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.

1. (a) Let A be an operator on a finite dimensional vector space. Its Hermitian conjugate A^{\dagger} satisfies the following condition

$$\langle \phi | A^{\dagger} | \psi \rangle^* = \langle \psi | A | \phi \rangle$$

for all vectors $|\phi\rangle$, $|\psi\rangle$ in the space. Use this to show that if matrix M_A is a matrix representation of A, the equivalent matrix representation of A^{\dagger} will be the complex conjugate transpose of M_A .

[2]

(b) The Pauli matrices,

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

are both Hermitian and unitary. Prove that any operator which is both Hermitian and unitary is self-inverse.

[2]

(c) Consider the matrix $B = a\mathbb{1} + b\sigma_x$, where a and b are real numbers and $\mathbb{1}$ is the 2×2 identity matrix. What conditions must a and b satisfy such that B is i) Hermitian ii) unitary iii) Hermitian and unitary.

[6]

(d) Given that $\sigma_x \sigma_z = -\sigma_z \sigma_x$, show that $(\sigma_x + \sigma_z)/\sqrt{2}$ is self-inverse and hence that

$$e^{i\alpha(\sigma_x + \sigma_z)/\sqrt{2}} = \cos(\alpha)\mathbb{1} + i\sin(\alpha)\left(\frac{\sigma_x + \sigma_z}{\sqrt{2}}\right).$$

Recall
$$e^x = \sum_{j=0}^{\infty} x^j/(j!)$$
, $\sin(x) = \sum_{j=0}^{\infty} (-1)^j (x)^{2j+1}/((2j+1)!)$ and $\cos(x) = \sum_{j=0}^{\infty} (-1)^j (x)^{2j}/((2j)!)$.

(e) For a d-dimensional vector space, let $|\alpha_j\rangle$ and $|\beta_j\rangle$ for $j=1,2,3,\ldots n$ be two distinct orthonormal bases. Let U be the operator which transforms $|\alpha_j\rangle$ to $|\beta_j\rangle$, i.e.

$$|\beta_j\rangle = U |\alpha_j\rangle$$

Show that the matrix elements of U with respect to basis $|\alpha_j\rangle$ are given by $U_{j,k} = \langle \alpha_j | \beta_k \rangle$ and hence that U is unitary. [6]

- 2. (a) Describe two applications of the WKB approximation and describe 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

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

With reference to the equivalent wave-function obtained in the special case where $V(x) = V_0$ is constant, explain why one might expect the terms in the wavefunction to be proportional to i) $\exp\left[\pm i\int p(x')dx'/\hbar\right]$ and ii) $1/\sqrt{p(x)}$.

- [3]
- (c) Explain why wave-functions of this form cannot be good approximations to physical states at classical turning points.
- [2]

[6]

(d) 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 position of classical turning points and n = 0, 1, 2, ... is a non-negative integer.

You may use the WKB connection formulae:

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

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

and the trigonometric identity: $\sin(A+B) = \sin(A)\cos(B) + \cos(A)\sin(B)$.

- (e) Consider a quantum well described by the potential $V(x) = \kappa x^2$ for |x| < a and $V(x) = \kappa a^2$ for $|x| \ge a$. Given $a^2 \sqrt{\kappa m}/\hbar = 4$, show that the well has 3 bound states, and calculate the ratios between their energies and κa^2 .
 - You may use the standard integral $\int_{-1}^{+1} (1 y^2)^{1/2} dy = \frac{\pi}{2}$. [6]

(a) Explain the meaning of the terms CSCO and tensor product, and their role in the addition of angular momentum in quantum mechanics.

[5]

[2]

[4]

(b) The angular momentum-like operator $\hat{L} = \hat{L}_x \vec{i} + \hat{L}_y \vec{j} + \hat{L}_z \vec{k}$ satisfies standard angular momentum-like commutation relations, $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$, and cyclic permutations thereof.

- The state $|l, m_l\rangle$ is the eigenstate of \hat{L}^2 and \hat{L}_z corresponding to quantum numbers l and m_l . Write down the eigenvalues of \hat{L}^2 and \hat{L}_z for $|l, m_l\rangle$. What is the allowed range of values that the quantum numbers l and m_l may take?
- (c) The operator $\hat{L}_{-} = \hat{L}_{x} i\hat{L}_{y}$ is known as a "lowering operator" due to its action on $|l, m_l\rangle$,

 $\hat{L}_{-}|l,m_l\rangle = c_{lm_l}|l,m_l-1\rangle$

where c_{l,m_l} is a constant. By using the identity $\hat{L}_-^{\dagger}\hat{L}_- = \hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z$ show that $|c_{l,m_l}|^2 = \hbar^2 (l(l+1) - m_l(m_l-1)).$

(d) An important application of the addition of angular momentum is spin-orbit coupling. Let $\hat{L} = \hat{L}_x \vec{i} + \hat{L}_y \vec{j} + \hat{L}_z \vec{k}$ and $\hat{S} = \hat{S}_x \vec{i} + \hat{S}_y \vec{j} + \hat{S}_z \vec{k}$ be, respectively, the orbital angular momentum and spin operators for an electron. Let $\hat{J} = \hat{L} \otimes \mathbb{1} + \mathbb{1} \otimes \hat{S}$ represent the sum of these quantities.

The operators \hat{J}^2 , \hat{J}_z , \hat{L}^2 and \hat{S}^2 form a CSCO. The joint eigenstates of this CSCO can be expressed in terms of the eigenstates of the CSCO \hat{L}^2 , \hat{L}_z , \hat{S}^2 and \hat{S}_z , $|l, m_l\rangle \otimes |s, m_s\rangle$. For example,

$$\left| j = \frac{3}{2}, m_j = \frac{3}{2}, l = 1, s = \frac{1}{2} \right\rangle = \left| l = 1, m_l = 1 \right\rangle \otimes \left| s = \frac{1}{2}, m_s = \frac{1}{2} \right\rangle$$

and

$$\begin{aligned} \left| j = \frac{1}{2}, m_j = \frac{1}{2}, l = 1, s = \frac{1}{2} \right\rangle \\ &= \sqrt{\frac{2}{3}} \left| l = 1, m_l = 1 \right\rangle \otimes \left| s = \frac{1}{2}, m_s = -\frac{1}{2} \right\rangle - \sqrt{\frac{1}{3}} \left| l = 1, m_l = 0 \right\rangle \otimes \left| s = \frac{1}{2}, m_s = \frac{1}{2} \right\rangle \end{aligned}$$

Derive a normalised expression for the state $\left|j=\frac{3}{2},m_j=\frac{1}{2},l=1,s=\frac{1}{2}\right\rangle$ expressed in the $|l, m_l\rangle \otimes |s, m_s\rangle$ basis. [4]

- (e) What is the expectation value of the operator $\hat{L}_z \otimes \hat{S}_z$ for $|j = \frac{1}{2}, m_j = \frac{1}{2}, l = 1, s = \frac{1}{2}\rangle$? [2]
- (f) Explain how one would calculate the Clebsch-Gordon coefficients for the remaining joint eigenstates of \hat{J}^2 , \hat{J}_z , \hat{L}^2 and \hat{S}^2 for $l=1, s=\frac{1}{2}$. [3]

4. (a) Consider a Hamiltonian of the form $\hat{H} = \hat{H}_0 + \lambda \hat{V}(t)$, where \hat{H}_0 is a time-independent operator with eigenstates $|\phi_k\rangle$ and corresponding eigenvalues E_k . In Dirac's method of variation of constants, we write a general state evolving in time in the form $|\psi(t)\rangle = \sum_k c_k(t) \exp[(-iE_k t)/\hbar] |\phi_k\rangle$.

Show that substituting this ansatz into the time-dependent Schrödinger equation leads to the following set of coupled differential equations:

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

where $\omega_{mk} = (E_m - E_k)/\hbar$ and $V_{mk} = \langle \phi_m | \hat{V} | \phi_k \rangle$.

(b) By writing $c_k(t)$ as a power series $c_k(t) = \sum_j \lambda^j c_m^{(j)}(t)$ derive the following expressions for the 0th and 1st order terms in the series,

$$\dot{c}_m^{(0)}(t) = 0 \qquad \dot{c}_m^{(1)}(t) = \frac{1}{i\hbar} \sum_k \exp\left[iw_{mk}t\right] V_{mk}(t) c_k^{(0)}(t).$$

(c) A spin-1 particle is held in a strong magnetic field in the z-direction. Immediately prior to time $t = -t_0$, a measurement of its spin indicates that it is in the state $|s = 1, m_s = 1\rangle$. At $t = -t_0$ the experiment is perturbed by a weak magnetic field in the x-direction which ramps up to a maximum and then decays back down to zero at time $t = t_0$.

The resulting Hamiltonian is $H = \Omega \hat{S}_z + \lambda(t) \hat{S}_x$ where $\lambda(t) = \lambda_0 (1 - |t|/t_0)$ for $|t| < t_0$ and $\lambda(t) = 0$ for $|t| \ge t_0$ and $|\lambda_0| \ll \Omega$. Using perturbation theory, show that (to first-order) the probability that a measurement on the spin at time $t = t_0$ will indicate $m_s = 0$ is:

$$P_{1\to 0}^{(1)} = 2 \left| \frac{\lambda_0}{\Omega^2 t_0} \right|^2 (1 - \cos(\Omega t_0))^2.$$

You may find the following spin-1 matrix representations of \hat{S}_z and \hat{S}_x :

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

and the following indefinite integral helpful:

$$\int e^{iat}(1-bt)dt = \frac{-e^{iat}}{a^2}(b+ia(1-bt)) + c.$$

(d) Without detailed calculation, explain why, in this example, second order perturbation theory is required to see a non-zero transition probability to the state $|s=1, m_s=-1\rangle$.

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[8]

[6]

[4]

5. (a) Describe the significance of the scattering cross-section in a scattering experiment, and explain why it has the units of area.

[4]

(b) Under what conditions can the state of a beam of particles be well-approximated by a single particle wave-function $\psi(\vec{r})$?

[2]

(c) For the scattering of a spinless particle from a finite scattering region, it can be shown that the following wavefunction is a solution of the time-independent Schrödinger equation in the limit $r \to \infty$.

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

where $k = |\vec{k}|$ and where the energy $E = \hbar^2 k^2/2m$. Explain the physical significance of the terms in this expression.

[3]

(d) In this regime, the differential cross-section is related to the $f(k,\theta,\phi)$ via $\partial \sigma/\partial \Omega = |f(k,\theta,\phi)|^2$. In a scattering experiment a beam of helium atoms is incident upon a stationary target. The differential cross-section is observed to have the following angular dependence.

$$\frac{\partial \sigma}{\partial \Omega} = A + B\cos(\theta) + C\cos^2(\theta) + D\cos^3(\theta) + E\cos^4(\theta)$$

Which partial waves have contributed to this scattering process? The first four Legendre polynomials are as follows:

[4]

$$P_0(x) = 1$$
 $P_1(x) = x$ $P_2(x) = \frac{1}{2}(3x^2 - 1)$ $P_3(x) = \frac{1}{2}(5x^3 - 3x).$

(e) The energy of this beam is reduced, and new measurements of the differential cross-section show that it no longer has any angular dependence. Which partial wave now dominates the scattering process?

The incident energy of each particle is now 3.32×10^{-27} J. If the total measured cross-section is 10^{-15} m² what is the phase-shift associated with the dominant partial wave?

[7]

The mass of a helium atom is 6.65×10^{-27} kg, and \hbar is 1.05×10^{-34} J s. You may use the relationship $f_l(k) = \frac{2l+1}{2ik} \left(e^{2i\delta_l(k)} - 1\right)$.

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END OF PAPER