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.

[Part marks]

1. The time-independent Hamiltonian operator H has a lowest energy eigenvalue E_0. Show that, for any normalizable function ϕ that satisfies the boundary conditions, the expectation value of H satisfies

$$\langle H \rangle_\phi \equiv \frac{\int \phi^* H \phi \, \mathrm{d}\tau}{\int \phi^* \phi \, \mathrm{d}\tau} \geq E_0,$$

where the integration is over the allowed range of coordinates.
Explain how a useful limit on the ground state energy of the system can be obtained from this expression. **[6]**

A particle of mass m interacts through an attractive central potential of the Yukawa type,

$$V(\mathbf{r}) = -V_0 \frac{\mathrm{e}^{-r/a}}{(r/a)}, \qquad \text{with } a \text{ a constant and } V_0 > 0.$$

For states with zero angular momentum use a trial function of the form

$$\phi(\mathbf{r}) = C\mathrm{e}^{-\lambda r/2a},$$

with λ as a dimensionless parameter, to show that

$$\langle H \rangle_\phi = \frac{\hbar^2}{2m}\frac{\lambda^2}{4a^2} - V_0 \frac{\lambda^3}{2(\lambda+1)^2}.$$ **[9]**

Show that the optimum value of the energy is obtained when λ satisfies

$$\frac{2ma^2}{\hbar^2} V_0 = \frac{(\lambda+1)^3}{\lambda(\lambda+3)}.$$ **[2]**

Find the condition on λ and hence that satisfied by V_0 and a for the ground state to be just bound. **[3]**

$\int_0^\infty r^n \mathrm{e}^{-\alpha r} \, \mathrm{d}r = \frac{n!}{\alpha^{n+1}}$, for n a positive integer and $\alpha > 0$.

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}.$$

2. The Cartesian components of the orbital and spin angular momentum operators, $\mathbf{L}$ and $\mathbf{S}$ respectively, satisfy the commutation relations

$$[L_x, L_y] = i\hbar L_z; \qquad [S_x, S_y] = i\hbar S_z; \qquad \left[\mathbf{L}^2, L_x\right] = 0; \qquad \text{and} \qquad \left[\mathbf{S}^2, S_y\right] = 0,$$

with cyclic permutation of the indices x, y, z. The orbital angular momentum and spin of a particle couple to give a total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Show that the operator $\mathbf{L} \cdot \mathbf{S}$ does **not** commute with L_z or S_z but **does** commute with J_z, $\mathbf{L}^2$, $\mathbf{S}^2$ and $\mathbf{J}^2$.

Show that $\mathbf{L} \cdot \mathbf{S}$ can be expressed as

$$\mathbf{L} \cdot \mathbf{S} = \tfrac{1}{2}\left(L_+ S_- + L_- S_+\right) + L_z S_z,$$

where L_+, S_+ and L_-, S_- are the raising and lowering operators for orbital (L) and spin (S) angular momenta respectively. **[5]**

For a particle of spin $\frac{1}{2}$ the eigenstates of $(\mathbf{L}^2, L_z)$ and $(\mathbf{S}^2, S_z)$ denoted by $|\ell, m\rangle$ and $|\frac{1}{2}, \pm\frac{1}{2}\rangle$, respectively, satisfy

$$\mathbf{L}^2|\ell, m\rangle = \ell\,(\ell+1)\,\hbar^2|\ell, m\rangle; \qquad L_z|\ell, m\rangle = m\hbar|\ell, m\rangle,$$

$$\mathbf{S}^2|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle = \tfrac{3}{4}\hbar^2|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle; \qquad S_z|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle = \pm\tfrac{1}{2}\hbar|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle.$$

From these states may be formed two orthonormal basis states

$$|\phi_1\rangle = |\ell, m - \tfrac{1}{2}\rangle|\tfrac{1}{2}, \tfrac{1}{2}\rangle \qquad \text{and} \qquad |\phi_2\rangle = |\ell, m + \tfrac{1}{2}\rangle|\tfrac{1}{2}, -\tfrac{1}{2}\rangle$$

which are eigenstates of J_z with eigenvalue $m\hbar$. Show that

$$\begin{aligned}
(\mathbf{L} \cdot \mathbf{S})\,|\phi_1\rangle &= \frac{\hbar^2}{2}\left(m - \tfrac{1}{2}\right)|\phi_1\rangle + \frac{\hbar^2}{2}\left[\left(\ell + \tfrac{1}{2}\right)^2 - m^2\right]^{1/2}|\phi_2\rangle, \\
(\mathbf{L} \cdot \mathbf{S})\,|\phi_2\rangle &= \frac{\hbar^2}{2}\left[\left(\ell + \tfrac{1}{2}\right)^2 - m^2\right]^{1/2}|\phi_1\rangle - \frac{\hbar^2}{2}\left(m + \tfrac{1}{2}\right)|\phi_2\rangle.
\end{aligned}$$

[6]

Hence show that with $|\phi_1\rangle$ and $|\phi_2\rangle$ as a basis the matrix representation of $\mathbf{L} \cdot \mathbf{S}$ is

$$\mathbf{L} \cdot \mathbf{S} = \frac{\hbar^2}{2}\begin{pmatrix} \left(m - \frac{1}{2}\right) & \left[\left(\ell + \frac{1}{2}\right)^2 - m^2\right]^{1/2} \\ \left[\left(\ell + \frac{1}{2}\right)^2 - m^2\right]^{1/2} & -\left(m + \frac{1}{2}\right) \end{pmatrix},$$

and that the eigenvalues of $\mathbf{L} \cdot \mathbf{S}$ are $\frac{1}{2}\ell\hbar^2$ and $-\frac{1}{2}(\ell+1)\,\hbar^2$. **[6]**

By considering $|\psi\rangle$ as a linear combination of $|\phi_1\rangle$ and $|\phi_2\rangle$ determine the corresponding total angular momentum quantum numbers j from $\mathbf{J}^2|\psi\rangle = j\,(j+1)\,\hbar^2|\psi\rangle$.

[3]

Note: $[AB, C] = A\,[B, C] + [A, C]\,B$.

The angular momentum raising and lowering operators $L_\pm = L_x \pm iL_y$ acting on a state $|\ell, m\rangle$ give $L_\pm|\ell, m\rangle = \left[\ell\,(\ell+1) - m\,(m \pm 1)\right]^{1/2}\hbar|\ell, m \pm 1\rangle$ and $S_+|\frac{1}{2}, -\frac{1}{2}\rangle = \hbar|\frac{1}{2}, \frac{1}{2}\rangle$, $S_-|\frac{1}{2}, \frac{1}{2}\rangle = \hbar|\frac{1}{2}, -\frac{1}{2}\rangle$.

3. A system at time t_0 is in a discrete eigenstate $|i\rangle$ with energy E_i of a time-independent Hamiltonian H_0. It is subjected to a weak, time-dependent perturbation $\lambda H'(t)$. Assume that the general solution of the time-dependent Schrödinger equation can be written in the form

$$\psi(\mathbf{r},t) = \sum_n c_n(t)\,\phi_n(\mathbf{r})\,\mathrm{e}^{-iE_n t/\hbar},$$

where ϕ_n are eigenfunctions of H_0 with eigenvalues E_n. Show that the probability, $P_k(t)$, that at a later time t the system will have made a transition to a state $|k\rangle$ $(k \neq i)$ of H_0 with energy E_k is given, to lowest order in λ, by

$$P_k(t) = |c_k(t)|^2$$

where

$$c_k(t) = \frac{1}{i\hbar}\int_{t_0}^{t} \langle k|\lambda H'(t')|i\rangle \mathrm{e}^{i\omega_{ki}t'}\mathrm{d}t'$$

with $\omega_{ki} = (E_k - E_i)/\hbar$. **[9]**

A particle of mass m is bound in a one-dimensional infinite potential well

$$V(x) = \begin{cases} 0 & |x| \leq a, \\ \infty & |x| > a. \end{cases}$$

The orthonormal eigenfunctions $\psi_n(x)$ satisfying $H_0\psi_n = E_n\psi_n$ where H_0 is the Hamiltonian for the system are the even and odd functions

$$\begin{aligned} \psi_n(x) &= \tfrac{1}{\sqrt{a}}\cos\left(\tfrac{n\pi x}{2a}\right) \qquad n = 1,3,5,\ldots, \\ \psi_n(x) &= \tfrac{1}{\sqrt{a}}\sin\left(\tfrac{n\pi x}{2a}\right) \qquad n = 2,4,6,\ldots, \end{aligned}$$

respectively, with corresponding energy eigenvalues $E_n = \dfrac{n^2\pi^2\hbar^2}{8ma^2}$. At large negative times the particle is in its ground state. It is acted upon by a time-dependent perturbation

$$H'(t) = A\sin\left(\frac{3\pi x}{2a}\right)\mathrm{e}^{-\gamma|t|}, \qquad \gamma > 0.$$

To which states can the particle be excited to lowest order in A? **[4]**

Calculate the probabilities that as $t \to \infty$ the particle has been excited to each of these states. **[7]**

NOTE: $2\sin A\cos B = \sin(A+B) + \sin(A-B)$
and $2\sin A\sin B = \cos(A-B) - \cos(A+B)$

4. Show that under a unitary transformation U of the states $|a\rangle$ and $|b\rangle$ (a) their scalar product is invariant, (b) the eigenvalues of an operator A are preserved if it transforms as $UAU^\dagger$.

Explain, making reference to state vectors and operators, what is meant by the Schrödinger picture in quantum mechanics. How are the state vectors and operators in the Heisenberg picture related to their counterparts in the Schrödinger picture? **[6]**

The state vector $|\psi_S(t)\rangle$ of a physical system in the Schrödinger picture with a Hamiltonian H_0 evolves according to

$$|\psi_S(t)\rangle = U_0(t,t_0)\,|\psi_S(t_0)\rangle, \qquad U_0(t_0,t_0) = 1,$$

where $U_0(t,t_0)$ is the unitary evolution operator and t_0 is an arbitrary reference time. Show that the evolution operator satisfies the differential equation

$$i\hbar\frac{\partial U(t,t_0)}{\partial t} = H_0 U(t,t_0).$$

If H_0 is time-independent, show that a formal solution of the Schrödinger equation is

$$|\psi_S(t)\rangle = \mathrm{e}^{-iH_0(t-t_0)/\hbar}|\psi_S(t_0)\rangle.$$

[4]

The system is acted on by a perturbation $V(t)$ so that the Hamiltonian becomes

$$H(t) = H_0 + \lambda V(t),$$

where λ is a dimensionless parameter. The state vector $|\psi_I(t)\rangle$ in the 'interaction picture' is defined by

$$|\psi_I(t)\rangle = U_0^\dagger(t,t_0)\,|\psi_S(t)\rangle,$$

where $|\psi_S(t)\rangle$ obeys

$$i\hbar\frac{\partial|\psi_S(t)\rangle}{\partial t} = [H_0 + \lambda V(t)]\,|\psi_S(t)\rangle.$$

Show that the equation of motion for the state vector $|\psi_I(t)\rangle$ is

$$i\hbar\frac{\partial|\psi_I(t)\rangle}{\partial t} = \lambda V_I(t)\,|\psi_I(t)\rangle,$$

where $V_I(t) = U_0^\dagger(t,t_0)\,V(t)\,U_0(t,t_0)$.

Hence show that $|\psi_I(t)\rangle$ is given by the recursive integral equation

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t}\lambda V_I(t')\,|\psi_I(t')\rangle \mathrm{d}t'.$$

[6]

If the system is initially at time $t_0 = 0$ in an eigenstate $|s\rangle$ of H_0 with energy E_s show that, to first order in λ,

$$|\psi_I(t)\rangle = |s\rangle - \frac{i\lambda}{\hbar}\sum_n\int_0^t \mathrm{e}^{i(E_n-E_s)t'/\hbar}|n\rangle\langle n|V(t')\,|s\rangle \mathrm{d}t'.$$

[4]

5. The wave function

$$\psi(\mathbf{r}) = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\,\frac{\mathrm{e}^{ikr}}{r},$$

is an asymptotic form of a solution of the Schrödinger equation describing the elastic scattering of a beam of spinless particles of mass m, momentum $\hbar\mathbf{k}$, by a central potential of finite range a. What do the two terms on the right-hand side of this expression represent? Identify the scattering amplitude and state, mathematically, its relationship to the differential cross section $\mathrm{d}\sigma/\mathrm{d}\Omega$.
For elastic scattering, the partial wave expansion for $f(\theta)$ is

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\,\mathrm{e}^{i\delta_\ell(k)}\sin\delta_\ell(k)\,P_\ell(\cos\theta)$$

where P_ℓ is a Legendre polynomial and δ_ℓ is the ℓ-th partial wave phase shift. Show that the total cross section, σ, is given by

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell(k).$$

For what values of the incident momentum is s-wave scattering dominant? Give briefly a semi-classical argument to support this value. **[6]**

The reduced radial wave function $u_0(r)$ describing the scattering of a beam of spinless particles of mass m, energy E from a **repulsive** square-well potential

$$V(r) = \begin{cases} V_0 & 0 \le r \le a; \qquad V_0 > 0, \\ 0 & r > a, \end{cases}$$

obeys the differential equation

$$\frac{\mathrm{d}^2 u_0(r)}{\mathrm{d}r^2} + \frac{2m}{\hbar^2}(E - V_0)\,u_0(r) = 0.$$

Show that the s-wave phase shift δ_0 satisfies, for $E > V_0$, (case A)

$$Q\cot Qa = k\cot(ka + \delta_0),$$

and for (case B), $E < V_0$,

$$K\coth Ka = k\cot(ka + \delta_0),$$

where $Q^2 = k^2 - K_0^2$, $K^2 = -Q^2$, $k^2 = 2mE/\hbar^2$ and $K_0^2 = 2mV_0/\hbar^2$. **[5]**

In case B, if $V_0 \to \infty$ (the impenetrable sphere) show that

$$\delta_0(k) = -ka.$$

State the effective range expansion for low-energy scattering. Show that for scattering from the impenetrable sphere the scattering length $A_0 = a$, the effective range $r_0 = 2a/3$ and the total cross section $\sigma = 4\pi a^2$. **[5]**

In case A, $(E > V_0)$, show that the ratio, D, of the amplitude of the wave function inside the potential to that outside is given by

$$D^2 = \frac{1}{1 - \frac{K_0^2}{k^2}\cos^2 Qa}.$$

This ratio has minima at $Qa = \left(n + \frac{1}{2}\right)\pi$ and maxima in the neighbourhood of $Qa = n\pi$ (close to the singularities of the logarithmic derivative of the radial wave function at $r = a$). Give a qualitative explanation for these maxima.
For $K_0 a = 4$ the first maximum occurs for $ka \simeq 5.2$. Discuss briefly whether this enhancement would or would not give rise to a significant feature in an experimental measurement of the total cross section. **[4]**

Note: $\int_{-1}^{1} P_\ell(\cos\theta)\, P_{\ell'}(\cos\theta)\, \mathrm{d}(\cos\theta) = \frac{2}{2\ell+1}\delta_{\ell\ell'}$;
$\sin ix = i\sinh x$; $\cos ix = \cosh x$
$\cot x \simeq \frac{1}{x} - \frac{x}{3}$ for small x.

END OF PAPER