac{B}{\sqrt{p(x)}} \exp\left[-i \int^x p(x')dx'/\hbar\right], \quad (3)$$

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

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

ii. Explain why wave-functions of this form cannot be good approximations to physical states at classical turning points. **[2]**

(c) For a quantum well with smooth sides show that 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.

You will find WKB connection formulae in the rubric at the beginning of this paper. **[7]**

(d) 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

$$\int \left(1 - \kappa\sqrt{x}\right)^{1/2} dx = \frac{-4}{15\kappa^2}(1 - \kappa\sqrt{x})^{3/2}(2 + 3\kappa\sqrt{x}) + c\,,$$

without proof. **[7]**

3. (a) A projector is an operator P which satisfies the property $P^2 = P$. Show that if P is a projector, the operator $\mathbb{1} - P$ is also a projector. **[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 the operator on its right hand side leaves a general state vector in this space invariant. **[3]**

(c) Using the closure relation or otherwise show that every linear operator O acting on the vector space may be expressed:

$$O = \sum_{j=1}^{d} \sum_{k=1}^{d} O_{j,k} |\phi_j\rangle \langle\phi_k| \ ,$$

where $O_{j,k} = \langle\phi_j| O |\phi_k\rangle$. **[2]**

(d) Every Hermitian operator H can be written in a spectral decomposition, $H = \sum_j \lambda_j P_j$ where λ_j are real scalars and P_j are projectors. We shall consider a three-dimensional system. Its state space has orthonormal basis $|\phi_1\rangle$, $|\phi_2\rangle$ and $|\phi_3\rangle$. Consider the following Hermitian operator:

$$M_1 = |\psi_1\rangle \langle\psi_1| - |\psi_2\rangle \langle\psi_2| - |\psi_3\rangle \langle\psi_3| \, ,$$

where $|\psi_1\rangle = (1/\sqrt{3})(|\phi_1\rangle + |\phi_2\rangle + |\phi_3\rangle)$, $|\psi_2\rangle = (1/\sqrt{6})(2\,|\phi_1\rangle - |\phi_2\rangle - |\phi_3\rangle)$ and $|\psi_3\rangle = (1/\sqrt{2})(|\phi_2\rangle - |\phi_3\rangle)$ are orthonormal eigenvectors of M_1.

Determine the eigenvalues of M_1 and the degeneracy of each eigenvalue. Hence, write down the scalars λ_j and the projectors P_j which make up the spectral decomposition of M_1 (expressed in a matrix representation in terms of basis states $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$). **[6]**

(e) A system is prepared in state $|\chi\rangle = (1/\sqrt{2})(|\phi_1\rangle + |\phi_2\rangle)$ and a measurement, represented by operator M_1 (defined above) is made. If the outcome of this measurement is -1, what is the (normalised) state of the system after the measurement? **[3]**

(f) The system is prepared in $|\chi\rangle$ again and a new experiment is performed where two measurements are made sequentially, M_1, defined above, and M_2, defined below, (M_1 is made first).

$$M_2 = |\psi_1\rangle \langle\psi_1| + |\psi_2\rangle \langle\psi_2| - |\psi_3\rangle \langle\psi_3| \ ,$$

If we write the measurement outcomes of the two measurements as pairs e.g. $(+1, -1)$, which of the following sequences of measurements will never be observed and why? $(+1, +1)$, $(+1, -1)$, $(-1, +1)$, $(-1, -1)$. Explain why this fact is true for any initial state. **[4]**

4. (a) The interaction picture is often employed to describe the dynamics of a system whose Hamiltonian has the form $H = H_0 + \lambda V$, where H_0 is solved, i.e. its eigenstates $|\phi_j\rangle$ and eigenenergies E_j are known.
Given that the state $|\psi_I(t)\rangle$ in the interaction picture is related to the state $|\psi_S(t)\rangle$ in the standard Schrödinger picture via $|\psi_I(t)\rangle = U_0(t)^\dagger |\psi_S(t)\rangle$, where $U_0(t) = \exp[-i(t/\hbar)H_0]$, show that the $|\psi_I(t)\rangle$ will evolve according to the following equation:

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = U_0(t)^\dagger \lambda V U_0(t)|\psi_I(t)\rangle \ .$$

You may use without proof the operator identity $(\partial/\partial t)\exp[At] = A\exp[At]$. **[5]**

(b) A system subjected to a time-dependent perturbation is described by a Hamiltonian: $H = H_0 + \lambda V(t)$, where H_0 is solved. By describing the state of the system in the interaction picture as, $|\psi_I(t)\rangle = \sum_j c_j(t)|\phi_j\rangle$, show that the coefficients $c_j(t)$ satisfy the following equations of motion,

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

defining all the symbols in this expression. **[4]**

(c) In perturbation theory, we expand $c_j(t)$ as a power series in λ, $c_j(t) = \sum_{m=0}^{\infty}\lambda^m c_j^{(m)}$. Show that 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]**

(d) The states $|\uparrow\rangle$ and $|\downarrow\rangle$ form an orthonormal basis for a spin-half particle. Such a particle is in state $|\uparrow\rangle$ at time $t = 0$. In an experiment, the particle is trapped and exposed to magnetic fields. Initially, the magnetic field has components solely in the z-direction, and the Hamiltonian is $H_0 = \hbar\kappa\sigma_z$. 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 $V = \hbar g(\cos(\omega t)\sigma_x + \sin(\omega t)\sigma_y)$ where $g \ll \kappa$.

i. 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 $|\downarrow\rangle$ is

$$|g|^2\tau^2\mathrm{sinc}^2\frac{(\omega - 2\kappa)\tau}{2}\,,$$

[7]

ii. In the long time limit, how must ω and κ be related, to ensure there is a non-negligible first order transition probability? **[2]**

5. (a) Show that, for any time-independent linear operator A, the following identity holds:

$$\frac{\partial}{\partial t}\exp[At] = A\exp[At]\,.$$

[3]

(b) Show that $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$ is a solution of the time-dependent Schrödinger equation for any time-independent Hamiltonian H, where $U(t) = \exp[-iHt/\hbar]$. **[2]**

(c) We say that two operators A and B anti-commute when $AB + BA = 0$. Show that the Pauli operators σ_x, σ_y and σ_z each pairwise anti-commute (i.e. σ_x anti-commutes with σ_y, σ_x anti-commutes with σ_z, σ_y anti-commutes with σ_z). **[3]**

(d) In an experiment, at time $t = 0$ a spin-half particle is trapped and prepared in state $|\psi(0)\rangle = |{\uparrow}\rangle$. It is exposed to a magnetic field such that its Hamiltonian is $H = \hbar g(\sigma_x + \sigma_y + \sigma_z)$.

i. Obtain the evolution operator $U(t)$ for this Hamiltonian, and hence write down the time-evolved state vector for the particle $|\psi(t)\rangle$. You may use without proof the identity, $\exp[iA\alpha] = \cos(\alpha)\mathbb{1} + i\sin(\alpha)A$, which holds for all self-inverse linear operators A and scalars α. **[5]**

ii. Will the system ever evolve so that its state is orthogonal to the initial state $|{\uparrow}\rangle$? If so, describe the time at which this happens. If not, show why not. **[3]**

(e) A student tries a different approach to solving this Hamiltonian. Inspired by the Suzuki-Trotter approximation, the student utilises the approximate operator $\tilde{U}_1(t) = \exp[-ig\sigma_x t]\exp[-ig\sigma_y t]\exp[-ig\sigma_z t]$.

i. Show that this approximation for $U(t)$ is correct to first order in t only. **[3]**

ii. Use your knowledge of the Suzuki-Trotter approximation to propose an approximate evolution operator $\tilde{U}_2(t)$ correct to second order in t. *Do not* provide explicit calculations to verify the order of this approximation. **[1]**

 END OF PAPER