PH 204: Quantum Mechanics II

1. Generators of $SO(3)$ and $SU(2)$:

   (i) $SO(3)$ is the group consisting of 3×3 real orthogonal matrices with determinant equal to 1. Consider an element of this group called M which lies near the identity, i.e., $M = I + iA$, where I is the identity matrix and all the matrix elements of A are small and imaginary (since M is real). Using the condition of orthogonality, show that, to first order, A must be antisymmetric. Hence show that it must be of the form $A = \epsilon_x T_x + \epsilon_y T_y + \epsilon_z T_z$, where the ϵ_j's are real parameters and T_j's are the matrices discussed in the class. Thus these matrices are the generators of $SO(3)$. (To obtain the usual Lie algebra of the rotation group, we have to take $\hbar$ times these matrices).

   (ii) $SU(2)$ is the group consisting of 2×2 unitary matrices with determinant equal to 1. Consider an element of this group called M which lies near the identity, i.e., $M = I + iA$, where I is the identity matrix and all the matrix elements of A are small. Using the conditions of unitarity and the determinant $= 1$, show that, to first order, A must be Hermitian and its trace must be zero. Hence show that it must be of the form $A = \epsilon_x \sigma^x + \epsilon_y \sigma^y + \epsilon_z \sigma^z$, where the ϵ_j's are real parameters and σ_j's are the Pauli matrices. Thus the generators of $SU(2)$ are the Pauli matrices. (To obtain the usual Lie algebra of the rotation group, we have to take $\hbar/2$ times these matrices).

2. Dirac equation in two dimensions:

   Consider the Hamiltonian for a spin-1/2 particle moving in two dimensions

$$H \;=\; -i\hbar c \,(\sigma^x \frac{\partial}{\partial x} \;+\; \sigma^y \frac{\partial}{\partial y}) \;+\; mc^2 \sigma^z,$$

   where m is the mass of the particle and c is the speed of light.

   (i) Given the Dirac equation $i\hbar \partial\psi/\partial t = H\psi$, where ψ is a two-component wave function, find the relation between the energy E and the momentum $\vec{p} = (p_x, p_y)$, assuming that $\psi \;=\; \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} e^{(i/\hbar)(p_x x + p_y y - Et)}$ is a solution of the Dirac equation.

   (ii) Now introduce a vector potential $\vec{A} = (A_x, A_y)$. If the charge of the particle is q, the Hamiltonian is given by

$$H \;=\; c\,[\sigma^x \,(-i\hbar \frac{\partial}{\partial x} \;-\; \frac{q}{c} A_x) \;+\; \sigma^y \,(-i\hbar \frac{\partial}{\partial y} \;-\; \frac{q}{c} A_y)] \;+\; mc^2 \sigma^z.$$

   If there is a magnetic field $\vec{B} = B\hat{z}$, show that

$$H^2 \;=\; m^2 c^4 \;+\; c^2 [(-i\hbar \frac{\partial}{\partial x} \;-\; \frac{q}{c} A_x)^2 \;+\; (-i\hbar \frac{\partial}{\partial y} \;-\; \frac{q}{c} A_y)^2] \;-\; 2qcB\; S^z,$$

where $S^z = (\hbar/2)\sigma^z$ is the component of the spin along the $\hat{z}$ axis. Taking the positive square root of H^2 and expanding in powers of $1/mc^2$ gives $mc^2 + H_{NR}$, where the non-relativistic Hamiltonian is given by

$$H_{NR} = \frac{1}{2m}\,[(-i\hbar\frac{\partial}{\partial x} - \frac{q}{c}A_x)^2 + (-i\hbar\frac{\partial}{\partial y} - \frac{q}{c}A_y)^2] - \frac{qB}{mc}\,S^z$$

plus higher order terms. This implies that the gyromagnetic ratio of the particle is given by $g = 2$.

(iii) For the same magnetic field, choose the vector potential to be $A_x = 0$ and $A_y = Bx$. Assuming that $\psi = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix} e^{(i/\hbar)(p_y y - Et)}$ is a solution of the Dirac equation, find the energy spectrum (take $qB > 0$).

Show that when $mc^2 \gg \sqrt{2\hbar qcB}$, we find that the positive energies are given by $E = mc^2 +$ the Landau spectrum that we got in QM I for a spin-1/2 particle with $g = 2$, while if $m = 0$, we obtain a completely different dependence of the energy spectrum on the magnetic field (this is relevant for graphene, with c replaced by the velocity v in graphene).

Hint: Note that the off-diagonal elements of the Hamiltonian, H_{12} and H_{21}, have the same commutation relation as $\sqrt{2\hbar qcB}$ times $a^\dagger$ and a respectively, where a and $a^\dagger$ are the lowering and raising operators of a simple harmonic oscillator. Taking $\psi_1 = \alpha\psi_n(x)$ and $\psi_2 = \beta\psi_{n-1}(x)$, where $\psi_n(x)$ is the n-th wave function of the harmonic oscillator, $n = 0, 1, 2, \cdots$, and α, β are some constants to be determined, the energies can be found as the eigenvalues of a 2×2 matrix.

3. Use the Bohr-Sommerfeld quantisation condition to find the energy levels of a particle moving in one dimension in a potential of the form $V(x) = \lambda\ |x/L|^\alpha$, where L has the dimensions of length, and λ and α are positive.

   (i) Show that E_n is given by $(n + 1/2)^\beta$ multiplied by some powers of $\hbar$, m, λ and L (which you have to calculate), and a dimensionless constant which contains the value of the integral $\int_0^1 dy\sqrt{1 - y^\alpha}$ (which you don't have to calculate). Find the value of β.

   (ii) Now consider the limit $\alpha \to \infty$. Then you can calculate the integral mentioned in (i) and find an explicit expression for E_n. For $n \gg 1$, show that this becomes identical to the energy levels of a particle in a box of a certain length. Can you argue why this should happen by looking at $V(x)$ in the limit $\alpha \to \infty$?

   Hint: What is the value of y^α in the limit $\alpha \to \infty$ if (i) $y < 1$ and (ii) $y > 1$?

4. Use the Bohr-Sommerfeld quantisation condition to find the energy levels of a particle moving in one dimension in a potential given by (i) $V(x) = \lambda\ |x|$, and (ii) $V(x) = \lambda x^4$, where $\lambda > 0$ in both cases. In the second case, use the fact that $\int_0^1 dx\sqrt{1 - x^4} \simeq 0.874$.

5. (i) Use the Bohr-Sommerfeld quantisation condition to find the energy levels of a particle

moving in one dimension in a potential given by

$$\begin{aligned} V(x) &= \frac{1}{2}\, m\omega_+^2 x^2 \quad \text{for} \quad x \geq 0, \\ &= \frac{1}{2}\, m\omega_-^2 x^2 \quad \text{for} \quad x \leq 0. \end{aligned}$$

(ii) What do you get for the cases (a) $\omega_+ = \omega_-$ and (b) ω_+ is finite but $\omega_- \to \infty$?

(iii) Is there another way to understand the result you got for the case $\omega_- \to \infty$?

6. WKB connection formulae when the potential is infinitely large on one side of a point:

   When $V(x) = \infty$ for $x < x_0$ and is finite for $x > x_0$, the connection formula turns out to be $\psi = 0$ for $x < x_0$ and

   $$\psi = \frac{1}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x_0}^{x} dx\ p(x)\right) = \frac{1}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_{x_0}^{x} dx\ p(x) - \frac{\pi}{2}\right),$$

   for $x > x_0$, where we assume that $p(x) = \sqrt{2m(E - V(x))}$ is real for $x > x_0$.

   When $V(x)$ is finite for $x < x_0$ and $= \infty$ for $x > x_0$, the connection formula is found to be

   $$\psi = \frac{1}{\sqrt{p(x)}} \sin\left(\frac{1}{\hbar}\int_{x}^{x_0} dx\ p(x)\right) = \frac{1}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int_{x}^{x_0} dx\ p(x) - \frac{\pi}{2}\right),$$

   for $x < x_0$ and $\psi = 0$ for $x > x_0$, where we assume that $p(x) = \sqrt{2m(E - V(x))}$ is real for $x < x_0$.

   Use the above connection formulae to find the WKB expressions for the energy levels of (i) a particle in a potential $V(x) = \infty$ for $x < 0$ and $(1/2)m\omega^2x^2$ for $x > 0$, and (ii) a particle in a box, $V(x) = 0$ for $0 < x < L$ and ∞ otherwise.

7. For a particle moving in one dimension in a confining potential $V(x)$ (where $V(-x) = V(x)$), the Bohr-Sommerfeld quantisation condition says that the energies E_n are given by $\int_{-x_n}^{x_n} dx\ \sqrt{2m\ (E_n\ -\ V(x))}\ =\ (n + 1/2)\pi\hbar$, where $n = 0, 1, 2, \cdots$, and $-x_n,\ x_n$ are the classical turning points where $V(-x_n) = V(x_n) = E_n$.

   (i) Use the above quantisation condition and a symmetry argument to find the energy levels of a particle in a potential which is ∞ for $x < 0$ and is $V(x)$ for $x > 0$.

   (ii) Use the result in part (i) to find the energy levels of a particle in a potential which is ∞ for $x < 0$ and is $(1/2)m\omega^2x^2$ for $x > 0$. Does this agree with the exact answer?

   (iii) Use the result in (i) to calculate the ground state energy of a neutron near the earth's surface. Denoting the vertical coordinate by x, the neutron sees a potential which is ∞ for $x < 0$ (where $x = 0$ denotes the surface of the earth) and is equal to mgx for $x > 0$, where the neutron mass $m \simeq 1.67 \times 10^{-27}$ Kg and $g \simeq 9.8$ m/sec^2. Express your answer in units of eV, where 1 eV $\simeq 1.60 \times 10^{-19}$ Joules. Also, $\hbar \simeq 1.05 \times 10^{-34}$ Joules-sec.

8. Consider a particle of mass m confined to a one-dimensional box given by $0 \leq x \leq L$. Let's pretend that we do not know the exact ground state wave function $\psi_0(x)$, but we know that ψ_0 must be zero at $x = 0$ and L. So let's try a simple wave function $\phi(x) = x(L-x)$ to estimate the ground state energy. (Note that this wave function does not have a parameter that can be varied). Normalise the wave function ϕ and then calculate $E = \langle\phi|H|\phi\rangle$, where $H = p^2/2m$. How well does this agree with the exact ground state energy E_0, i.e., what is the percentage error?

9. Use a variational wave function of the form

$$\psi(\vec{r}) \sim \exp(-\frac{\beta\vec{r}^2}{2}) ,$$

where β is a variational parameter, to estimate the ground state energy of the hydrogen atom. How does your answer compare with the exact result $E_0 = -me^4/2\hbar^2$, i.e., what is the percentage error?

10. Consider a particle moving on the circumference of a circle of length L so that its coordinate x lies in the range $[0, L]$ and the wave functions are periodic functions of x with period L. In the presence of a cosine potential, the Hamiltonian is given by

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} - \lambda\cos\left(\frac{2\pi x}{L}\right).$$

We will use the variational method to estimate the ground state energy of this system. Let's try a wave function of the form

$$\psi(x) = 1 + \alpha\cos\left(\frac{2\pi x}{L}\right),$$

where α is the variational parameter (assume that α is real).

(i) Calculate the variational energy

$$E(\alpha) = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}.$$

(ii) Minimise $E(\alpha)$ with respect to α to obtain an estimate for the ground state energy as a function of λ.

(iii) Now let's forget about the variational calculation. Use any method you like to estimate the ground state energy as accurately as you can in the limit $\lambda \to \infty$.

11. (i) Use the Thomas-Fermi method to find an expression for the ground state energy of N spin-1/2 noninteracting electrons placed in a simple harmonic potential in one dimension $V(x) = (1/2)m\omega^2x^2$. [Use the values of the following integrals: $\int_0^1 dy\ (1-y^2)^{1/2} = \pi/4$, $\int_0^1 dy\ (1-y^2)^{3/2} = 3\pi/16$, and $\int_0^1 dy\ y^2(1-y^2)^{1/2} = \pi/16$].

(ii) Calculate the exact ground state energy assuming that N is an even integer (so that all the occupied states are completely filled). How well do the Thomas-Fermi and exact results agree with each other?

12. Use the Thomas-Fermi method to find an expression for the ground state energy of N spin-1/2 noninteracting electrons placed in a simple harmonic potential in three dimensions $V(\vec{r}) = (1/2)m\omega^2\vec{r}^2$.

    How well does the Thomas-Fermi result agree with the exact result for $N = 112$? (The ground state of this system is non-degenerate since a certain number of shells are completely filled).

13. (i) Use the Thomas-Fermi method to find an expression for the ground state energy of N spin-1/2 noninteracting electrons placed in a simple harmonic potential in two dimensions $V(x, y) = (1/2)m\omega^2(x^2 + y^2)$.

    (ii) Calculate the exact ground state energy for $N = 20$. How well do the Thomas-Fermi and exact results agree with each other?

14. Suppose that an electron is placed in a three-dimensional simple harmonic potential $V(\vec{r}) = (1/2)\ m\omega^2\ \vec{r}^2$.

    (i) What are the energies of the four lowest lying states?

    (ii) What are the values of the orbital angular momentum in these four states?

    (iii) The spin-orbit coupling is given by $(1/2m^2c^2)\ \vec{\nabla}V \times \vec{p} \cdot \vec{S}$ for any potential V. For a central potential, $\vec{\nabla}V$ points along $\vec{r}$, hence $\vec{\nabla}V \times \vec{p}$ is proportional to $\vec{L}$. Use the result in (ii) to compute the change in the energies of the four states due to spin-orbit coupling. Note that these can be found exactly in this problem, you don't have to use perturbation theory.

    (iii) Now let us put N electrons in the above potential. What is the ground state degeneracy of the N-particle system if $N = 3,\ 4$ and 5 ?

    (Include the spin-orbit coupling discussed above but ignore the Coulomb interaction between the electrons).

15. Hund's rule:

    Consider the following three possible states of two electrons placed in the $l = 1$ states in some radial quantum number n of some atom.
    (i) both electrons are in the $l = 1,\ l_z = 1$ state, with their spins forming a singlet,
    (ii) one electron is in the $l = 1,\ l_z = 0$ and the other in the $l = 1,\ l_z = 1$ state in a symmetric combination, with their spins forming a singlet,
    (iii) one electron is in the $l = 1,\ l_z = 0$ and the other in the $l = 1,\ l_z = 1$ state in an antisymmetric combination, with their spins forming a triplet.
    These three states are degenerate if the Coulomb interaction between the electrons is ignored.

    Assuming that the Coulomb interaction between the two electrons is described by the 'simplified' Hamiltonian $H_{int} = U\ \delta^3(\vec{r}_1 - \vec{r}_2)$ (where $U > 0$, since the Coulomb interaction is repulsive), compute the expectation value of H_{int} in terms of U in the three states described above. Which state has the lowest energy? (We do not need to know the explicit forms of the spatial wave functions $\psi_{n,l,m}$ to answer this question).

16. Suppose that two distinguishable particles with the same mass interact with each other by a central potential. Let $f(\theta)$ denote the scattering amplitude in the centre of mass frame, where θ is the angle of scattering of either one of the particles. Now, if two electrons whose spins are unpolarised interact through the same central potential, show that the differential scattering cross-section is given by

$$\frac{d\sigma}{d\Omega} = \frac{3}{4}\,|f(\theta) - f(\pi-\theta)|^2 + \frac{1}{4}\,|f(\theta) + f(\pi-\theta)|^2.$$

17. For N spinless fermions in the lowest N energy states of the one-dimensional simple harmonic oscillator, show that the wave function is proportional to the Vandermonde determinant times a Gaussian, namely,

$$\psi \propto \left[\prod_{i<j} (x_i - x_j)\right] \exp\left(-\frac{m\omega}{2\hbar}\sum_{i=1}^{N} x_i^2\right).$$

18. For N spin-1/2 fermions occupying N states $\psi_1,\ \psi_2,\ \cdots,\ \psi_N$ (where the ψ_i's involve both space and spin and form an orthonormal set satisfying $\int d^3\vec{r}\psi_i^\dagger(\vec{r})\psi_j(\vec{r}) = \delta_{ij}$), we know that the normalised wave function $\Psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_N)$ is given by $1/\sqrt{N!}$ times a Slater determinant. The probability density for one of the electrons is defined to be

$$P(\vec{r}_1) = \int d^3\vec{r}_2\, d^3\vec{r}_3 \cdots d^3\vec{r}_N\ \Psi^\dagger\Psi.$$

Show that

$$P(\vec{r}_1) = \frac{1}{N}\sum_{i=1}^{N} \psi_i^\dagger(\vec{r}_1)\psi_i(\vec{r}_1) \quad \text{and} \quad \int d^3\vec{r}_1\, P(\vec{r}_1) = 1.$$

Hint: Prove this for $N = 2$ and then generalise the argument to any value of N.

19. We know that two non-identical spin-1 particles can combine to have a total angular momentum $j = 0, 1$ and 2. What are the possible values of j if the two particles are identical bosons, i.e., only those states are allowed which are symmetric under the exchange of the two particles? (In this problem, we are only considering spin angular momentum and ignoring any orbital angular momentum).

20. Consider three particles moving in one dimension with coordinates $X_1 < x < X_2$, where the heavy particles at $X_1,\ X_2$ have mass M each and the light particle at x has mass m, where $m \ll M$. Suppose that the Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2[(x - X_1 - a)^2 + (X_2 - x - a)^2] + \frac{P_1^2}{2M} + \frac{P_2^2}{2M}.$$

(i) Find the ground state energy of the light particle taking the coordinates $X_1,\ X_2$ to be fixed, and show that this produces a potential $V(X_1, X_2)$ between the heavy particles.

(ii) Now find all the energy levels of the system of two heavy particles.

21. Born-Oppenheimer approximation: Consider a heavy particle and a light particle moving in one dimension with coordinate, momentum and mass denoted by (X, P, M) and (x, p, m) respectively. Supposed that the Hamiltonian is

$$H = \frac{P^2}{2M} + \frac{1}{2}KX^2 + \frac{p^2}{2m} + \frac{1}{2}kx^2 + \lambda X x,$$

where λ satisfies $\lambda^2 \ll Kk$, and $k/m \gg K/M$ (so that the oscillation frequency of the light particle is much larger than that of the heavy particle).

(i) Find the ground state energy of the light particle taking X to be fixed, and show that this effectively decreases the value of K for the heavy particle by some amount. Now find the energy levels of the heavy particle.

(ii) Find the frequencies of the two normal modes of the system classically and show that the smaller frequency agrees with what you get from the quantum energy levels of the heavy particle found in (i), when $\lambda^2 \ll Kk$ and $k/m \gg K/M$.

22. Consider a diatomic molecule in which the nuclei have mass M each and the internuclear potential is of the form

$$V(R) = V_0 \left[\left(\frac{a}{R} \right)^2 - 2 \left(\frac{a}{R} \right) \right],$$

where R is the internuclear separation. Calculate the vibrational frequency and the rotational spectrum if the orbital angular momentum is given by $\vec{L}^2 = l(l+1)\hbar^2$.

Hint: Find the separation R_0 where $V(R)$ has a minimum and use that to compute the required moments of inertia and the rotational spectrum. Then expand around R_0 to second order in $R - R_0$ and use that simple harmonic potential to find the vibrational frequency.

23. In HCl, a number of absorption lines with wave numbers (in cm^{-1}) given by 83.03, 103.73, 124.30, 145.03, 165.61 and 185.86 have been observed. Assume that these correspond to transitions between different rotational levels and remember that in such transitions the angular momentum l changes by 1. Find the moment of inertia of a HCl molecule in units of Kg-m^2. Recall that $\hbar \simeq 1.05 \times 10^{-34}$ Joules-sec and $c \simeq 3.00 \times 10^8$ m/sec.

24. Rutherford experiment: Consider the scattering of an α-particle (with mass M and charge $-2e$) from an infinitely heavy atom (hence the recoil of the atom can be ignored). Assume that the atom has a point nucleus of charge Ze and an uniform spherically symmetric electron cloud of radius a surrounding it, so that the electron charge density $\rho(r)$ satisfies $(4\pi/3)a^3\rho(r) = -Ze$ for $r \leq a$, and $\rho(r) = 0$ for $r > a$. Use the Born approximation to calculate the differential scattering cross-section $d\sigma/d\Omega$ as a function of the scattering angle θ and the wave number k.

25. Consider scattering from a δ-function potential in three dimensions, $V(\vec{r}) = \lambda\delta^3(\vec{r})$. Use the Born approximation to compute the differential scattering cross-section $d\sigma/d\Omega$, and explain the form of its dependence on the polar angles θ and ϕ.

26. Consider scattering from two δ-function potentials located at the points $\pm a\hat{z}$ in three dimensions, i.e., the potential is $V(\vec{r}) = \lambda[\delta^3(\vec{r} - a\hat{z}) + \delta^3(\vec{r} + a\hat{z})]$.

    (i) Use the Born approximation to compute the differential scattering cross-section $d\sigma/d\Omega$ as a function of θ (the angle of scattering with respect to the $\hat{z}$-axis).

    (ii) Now integrate $d\sigma/d\Omega$ to find the total scattering cross-section σ. What is the value of the ratio $\sigma(ka \to \infty)/\sigma(ka \to 0)$? Can you give a physical explanation for this value?

27. Consider scattering from a hard sphere, i.e., from the potential

$$\begin{aligned} V(r) &= \infty \quad \text{for} \quad r < a, \\ &= 0 \quad \text{for} \quad r > a. \end{aligned}$$

    Find the phase shifts $\delta_l(k)$ in the limits $ka \ll 1$ and $ka \gg 1$. Then find the total scattering cross-section in the limits $ka \to 0$ and $ka \to \infty$.

28. For the scattering potential $V(r) = \hbar^2 c/(2mr^2)$ (with $c > 0$), calculate the phase shift $\delta_l(k)$ as a function of the angular momentum l. What is the total scattering cross-section?

29. (i) Derive an expression for the Born approximation for scattering in one dimension.

    Remember that there are only two scattering amplitudes in one dimension. Namely, if the initial wave function is $\psi_{initial} = e^{ikx}$, then the scattered wave function $\psi_{scattered} = \psi_{final} - \psi_{initial}$ is given by

$$\begin{aligned} \psi_{scattered} &= f_t \, e^{ikx} \quad \text{for} \quad x \to \infty \, , \\ &= f_r \, e^{-ikx} \quad \text{for} \quad x \to - \infty \, . \end{aligned}$$

    You have to find the Born approximation for f_t and f_r.

    (ii) Use the Born approximation to derive expressions for f_t and f_r for scattering from a δ-function potential, $V(x) = \lambda\delta(x)$. Show that these agree with the exact expressions if λ is small.

30. A tritium atom in its ground state (denoted ${}^3H(1\text{s})$) can decay into a helium ion (${}^3He^+$) after emitting an electron and an antineutrino. (Assume that the last two particles play no role in this problem). This decay is a sudden process on atomic time scales. Using the wave functions of one electron in the various atomic states, calculate the probabilities that immediately after the decay, the helium ion will be found in the $1s$ and $2s$ states respectively.

31. Rabi oscillations: Consider a two-level system whose Hamiltonian and wave function are respectively given by

$$H(t) = \begin{pmatrix} E_1 & \hbar\gamma e^{i\omega t} \\ \hbar\gamma e^{-i\omega t} & E_2 \end{pmatrix} \quad \text{and} \quad \psi(t) = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}.$$

(i) Find the general solution $\psi(t)$ of the Schrödinger equation $i\hbar\partial\psi/\partial t = H\psi$.

Hint: Assume that $\psi_1(t) = \chi_1(t)$ and $\psi_2(t) = \chi_2(t)e^{-i\omega t}$, and show that $\chi(t)$ satisfies the Schrödinger equation with a time-independent Hamiltonian H'. Show that H' can be written as $A\ I + B\ (\cos\theta\ \sigma^z + \sin\theta\ \sigma^x)$, and find the values of A, B, $\cos\theta$ and $\sin\theta$. Now find the general solution for $\chi(t)$ and hence $\psi(t)$.

(ii) Assume that the initial condition is $\psi_1(t=0) = 1$ and $\psi_2(t=0) = 0$. Show that $|\psi_1(t)|^2$ and $|\psi_2(t)|^2$ oscillate with the frequency $\Omega = 2\sqrt{\gamma^2 + \frac{1}{4}\left(\omega - \frac{E_2-E_1}{\hbar}\right)^2}$, and that $|\psi_2(t)|^2$ oscillates between zero and

$$\frac{\gamma^2}{\gamma^2 + \frac{1}{4}\left(\omega - \frac{E_2-E_1}{\hbar}\right)^2}\ .$$

Hence the amplitude of oscillation is maximum when $\omega = (E_2 - E_1)/\hbar$. This is called the resonance condition.

32. Show that

$$\lim_{t\to\infty} \frac{\sin^2(\omega t)}{\omega^2 t} = \pi\ \delta(\omega) \quad \text{and} \quad \lim_{t\to\infty} \frac{\sin(\omega t)}{\omega} = \pi\ \delta(\omega).$$

Hint: In the first case replace $1/\omega^2$ by $1/(\omega^2+\epsilon^2)$, and in the second case replace $1/\omega$ by $\omega/(\omega^2+\epsilon^2)$, where ϵ is a real and positive quantity which we will eventually take to zero. Then do an appropriate contour integral with some function $f(\omega)$ (which is well-behaved near $\omega = 0$) and show that we get $\pi f(0)$ in both cases.

33. Use the Fermi golden rule to derive the Born approximation result for the differential scattering cross-section $d\sigma/d\Omega = |f(\theta)|^2$ for scattering from a potential $V(\vec{r})$.

The derivation goes as follows. According to the Fermi golden rule, the transition rate to go from an initial state $\psi_{initial} = e^{i\vec{k}\cdot\vec{r}}$ (where $\vec{k} = k\hat{z}$) to a final state $\psi_{final} = e^{i\vec{k}'\cdot\vec{r}}$ (where the direction $\hat{k}'$ is described by polar angles θ, ϕ) is given by

$$\Gamma = \frac{2\pi}{\hbar} \int \frac{d^3\vec{k}'}{(2\pi)^3}\ |\langle\psi_{final}|V(\vec{r})|\psi_{initial}\rangle|^2\ \delta(E_{\vec{k}'} - E_{\vec{k}}).$$

Next, we write $d^3\vec{k}' = k'^2 dk' d\Omega$. Writing $\Gamma = \int d\Omega\ d\Gamma/d\Omega$, we get an expression for the differential transition rate $d\Gamma/d\Omega$ in terms of an integral over k'. We now do the integral over k'; the energy-conserving δ-function then tells us that $k' = k$ as we expect. Finally, we divide $d\Gamma/d\Omega$ by the initial flux $\hbar k/m$ (since $\vec{J}_{initial} = (\hbar k/m)\hat{z}$) to obtain an expression for $d\sigma/d\Omega$. This should agree with what we got earlier from the Born approximation.

34. A hydrogen atom, which is in its ground state at time $t = -\infty$, is placed in an electric field of the form

$$\vec{E} = \frac{\lambda}{\pi}\ \frac{\tau}{t^2 + \tau^2}\ \hat{z}\ .$$

Find the probability, to order λ^2, of finding the hydrogen atom in the $2p$ state (with $m = 0$) at time $t = \infty$. What does the probability tend to in the limit $\tau \to 0$, which corresponds to an impulse field $\vec{E} = \lambda\delta(t)\hat{z}$?
Express all your answers in terms of $|\langle\psi_{2p,m=0}|z|\psi_{1s}\rangle|^2 = Ka_0^2$, where $K = (8/9)^5$.

35. A particle in a one-dimensional simple harmonic potential is subjected to a force $F(t) = f cos(\gamma t)$ for a period of time $0 < t < T$, where γ may be different from the frequency ω of the harmonic oscillator, and T is finite.

    (i) If the particle is in the ground state at time $t < 0$, what is the probability of finding it in the first excited state at $t > T$ to second order in f ?

    (ii) How does the probability behave with T if $\gamma = \omega$?

    (iii) What happens in the cases $\gamma \neq \omega$ and $\gamma = \omega$ in the limit $T \to \infty$?

36. A particle is in the ground state of the Hamiltonian H of a shifted harmonic oscillator in one dimension, where

$$\begin{aligned} H &= H_0 - \lambda x \ , \\ \text{and } H_0 &= \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \ , \end{aligned}$$

    at time $t < 0$. At time $t = 0$, λ is suddenly reduced to zero. What is the probability of finding the particle in the n-th eigenstate of H_0 at time $t > 0$?

37. At time $t < 0$, a particle is in the ground state of the one-dimensional potential

$$\begin{aligned} V(x) &= 0 \quad \text{for} \quad 0 < x < L \ , \\ &= \infty \quad \text{otherwise} \ . \end{aligned}$$

    At $t = 0$, the potential is suddenly changed to the form

$$\begin{aligned} V(x) &= 0 \quad \text{for} \quad 0 < x < L' \ , \\ &= \infty \quad \text{otherwise} \ , \end{aligned}$$

    where $L' > L$. Find the probabilities of finding the particle in the different eigenstates of the new Hamiltonian at $t > 0$.

    How would the answer change if the potential is changed adiabatically?

38. Thomson scattering: Consider the elastic scattering of a high energy photon from an electron in an atom. (Ignore the spin of the electron in this problem). If the photon energy is much larger than the atomic binding energies (but much smaller than the rest energy of the electron), it is sufficient to do first-order perturbation theory with the term $(e^2/2mc^2)\vec{A}_{qu}^2$. (The contribution of the second-order perturbation due to $-(e/mc)\vec{A}_{qu} \cdot \vec{p}$ is negligible due to the large energy denominator which appears in that calculation). Assume also that the atomic state does not change as a result of the scattering, and that

the wavelengths of the initial and final photons are much larger than the length scale of the atomic wave functions.

(i) If $\vec{\epsilon}_{\vec{k},\lambda}$ and $\vec{\epsilon}_{\vec{k}',\lambda'}$ denote the initial and final polarisation vectors, show that the differential scattering cross-section is

$$\frac{d\sigma}{d\Omega} = r_0^2 \, |\vec{\epsilon}^{\,*}_{\vec{k}',\lambda'} \cdot \vec{\epsilon}_{\vec{k},\lambda}|^2 \, ,$$

which is independent of the atomic state of the electron. Here, $r_0 = e^2/(mc^2)$ is called the classical radius of the electron. What is its numerical value?

(ii) Compute the total unpolarised scattering cross-section by summing over the final polarisations and averaging over the initial polarisations with equal probability.

(iii) Show that for 90° scattering of the photon, the final photon is linearly polarised along the direction $\vec{k} \times \vec{k}'$.

39. The process in the previous problem is called Compton scattering if the electron is free, i.e., not inside an atom. If the initial and final wavelengths of the photon are λ and λ', and the angle of scattering of the photon is θ, use the relativistic relation between the energy and momentum of the electron, $E = \sqrt{p^2c^2 + m^2c^4}$, to show that

$$\lambda' = \lambda + \frac{h}{mc} \, (\, 1 - \cos\theta \,) \, .$$

(Hence h/mc is called the Compton wavelength of the electron).

40. Calculate the unpolarised decay rate and life-time for the transition from the $1s(j = 1)$ state of the hydrogen atom to the $1s(j = 0)$ state plus a photon due to the term $(e\hbar/2mc)\vec{\sigma} \cdot \vec{\nabla} \times \vec{A}_{qu}$. Express your answer in terms of the energy difference ΔE between the $1s(j = 1)$ and $1s(j = 0)$ states (i.e., the hyperfine splitting), and ignore the coupling of the proton spin to $\vec{A}_{qu}$ since the proton is much more massive than the electron. [Do not calculate the decay rates for each of the 6 possible polarisations (3 for the initial state of the hydrogen atom ($j_z = 0, \pm 1$) times 2 for the polarisation of the final photon); just take the unpolarised expression given in class and do the calculation].

41. Consider a simplified version of the photoelectric effect in which an electron can only move in one dimension but the quantized electromagnetic field is in three dimensions. Suppose that the electron is initially in a bound state with normalised wave function $\psi_0(x) = \sqrt{\beta} e^{-\beta|x|}$ and energy $E_0 = -\hbar^2\beta^2/(2m)$. Let a photon with wave vector $\vec{k} = k(\sin\theta, 0, \cos\theta)$ be incident on the electron. (You can use the polarisation vectors given in question 4 (i) above). Assume that the photon has energy larger than $-E_0$. You have to calculate the transition rate for the electron to absorb the photon and end up in a final state with momentum p_f (hence $\psi_{p_f}(x) = e^{ip_f x/\hbar}$ and $E_f = p_f^2/(2m)$).

(i) Calculate the matrix element $\langle \psi_{p_f} | (e/mc) A_x \hat{p}_x | \psi_0 + \text{photon} \rangle$, where A_x is the $\hat{x}$-component of the quantized vector potential $\vec{A}$, and $\hat{p}_x = -i\hbar\partial/\partial x$ is the electron momentum operator. (Note that $A_y, A_z, \hat{p}_y, \hat{p}_z$ do not appear in this problem since the electron can only move along the $\hat{x}$-axis).

(ii) Now use the Fermi golden rule to integrate over the final momentum of the electron and thus obtain the transition rate Γ. (You have to sum over left and right circularly polarisations of the incident photon with probability 1/2 each. Also, note that the final electron momentum can have two possible values, $p_f > 0$ and $p_f < 0$). How does Γ depend on the angle θ ?

42. Heisenberg operator: For a time-independent Hamiltonian H, the Heisenberg operator $\mathcal{O}(t)$ is related to the Schrödinger operator $\mathcal{O}$ as $\mathcal{O}(t) = e^{iHt/\hbar}\mathcal{O}e^{-iHt/\hbar}$. For a simple harmonic oscillator in one dimension, show that the Heisenberg lowering and rising operators are given by

$$a(t) \; = \; a \, e^{-i\omega t} \quad \text{and} \quad a^\dagger(t) \; = \; a^\dagger \, e^{i\omega t}.$$

43. Bogoliubov transformation:

(a) Given two operators a and $a^\dagger$ satisfying $[a, a^\dagger] = 1$, consider the Hamiltonian

$$H \;=\; \mu \, a^\dagger a \;+\; \nu \, aa \;+\; \nu^* \, a^\dagger a^\dagger \;,$$

where μ is real and positive, but ν may be complex.

(i) Diagonalise the Hamiltonian, i.e., write it in the form $\mu' b^\dagger b + \alpha$, where b and $b^\dagger$ are linearly related to a and $a^\dagger$ and satisfy $[b, b^\dagger] = 1$, and μ' and α are related to μ and ν in some way.

(ii) Find the ground state energy and the expectation value of $\hat{N}$ in the ground state, where $\hat{N} = a^\dagger a$.

(iii) Given a value of μ, is the problem well-defined for all values of ν? If not, why not? (It may become easier to answer this question after you do part (iv) below).

(iv) Assuming that this system describes a simple harmonic oscillator, write a and $a^\dagger$ in terms of x and p and find the oscillation frequency ω' classically. Show that this agrees with $\mu'/\hbar$.

(b) Given four operators a_1, $a_1^\dagger$, a_2, and $a_2^\dagger$, satisfying $\{a_i, a_j^\dagger\} \equiv a_i a_j^\dagger + a_j^\dagger a_i = \delta_{ij}$ (and all other anticommutators are equal to zero), consider the Hamiltonian

$$H \;=\; \mu \, (a_1^\dagger a_1 \;+\; a_2^\dagger a_2) \;+\; \nu \, a_1 a_2 \;+\; \nu^* \, a_2^\dagger a_1^\dagger \;,$$

where μ must be real (but need not be positive), but ν may be complex.

(i) Diagonalise the Hamiltonian, i.e., write it in the form $\mu'(b_1^\dagger b_1 + b_2^\dagger b_2) + \alpha$, where $b_i, b_i^\dagger$ satisfy the same anticommutation relations amongst each other as $a_i, a_i^\dagger$.

(ii) Answer the same questions as in parts (ii) and (iii) of question (a), except that $\hat{N} = a_1^\dagger a_1 + a_2^\dagger a_2$ here.

44. Consider a particle moving in one dimension with the Hamiltonian $H = (p^2/2m) + V(x)$. Assume that the potential is such that H has only discrete eigenstates which are labelled as $|n>$ (with energy E_n). Show that

$$[[H, x], x] \;=\; -\frac{\hbar^2}{m} \; .$$

Use this relation to show that for any eigenstate $|a>$ of H,

$$\sum_n (E_n \; - \; E_a) \; | < n|x|a > |^2 \;=\; \frac{\hbar^2}{2m} \; .$$

This is called the Thomas-Reiche-Kuhn sum rule.

45. (i) Use the expression for the second quantised vector potential $\vec{A}(\vec{r}, t)$, with δ-function normalisation, to compute the equal time commutation relations $[E_i(\vec{r}, t), E_j(\vec{r}\,', t)]$, $[E_i(\vec{r}, t), B_j(\vec{r}\,', t)]$ and $[B_i(\vec{r}, t), B_j(\vec{r}\,', t)]$, where E_i and B_i denote the components of the electric and magnetic fields respectively. Verify that

$$[\; E_i(\vec{r}, t) \; , \; B_j(\vec{r}\,', t) \;] \;=\; -\, i4\pi\hbar c \sum_k \epsilon_{ijk} \frac{\partial}{\partial r^k} \, \delta^3(\vec{r} \; - \; \vec{r}\,') \; ,$$

while the other two commutators are zero.

Qualitatively, what do these relations imply about the simultaneous measurability of $\vec{E}$ and $\vec{B}$?

(ii) Calculate the expectation value of $\vec{E}(\vec{r}, t) \cdot \vec{E}(\vec{r}\,', t)$ in the vacuum state. What is the value of this for $\vec{r} = \vec{r}\,'$?

46. Consider the hypothetical case of a photon with mass m. In the presence of classical charge and current densities ρ and $\vec{J}$, the Maxwell equations take the form

$$\begin{aligned}
\vec{\nabla} \cdot \vec{E} \;&=\; 4\pi\rho \; - \; \frac{m^2 c^2}{\hbar^2} \phi \; , \\
\vec{\nabla} \times \vec{B} \;&=\; \frac{1}{c}\frac{\partial \vec{E}}{\partial t} \; + \; \frac{4\pi}{c} \vec{J} \; - \; \frac{m^2 c^2}{\hbar^2} \vec{A} \; , \\
\vec{\nabla} \cdot \vec{B} \;&=\; 0 \; , \quad \text{and} \quad \vec{\nabla} \times \vec{E} \; + \; \frac{1}{c}\frac{\partial \vec{B}}{\partial t} \;=\; 0 \; ,
\end{aligned}$$

where $\vec{E} = -\vec{\nabla}\phi - (1/c)\partial\vec{A}/\partial t$ and $\vec{B} = \vec{\nabla} \times \vec{A}$ as usual.

(Note that the Maxwell equations are gauge invariant only if $m = 0$).

(i) Using the above equations, show that the equation of continuity $\vec{\nabla} \cdot \vec{J} + \partial\rho/\partial t = 0$ automatically implies that $\vec{\nabla} \cdot \vec{A} + (1/c)\partial\phi/\partial t = 0$.

(ii) Show that the Maxwell equations are exactly the Euler-Lagrange equations of motion which follow from the Lagrangian

$$L \;=\; \int d^3\vec{r} \, \Big[\frac{1}{8\pi} \, (\vec{E}^2 \; - \; \vec{B}^2) \; + \; \frac{m^2 c^2}{8\pi\hbar^2} \, (\phi^2 \; - \; \vec{A}^2) \; - \; \phi\rho \; + \; \frac{1}{c} \, \vec{J} \cdot \vec{A} \Big].$$

(iii) If $\rho = Q\ \delta^3(\vec{r})$ and $\vec{J} = 0$, verify that a solution of the Maxwell equations is

$$\phi \ = \ Q\ \frac{e^{-mcr/\hbar}}{r}\ , \qquad \text{and} \quad \vec{A} = 0\ .$$

(iv) If ρ and $\vec{J}$ are zero, verify that the Maxwell equations have solutions of the form

$$\begin{aligned} \vec{E} &= \vec{\epsilon}_{\vec{k},\lambda}\ e^{i(\vec{k}\cdot\vec{r}-\omega_{\vec{k}}t)}\ +\ \text{complex conjugate}\ , \\ \vec{B} &= \frac{c}{\omega_{\vec{k}}}\ \vec{k}\times\vec{\epsilon}_{\vec{k},\lambda}\ e^{i(\vec{k}\cdot\vec{r}-\omega_{\vec{k}}t)}\ +\ \text{complex conjugate}\ , \end{aligned}$$

where $\hbar\omega_{\vec{k}} = \left[\hbar^2\vec{k}^2c^2 + m^2c^4\right]^{1/2}$, and $\vec{\epsilon}_{\vec{k},\lambda}$ can take three possible values. For instance, if $\vec{k} = (0,0,0)$, then $\vec{\epsilon}_{\vec{k},\lambda}$ can take the values $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$.

47. Lagrangian for the Schrödinger equation: Given a field $\psi(\vec{r},t)$ and its complex conjugate $\psi^*(\vec{r},t)$, consider the Lagrangian

$$L \ = \ \int d^3\vec{r}\ [i\hbar\ \psi^* \frac{\partial\psi}{\partial t}\ -\ \psi^*\ \frac{\vec{p}^2}{2m}\ \psi\ -\ V(\vec{r},t)\ \psi^*\psi],$$

where $\vec{p}^2 = -\hbar^2\vec{\nabla}^2$. Show that the Euler-Lagrangian equation for ψ^*, given by $\delta L/(\delta\partial\psi^*/\partial t) = \delta L/\delta\psi^*$, leads to the Schrödinger equation for ψ.

Calculate the momentum conjugate to ψ defined as $\Pi = \delta L/(\delta\partial\psi/\partial t)$. Then find an expression for the Hamiltonian

$$H \ = \ \left[\ \int d^3\vec{r}\ \Pi\ \frac{\partial\psi}{\partial t}\ \right]\ -\ L.$$

[We have ignored spin in this problem but it can be easily included. For a spin-1/2 particle, we allow ψ to be a column with two entries corresponding to the spin-up and spin-down components, and replace ψ^* by $\psi^\dagger$ in the Lagrangian given above].

48. Consider the second quantised theory of the electron (ignore spin in this problem). The electron field is given by

$$\Psi(\vec{r},t) \ = \ \int \frac{d^3\vec{p}}{(2\pi\hbar)^3}\ c_{\vec{p}}\ \exp\ [\frac{i}{\hbar}\ (\vec{p}\cdot\vec{r}\ -\ E_{\vec{p}}\ t)]\ ,$$

where $E_{\vec{p}}$ is some function of $\vec{p}$ (which we don't need to know), $\{c_{\vec{p}\,'}, c^\dagger_{\vec{p}}\} = (2\pi\hbar)^3\ \delta^3(\vec{p} - \vec{p}\,')$, and all other anticommutators are zero.

(i) Show that $\{\Psi(\vec{r}_1,t)\ ,\ \Psi^\dagger(\vec{r}_2,t)\} \ = \ \delta^3(\vec{r}_1 - \vec{r}_2)$.

(ii) The number, Hamiltonian and momentum operators are given by

$$\mathcal{N} = \int \frac{d^3\vec{p}}{(2\pi\hbar)^3}\ c^\dagger_{\vec{p}}c_{\vec{p}}\ , \quad \mathcal{H} = \int \frac{d^3\vec{p}}{(2\pi\hbar)^3}\ E_{\vec{p}}\ c^\dagger_{\vec{p}}c_{\vec{p}} \quad \text{and} \quad \vec{\mathcal{P}} = \int \frac{d^3\vec{p}}{(2\pi\hbar)^3}\ \vec{p}\ c^\dagger_{\vec{p}}c_{\vec{p}}\ .$$

Show that

$$[\mathcal{N}\ ,\ \Psi]\ =\ -\Psi\ ,\qquad [\mathcal{H}\ ,\ \Psi]\ =\ -i\hbar\ \partial\Psi/\partial t\quad \text{and}\quad [\vec{\mathcal{P}}\ ,\ \Psi]\ =\ i\hbar\vec{\nabla}\Psi.$$

Hint: You have to use the identity $[AB, C] = A\{B, C\} - \{A, C\}B$.

(iii) Consider a two-particle state defined as

$$\mid \vec{p}_1,\ \vec{p}_2 > \ =\ c^\dagger_{\vec{p}_2}\ c^\dagger_{\vec{p}_1}\mid vacuum > .$$

Show that

$$\begin{aligned}
\mathcal{N}\mid \vec{p}_1,\ \vec{p}_2 > &=\ 2\mid \vec{p}_1,\ \vec{p}_2 >,\\
\mathcal{H}\mid \vec{p}_1,\ \vec{p}_2 > &=\ (E_{\vec{p}_1} + E_{\vec{p}_2})\mid \vec{p}_1,\ \vec{p}_2 >,\\
\vec{\mathcal{P}}\mid \vec{p}_1,\ \vec{p}_2 > &=\ (\vec{p}_1 + \vec{p}_2)\mid \vec{p}_1,\ \vec{p}_2 > .
\end{aligned}$$

(iv) Show that the two-particle wave function is given by

$$\begin{aligned}
&< vacuum \mid \Psi(\vec{r}_1, t)\ \Psi(\vec{r}_2, t)\mid \vec{p}_1,\ \vec{p}_2 >\\
&= \Big[\exp[\frac{i}{\hbar}(\vec{p}_1\cdot\vec{r}_1 + \vec{p}_2\cdot\vec{r}_2)]\ -\ \exp[\frac{i}{\hbar}(\vec{p}_1\cdot\vec{r}_2 + \vec{p}_2\cdot\vec{r}_1)]\Big]\ \exp[-\frac{it}{\hbar}(E_{\vec{p}_1} + E_{\vec{p}_2})].
\end{aligned}$$

Note that this is antisymmetric under the exchange $\vec{r}_1 \leftrightarrow \vec{r}_2$.

49. Bogoliubov transformation for electrons:

Given four operators $c_1,\ c_2,\ c_1^\dagger$ and $c_2^\dagger$ satisfying $\{c_i, c_j^\dagger\} = \delta_{ij},\ \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$, consider the Hamiltonian

$$H\ =\ \mu\ (c_1^\dagger c_1\ +\ c_2^\dagger c_2)\ +\ \nu\ c_1 c_2\ +\ \nu\ c_2^\dagger c_1^\dagger,$$

where both μ and ν are real and positive.

(i) Diagonalise the Hamiltonian, i.e., write it in the form $\mu'(d_1^\dagger d_1 + d_2^\dagger d_2) + \alpha$, where

$$d_1\ =\ \cos\theta\ c_1\ +\ \sin\theta\ c_2^\dagger,\quad d_2\ =\ \cos\theta\ c_2\ -\ \sin\theta\ c_1^\dagger,$$

and $\{d_i, d_j^\dagger\} = \delta_{ij},\ \{d_i, d_j\} = \{d_i^\dagger, d_j^\dagger\} = 0$, θ is a real parameter that you have to find, and μ' and α are related to μ and ν in some way.

(ii) Find the ground state energy and the expectation value of $\hat{N}$ in the ground state, where $\hat{N} = c_1^\dagger c_1 + c_2^\dagger c_2$.

Note that the above problem is well-defined for all values of μ and ν, unlike the Bogoliubov transformation for operators which satisfy commutation relations (like the creation and annihilation operators of photons) where the problem is well-defined only if μ and ν satisfy some relation. Also, the Bogoliubov transformation in that problem involves $\cosh\theta$ and $\sinh\theta$ instead of $\cos\theta$ and $\sin\theta$.

The Bogoliubov transformation for electrons is used in the theory of superconductivity, and there the operator $c_2^\dagger c_1^\dagger$ creates a pair of electrons called a Cooper pair.

50. Suppose that the density matrix of a spin-1/2 particle is given by $\rho = (1/2)(I \ + \ a_1\sigma^x \ + \ a_2\sigma^y \ + \ a_3\sigma^z)$, where I denotes the 2×2 identity matrix, the σ^i's are Pauli matrices, and the a_i's are real numbers.

(i) What is the condition that the a_i must satisfy so that ρ satisfies all the properties of a density matrix?

(ii) What is the condition that the a_i must satisfy so that ρ describes a pure state?

(iii) Suppose that the particle is governed by a Hamiltonian $H = \hbar\omega\sigma^z$, where ω is a constant. Then ρ will still have the form $(1/2)(I + a_1\sigma^x + a_2\sigma^y + a_3\sigma^z)$, but the a_i's will vary with time. Find expressions for $(a_1(t), a_2(t), a_3(t))$ in terms of $(a_1(0), a_2(0), a_3(0))$.

51. Consider a system with three spin-1/2 objects which are labelled as 1, 2 and 3. Suppose that the wave function of the system is

$$|\psi\rangle \ = \ a \, | \downarrow_1 \ \uparrow_2 \ \uparrow_3\rangle \ + \ b \, | \uparrow_1 \ \downarrow_2 \ \uparrow_3\rangle \ + \ c \, | \uparrow_1 \ \uparrow_2 \ \downarrow_3\rangle,$$

where $|a|^2 + |b|^2 + |c|^2 = 1$.

(i) Find the reduced density matrix of spin 1 by summing over the states of spins 2 and 3.

(ii) Use this to calculate the entanglement entropy between spin 1 and the other two spins.

(iii) Use the result in part (ii) to find the entanglement entropy if $a = 0$.
Can you give a simple understanding of your answer?

52. Consider a system with four spin-1/2 objects which are labelled as 1, 2, 3 and 4. Suppose that the wave function of the system is

$$\begin{aligned} |\psi\rangle \ &= \ a \, | \downarrow_1 \ \uparrow_2 \ \uparrow_3 \ \uparrow_4\rangle \ + \ b \, | \uparrow_1 \ \downarrow_2 \ \uparrow_3 \ \uparrow_4\rangle \\ &\quad + c \, | \uparrow_1 \ \uparrow_2 \ \downarrow_3 \ \uparrow_4\rangle \ + \ d \, | \uparrow_1 \ \uparrow_2 \ \uparrow_3 \ \downarrow_4\rangle, \end{aligned}$$

where $|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1$.

(i) Find the reduced density matrix of spin 1 by summing over the states of spins 2, 3 and 4. Use this to calculate the entanglement entropy between spin 1 and the other three spins.

(ii) Considering spins 1 and 2 as part I of the system and spins 3 and 4 as part II, calculate the reduced density matrix of part I. Use this to calculate the entanglement entropy between parts I and II.

53. (i) Use any method you like to show that

$$\sum_{n=-\infty}^{\infty} e^{iny} \ = \ 2\pi \sum_{n=-\infty}^{\infty} \delta(y \ - \ 2\pi n).$$

(ii) Multiply both sides with $\exp[i(n+b)y - ay^2/2]$ and integrate over y from $-\infty$ to ∞ to prove the Poisson resummation formula

$$\sum_{n=-\infty}^{\infty} \exp \left(-\frac{1}{2a}(n+b)^2\right) = \sqrt{2\pi a} \sum_{n=-\infty}^{\infty} \exp \left(i2\pi nb - 2\pi^2 n^2 a\right),$$

where $a,\ b$ can be complex numbers, but the real part of a should not be negative (so that we can use the identity $\int_{-\infty}^{\infty} dy\ e^{-ay^2/2} = \sqrt{2\pi/a}$).

(iii) Substitute $a = i\hbar t/(mL^2)$ and $b = (x' - x)/L$ in the Poisson resummation formula to show that

$$\sum_{n=-\infty}^{\infty} \sqrt{\frac{m}{i2\pi\hbar t}} \exp \left[\frac{im}{2\hbar t}(x' - x + nL)^2\right]$$
$$= \sum_{n=-\infty}^{\infty} \frac{1}{L} \exp \left[i\frac{2\pi n}{L}(x' - x) - \frac{it}{\hbar} \frac{(2\pi n\hbar/L)^2}{2m}\right].$$

This formula will be required later when we use path integrals to study the problem of a particle moving on a circle with circumference L.

54. Consider the Dirac equation in $1+1$ dimensions with mass $m = 0$ and a potential $V(x)$. Hence $i\hbar\partial\psi/\partial t = H\psi$, where

$$H = -ic\hbar\sigma^x \frac{\partial}{\partial x} + V(x).$$

Since σ^x commutes with H, solutions of the Dirac equations corresponding to eigenvalues $+1$ and -1 of σ^x decouple from each other. We will concentrate on solutions with eigenvalue $+1$ of σ^x in this problem

(i) Show that solutions of the Dirac equation with eigenvalue $+1$ of σ^x and energy E can be written as

$$\psi(x,t) = f(x)\, e^{-iEt/\hbar} \begin{pmatrix} 1 \\ 1 \end{pmatrix},$$

where $f(x)$ has only one component, depends only on x, and satisfies the equation

$$-ic\hbar\frac{\partial f}{\partial x} + Vf = Ef.$$

(ii) Suppose that the potential $V(x)$ is non-zero only in the region $0 < x < L$. (We will not need the exact form of $V(x)$ in this problem). Assuming that the energy $E > 0$, use part (i) to find the general solution for $f(x)$ in the three regions $x < 0$, $0 < x < L$ and $x > L$. (The solution in the region $0 < x < L$ will depend on $V(x)$ in some way).

(iii) Now suppose that there is a wave incident from $x = -\infty$ so that $f(x) = e^{ipx/\hbar}$ for $x < 0$ and $t_p e^{ipx/\hbar}$ for $x > L$, where t_p is the transmission amplitude. Find p in terms of E. Next, find the general solution in the region $0 < x < L$ and match the wave functions at $x = 0$ and $x = L$ to find t_p and the transmission probability $|t_p|^2$. (Note that there is no reflected wave and the wave is completely transmitted regardless of the form of $V(x)$. This is the simplest example of a phenomenon called Klein tunnelling: a massless particle satisfying the Dirac equation can transmit perfectly through any potential barrier).