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Homework-1

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1. Consider an infinite square well potential as

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

Applying a  $\delta$ -perturbation as  $V_1(x) = V_0 L \delta(x - L/2)$ , where  $V_0$  has the dimesnion of energy.

- (a) Show that the first-order corrections to the energies are

$$E_n^{(1)} = V_0 [1 - (-1)^n].$$

- (b) Show that the first-order correction to the ground state wave function is

$$\psi_1^{(1)}(x) \simeq \frac{V_0}{4E_1^{(0)}} \sqrt{\frac{2}{L}} \left[ \sin\left(\frac{3\pi x}{L}\right) - \frac{1}{3} \sin\left(\frac{5\pi x}{L}\right) + \frac{1}{6} \sin\left(\frac{7\pi x}{L}\right) - \frac{1}{10} \sin\left(\frac{9\pi x}{L}\right) + \dots \right],$$

where  $E_1^{(0)} = (\pi\hbar)^2/(2ML^2)$ .

- (c) Plot  $\psi_1^{(0)}(x)$ ,  $\psi_1^{(1)}(x)$  and  $\psi(x) = \psi_1^{(0)}(x) + \psi_1^{(1)}(x)$ .

- (d) Show that the second-order energy corrections for odd  $n$  are

$$E_n^{(2)} = \frac{(2V_0)^2}{E_1^{(0)}} \sum_{l \neq n, l: \text{odd}} \frac{1}{n^2 - l^2},$$

2. Consider two identical spin-zero bosons kept in one-dimensional harmonic potential well. The interaction between two bosons is given by  $V(x_1, x_2) = -V_0 a_0 \delta(x_1 - x_2)$ . Here  $V_0$  is a constant having dimension of energy and  $a_0 = \sqrt{\hbar/(m\omega)}$  is the oscillator length scale.

- (a) For non-interacting case, obtain the ground and first excited state energies and the corresponding eigenfunctions (in terms of the oscillator functions).
- (b) Calculate the first-order correction to the ground state and excited state energies, due to the two-body interaction  $V(x_1, x_2)$ .
- (c) Calculate the first-order correction to the ground state and excited state wavefunctions, due to the two-body interaction  $V(x_1, x_2)$ .

3. Consider a charge particle (mass  $m$  and charge  $q$ ) is performing a simple harmonic motion with the oscillation frequency  $\omega$  along  $x$ -axis. It is subjected to a constant electric field  $\mathbf{E} = E_0 \hat{x}$ . The quantum mechanical Hamiltonian for this system is

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 - q E_0 x.$$

- (a) Solve this problem exactly.

- (b) Treat the dipole interaction energy term as a perturbation and solve the problem perturbatively (up to second-order energy correction and first-order correction to the eigenstates).
  - (c) Show that the perturbative results are in agreement with the series expansion of the exact results.
4. Consider an anharmonic oscillator as described by

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}\lambda \frac{m^{3/2}\omega^{5/2}}{\hbar^{1/2}} x^3,$$

where  $\lambda \ll 1$  so that the cubic term can be treated as a perturbative term.

- (a) Express the Hamiltonian  $H$  in terms of dimensionless variable  $\eta = x/a_0$  with  $a_0 = \sqrt{\hbar/(m\omega)}$ .
- (b) Plot the potential energy  $V(\eta)$  for  $\lambda = 0.1, 0.15, 0.5$ :

$$V(\eta) = \frac{1}{2}\hbar\omega [\eta^2 + \lambda\eta^3].$$

Comment on the behaviour of the potential energy on the negative  $\eta$  axis side for three different  $\lambda$  values. Under what condition on  $\lambda$ , the perturbative analysis will be valid?

- (c) Obtain first-order and second-order energy corrections.
  - (d) Obtain the first-order correction to the eigenstates.
5. Consider another anharmonic oscillator as described by

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \frac{1}{2}\lambda \frac{m^2\omega^3}{\hbar} x^4,$$

where  $\lambda \ll 1$  so that the quartic term can be treated as a perturbative term.

- (a) Express the Hamiltonian  $H$  in terms of dimensionless variable  $\eta = x/a_0$  with  $a_0 = \sqrt{\hbar/(m\omega)}$ .
- (b) Plot the effective potential energy  $V(\eta)$ :

$$V(\eta) = \frac{1}{2}\hbar\omega [\eta^2 + \lambda\eta^4].$$

- (c) Show that the first-order energy correction to the  $n$ -th level is

$$E_n^{(1)} = \frac{3\lambda\hbar\omega}{8}(2n^2 + 2n + 10).$$

Note that the energy levels are enhanced because the quartic potential compressed the harmonic potential.

- (d) Show that the second-order energy correction to the ground state is

$$E_0^{(2)} = -\frac{21\lambda\hbar\omega}{16}.$$

Note that the second-order energy correction to the ground state is always negative.

- (e) Show that the first-order correction to the ground state wavefunction is

$$\phi_0^{(1)}(x) = -\frac{\lambda}{16} \left[ 6\sqrt{3}\phi_2^{(0)}(x) + \sqrt{6}\phi_4^{(0)}(x) \right],$$

where  $\phi_n^{(0)}(x)$  are the normalized oscillator states.

- (f) Plot  $\phi_0^{(0)}(x)$ ,  $\phi_0^{(1)}(x)$  and  $\phi_0(x) = \phi_0^{(0)}(x) + \phi_0^{(1)}(x)$ .  
 (g) Obtain low-lying energy eigenvalues and the corresponding eigenstates using exact diagonalization method. [Exact diagonalization is a numerical technique for obtaining the eigenvalues and the eigenstates of a given quantum Hamiltonian].

HINT: For  $\lambda = 0$ , the system reduces to the simple harmonic oscillator problem whose eigenvalues and eigenfunctions are exactly known:  $\epsilon_n = \hbar\omega(n + 1/2)$  and the oscillator wavefunctions  $\phi_n(x)$ . The unperturbed wavefunctions can be used as a basis states and the most general wavefunction for  $\lambda \neq 0$  can be assumed to be of the form

$$\psi(x) = \sum_{n=0}^{\infty} c_n \phi_n(x).$$

Acting the total Hamiltonian  $H$  on  $\psi(x)$ , multiplying  $\phi_m^*(x)$  from left and integrating over all space, you will get

$$[(n + 1/2) - E]c_n + \frac{\lambda}{2} \sum_m c_m M_{nm} = 0,$$

where the matrix elements  $M_{nm}$  are given by

$$M_{nm} = \int_{-\infty}^{\infty} \phi_m(\eta) \eta^4 \phi_n(\eta) d\eta.$$

6. Consider a two-dimensional anisotropic harmonic oscillator

$$H = -\frac{\hbar^2}{2m} \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] + \frac{1}{2}m\Omega^2 (x^2 + y^2) + \frac{1}{2}m\omega_0^2 xy.$$

- (a) Obtain energy levels and the corresponding eigenstates exactly.  
 (b) Assuming  $\omega_0 \ll \Omega_0$  and treat the term  $H' = \frac{1}{2}m\omega_0^2 xy$  as a perturbation. Obtain energy corrections up to second-order and the eigenstates up to first-order.  
 (c) Show that the perturbative results are in agreement with the series expansion of the exact results.
7. Consider an electron's spin is interacting with the static magnetic field  $\mathbf{B} = B_x \hat{x} + B_z \hat{z}$  with  $B_x < B_z$ . The Hamiltonian for the spin degree of freedom can be written as

$$H = \hbar\omega_z \sigma_z + \hbar\omega_x \sigma_x,$$

where  $\omega_z = eB_z/(2m)$  and  $\omega_x = eB_x/(2m)$  with  $\omega_z > \omega_x$ . Here  $\sigma_z$  and  $\sigma_x$  are the usual Pauli matrices.

- (a) Obtain energy levels and the corresponding eigenstates exactly.

- (b) Treat the term  $\omega_x \sigma_x$  as a perturbation and obtain energy corrections up to second-order and the eigenstates up to first-order.
- (c) Show that the perturbative results are in agreement with the series expansion of the exact results.

## 8. Fine structure electronic energy levels of hydrogenic atoms:

- (a) Write down the relativistic expression for the kinetic energy in terms of the relativistic momentum ( $m_e c$ ). Here  $m_e$  is the mass of the electron and  $c$  is the velocity of light. In the non-relativistic limit ( $p \ll m_e c$ ), show that the lowest-order relativistic correction to the kinetic energy in one-electron atom is

$$E_{\text{kin}} = -E_n \left( \frac{Z\alpha}{n} \right)^2 \left[ \frac{3}{4} - \frac{n}{l+1/2} \right].$$

- (b) The spin-orbit interaction term is given as

$$H_{\text{so}} = \frac{1}{2m_e^2 c^2} \frac{1}{r} \frac{dV(\mathbf{r})}{dr} \mathbf{L} \cdot \mathbf{S}.$$

Show that components of  $\mathbf{L}$  and  $\mathbf{S}$  do not commute with  $H_{\text{so}}$ , but the total angular momentum of the electron  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  does commute with the  $H_{\text{so}}$ .

- (c) Show that the spin-orbit correction to the electronic energy levels are

$$\begin{aligned} E_{\text{so}} &= -E_n \left( \frac{Z\alpha}{n} \right)^2 \left[ \frac{n}{2(l+1/2)(l+1)} \right]; & j = l + 1/2 \\ &= E_n \left( \frac{Z\alpha}{n} \right)^2 \left[ \frac{n}{2l(l+1/2)} \right]; & j = l - 1/2 \end{aligned}$$

- (d) **Darwin term:** For a relativistic particle, its position rapidly oscillates with the amplitude  $\lambda_c = \hbar/(m_e c)$ , ( $\lambda_c$  is the Compton wavelength) due to interference between positive and negative energy states. In other words, the instantaneous position of the relativistic particle can not be defined more precisely than within the volume  $V_c = (4\pi/3)\lambda_c^3$ . Therefore, the Coulomb potential  $V(r)$  can not be the actual potential. It must be modified to take into account of the intrinsic oscillation of the particle's position.

Show that the smeared average of the potential  $V(\mathbf{r})$  over a sphere of radius  $\lambda_c$  is

$$\bar{V}(\mathbf{r}) = \frac{3}{4\pi\lambda_c^3} \int_{V_c} V(\mathbf{r} + \mathbf{r}') d^3 r' \simeq V(\mathbf{r}) + \frac{\lambda_c^2}{10} \nabla_{\mathbf{r}}^2 V(\mathbf{r}) + \dots$$

The second term on the right hand side is the Darwin term, but the factor 1/10 should be replaced by 1/8 if we obtain the term from the Dirac equation.

- (e) Show that the Darwin correction to the electronic energy levels is

$$E_D = -E_n \frac{(Z\alpha)^2}{n}, \quad l = 0.$$

(f) Show that the total energy correction is

$$E_{nj} = (E_{\text{kin}} + E_{\text{so}} + E_D) = E_n \left( \frac{Z\alpha}{n} \right)^2 \left[ \frac{n}{j+1/2} - \frac{3}{4} \right]$$

for **all** values of  $l$ . Note that the individual corrections depend on  $l$ , but the total correction does not depend on  $l$ . [Hint: Note that  $j = l \pm 1/2$ ; treat the  $j = l + 1/2$  and  $j = l - 1/2$  separately. You will get the same final answer either way.]

(g) The exact fine-structure energy for hydrogenic atom obtained by solving the relativistic Dirac equation is

$$E_{nj}^{\text{exact}} = m_e c^2 \left( \left[ 1 + \left( \frac{Z\alpha}{n - (j+1/2) + \sqrt{(j+1/2)^2 - Z^2\alpha^2}} \right)^2 \right]^{-1/2} - 1 \right).$$

Expand in powers of  $Z\alpha$  [upto order  $(Z\alpha)^4$ ] and show that you get

$$E_{nj}^{\text{exact}} \simeq E_n \left[ 1 + \left( \frac{Z\alpha}{n} \right)^2 \left[ \frac{n}{j+1/2} - \frac{3}{4} \right] \right],$$

which matches exactly with the perturbative results. Note that  $Z\alpha < 1$  as long as  $Z < 137$ .

9. **Isotope Shifts:** The protons in the nucleus are distributed in a finite volume. The electrostatic potential inside the nucleus is different from  $1/r$  law. Actual potential depends on the proton distribution within the nucleus. For simplicity, consider the nuclear charge is distributed uniformly within a sphere of radius  $R = r_0 A^{1/3}$ , where  $A$  is the atomic mass number and  $r_0 \sim 1.2 \times 10^{-15}$  fm.

(a) Show that, in this simple model, the electrostatic potential due to the nucleus of charge  $Ze$  is

$$\begin{aligned} V_0(r) &= \frac{Ze^2}{4\pi\epsilon_0 2R} \left( \frac{r^2}{R^2} - 3 \right), & r \leq R \\ &= -\frac{Ze^2}{4\pi\epsilon_0 r}, & r \geq R. \end{aligned}$$

(b) Calculate the first-order energy shift  $\Delta E$  to electronic energy levels of hydrogenic atoms.

(c) Estimate  $\Delta E$  for hydrogen atom and muonic atom.

(d) Calculate the first-order energy correction due to the Darwin term  $H_D = \frac{\lambda_c^2}{8} \nabla_{\mathbf{r}}^2 V_0(\mathbf{r})$ . Here  $\lambda_c$  is the Compton wavelength.

[You may use the condition  $R \ll a_0$  to evaluate the integral approximately. This calculation will give you a correction to  $E_D$  (obtained in the class based on point nucleus) due to finite size of the nucleus].

10. Show that in the linear Stark effect the  $n = 3$  level of a hydrogenic atom is splitting into five equally spaced levels. Calculate the expression for the level separation as a function of the electric field strength.

11. **Quenching of orbital angular momentum:** In a crystal, the electric field of neighboring ions perturbs the energy levels of an atom. As a crude model, imagine that a hydrogen atom in  $n = 2, l = 1$  state is surrounded by three pairs of point charges. Ignore spin of the electron. Now the potential energy of the electron due to the field arising from the atom's surroundings is of the following form:

$$H' = ax^2 + by^2 - (a + b)z^2,$$

where  $a$  and  $b$  are two constants with  $a > b$ . Show that the  $l = 1$  level of a hydrogenic atom splits into three distinct levels for  $a \neq b$ . Show that each state has a wave function of the form

$$\Psi(\mathbf{r}) = (\alpha x + \beta y + \gamma z)f(r),$$

where  $f(r)$  is a common function and each level has its own set of constants  $\alpha$ ,  $\beta$ , and  $\gamma$ . Show that  $\langle \Psi(\mathbf{r}) | \mathbf{L} | \Psi(\mathbf{r}) \rangle = 0$  for all the three states. This is known as the **quenching of orbital angular momentum** due to the strong crystal fields.

[Answer: The splitted energy levels are  $\epsilon_1 = -12a_0^2(a + b)$ ,  $\epsilon_2 = 12a_0^2b$  and  $\epsilon_3 = 12a_0^2a$ . Here  $a_0$  is the Bohr radius. The corresponding  $(\alpha, \beta, \gamma)$  are  $(1, 0, 0)$ ,  $(0, 1, 1)$  and  $(0, -1, 1)$ , respectively].

12. Consider an electron ( $q = -e$ ) moving on  $xy$  plane subjected to the uniform magnetic field  $\mathbf{B} = B\hat{z}$ .

- (a) Using the Landau gauge for the vector potential  $\mathbf{A} = Bx\hat{y}$ , show that its Hamiltonian is

$$H_0 = \frac{p_x^2}{2m} + \frac{(p_y + eBx)^2}{2m}.$$

- (b) Since the Hamiltonian  $H_0$  commutes with the momentum operator  $p_y$ ,  $[H_0, p_y] = 0$ , the total wave function can be decomposed as  $\psi(x, y) = \phi(x)e^{ik_y y}$ , where  $k_y$  is a number. Using this fact, show that the two-dimensional Hamiltonian  $H_0$  reduces to the following one-dimensional Hamiltonian:

$$H_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega_c^2(x + k_y l_0)^2.$$

Here  $\omega_c = eB/m$  and  $l_0 = \sqrt{\hbar/(eB)}$ .

Introducing the bosonic ladder operators as

$$b = \frac{1}{\sqrt{2}} \left[ \frac{\xi}{l_0} + i \frac{p_\xi}{p_0} \right], \quad b^\dagger = \frac{1}{\sqrt{2}} \left[ \frac{\xi}{l_0} - i \frac{p_\xi}{p_0} \right],$$

where  $\xi = x + k_y l_0^2$  and  $p_0 = \sqrt{\hbar m \omega_c}$ . Note that the origin of the coordinate system has been shifted along  $x$ -axis by a constant amount  $k_y l_0$ , such that the minimum of effective potential is at  $\xi = 0$ .

Show that the Hamiltonian can be expressed as

$$H_0 = \left( b^\dagger b + \frac{1}{2} \right) \hbar \omega_c.$$

Therefore its energy levels are  $E_n = (n + 1/2)\hbar\omega_c$  and the corresponding eigenfunctions are the oscillator wavefunctions  $\phi_n(\xi/l_0)$ .

- (c) Applying an in-plane electric field  $\mathbf{E} = E_x \hat{x}$ , so the dipole interaction term is  $V = eE_x x$ . Now the total Hamiltonian is  $H = H_0 + V$  which can be solved exactly. Show that the energy levels are

$$E_n = (n + 1/2)\hbar\omega_c - \hbar k_y v_d + \frac{1}{2}mv_d^2,$$

where  $v_d = E_x/B$  and the corresponding eigenfunctions are

- (d) Treat the dipole potential energy  $V = eE_x x$  as a perturbative term in the total Hamiltonian  $H$ .

Calculate the first-order and second-order energy corrections and compare with the exact result.

Calculate the first-order correction to the unperturbed eigenstate  $\phi_n$  and compare with the exact result.

13. **A Dirac electron subjected to crossed magnetic and electric fields:** Consider the Dirac electron (on a graphene sheet) in  $xy$  plane subject to constant magnetic field ( $\mathbf{B} = B\hat{z}$ ) is described by the Hamiltonian

$$H_0 = \hbar v_f \boldsymbol{\sigma} \cdot (\mathbf{k} + e\mathbf{A}/\hbar), \quad (1)$$

where  $\boldsymbol{\sigma}$  is the Pauli matrices and  $\mathbf{A}$  is the vector potential. For convenience, we choose  $\mathbf{A} = Bx\hat{y}$ . One can solve this Hamiltonian exactly [see “Graphene: Carbon in Two Dimesions” by M. I. Katsnelson, Cambridge University Press]. The energy levels are

$$E_n^{(0)} = \hbar\omega_c \sqrt{2n}, \quad n = 0, 1, 2, \dots$$

and the corresponding eigenstates are

$$\psi_{n,k_y}^{(0)}(x, y) = \frac{e^{ik_y y}}{\sqrt{2L_y}} \begin{pmatrix} \phi_{n-1}(\xi/l_0) \\ i\phi_n(\xi/l_0) \end{pmatrix}.$$

Here  $\omega_c = v_f/l_0$  with  $l_0 = \sqrt{\hbar/(eB)}$  and  $\phi_n(\xi)$  are the normalized oscillator wavefunctions with  $\xi = (x + k_y l_0^2)$ . Note that  $\phi_{-1}(\xi) = 0$ .

Applying an in-plane electric field  $\mathbf{E} = E_x \hat{x}$ , so the dipole interaction term is  $V = eE_x x \sigma_0$ , where  $\sigma_0$  is the  $2 \times 2$  identity matrix. Now the total Hamiltonian is  $H = H_0 + V$  which can be solved exactly using the Lorentz boost transformation [V Lukose, R. Shankar and G. Baskaran, Phys. Rev. Lett. **98**, 116802 (2007)]. The exact energy levels of the Hamiltonian  $H$  are given by

$$E_n = \hbar\omega_c \sqrt{2n} (1 - \beta^2)^{3/4} - \hbar v_f k_y \beta,$$

where  $\beta = v_d/v_f = E_x/(v_f B)$ . For typical experimental parameters,  $\beta \ll 1$ . Therefore we can have Taylor series expansion (keeping upto quadratic in  $\beta$ ) of the exact energy levels as

$$\begin{aligned} E_n &\simeq \hbar\omega_c \sqrt{2n} - \hbar v_f k_y \beta - \hbar\omega_c \sqrt{2n} \frac{3}{4} \beta^2 + \dots \\ &\simeq E_n^{(0)} - \hbar v_f k_y \beta - \frac{3E_n^{(0)}}{4} \beta^2 + \dots \end{aligned} \quad (2)$$

- (a) Treat the dipole energy term  $V = eE_x x \sigma_0 = \sigma_0 \hbar \omega_c (x/l_0) \beta$  as a perturbation to  $H_0$ . Obtain the first-order and second-order energy corrections for  $n > 0$  and compare with the series expansion of the exact result for  $n = 1, 2, 3$  and 4.

**Answers:**

$$\begin{aligned} E_n^{(1)} &= -\hbar v_f k_y \beta. \\ E_n^{(2)} &= \beta^2 \hbar \omega_c \left[ \frac{4n(\sqrt{n-1} - \sqrt{n+1}) - 6\sqrt{n} - \sqrt{n-1} - \sqrt{n+1}}{8\sqrt{2}} \right]. \end{aligned}$$

- (b) Show that for large  $n$  ( $n \rightarrow \infty$ ),

$$E_n^{(2)} \sim -E_n^{(0)} \frac{\beta^2}{2}.$$

14. **The Aharonov-Bohm ring geometry subjected to crossed magnetic and electric fields:** Consider an electron of charge  $e$  and mass  $M$  is free to move on a circle of radius  $R$  and negligible width. This ring is lying on  $xy$  plane and subjected to the uniform magnetic field  $\mathbf{B} = B\hat{z}$  perpendicular to the ring. We will consider the magnetic vector potential  $\mathbf{A} = (Br/2)\hat{\phi}$  in the circular gauge owing to the circular symmetry of the given problem.

- (a) Show that the Hamiltonian for the electron is

$$H_0 = \frac{\hbar^2}{2MR^2} \left( i \frac{\partial}{\partial \phi} + \frac{\Phi}{\phi_0} \right)^2.$$

Here  $\Phi = B\pi R^2$  is the total magnetic flux passing through the ring and  $\phi_0 = h/e$  is the unit of magnetic flux quanta.

- (b) Show that you will get the same Hamiltonian if you consider an infinitely long solenoid of radius  $R_s (< R)$  oriented along  $z$  axis placed at the center of the ring. In this case,  $\Phi$  will be replaced by  $\Phi_s = \pi R_s^2 B_s$ , where  $B_s = \mu_0 n_s I$  is the magnetic field inside the solenoid. Here  $n_s$  is the number of turns per unit length and  $I$  is the current flowing along the wire of the solenoid.
- (c) Show that the energy levels are

$$E_m^{(0)} = \frac{\hbar^2}{2MR^2} \left( m - \frac{\Phi}{\phi_0} \right)^2$$

and the corresponding normalized eigenstates

$$\langle \phi | m \rangle = \frac{1}{\sqrt{2\pi}} e^{im\phi}, \quad m \in Z.$$

- (d) Sketch/plot  $E_m$  (in units of  $\epsilon_0 = \hbar^2/(2MR^2)$ ) vs  $\Phi/\phi_0$  for different values of  $m$ . Identify the ground state and first excited state for a given  $\frac{\Phi}{\phi_0}$ .

Important observations:

Two successive angular momentum states  $|m\rangle$  and  $|m+1\rangle$  are crossing whenever  $\Phi/\phi_0 = m + 1/2$ .

In presence of the magnetic field,  $E_{+|m|}^{(0)} < E_{-|m|}^{(0)}$ , implying the magnetic field breaks the degeneracy.

For  $\mathbf{B} = 0$ , the ground state ( $m = 0$ ) has zero angular momentum. For  $\mathbf{B} \neq 0$ , the ground state ( $m = 0$ ) has finite angular momentum which gives rise to a persistent current.



- (e) Choosing magnetic field such that  $\Phi/\phi_0 = (m + 1/2) + \delta$  with  $\delta \ll 1$ , representing two energy levels slightly away from the degeneracy at  $\Phi/\phi_0 = (m + 1/2)$ . Show that energies and the corresponding eigenvectors of the two states at  $\Phi/\phi_0 = (m + 1/2) + \delta$  are

$$\begin{aligned} E_m^{(0)} &= \epsilon_0 \left( \frac{1}{2} + \delta \right)^2, & |m\rangle &= \frac{1}{\sqrt{2\pi}} e^{im\phi} \\ E_{(m+1)}^{(0)} &= \epsilon_0 \left( \frac{1}{2} - \delta \right)^2, & |m+1\rangle &= \frac{1}{\sqrt{2\pi}} e^{i(m+1)\phi}. \end{aligned} \quad (3)$$

- (f) Constructing a subspace spanned by the vectors  $|m\rangle$  and  $|m+1\rangle$ . What will be the matrix representation of  $H_0$  in this subspace? Express in terms of the Pauli matrices and identity matrix.
- (g) Now we apply an in-plane weak electric field  $\mathbf{E} = \hat{\mathbf{i}}E_1 \cos \phi + \hat{\mathbf{j}}E_2 \sin \phi$ , where  $\phi$  is the azimuthal angle. Show that the dipole interaction energy due to electric field is

$$H_1 = -eR(E_1 \cos \phi + E_2 \sin \phi).$$

What will be the matrix representation of  $H_1$  in the subspace defined earlier. Express in terms of the Pauli matrices and identity matrix.

- (h) Express the full Hamiltonian  $H = H_0 + H_1$  in a matrix form. Obtain eigenvalues and the eigenvectors.
- (i) Show that there is an energy gap at the level crossing is  $eR\sqrt{E_1^2 + E_2^2}$ , independent of  $m$ .

15. **Jaynes-Cummings model:** The Jaynes-Cummings (JC) Hamiltonian describes a two-level system interacting with the quantized electromagnetic field of a single mode. This model Hamiltonian has great importance in atomic physics, solid state physics, and quantum optics.

The JC model Hamiltonian is given by  $H_{JC} = H_0 + H_{\text{int}}$ , where

$$\begin{aligned} H_0 &= \hbar\omega_c \left( a^\dagger a + \frac{1}{2} \right) + \hbar\omega_a \frac{\sigma_z}{2} \\ H_{\text{int}} &= \frac{\hbar g}{2} (a\sigma_+ + a^\dagger\sigma_-). \end{aligned}$$

The first term in the free Hamiltonian  $H_0$  describes the quantized electromagnetic field with the energy  $\hbar\omega_c$ , whereas the second term describes a two-level system (TLS) with the energy separation  $\hbar\omega_a$ . Finally,  $H_{\text{int}}$  describes the interaction between TLS and the EM field. Here  $a^\dagger$  and  $a$  are the EM field mode creation and annihilation operators respectively, acting on the  $n$ -th oscillator states  $|n\rangle$  satisfying the properties:  $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$  and  $a|n\rangle = \sqrt{n}|n-1\rangle$ . Also,  $\sigma_\pm = (\sigma_x \pm i\sigma_y)/2$  represent raising and lowering operators in the Hilbert space spanned by  $(1,0)^T$  and  $(0,1)^T$ , where  $\mathcal{T}$  represents the transpose operation.

We are interested in the two regimes: (i) at resonance,  $\omega_c = \omega_a = \omega$  and (ii) nearly resonance,  $\omega_c \sim \omega_a$ .

- (a) Show that  $[H_0, H_{\text{int}}] = 0$  and  $[H_0, H_{JC}] = 0$  at resonance.
- (b) Show that the total number of excitation quanta is conserved,  $[N, H] = 0$ , where  $N = a^\dagger a + \sigma_+ \sigma_-$  is a constant of motion at resonance.

- (c) Show that doubly degenerate eigenvalues of  $H_0$  at resonance are  $E_n = (n+1)\hbar\omega$  and the corresponding eigenstates are

$$|\chi_n^+\rangle = |n\rangle \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} |n\rangle \\ 0 \end{pmatrix}, \quad |\chi_n^-\rangle = |n+1\rangle \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ |n+1\rangle \end{pmatrix}$$

for all the harmonic oscillator states  $|n\rangle$ . Here  $|\chi_n^+\rangle$  represents the TLS is in the excited state and  $n$  photons and  $|\chi_n^-\rangle$  represents the TLS is in the ground state and  $(n+1)$  photons.

Show that the ground state energy of the whole system is  $\epsilon_0 = 0$  and the corresponding state is  $(0, |0\rangle)$ .

- (d) In the off-resonant condition, the Hamiltonian  $H_0$  can be written as

$$H_0 = \hbar\omega_c \left( a^\dagger a + \frac{1}{2} + \frac{\sigma_z}{2} \right) + \frac{\hbar\delta}{2} \sigma_z,$$

where  $\delta = \omega_a - \omega_c$  is the detuning frequency. Show that the two eigenstates  $|\chi_n^\pm\rangle$  now have different eigenvalues

$$\tilde{E}_n^\pm = (n+1)\hbar\omega_c \pm \hbar\frac{\delta}{2}.$$

So the degeneracy is removed due to non-zero  $\delta$ . It provides  $n$  dimensional orthogonal Hilbert sub-spaces of dimension  $2 \times 2$ .

- (e) The interacting part  $H_{\text{int}}$  is an unique entangled state of TLS and EM field:  $H_{\text{int}}$  couples only those states that belong to a single subspace of dimension  $2 \times 2$ . It is sufficient to consider eigenspace of  $H_0$  at a given number of photons  $n$ :  $\{|\chi_n^+\rangle, |\chi_n^-\rangle\}$  with  $n = 0, 1, 2, \dots$ . Within each of these subspaces, show that the matrix representation of  $H_{JC}$  is

$$[H_{JC}]_n = \hbar \begin{pmatrix} (n+1)\omega_c + \frac{\delta}{2} & \frac{g}{2}\sqrt{n+1} \\ \frac{g}{2}\sqrt{n+1} & (n+1)\omega_c - \frac{\delta}{2} \end{pmatrix}$$

Show that the energy eigenvalues of  $H_{JC}$  for a given  $n$  are

$$E_n^\pm = (n+1)\hbar\omega_c \pm \frac{1}{2}\hbar\Omega_n,$$

where  $\Omega_n = \sqrt{\delta^2 + (n+1)g^2}$  is the Rabi frequency. At resonance ( $\delta = 0$ ), the splitting energy is

$$\Delta E_n = E_n^+ - E_n^- = \hbar g \sqrt{n+1}.$$

So  $\Delta E_n \propto \sqrt{n}$ , not  $n$ .

- (f) Show that the corresponding eigenvectors are

$$\begin{aligned} |n, +\rangle &= \cos(\theta_n/2) |\chi_n^+\rangle + \sin(\theta_n/2) |\chi_n^-\rangle, \\ |n, -\rangle &= \sin(\theta_n/2) |\chi_n^+\rangle - \cos(\theta_n/2) |\chi_n^-\rangle, \end{aligned} \quad (4)$$

where  $\theta_n = \tan^{-1}(\sqrt{n+1}g/\delta)$ .

- (g) Near the resonance  $\omega_a \sim \omega_c$ , so  $\delta \rightarrow 0$ , Assuming that  $g \ll \omega_c$  and  $H_{\text{int}}$  can be treated as a perturbation. Calculate first-order and second-order energy corrections to the unperturbed energy levels. Compare with the series expansion of the exact results.

Department of Physics, IIT-Kanpur

Instructor: Tarun Kanti Ghosh

Quantum Mechanics-II (PHY432)

AY 2024-25, SEM-II

Homework-2

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1. Consider a hydrogenic Hamiltonian (including the electron's spin magnetic moment) in presence of a static and uniform magnetic field  $\mathbf{B} = \nabla \times \mathbf{A}$ . Here  $\mathbf{A} = (\mathbf{B} \times \mathbf{r})/2$  is the vector potential.
  - (a) Show that the diamagnetic term can be neglected compared to the paramagnetic term if  $B \ll Z^2 10^6 / n^4$ .
  - (b) Now write down the full Hamiltonian by adding the three fine-structure correction terms.
2. **Weak-field Zeeman effect:** This is also known as Anomalous Zeeman effect.
  - (a) Find out the critical magnetic field ( $B_c$ ) below which the Zeeman interaction energy is less than the fine structure energy correction.
  - (b) What are the "good" quantum numbers in this case?
  - (c) The total magnetic moment of an electron in hydrogenic atoms is

$$\boldsymbol{\mu} = -\frac{\mu_B}{\hbar}(\mathbf{L} + 2\mathbf{S}),$$

where  $\mu_B$  is the Bohr magneton.

The quantum projection theorem (or Wigner-Eckart theorem) is given by

$$\langle jm_j | \mathbf{V} | jm_j \rangle = \frac{\langle jm_j | \mathbf{V} \cdot \mathbf{J} | jm_j \rangle \langle jm_j | \mathbf{J} | jm_j \rangle}{j(j+1)\hbar^2}.$$

Here  $\mathbf{V}$  is any vector operator and  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ . Using this theorem, show that the magnetic moment  $\boldsymbol{\mu}$  can be expressed as  $\boldsymbol{\mu} = -g_e \mu_B \mathbf{J} / \hbar$ , where the effective Lande- $g$  factor is

$$g_e = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)}.$$

Note that this expression of  $g_e$  is valid for weak magnetic field as well as for low values of  $Z$ .

[Hint: see Griffiths quantum mechanics book, page 289 (second edition)].

- (d) In the weak-field case, the perturbative Zeeman term can be written as

$$H_z = g_e \mu_B B J_z.$$

Calculate the Zeeman energy splitting of  $|nl\rangle$  and  $|np\rangle$  states. Compare these results with that obtained in class in different methods.

3. **Zeeman splitting for an arbitrary magnetic field  $B$ :** One can solve the Zeeman effect problem by diagonalizing the full Hamiltonian  $H = H_0 + H_{fs} + H_Z$  for an arbitrary magnetic field  $B$ . Consider the hydrogen atom in the first excited state ( $n = 2$ ). There are 8 degenerate states in this level. Use  $|jm_j\rangle$  as basis states for degenerate perturbation theory. Use the

Clebsch-Gordan co-efficients to express  $|jm_j\rangle$  as a linear combination of  $|lm_l\rangle$  and  $|sm_s\rangle$  states:

$$|jm_j\rangle = \sum_{m_l=m_l+m_s} C_{l,s,j}^{m_l,m_s} |lm_l, m_s\rangle.$$

For any  $l$  and  $s = 1/2$ , the  $|jm_j\rangle$  states as a linear combination of  $|lm_l m_s\rangle$  are given by

$$|j = l \pm \frac{1}{2}, m_j\rangle = \pm \sqrt{\frac{l \pm m_j + \frac{1}{2}}{2l+1}} |l \frac{1}{2} m_l = m_j - \frac{1}{2}, +\frac{1}{2}\rangle + \sqrt{\frac{l \mp m_j + \frac{1}{2}}{2l+1}} |l \frac{1}{2} m_l = m_j + \frac{1}{2}, -\frac{1}{2}\rangle.$$

[Hint: In order to solve the following problems, see Griffiths quantum mechanics book, page 293 (second edition)].

- Calculate the Zeeman energy levels for any arbitrary magnetic field  $B$ .
- Plot the Zeeman energy levels as a function of the field  $B$ .
- Now take two limiting cases: weak field and strong field. Compare your results of the limiting cases with that of obtained in class.

[Hint: see Griffiths quantum mechanics book, page 293 (second edition)].

- Zeeman effect in the hyperfine states:** Consider the ground state of a hydrogen atom in presence of a static and uniform magnetic field  $\mathbf{B} = B\hat{z}$ .

The effective Hamiltonian can be written as

$$H = \frac{A}{\hbar^2} \mathbf{I} \cdot \mathbf{S} + \frac{a}{\hbar} S_z - \frac{b}{\hbar} I_z, \quad (1)$$

where  $a = g_e \mu_B B$  and  $b = g_p \mu_N B$ .  $\mathbf{I} \cdot \mathbf{S}$  can be written in terms of the raising and lowering ladder operators:  $\mathbf{I} \cdot \mathbf{S} = I_z S_z + (I_+ S_- + I_- S_+)/2$ . We choose the following states as a basis states to diagonalize the above Hamiltonian:  $|M_I M_S\rangle : |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle$ . The most general wavefunction is

$$\Psi = d_1 |\uparrow\uparrow\rangle + d_2 |\downarrow\downarrow\rangle + d_3 |\uparrow\downarrow\rangle + d_4 |\downarrow\uparrow\rangle. \quad (2)$$

The spatial part of the wave function does not matter here because the Hamiltonian is space independent.

- Show that the matrix representation of  $H$  in the above basis states (maintain the order) can be written as

$$M = \begin{bmatrix} \frac{A}{4} + \frac{(a-b)}{2} & 0 & 0 & 0 \\ 0 & \frac{A}{4} - \frac{(a-b)}{2} & 0 & 0 \\ 0 & 0 & -\frac{A}{4} - \frac{(a+b)}{2} & \frac{A}{2} \\ 0 & 0 & \frac{A}{2} & -\frac{A}{4} + \frac{(a+b)}{2} \end{bmatrix}.$$

- Show that the eigenvalues are

$$E_{\pm} = \frac{A}{4} \pm \frac{(a-b)}{2} \quad (3)$$

$$\epsilon_{\pm} = -\frac{A}{4} \pm \sqrt{\frac{A^2}{4} + \frac{(a+b)^2}{4}}. \quad (4)$$

Obtain the corresponding eigenvectors.

- (c) Plot the Zeeman energy levels as a function of  $B$ . Indicate each level by the quantum numbers.
- (d) Obtain the energy levels in the two limiting cases: (i) weak-field and (ii) strong field.

[This problem is important if you want to understand how to trap alkali atoms magnetically. The wavelength (21 cm) corresponding to the hyperfine transition in the ground state of hydrogen atom can be measured with very high accuracy. An atomic clock and MASER can be made based on the hyperfine transition in the ground state of atomic hydrogen.]

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Homework problems  
PHY 432

**Department of Physics, IIT-Kanpur**

Instructor: Tarun Kanti Ghosh

Quantum Mechanics-II (PHY432)

AY 2024-25, SEM-II

**Homework-1**

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1. A one-dimensional harmonic oscillator (with oscillator frequency  $\omega$ ) is subjected to the following force

$$\mathbf{F}(t) = F_0 \frac{\tau/\omega}{t^2 + \tau^2} \hat{\mathbf{x}}, \quad -\infty < t < +\infty.$$

Here  $\tau$  is a time constant. The time-dependent perturbation is

$$V(t) = \frac{F_0 \tau}{\omega} \frac{x}{t^2 + \tau^2}, \quad -\infty < t < +\infty.$$

The oscillator is prepared in the ground state at  $t = -\infty$ .

- (a) Within the first-order time-dependent perturbation theory, calculate the transition probability to other excited states at  $t = \infty$ .

$$P_{10} = |c_1^{(1)}(t \rightarrow \infty)|^2 = \frac{(F_0 \pi)^2}{2m \hbar \omega^3} e^{-2\omega\tau}.$$

- (b) Analyse the result for the following limiting cases: (i)  $\omega\tau \ll 1$  and (ii)  $\omega\tau \gg 1$ .

- (c) When  $\tau \rightarrow 0$ , the time-dependent perturbation can be re-written as

$$V(t) = \frac{F_0 \pi}{\omega} \delta(t).$$

Calculate the transition probability for the  $\delta$  perturbation and compare with the previous result for  $\omega\tau \ll 1$  case.

2. Consider a one-dimensional quantum harmonic oscillator with the oscillation frequency  $\omega$  is perturbed during  $t = 0$  to  $t = T$  and it is given by

$$V(t) = \lambda m \omega^2 x^2, \quad 0 < t \leq T.$$

Here  $\lambda < 1$  and  $T$  is some time-scale, not necessarily to be the time-period of the oscillator.

- (a) Obtain the allowed transitions from the initial state  $|i\rangle$  to the final state  $|f\rangle \neq |i\rangle$ .

- (b) Show that the first-order transition probability is

$$P_{fi} = \frac{4|V_{fi}|^2}{\hbar^2 \omega_{fi}^2} \sin^2(\omega_{fi} T/2).$$

3. A quantum harmonic oscillator is subjected to a time-periodic  $\delta$  kicks with the periodicity  $T$  as given by

$$\mathbf{F}(t) = \frac{F_0}{\omega} \sum_{k=0}^{\infty} p^k \delta(t - kT) \hat{\mathbf{x}}.$$

Here  $p < 1$  and the factor  $p^k$  is implying that kick is reduced at each time interval. The oscillator is prepared in a state  $|n\rangle$  at  $t = 0$ . Within the first-order time-dependent perturbation

theory, calculate the transition probability to other states  $|m\rangle \neq |n\rangle$  at  $t = \infty$ . Analyse the result for the two limiting cases: (i)  $\omega T \ll 1$  and (ii)  $\omega T \gg 1$ .

Repeat the same problem for the  $\delta$  kicks applied over a finite time  $NT$  as described by

$$\mathbf{F}(t) = \frac{F_0}{\omega} \sum_{k=0}^{N-1} \delta(t - kT) \hat{\mathbf{x}}.$$

4. A hydrogen atom in its ground state is subjected to the electric field  $\mathbf{E} = E_0 e^{-t/\tau} \theta(t) \hat{\mathbf{r}}$ , where  $\hat{\mathbf{r}}$  is the unit vector in the radial direction.
  - (a) Calculate the transition amplitude from the initial state  $|100\rangle$  to the final states  $|2lm\rangle$ , within the first-order time-dependent perturbation theory. For  $n = 2$ :  $l = 0, 1$  and for  $l = 1$ :  $m = -1, 0, 1$ .
  - (b) Repeat the same problem if the electric field is given as

$$\mathbf{E} = E_0 \cos(\Omega t) e^{-t/\tau} \theta(t) \hat{\mathbf{r}}.$$

5. Consider a one-dimensional quantum harmonic oscillator with the oscillation frequency  $\omega$  is perturbed by

$$V(t) = \frac{1}{2} m \omega^2 x^2 \cos(\Omega t) e^{-t/\tau} \theta(t)$$

Here  $\Omega$  and  $\tau$  are positive constants.

- (a) Calculate the probability of transition from the state  $|n\rangle$  and to the state  $|m\rangle$ .
  - (b) Find out the selection rules for which the transitions are allowed.
  - (c) Analyze the features that may arise when  $\Omega \rightarrow \omega$  and  $\tau \rightarrow 0$  as well as  $\tau \rightarrow \infty$ .
6. **Dynamics of a two-level quantum system:** Consider a quantum system with just two energy levels  $E_0$  and  $E_1 > E_0$  with corresponding states  $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$  and  $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ , respectively.

The Hamiltonian can be expressed as

$$H_0 = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix} \quad (1)$$

For example, an electron's spin in presence of  $\mathbf{B} = B_z \hat{\mathbf{z}}$ :  $H_0 = -(g\mu_B B_z/2)\sigma_z$  with  $E_0 = -(g\mu_B B_z/2)$  and  $E_1 = +(g\mu_B B_z/2)$ . Here we are assuming  $q = +e$ .

- (a) Applying a rotating magnetic field:

$$\mathbf{B}(t) = B_0 [\cos(\omega t + \phi) \hat{\mathbf{x}} - \sin(\omega t + \phi) \hat{\mathbf{y}}],$$

where  $\phi$  is a constant phase angle. It interacts with the electron's spin. Show that the time-dependent perturbation takes the following form:

$$V(t) = \begin{pmatrix} 0 & \delta e^{i\omega t} \\ \delta^* e^{-i\omega t} & 0 \end{pmatrix}.$$

Here  $\delta = |\delta| e^{i\phi} = (g\mu_B B_0/2) e^{i\phi}$  is a time-independent complex number with the constant phase  $\phi$ . This perturbation induces a transition between the two states.

- (b) Express the total Hamiltonian  $H(t) = H_0 + V(t)$  in terms of the Pauli matrices and  $2 \times 2$  identity matrix  $\sigma_0$ .
- (c) Express the total Hamiltonian  $H(t)$  in terms of the four matrix operators:  $|0\rangle\langle 0|, |0\rangle\langle 1|, |1\rangle\langle 0|, |1\rangle\langle 1|$ .
- (d) Obtain the time-dependent perturbation  $V(t)$  in the Interaction representation i.e.

$$V_I(t) = e^{iH_0 t} V(t) e^{-iH_0 t}.$$

- (e) The most general state can be written in the Interaction representation as

$$|\psi(t)\rangle_I = c_0(t)|0\rangle + c_1(t)|1\rangle,$$

where the coefficients  $c_0(t)$  and  $c_1(t)$  satisfy the normalization condition  $|c_0(t)|^2 + |c_1(t)|^2 = 1$ . The initial conditions are given by  $c_0(0) = 1$  and  $c_1(0) = 0$ .

Show that the time-evolution of the expansion coefficients can be obtained as

$$\begin{aligned} c_0(t) &= e^{i(\omega - \omega_{10})t} \left[ \cos(\Omega t) - i \frac{(\omega - \omega_{10})}{2\Omega} \sin(\Omega t) \right], \\ c_1(t) &= -\frac{i\delta^*}{\hbar\Omega} \sin(\Omega t), \end{aligned}$$

with the Rabi frequency  $\Omega$  is given by

$$\Omega = \sqrt{\frac{|\delta|^2}{\hbar^2} + \frac{(\omega - \omega_{10})^2}{4}}.$$

- (f) Show that the probability of finding the system at level  $|1\rangle$  at time  $t$  is

$$|c_1(t)|^2 = \frac{|\delta|^2}{|\delta|^2 + \hbar^2(\omega - \omega_{10})^2/4} \sin^2(\Omega t)$$

and the probability of finding the system at level  $|0\rangle$  at time  $t$  is

$$|c_0(t)|^2 = 1 - |c_1(t)|^2.$$

It clearly shows that there is a transfer of probability as time goes on. The amplitude of the probability has the Lorentzian shape.

**Off-resonance case:** For  $\omega \neq \omega_{10}$ , the probability  $c_1$  will never reach to one since the amplitude of  $|c_0(t)|^2 < 1$  at all times.

**On-resonance case:** Maximum transition probability, i.e. unit probability can be achieved at resonance  $\omega = \omega_{10}$  and at times  $t_n$  satisfying the condition  $\sin(|\delta|t/\hbar) = 1$ , or

$$t_n = \frac{\hbar}{|\delta|} (n + 1/2)\pi, \quad n = 0, 1, 2, \dots$$

- (g) Plot the  $|c_1(t)|^2$  and  $|c_0(t)|^2$  as a function of  $\omega_x t$  for the two cases: (i) on-resonance and (ii) off-resonance. Here  $\omega_x = g\mu_B B_0/(2\hbar)$ .
- (h) Construct the spinors  $|\psi(t)\rangle_I$  and  $|\psi(t)\rangle_S$ .
- (i) Calculate expectation value of  $\boldsymbol{\sigma}$  in both the representations i.e. Interaction as well as Schrödinger representations. Are the expectation values same?



- (j) Plot the expectation values of the Pauli matrices ( $\langle \sigma_j \rangle$  with  $j = x, y, z$ ) as a function of  $\omega_x t$  for the two cases: (i) on-resonance and (ii) off-resonance. Here  $\omega_x = g\mu_B B_0 / (2\hbar)$ .
- (k) Calculate the transition probability from the state  $|0\rangle$  to the state  $|1\rangle$  using the first-order perturbation theory and compare with the exact results.

**7. Dynamics of a three-level quantum system:** Consider a quantum system with just three energy levels  $E_1$ ,  $E_2$  and  $E_3$  with corresponding states  $|1\rangle$ ,  $|2\rangle$  and  $|3\rangle$ , respectively. Assuming  $E_3 > E_2 > E_1$ . The Hamiltonian can be expressed as

$$H_0 = \begin{pmatrix} E_1 & 0 & 0 \\ 0 & E_2 & 0 \\ 0 & 0 & E_3 \end{pmatrix} \quad (2)$$

Applying a time-dependent perturbation of the following form:

$$V(t) = \begin{pmatrix} 0 & \delta^* e^{-i\omega t} & 0 \\ \delta e^{i\omega t} & 0 & \delta^* e^{-i\omega t} \\ 0 & \delta e^{i\omega t} & 0 \end{pmatrix}.$$

Here  $\delta = |\delta|e^{i\phi}$  is an time-independent complex number with the constant phase  $\phi$ . This perturbation induces a transition among the three states.

- (a) First obtain the eigenvectors  $|n\rangle$  with  $n = 1, 2, 3$ , correspond to the energy eigenvalues  $E_n$  for  $H_0$ .
- (b) Express the total Hamiltonian  $H(t) = H_0 + V(t)$  in terms of the spin-1 matrices and  $3 \times 3$  identity matrix  $S_0$ .
- (c) Express the total Hamiltonian  $H(t)$  in terms of the nine matrix operators:  $|1\rangle\langle 1|, |1\rangle\langle 2|, |1\rangle\langle 3|, |2\rangle\langle 1|, |2\rangle\langle 2|, |2\rangle\langle 3|, |3\rangle\langle 1|, |3\rangle\langle 2|, |3\rangle\langle 3|$ .
- (d) Obtain the time-dependent perturbation  $V(t)$  in the Interaction representation i.e.

$$V_I(t) = e^{iH_0 t} V(t) e^{-iH_0 t}.$$

- (e) The most general state can be written in the Interaction representation as

$$|\psi(t)\rangle_I = c_1(t)|1\rangle + c_2(t)|2\rangle + c_3(t)|3\rangle,$$

where the coefficients  $c_1(t)$ ,  $c_2(t)$  and  $c_3(t)$  satisfy the normalization condition  $|c_1(t)|^2 + |c_2(t)|^2 + |c_3(t)|^2 = 1$ .

- (a) Obtain coupled equations of motion of the expansion coefficients.
- (b) The initial conditions are given by  $c_1(0) = 1$  and  $c_2(0) = c_3(0) = 0$ . Check if you can solve the time-evolution of the expansion coefficients exactly or not.
- (c) Within the first-order time-dependent perturbation theory, calculate the transition probabilities  $P_{21}(t)$ ,  $P_{31}(t)$  and  $P_{32}(t)$ . [Convention:  $P_{f \leftarrow i} = P_{fi}$ ]

Department of Physics, IIT-Kanpur

Instructor: Tarun Kanti Ghosh

Quantum Mechanics-II (PHY432)

AY 2024-25, SEM-II

Homework-4

1. Consider a **free** electron interacting with a single photon of energy  $\hbar\omega$ . For the time being, assume a free electron can absorb or emit a photon. The initial and final wave functions can be taken to be  $\psi_i \sim e^{i\mathbf{k}_i \cdot \mathbf{r}}$  and  $\psi_f \sim e^{i\mathbf{k}_f \cdot \mathbf{r}}$ , respectively. Here  $\mathbf{k}_i$  and  $\mathbf{k}_f$  are the initial and final wavevectors of the free electron.

Using the most general expression of the transition rates for the absorption and emission, show that a free electron can not absorb or emit a photon.

2. **Equivalence between “potential picture” and “field picture” of the atom-field interaction.** Here “atom-field” interaction means interaction between an atom and an electromagnetic field. The vector potential responsible for the spontaneous emission is given by

$$\mathbf{A}(\mathbf{r}, t) = \sqrt{\frac{2\hbar}{V\epsilon_0\omega}} \frac{1}{2} \sum_{p=1,2} \boldsymbol{\epsilon}_p e^{-i(\mathbf{k} \cdot \mathbf{r} - \omega t)}.$$

Within the dipole approximation  $e^{-i\mathbf{k} \cdot \mathbf{r}} \sim 1$ , the vector potential is reduced to

$$\mathbf{A}(\mathbf{r}, t) = \sqrt{\frac{\hbar}{2V\epsilon_0\omega}} \sum_{p=1,2} \boldsymbol{\epsilon}_p e^{i\omega t}.$$

The corresponding electric field is

$$\mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{A}(\mathbf{r}, t)}{\partial t} = -i\sqrt{\frac{\hbar\omega}{2V\epsilon_0}} \sum_{p=1,2} \boldsymbol{\epsilon}_p e^{i\omega t}$$

and the magnetic field is  $\mathbf{B}(\mathbf{r}, t) = 0$ .

- (a) The atom-field interaction term in terms of vector potential is given by

$$H_{\text{int}}^{\text{pot}} = \frac{e}{m} \mathbf{A}(\mathbf{r}, t) \cdot \mathbf{p},$$

where  $\mathbf{A}(\mathbf{r}, t)$  is the vector potential generating both the electric and magnetic fields, whereas the momentum operator  $\mathbf{p}$  is acting on the atomic states.

Within the first-order time-dependent perturbation theory, show that the total spontaneous emission rate for unpolarized radiation is

$$\widetilde{W}_{\text{spont}} = \frac{4\alpha}{3c^2} \omega_{if}^3 |\mathbf{r}_{fi}|^2,$$

where  $\alpha = e^2/(4\pi\epsilon_0\hbar c)$  is the fine structure constant.

- (b) The atom-field interaction term  $H_{\text{int}}$  can also be expressed in terms of the electric field, instead of vector potential, as

$$H_{\text{int}}^{\text{field}} = e\mathbf{r} \cdot \mathbf{E}(\mathbf{r}, t),$$

where the electric field is  $\mathbf{E}(\mathbf{r}, t) = -\frac{\partial \mathbf{A}}{\partial t}$ .

Calculate the emission rate using  $H_{\text{int}}^{\text{field}}$  and compare with the previous result.

3. Consider an electron ( $q = -e$ ) is trapped in a one-dimensional harmonic oscillator potential  $V(x) = \frac{1}{2}m_e\omega_0^2x^2$ .

- (a) Obtain the spontaneous emission rate for the transition from the excited state  $|n\rangle$  to the lower state  $|n-m\rangle$ . Note that the emitted photon has the same frequency as the classical oscillator.

Answer:

$$W_{\text{spon}} = \frac{4n\alpha\hbar\omega_0^2}{6m_e c^2} = \frac{ne^2\omega_0^2}{6\pi\epsilon_0 m_e c^3}.$$

- (b) Show that the radiated power is

$$P = \hbar\omega_0 W_{\text{spon}} = \frac{e^2\omega_0^2(n\hbar\omega_0)}{6\pi\epsilon_0 m_e c^3}.$$

According the classical electrodynamics, power radiated by an oscillating electron is

$$P_{\text{classical}} = \frac{e^2 a^2}{6\pi\epsilon_0 c^3},$$

where  $a$  is the acceleration. Compare the quantum result with that of the classical result.

- (c) Estimate the spontaneous emission rate and life time of the excited state if  $|n=3\rangle$  for  $\omega_0 = 10^{14}$  rad/sec.
- (d) Check whether the dipole approximation is valid or not in this problem.
4. Consider the transition from  $2p$  states to  $1s$  state in a hydrogen atom. Assuming all the three sub-levels of  $2p$  state are equally populated. Total spontaneous emission rate can be written as

$$W_{\text{spon}} = \frac{4\alpha}{3c^2}\omega_{if}^3 |\mathbf{r}_{fi}|^2 \rightarrow \frac{4\alpha}{3c^2}\omega_{if}^3 \frac{1}{3} \sum_{m=0,\pm 1} |\mathbf{r}_{fi}|^2.$$

Here  $\alpha = e^2/(4\pi\epsilon_0\hbar c)$ ,  $|i\rangle = |2, 1, m\rangle$  with  $m = 0, \pm 1$  and  $|f\rangle = |1, 0, 0\rangle$ . Calculate

$$\widetilde{W}_{\text{spon}} = \frac{4\alpha}{9c^2}\omega_{if}^3 \sum_{m=0,\pm 1} |\mathbf{r}_{fi}|^2.$$

Hint:

$$|\hat{\mathbf{r}}_{fi}|^2 = |\langle f|\hat{\mathbf{r}}|i\rangle|^2 = |\langle f|\sin\theta\cos\phi|i\rangle|^2 + |\langle f|\sin\theta\sin\phi|i\rangle|^2 + |\langle f|\cos\theta|i\rangle|^2.$$

5. Consider an isotropic two-dimensional harmonic oscillator.
6. The vector potential operator  $\mathbf{A}(\mathbf{r}, t)$  for a monochromatic electromagnetic field with frequency  $\omega$  confined in cube of volume  $V = L^3$  is given by

$$\mathbf{A}(\mathbf{r}, t) = \sqrt{\frac{2\hbar}{V\epsilon_0\omega}} \frac{1}{2} \sum_{p=1,2} \boldsymbol{\epsilon}_p \left[ a e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)} + a^\dagger e^{-i(\mathbf{k}\cdot\mathbf{r}-\omega t)} \right].$$

Calculate the electric field operator  $\mathbf{E}(\mathbf{r}, t)$  and the magnetic field operator  $\mathbf{B}(\mathbf{r}, t)$ .

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**Homework-5 (Classical and quantum scattering )**

1. Consider a classical scattering process by a 3D hard sphere of radius  $R$  as shown in the diagram [Fig. 1]. The hard sphere potential is given by  $V(r) = \infty$  for  $r \leq R$ , otherwise zero.

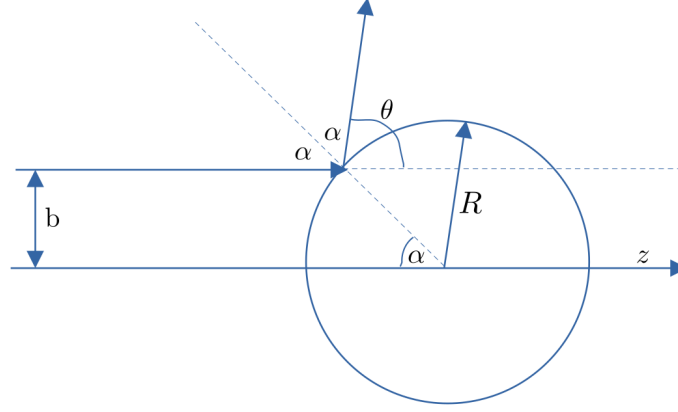


Figure 1: Sketch of a scattering event from a hard sphere scatterer.

- (a) Obtain the relation between the impact parameter  $b$  and the scattering angle  $\theta$  as shown in the diagram.
  - (b) Calculate the differential scattering cross-section  $D(\theta) \equiv \frac{d\sigma}{d\Omega}$ . Here  $d\sigma = b db d\phi$  and  $d\Omega = \sin\theta d\theta d\phi$ . Note that  $\frac{d\sigma}{d\Omega}$  is not the usual derivative!
  - (c) Calculate the total scattering cross-section  $\sigma_T = \int D(\theta) d\Omega$ .
2. Consider a classical scattering process by a 2D hard disk of radius  $R$ .

- (a) Draw a sketch of a scattering event from a hard disk scatterer. Obtain the relation between the impact parameter  $b$  and the scattering angle  $\phi$ . Here the incident particles are moving along  $x$  axis and the scattering angle  $\phi$  is measured with respect to the  $x$ -axis.
- (b) Show that the “differential scattering cross-section” is

$$D(\phi) \equiv \frac{db}{d\phi} = \frac{R}{2} \left| \sin \frac{\phi}{2} \right|.$$

Note the dimension of the differential scattering cross-section.

- (c) Show that the total scattering cross-section is  $\sigma_T = \int D(\phi) d\phi = 2R$ .
3. **Rutherford scattering:** Consider an incident particle of charge  $q_1$  with kinetic energy  $E$  scatters a heavy particle of charge  $q_2$ . Here the scattering potential is the Coulomb potential between the two charges.

- (a) Show that the impact parameter  $b$  can be obtained as

$$b = \frac{q_1 q_2}{8\pi\epsilon_0 E} \cot(\theta/2),$$

where  $\theta$  is the scattering angle.

- (b) Show that the differential scattering cross-section is

$$D(\theta) = \left[ \frac{q_1 q_2}{16\pi\epsilon_0 E \sin^2(\theta/2)} \right]^2.$$

- (c) You will see that the total cross-section is not finite. This is because the Coulomb potential has infinite range.

[It is not easy to solve this problem. See the classical mechanics book by Goldstein or any other standard books].

4. **Partial wave analysis:** Consider a particle with energy  $E = \hbar^2 k^2 / (2m)$  is moving towards a static hard-sphere of radius  $R$ . Our aim is to calculate scattering cross-section quantum mechanically.

- (a) The most general solution outside the hard-sphere potential ( $r > R$ ) can be written as

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos \theta) [a_l j_l(kr) + b_l n_l(kr)],$$

As  $r \rightarrow \infty$ , the asymptotic expressions of  $j_l(x)$  and  $n_l(x)$ :

$$j_l(x) \sim \frac{\sin(x - l\pi/2)}{x}, \quad n_l(x) \sim -\frac{\cos(x - l\pi/2)}{x}.$$

Use these asymptotic expressions, show that  $\psi(\mathbf{r})$  in the asymptotic limit can be expressed as

$$\psi(\mathbf{r}) \sim \sum_{l=0}^{\infty} \frac{(2l+1)}{2i} P_l(\cos \theta) \left[ (a_l - ib_l) \frac{e^{ikr}}{kr} + (-1)^{l+1} (a_l + ib_l) \frac{e^{-ikr}}{kr} \right].$$

- (b) The scattering amplitude  $f(\theta)$ , which is the coefficient of the outgoing wave ( $\frac{e^{ikr}}{kr}$ ) must be a purely imaginary, so we can write  $a_l - ib_l = e^{2i\delta_l}$  and  $a_l + ib_l = 1$ . Show that

$$a_l = \cos \delta_l e^{i\delta_l}, \quad b_l = -\sin \delta_l e^{i\delta_l}.$$

these expansion coefficients are obtained using the asymptotic limits of  $j_l$  and  $n_l$ . But they will be equally valid for all range of  $r > R$ . Moreover, we will see that  $l = 0$  is the most dominating term and the asymptotic expressions for  $l = 0$  match exactly with the exact expressions. Thus we can safely use the expressions of  $a_l$  and  $b_l$ . Also,  $\psi(r)$  we are considering for  $r > R$ , for large  $R$  asymptotic expressions are matching quite well.

Therefore the most general solution outside the hard-sphere potential ( $r > R$ ) can be re-written as

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos \theta) e^{i\delta_l} [\cos \delta_l j_l(kr) - \sin \delta_l n_l(kr)],$$

- (c) Using the boundary condition,  $\psi(r = R) = 0$ , show that

$$\tan \delta_l = \frac{j_l(kR)}{n_l(kR)}.$$

- (d) Calculate the phase shifts  $\delta_l$  for the first three partial waves ( $l = 0, 1, 2$ ) for (i)  $kR = \pi/6$  and (ii)  $kR = \pi/4$ .
- (e) **Low-energy approximation:** In the low-energy limit,  $kR \ll 1$ , we know

$$j_l(kR) \sim \frac{(kR)^l}{(2l+1)!!}, \quad n_l(kR) \sim -\frac{(2l-1)!!}{(kR)^{l+1}}.$$

Show that in the low-energy limit ( $kR \ll 1$ ) the phase shift is

$$\delta_l \sim -\frac{(kR)^{2l+1}}{(2l+1)!!(2l-1)!!}.$$

It clearly shows that the maximum phase shift occurs for  $l = 0$  and it decreases with increase of  $l$ . The maximum phase shift is  $\delta_0 = -kR$ .

As  $l$  increases, the wavefunction sprades away from the scatterer and so the overlap with the potential decreases. This lead to a smaller phase shift.

- (f) We know that the total cross-section is

$$\sigma_T = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l.$$

Calculate  $\sigma_T$  keeping contributions from the first three partial waves for (i)  $kR = \pi/6$  and  $kR = \pi/4$ .

- (g) Using the trigonometric relation,  $\sin^2 \delta_l = \tan^2 \delta_l / (1 + \tan^2 \delta_l)$ , show that the total cross-section in the low-energy limit is

$$\sigma_T \sim 4\pi R^2 [1 + \mathcal{O}(kR)^4 + \dots].$$

This is four times larger than the classical result.

5. Consider a scattering process by a spherically symmetric potential well

$$\begin{aligned} V(r) &= -V_0, & r \leq R \\ &= 0, & r > R. \end{aligned}$$

Show that in the low-energy limit  $kR \ll 1$ , the total cross-section for  $l = 0$  partial wave is given by

$$\sigma_T = 4\pi R^2 \left[ 1 - \frac{\tan(qR)}{qR} \right]^2,$$

where  $q^2 = 2m(E + V_0)/\hbar^2 = k^2 + 2mV_0/\hbar^2$  with  $m$  being mass of the incident particle.

6. Consider a scattering process by a three-dimensional  $\delta$ -function shell of radius  $R$  as described by  $V(r) = V_0\delta(r - R)$ .

- (a) Show that the s-wave phase shift  $\delta_0$  is given by

$$\sin^2 \delta_0 = \frac{\beta^2 \sin^4 x}{x^2 + x\beta \sin(2x) + \beta^2 \sin^2 x}.$$

Here  $x = kR$  and  $\beta = 2mV_0R/\hbar^2$ .

- (b) Show that the total cross-section in the low-energy limit is

$$\sigma_T = 4\pi R^2 \left[ \frac{\beta}{1 + \beta} \right]^2.$$

7. Show that

$$G(\mathbf{r}, \mathbf{r}') \equiv \int \frac{d^3 k'}{(2\pi)^3} \left[ \frac{e^{i\mathbf{k}' \cdot (\mathbf{r} - \mathbf{r}')}}{k^2 - (k')^2 \pm i\epsilon} \right] = -\frac{1}{4\pi} \frac{e^{\pm ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}$$

8. Show that

$$\psi(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} + \frac{2m}{\hbar^2} \int d^3 r' \left[ -\frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|} \right] V(\mathbf{r}') \psi(\mathbf{r}')$$

is the solution of the following Schrödinger equation

$$\left[ -\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}),$$

with  $E = \hbar^2 k^2 / (2m)$ .

9. **Born approximation:** The scattering amplitude within the first-order Born approximation is given by

$$f_B(\theta) = -\frac{m}{2\pi\hbar^2} \int d^3 r' e^{i\mathbf{q} \cdot \mathbf{r}'} V(\mathbf{r}').$$

Here  $m$  is the mass of the incident particle,  $V(\mathbf{r})$  is the scattering potential,  $\mathbf{q} = \mathbf{k}_s - \mathbf{k}$  is the change in the wave vector and  $q^2 = 2k^2(1 - \cos \theta)$ .

- (a) Calculate the scattering amplitude within the Born approximation for the following scattering potential:

$$V(\mathbf{r}) = V_0 \lambda^3 \delta^3(\mathbf{r}), \quad V(\mathbf{r}) = V_0 \lambda^5 \nabla^2 \delta^3(\mathbf{r}), \quad V(\mathbf{r}) = V_0 e^{-r^2/(4\lambda^2)}.$$

Here  $V_0$  has the dimension of energy and  $\lambda$  has the dimension of length.

- (b) **Soft sphere potential:** Consider the following finite spherical potential barrier:

$$\begin{aligned} V(r) &= V_0, & r &\leq R \\ &= 0, & r &> R. \end{aligned}$$

- (i) Show that the scattering amplitude is

$$f_B(\theta) = -\frac{2mV_0R^3}{\hbar^2} \left[ \frac{\sin(qR) - (qR) \cos(qR)}{(qR)^3} \right],$$

where  $q = 2k \sin(\theta/2)$ .

For a given  $kR = 1/2$ , find the scattering angles  $\theta$  at which  $f_B(\theta) = 0$ .

- (ii) Show that the total scattering cross-section is

$$\sigma_T = \pi R^2 \left[ \frac{2mV_0 R^2}{\hbar^2} \right]^2 F(d),$$

where the function  $F(d)$  is given by

$$F(d) = \left[ \frac{2d^4 - 2d^2 - 1 + 2d \sin(2d) + \cos(2d)}{d^6} \right],$$

with  $d = 2kR$ .

- (iii) Plot  $F(d)$  vs  $d$ . Show that  $F(d) \sim 4/9 - 2d^2/(45) + \dots$  as  $d \rightarrow 0$ . [Take the limit  $d \rightarrow 0$  carefully].

From the plot, show that the maximum value of  $F(d)$  is  $4/9$  at  $d = 0$ .

- (iv) Show that the maximum total cross-section is

$$\sigma_T^{\max} = 4\pi R^2 \left[ \frac{V_0}{3} \frac{2mR^2}{\hbar^2} \right]^2.$$

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**Homework-6 (Relativistic quantum mechanics)**

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1. **Klein-Gordon equation:** The Klein-Gordon (KG) equation is given by

$$\frac{1}{c^2} \frac{\partial^2 \psi(\mathbf{r}, t)}{\partial t^2} = \nabla^2 \psi(\mathbf{r}, t) - \left( \frac{m_e c}{\hbar} \right)^2 \psi(\mathbf{r}, t),$$

where  $\psi(\mathbf{r}, t)$  is a single-component wave function.

- (a) Obtain the following continuity equation from the KG equation:

$$\frac{\partial P}{\partial t} + \nabla \cdot \mathbf{J} = 0,$$

where the probability density is given by

$$P(\mathbf{r}, t) = \frac{i\hbar}{2m_e c^2} \left[ \psi^*(\mathbf{r}, t) \frac{\partial \psi(\mathbf{r}, t)}{\partial t} - \psi(\mathbf{r}, t) \frac{\partial \psi^*(\mathbf{r}, t)}{\partial t} \right]$$

and the probability current density is given by

$$\mathbf{J}(\mathbf{r}, t) = \frac{\hbar}{2im_e} [\psi^*(\mathbf{r}, t) \nabla \psi(\mathbf{r}, t) - \psi(\mathbf{r}, t) \nabla \psi^*(\mathbf{r}, t)].$$

- (b) Show that the probability density is negative for negative energy branch.  
What will be the probability density if  $\psi(\mathbf{r}, t)$  is real?
- (c) Can we obtain/define a velocity operator from the KG equation?

2. **Properties of the Dirac matrices:** The Dirac matrices are given as

$$\alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad (1)$$

where  $j = x, y, z$ , Pauli matrices  $\sigma_j$ ,  $2 \times 2$  null matrix  $0$  and  $2 \times 2$  identity matrix  $I$ .

- (a) Check that  $\alpha_j^2 = I_{4 \times 4}$  and  $\beta^2 = I_{4 \times 4}$ .
- (b) Show that  $\{\alpha_i, \alpha_j\} = 2I_{4 \times 4} \delta_{ij}$  and  $\{\alpha_i, \beta\} = 0$ .
- (c) Show that

$$\alpha_j \alpha_k = i \epsilon_{jkl} \begin{pmatrix} \sigma_l & 0 \\ 0 & \sigma_l \end{pmatrix},$$

where  $j, k, l : x, y, z$ .

3. The Dirac equation for a free particle is given by

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = H \psi(\mathbf{r}, t),$$

where the Dirac Hamiltonian  $H$  is given by

$$H = c \boldsymbol{\alpha} \cdot \mathbf{p} + \beta m_e c^2$$

and the Dirac spinor is represented as  $\psi^\dagger = (\psi_1^*, \psi_2^*, \psi_3^*, \psi_4^*)$ .

- (a) Write down the Dirac equation explicitly in  $4 \times 4$  matrix form.
- (b) Show that the velocity operator for a Dirac particle is  $\hat{\mathbf{v}} = c\boldsymbol{\alpha}$ .  
Note that the velocity operator in Dirac theory is a purely matrix operator  $\boldsymbol{\alpha}$ , as opposed to the differential operator (in real space) in non-relativistic case.
- (c) Obtain the following continuity equation from the Dirac equation:

$$\frac{\partial P}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{J} = 0,$$

where  $P$  is the probability density and  $\mathbf{J}$  is the probability current density. Show that the expressions of  $P$  and  $\mathbf{J}$  are  $P(\mathbf{r}, t) = \psi^\dagger(\mathbf{r}, t)\psi(\mathbf{r}, t)$  and  $\mathbf{J}(\mathbf{r}, t) = c\psi^\dagger(\mathbf{r}, t)\boldsymbol{\alpha}\psi(\mathbf{r}, t)$ . Here  $\psi(\mathbf{r}, t)$  is the four-component Dirac spinor.

#### 4. Total angular momentum is a constant of motion:

- (a) Show that the orbital angular momentum  $\mathbf{L} = \mathbf{r} \times \mathbf{p}$  is not a conserved quantity:  $[\mathbf{L}, H] = i\hbar c(\boldsymbol{\alpha} \times \mathbf{p})$ .  
**Orbital angular momentum is not a good quantum number for the Dirac equation.**
- (b) Defining  $\mathbf{S} = (\hbar/2)\boldsymbol{\Sigma}$ , where components of the operator  $\boldsymbol{\Sigma}$  are  $\Sigma_x = -i\alpha_y\alpha_z$ ,  $\Sigma_y = -i\alpha_z\alpha_x$  and  $\Sigma_z = -i\alpha_x\alpha_y$ . Show that

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}.$$

- (c) Find the eigenvalues of  $\mathbf{S}$ . Show that  $\mathbf{S}^2 = \frac{3\hbar^2}{4}I_{4 \times 4}$ .  
So it proves that  $S = \hbar/2$  and the Dirac equation describes particles with spin  $1/2$ . Thus  $\mathbf{S}$  is the spin angular momentum operator for spin  $1/2$  particle.
- (d) Show that the total angular momentum is  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  is a constant of motion:  $[\mathbf{J}, H] = 0$ .  
**Total angular momentum is a good quantum number for the Dirac equation.**
- (e) Show that the operator  $\mathbf{S} \cdot \mathbf{p}$  is a constant of motion:  $[H, \mathbf{S} \cdot \mathbf{p}] = 0$ .
- (f) Helicity is defined as the projection of the spin along the motion of the particle. Mathematically, the helicity operator is defined as

$$\hat{h} = \frac{\boldsymbol{\Sigma} \cdot \hat{\mathbf{p}}}{|\mathbf{p}|}.$$

Find the eigenvalues and the eigenfunctions of the helicity operator  $\hat{h}$ .

**Helicity is also a good quantum number.**

#### 5. Non-relativistic approximation to the Dirac equation:

- (a) The Dirac equation for an electron in a hydrogen atom is given by

$$[c\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m_e c^2 + V(r)]\Psi(\mathbf{r}) = E\Psi(\mathbf{r}),$$

where  $E$  is the total energy,  $V(r)$  is the Coulomb interaction between nucleus and the electron and  $\Psi(\mathbf{r}) = (\psi(\mathbf{r}), \chi(\mathbf{r}))$  with  $\psi(\mathbf{r})$ , and  $\chi(\mathbf{r})$  are being two-component spinors. Show that in the non-relativistic limit ( $p \ll m_e c$ ), it is reduced to the Schrödinger equation for the hydrogen atom along with the three relativistic correction terms.

- (b) Consider an electron described by the Dirac equation is subjected to the magnetic field  $\mathbf{B}$ . The Dirac equation is given by

$$[c\boldsymbol{\alpha} \cdot (\mathbf{p} + e\mathbf{A}) + \beta m_e c^2] \Psi(\mathbf{r}) = E \Psi(\mathbf{r}),$$

where  $\mathbf{A}$  is a vector potential corresponding to the magnetic field  $\mathbf{B}$  and  $E$  is the total energy. Here  $\Psi(\mathbf{r}) = (\psi(\mathbf{r}), \chi(\mathbf{r}))$  with  $\psi(\mathbf{r})$ , and  $\chi(\mathbf{r})$  are being two-component spinors. Show that in the non-relativistic limit, it reduces to

$$\left[ \frac{(\mathbf{p} + e\mathbf{A})^2}{2m_e} + g \frac{e}{2m_e} \mathbf{S} \cdot \mathbf{B} \right] \psi(\mathbf{r}) = \epsilon \psi(\mathbf{r}),$$

where  $g = 2$ ,  $\mathbf{S} = (\hbar/2)\boldsymbol{\sigma}$  and  $\epsilon = E - m_e c^2$  is the energy measured with respect to the rest mass energy.

It clearly demonstrate how the Zeeman interaction energy appears along with the correct  $g$ -factor and the spin angular momentum operator  $\mathbf{S} = (\hbar/2)\boldsymbol{\sigma}$ .