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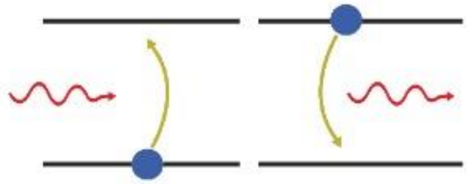

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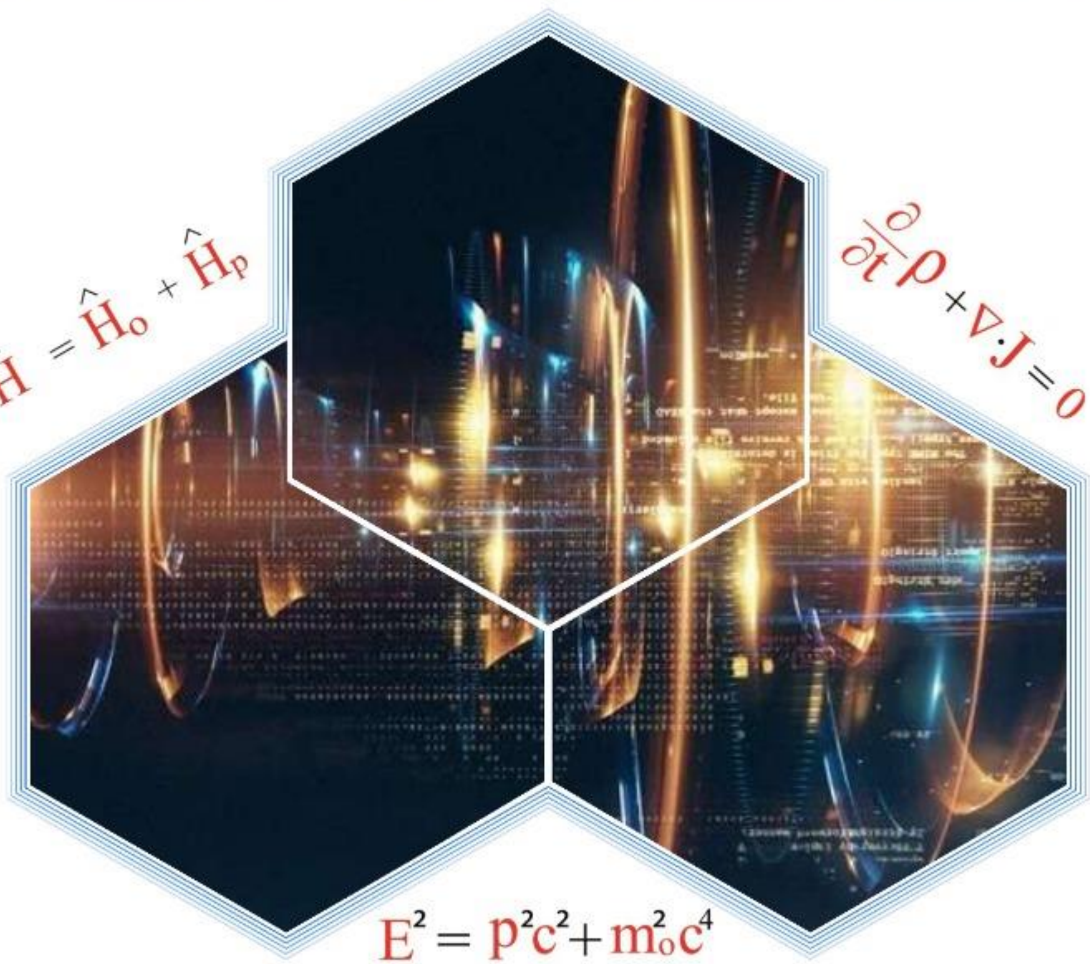
QUANTUM MECHANICS-II

For BS/M.Sc Physics Programme 4th Edition

$\hat{H} = \hat{H}_o + \hat{H}_p$



$\frac{\partial}{\partial t}\rho + \nabla \cdot J = 0$

$E^2 = p^2c^2 + m_o^2c^4$

Dr. R. M. Arif Khalil
Dr. Syed Hamad Bukhari
Hafiz Umer Farooq

TEACH YOURSELF

QUANTUM MECHANICS-II

3rd Edition

For **BS/M.Sc. Physics** students of all Pakistani Universities/Colleges

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Dr. R. M. Arif Khalil
Department of Physics
Bahauddin Zakariya University, Multan

&

Dr. Syed Hamad Bukhari
Department of Physics
G.C. University Faisalabad, Sub-Campus, Layyah

&

Hafiz Umer Farooq
Department of Physics
Govt. Graduate College of Science, Multan

•

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Contents

Chapter 1

Identical Particles

SOLVED PROBLEMS

Problem 1.1- Consider a one-dimensional infinite square well of width 1cm with free electrons in it. If its Fermi energy is 2eV, what is the number of electrons inside the well?

Solution

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

where, $n = 1, 2, 3, \ldots$ shows energy levels. Each level accommodate two electrons, one spin up and the other spin down. If the highest filled level is n, then the Fermi energy, $E_F = E_n$.

$$n^2 = \frac{2ma^2E_F}{\pi^2\hbar^2}$$

$$n^2 = \frac{\left(2\times 1.6\times 10^{-19}J\right)\times 2\times\left(9.1\times 10^{-31}Kg\right)(0.01m)^2}{(3.14)^2\left(1.05\times 10^{-34}Js\right)^2}$$

$$n^2 = 5.3475\times 10^{14} \quad\longrightarrow\quad n \;=\; 2.31\times 10^7$$

The number of electrons (n) inside the well $= 4.62\times 10^7$.

Problem 1.2- N non-interacting bosons are in an infinite potential well defined by $V(x) = 0$ for $0 < x < a$; $V(x) = \infty$ for $x < 0$ and for $x > a$. Find the ground state energy of the system. What would be the ground state energy if the particles are fermions?

Solution

The energy eigenvalue of a particle in the infinite square well is given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

As the particles are bosons, all the N-particles will be in the $n = 1$ state. Hence the total energy of system

$$E'_{n_1,n_2,n_3\ldots n_N} = \frac{\pi^2\hbar^2}{2ma^2}(1^2 + 1^2 + 1^2 \ldots 1^2)$$

$$E = \frac{N\pi^2\hbar^2}{2ma^2}$$

If the particles are fermions, a state can have only two of them, one spin up and the other spin down. Therefore, the lowest $\frac{N}{2}$ states will be filled. The total ground state energy will be

$$2\varepsilon_1 + 2\varepsilon_2 + 2\varepsilon_3 + \ldots + 2\varepsilon_{\frac{N}{2}} = E^1 = \frac{\pi^2\hbar^2}{2ma^2}\Big[(1^2+1^2) + (2^2+2^2) + \ldots\Big]$$

$$\because\ 1^2 + 2^2 + \ldots n^2 = \frac{1}{6}n(n+1)(2n+1) = \frac{2\pi^2h^2}{2ma^2}\left[1^2 + 2^2 + \ldots + \left(\frac{N}{2}\right)^2\right]$$

$$E^\circ = \frac{N^3\pi^2\hbar^2}{24\,ma^2}$$

Problem 1.3- Sixteen non-interacting electrons are confined in a potential $V(x) = \infty$ for $x < 0$ and $x > a$; $V(x) = 0$, for $0 < x < a$. **(i)** What is the energy of the least energetic electron in the ground state? **(ii)** What is the energy of the most energetic electron? **(iii)** What is the Fermi energy E_F of the system?

Solution

(i) The least energetic electron in the ground state is given by

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

(ii) In the given potential, the energy eigenvalue is

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

As two electrons can go into each of the states $n = 1, 2, 3, \ldots$ the highest filled level will have $n = 8$ and its energy will be

$$E_8 = \frac{8^2\pi^2\hbar^2}{2ma^2}$$

(iii) The energy of the highest filled state is the Fermi energy E_F. Hence,

$$E_f = \frac{n^2\pi^2\hbar^2}{2ma^2}$$
$$E_f = \frac{64\pi^2\hbar^2}{2ma^2} = \frac{32\pi^2\hbar^2}{ma^2}$$

Each state has 2 electrons

$$E_f = \frac{64\pi^2\hbar^2}{ma^2}$$

Problem 1.4- Prove that it is impossible to construct a completely anti-symmetric spin function for three electrons. (Concept: Because electrons has only two spin orientations)

Solution

Let a, b, c stands for three functions and 1,2,3 for three identical particles. In the function $a(1)\,b(2)\,c(3)$, particle 1 is in a, particle 2 is in b, and particle 3 is in c. Let us proceed without specifying that these functions correspond to space or spin functions. The third-order slater determinant for the case is

$$= \frac{1}{\sqrt{6}}\begin{vmatrix} a(1) & a(2) & a(3) \\ b(1) & b(2) & b(3) \\ c(1) & c(2) & c(3) \end{vmatrix}$$

This is completely anti-symmetrized as interchange of two spins amount to interchanging two columns of the determinant, which multiplies it by -1. Let us now specify the functions a, b, c as that due to electron spins. Let $a = \alpha, b = \beta, c = \beta$ in the above determinant. The determinant reduces to

$$= \frac{1}{\sqrt{6}} \begin{vmatrix} \alpha(1) & \alpha(2) & \alpha(3) \\ \beta(1) & \beta(2) & \beta(3) \\ \beta(1) & \beta(2) & \beta(3) \end{vmatrix}$$

As the second and third rows of the determinant are identical, its value is zero. In whatever way we select a, b, c, the two rows of the determinant will be equal. Therefore, we can not construct a completely anti-symmetric three-electron spin function.

Problem 1.5- The valence electron in the first excited state of an atom has the electronic configuration $3s^1, 3p^1$. **(i)** Under L-S coupling what value of L and S are possible? **ii** Write the spatial part of their wave-functions using the single particle functions $\psi_s(r)$ and $\psi_p(r)$.

Solution

i Electronic configuration $3s^1, 3p^1$. Hence $l_1 = 0, l_2 = 1$; $s_1 = \left(\frac{1}{2}\right), s_2 = \left(\frac{1}{2}\right)$; $L = 1, \quad S = 0, 1$ **ii** Taking exchange degeneracy into account, the two possible space functions are

$$\psi_s(r_1)\psi_p(r_2) \quad \text{and} \quad \psi_s(r_2)\psi_p(r_1)$$

The symmetric combination

$$\psi_s = \frac{1}{\sqrt{2!}}\left[\psi_s(r_1)\psi_p(r_2) + \psi_s(r_2)\psi_p(r_1)\right]$$

Anti-symmetric combination

$$\psi_{as} = \frac{1}{\sqrt{2!}}\left[\psi_s(r_1)\psi_p(r_2) - \psi_s(r_2)\psi_p(r_1)\right]$$

where N_s and N_{as} are normalization constants.

Problem 1.6- Specify the symmetry of the following functions

(a)- $\psi(x_1, x_2) = 4(x_1 - x_2)^2 + \frac{10}{x_1^2 + x_2^2}$

(b)- $\phi(x_1, x_2) = -\frac{3(x_1 - x_2)}{2(x_1 - x_2)^2 + 7}$

(c)- $\chi(x_1, x_2, x_3) = 6x_1x_2x_3 + \frac{x_1^2 + x_2^2 + x_3^2 - 1}{2x_1^3 + 2X_2^3 + 2X_3^3 + 5}$

Solution

(a)- The function $\psi(x_1, x_2)$ is symmetric, since $\psi(x_2, x_1) = \psi(x_1, x_2)$

(b)- The function $\phi(x_1, x_2)$ is antisymmetric, since $\phi(x_2, x_1) = -\phi(x_1, x_2)$, and ϕ is zero

(c)- The function $\chi(x_1, x_2, x_3)$ is symmetric because

$$\begin{aligned} \chi(x_1, x_2, x_3) &= \chi(x_1, x_3, x_2) = \chi(x_2, x_1, x_3) = \chi(x_2, x_3, x_1) \\ &= \chi(x_3, x_1, x_2) = \chi(x_3, x_2, x_1) \end{aligned}$$

Problem 1.7- Suppose we have two noninteracting particles, both of mass m in infinite square well. The one particle states are:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), \qquad E_n = n^2\left(\frac{\pi^2\hbar^2}{2mL^2}\right) = n^2K$$

Write wave functions:

- If particles are distinguishable.
- If particles are identical bosons.
- If particles are identical fermions.

Solution

If particles are distinguishable, composite wave functions are,

$$\psi_{n_1n_2}(x) = \psi_{n_1}(x)\psi_{n_2}(x), \qquad E_{n_1n_2} = (n_1^2 + n_2^2)k$$

For example the ground state is,

$$\psi_{11}(x) = \frac{2}{L} \sin\left(\frac{\pi x_1}{L}\right) \sin\left(\frac{\pi x_2}{L}\right), \qquad E_{11} = 2K$$

The first excited state is doubly degenerate;

$$\psi_{12}(x) = \frac{2}{L}\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right), \qquad E_{12} = 5K$$

$$\psi_{21}(x) = \frac{2}{L}\sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{\pi x_2}{L}\right), \qquad E_{21} = 5K \ \ \& \ \text{so on.}$$

If particles are identical bosons, the ground state is unchanged but 1st excited state is non-degenerate;

$$\frac{\sqrt{2}}{L}\left\{\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) + \sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{\pi x_2}{L}\right)\right\} \text{ with energy } 5K$$

If particles are identical fermions, the ground state is:

$$\frac{\sqrt{2}}{L}\left\{\sin\left(\frac{\pi x_1}{L}\right)\sin\left(\frac{2\pi x_2}{L}\right) - \sin\left(\frac{2\pi x_1}{L}\right)\sin\left(\frac{\pi x_2}{L}\right)\right\} \text{ with energy } 5K$$

Problem 1.8- Find the ground state energy and wave function of a system of N noninteracting identical particles that are confined to a one-dimensional, infinite well when the particles are (a) bosons and (b) spin $\frac{1}{2}$ fermions.

Solution

In the case of a particle moving in an infinite well, its energy and wave function are $\varepsilon_n = n^2\hbar^2\pi^2/(2ma^2)$ and $\psi_n(x_i) = \sqrt{2/a}\,\sin(n\pi x_i/2)$

(a)- In the case where the N particles are bosons, the ground state is obtained by pitting all the particles in the state $n = 1$, the energy and wave function are then given by

$$E^{(0)} = \varepsilon_1 + \varepsilon_1 + \varepsilon_1 + \cdots + \varepsilon_1 = N + \varepsilon_1 = \frac{N\hbar^2\pi^2}{2ma^2}$$

$$\psi^0(x_1, x_2\cdots, x_N) = \prod_{n=1}^{N}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{2}x_i\right) = \sqrt{\frac{2^N}{a^N}}\sin\left(\frac{\pi}{2}x_1\right)\sin\left(\frac{\pi}{2}x^2\right)\cdots\sin\left(\frac{\pi}{2}x_N\right)$$

(b)- In the case where the N particles are spin $\frac{1}{2}$ fermions, each level can be occupied by at most two particles having different spin states $\left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle$. The ground state is thus obtained by distributing the N particles among the $N/2$ lowest levels at a rate of two particles per level:

$$E^0 = 2 + \varepsilon_1 + 2 + \varepsilon_2 + 2 + \varepsilon_3 + \cdots + 2 + \varepsilon_{N/2} = 2\sum_{n=1}^{N/2} \frac{n^2\hbar^2\pi^2}{2ma^2} = \frac{\hbar^2\pi^2}{ma^2}\sum_{n=1}^{N/2} n^2.$$

If N is large we may calculate $\sum\limits_{n=1}^{N/2} n^2$ by using the approximation

$$\sum_{n=1}^{N/2} n^2 \simeq \int_1^{N/2} n^2 dn \simeq \frac{1}{3}\left(\frac{N}{2}\right)^3$$

hence the ground state will be given by

$$E^0 \simeq N^2 \frac{\hbar^2\pi^2}{24ma^2}$$

The average energy per particle is $E^0/N \simeq N^2\hbar^2\pi^2/(24ma^2)$. In the case where N is even, a possible configuration of the ground state wave function $\psi^0(x_1, x_2, \cdots, x_N)$ is given as follows

$$\frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_1(x_1)\chi(S_1) & \psi_1(x_2)\chi(S_2) & \dots & \psi_1(x_N)\chi(S_N) \\ \psi_1(x_1)\chi(S_1) & \psi_1(x_2)\chi(S_2) & \dots & \psi_1(x_N)\chi(S_N) \\ \psi_2(x_1)\chi(S_1) & \psi_2(x_2)\chi(S_2) & \dots & \psi_2(x_N)\chi(S_N) \\ \psi_2(x_1)\chi(S_1) & \psi_2(x_2)\chi(S_2) & \dots & \psi_2(x_N)\chi(S_N) \\ \psi_3(x_1)\chi(S_1) & \psi_3(x_2)\chi(S_2) & \dots & \psi_3(x_N)\chi(S_N) \\ \psi_3(x_1)\chi(S_1) & \psi_3(x_2)\chi(S_2) & \dots & \psi_3(x_N)\chi(S_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_{N/2}(x_1)\chi(S_1) & \psi_{N/2}(x_2)\chi(S_2) & \dots & \psi_{N/2}(x_N)\chi(S_N) \\ \psi_{N/2}(x_1)\chi(S_1) & \psi_{N/2}(x_2)\chi(S_2) & \dots & \psi_{N/2}(x_N)\chi(S_N) \end{vmatrix}$$

where $\chi(S_i) = \left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle$ is the spin state of the ith particle, with $i = 1, 2, 3, \cdots, N$. If N is odd then we need to remove the last row of the determinant.

Problem 1.9- An electron is in spin state

$$\chi = A \begin{pmatrix} 3i \\ 4 \end{pmatrix}$$

Normalize this state. Evaluate expectation values of S_x, S_y, S_z

Solution

To normalize the state, we apply normalization condition.

$$\chi^\dagger \chi = 1$$

$$\Rightarrow \; A\,A \begin{pmatrix} -3i & 4 \end{pmatrix} \begin{pmatrix} 3i \\ 4 \end{pmatrix} = 1$$

$$\Rightarrow \; |A|^2 (9+16) = 1 \quad \Rightarrow \; |A|^2 25 = 1 \quad \Rightarrow \; A = \frac{1}{5}$$

Expectation values of S_x, S_y, S_z are

$$\langle S_x \rangle = \chi^\dagger S_x \chi = \frac{1}{5} \begin{pmatrix} -3i & 4 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{5} \begin{pmatrix} 3i \\ 4 \end{pmatrix} = 0$$

$$\langle S_y \rangle = \chi^\dagger S_y \chi = \frac{1}{5} \begin{pmatrix} -3i & 4 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{1}{5} \begin{pmatrix} 3i \\ 4 \end{pmatrix} = -\frac{12}{25}\hbar$$

$$\langle S_z \rangle = \chi^\dagger S_z \chi = \frac{1}{5} \begin{pmatrix} -3i & 4 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{5} \begin{pmatrix} 3i \\ 4 \end{pmatrix} = -\frac{7}{50}\hbar$$

Problem 1.10- An electron is in spin state

$$\chi = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Evaluate expectation values of S_x, S_y, S_z

Solution

Expectation values of S_x, S_y, S_z are

$$\langle S_x \rangle = \chi^\dagger S_x \chi = \begin{pmatrix} 1 & 2 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = 2\hbar$$

$$\langle S_y \rangle = \chi^\dagger S_y \chi = \begin{pmatrix} 1 & 2 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = 0$$

$$\langle S_z \rangle = \chi^\dagger S_z \chi = \begin{pmatrix} 1 & 2 \end{pmatrix} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = -\frac{3}{2}\hbar \quad \text{as required}$$

$$\langle S^2 \rangle = \chi^\dagger S^2 \chi = \begin{pmatrix} 1 & 2 \end{pmatrix} \frac{3\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \frac{15}{4}\hbar \quad \text{as bonus}$$

Problem 1.11- Find the normalized wave function of a system of three identical bosons, which are given in one particle.

Solution

Let ψ_1, ψ_2, ψ_3 be normalized one particle states.

- If all three occupied states are different, then state function of system will be;

$$\psi = \frac{1}{\sqrt{3!}} \{\psi_1(1)\psi_2(2)\psi_3(3) + \psi_1(1)\psi_2(3)\psi_3(2) + \psi_1(3)\psi_2(2)\psi_3(1) + \psi_1(3)\psi_2(1)\psi_3(2)$$
$$+\psi_1(2)\psi_2(1)\psi_3(3) + \psi_1(2)\psi_2(3)\psi_3(1)\}$$

- If two of three filled states are identical e.g. $\psi_1(1) \neq \psi_2(2) = \psi_2(3)$, then state function of system will be;

$$\psi = \sqrt{\frac{2!}{3!}} \{\psi_1(1)\psi_2(2)\psi_3(2) + \psi_1(2)\psi_2(1)\psi_3(2) + \psi_1(2)\psi_2(2)\psi_3(1)\}$$

- If three are in same, then state function of system will be;

$$\psi = \psi_1(1)\psi_2(1)\psi_3(1)$$

Chapter 2

Approximation Methods

SOLVED PROBLEMS

Problem: 2.1- A trial function ϕ differs from an eigen-function ψ_E so that $\phi = \psi_E + \alpha\phi_1$, where ψ_E and ϕ_1 are orthonormal and $\alpha << 1$. Show that $\langle H \rangle$ differs from E only by a term of order α^2 and find this term. Given that $H\psi_E = E\psi_E$

Solution

$$\langle H \rangle = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{\langle (\psi_E + \alpha\phi_1) | H | (\psi_E + \alpha\phi_1) \rangle}{\langle (\psi_E + \alpha\phi_1) | (\psi_E + \alpha\phi_1) \rangle}$$

$$\langle H \rangle = \frac{\langle \psi_E | H | \psi_E \rangle + \alpha \langle \psi_E | H | \phi_1 \rangle + \alpha \langle \phi_1 | H | \psi_E \rangle + \alpha^2 \langle \phi_1 | H | \phi_1 \rangle}{\langle \psi_E | \psi_E \rangle + \alpha \langle \psi_E | \phi_1 \rangle + \alpha \langle \phi_1 | \psi_E \rangle + \alpha^2 \langle \phi_1 | \phi_1 \rangle}$$

Since H is Hermitian,

$$\langle \psi_E | H | \phi_1 \rangle = E \langle \psi_E | \phi_1 \rangle = 0$$

$$\langle H \rangle = \frac{E + \alpha^2 \langle \phi_1 | H | \phi_1 \rangle}{1 + \alpha^2} = E + \alpha^2 \langle \phi_1 | H | \phi_1 \rangle$$

As $1 + \alpha^2 \cong 1$. Hence the result $\langle H \rangle$ differs from E by the term $\alpha^2 \langle \phi_1 | H | \phi_1 \rangle$.

Problem: 2.2- The unperturbed wave-functions for harmonic oscillator is

$$\psi_n^{\circ}(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} - \exp\left(\frac{m\omega x^2}{2\hbar}\right)$$

If a small perturbation

$$V' = \begin{cases} \lambda x, x > 0 \\ 0, x \leq 0 \end{cases}$$

acts on the system, evaluate the first order correction to the ground state energy.

Solution

The given $H_{\circ}$ is the one dimensional simple harmonic oscillator. Hence the unperturbed ground state energy is

$$\psi_n^{\circ}(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \exp\left(\frac{m\omega x^2}{2\hbar}\right)$$

The first order correction to the energy is

$$\begin{aligned} E_n^{(1)} &= \langle \psi_{\circ}(x) | \lambda x | \psi_{\circ}(x) \rangle \\ &= \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \lambda \int_0^{\infty} x . \exp\left(-\frac{m\omega x^2}{\hbar}\right) dx \\ E_n^{(1)} &= \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \lambda \left(\frac{\hbar}{2m\omega}\right) = \frac{\lambda}{2}\sqrt{\frac{\hbar}{\pi m\omega}}. \end{aligned}$$

Problem: 2.3- Solve the following one-dimensional infinite potential well, which is modified at the bottom by a perturbation $V_p(x)$

$$V(x) = \begin{cases} 0, for 0 < x < a; \\ \infty, \text{elsewhere}; \end{cases}, \quad V_P(x) = \begin{cases} V_{\circ}, \ 0 \leq x \leq \frac{a}{2} \\ 0, \ \text{eleswhere} \end{cases}$$

Calculate the energy E_n. Using the WKB method and compare it with where the $V_{\circ} << 1$, the exact solution.

Solution

$V(x) = 0$ for $0 < x < a$ and $V(x) = \infty$ elsewhere. The turning points are $x_1 = 0$ and $x_2 = a$. The energy within the WKB approximation can be obtained using the quantization condition

$$\int_0^a P(E_n, x)dx = n\pi\hbar \qquad \because \; n = 1, 2, 3, \cdots$$

$$\int_0^{a/2} \sqrt{2m(E_n - V_\circ)}dx + \int_{a/2}^{a} \sqrt{2mE_n}dx = n\pi\hbar$$

$$\frac{a}{2}\sqrt{2m}\left(\sqrt{E_n - V_\circ} + \sqrt{E_n}\right) = n\pi\hbar$$

squaring on both side,

$$2\sqrt{E_n(E_n - V_\circ)} = a_n - 2E_n + V_\circ \qquad \because \; a_n \frac{2n^2\pi^2\hbar^2}{ma^2}$$

again squaring on both side

$$4E_n^2 - 4E_nV_\circ = a_n^2 + 4E_n^2 + V_\circ^2 - 4a_nE_n + 2a_nV_\circ - 4E_nV_\circ$$

$$E_n = \frac{a_n}{4} + \frac{V_\circ}{2} + \frac{V_\circ^2}{4a_n}$$

As $V_\circ$ is small so neglect $V_\circ^2/4a_n$. The exact solution gives

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \qquad n = 1, 2, 3, ...$$

The WKB solution has $\left(n + \frac{1}{2}\right)$ in place of n. Another major difference is the allowed values of n.

$$E_n^{\text{WKB}} = \frac{\pi^2\hbar^2}{2ma^2}n^2 + \frac{V_\circ}{2}$$

Problem: 2.4- Use the WKB method to calculate the transmission coefficient of a particle of mass m and energy E moving in the potential barrier

$$V(x) = \begin{cases} V_\circ - ax, x > 0 \\ 0, x < 0 \end{cases}$$

Solution

As the transmission coefficient is,

$$T = \exp^{-2\gamma} \qquad \because \; \gamma = \frac{1}{\hbar}\int_{x_1}^{x_2} \sqrt{2m(V(x)-E)}dx \tag{2.1}$$

where the turning point $x_1 = 0$. To get the other turning point, it is necessary that

$$\begin{aligned} E = V(x) =& V_\circ - ax_2 \\ x_2 =& \frac{V_\circ - E}{a} \end{aligned}$$

so, we get

$$\begin{aligned} \gamma =& \frac{1}{\hbar}\int_0^{\frac{V_\circ - E}{a}} \sqrt{2m(V(x)-E)}dx \\ =& \frac{\sqrt{2m}}{\hbar}\left|\frac{(V_\circ - ax - E)^{3/2}}{-\frac{3}{2}a}\right|_0^{\frac{V_\circ - E}{a}} \\ =& \frac{-2\sqrt{2m}}{3a\hbar}\left[\left(V_\circ - a\left(\frac{V_\circ - E}{a}\right) - E\right)^{3/2} - \left(V_\circ - E\right)^{3/2}\right] \\ \gamma =& \frac{-2\sqrt{2m}}{3a\hbar}\left[\left(0\right)^{3/2} - \left(V_\circ - E\right)^{3/2}\right] = \frac{2\sqrt{2m}}{3a\hbar}\left(V_\circ - E\right)^{3/2} \end{aligned}$$

Put in Eq.(2.1)

$$T = \exp\left[-\frac{4\sqrt{2m}}{3\hbar a}(V_\circ - E)^{\frac{3}{2}}\right]$$

Problem: 2.5- A particle of mass m moves in an infinite one-dimensional box of length $2a$ with a potential dip as defined by

$$V(x)=\begin{cases}\infty, a<x<-a\\ -V_\circ, -a<x<-\frac{a}{3}\\ 0, -\frac{a}{3}<x<a\end{cases}$$

Find the energy of the ground state corrected to first order.

Solution

The unperturbed part of the Hamiltonian is that due to a particle in an infinite potential defined by $V(x)$ for $-a<x<a$ and $V(x)=\infty$ otherwise. The unperturbed ground state energy and eigen-functions are

$$E_1=\frac{\pi^2\hbar^2}{8ma^2},\qquad \psi_1=\frac{1}{\sqrt{a}}\cos\frac{\pi x}{2a}$$

The perturbation $H'=-V_\circ$, $-a<x<-\frac{a}{3}$. The first order correction is

$$\begin{aligned}E^{(1)}&=-\frac{V_\circ}{a}\int_{-a}^{-\frac{a}{3}}\cos^2\frac{\pi x}{2a}dx=-\frac{V_\circ}{2a}\int_{-a}^{-\frac{a}{3}}\left(1+\cos\frac{\pi x}{a}\right)dx\\ &=-\frac{V_\circ}{a}\left|x\right|_{-a}^{-\frac{a}{3}}-\frac{V_\circ}{2a}\frac{a}{\pi}\left|\sin\frac{\pi x}{a}\right|_{-a}^{-\frac{a}{3}}\\ &=-\frac{V_\circ}{3}+\frac{V_\circ}{2\pi}\sin 60^\circ=-\frac{V_\circ}{3}+\frac{V_\circ}{2\pi}(0.866)\;=\;0.195V_\circ\end{aligned}$$

The ground state energy corrected to first order is

$$E=\frac{\pi^2\hbar^2}{8ma^2}=0.195V_\circ$$

Problem: 2.6- Use the WKB approximation to calculate the energy levels of a spinless particles of mass m moving in one-dimensional box with walls at $x = 0$ and $x = L$.

Solution

This potential has two rigid walls. One at $x = 0$ and the other at $x = L$. To find the energy levels, we make use of the quantization rule. Since the momentum is constant within the well $p(E, x) = \sqrt{2mE}$, we can easily infer the WKB energy expression of the particle within the well. The integral is quite simple to calculate

$$\int_0^L p dx = \sqrt{2mE} \int_0^L dx = L\sqrt{2mE}$$

Now since $\int_0^L p dx = n\pi\hbar$ we obtain,

$$L\sqrt{2mE_n^{WKB}} = n\pi\hbar$$

hence

$$E_n^{WKB} = \frac{\pi^2\hbar^2}{2mL^2}n^2$$

This is the exact value of the energy of a particle in an infinite well.

Problem: 2.7- Use the WKB approximation to calculate the energy levels of the s states of an electron that is bound to Ze nucleus.

Solution

The electron moves in the Coulomb field of the Ze nucleus: $V(r) = -Ze^2/r$. Since the electron is bound to the nucleus, it can be viewed as moving between two rigid walls $0 \leq r \leq a$ with $E = V(a),\ a = -Ze^2/E$; the energy of the electron is negative , $E < 0$.

The energy levels of the s states (i.e. $l = 0$) can thus be obtained from the equation below,

$$\int_{x_1}^{x^2} p(x)dx = n\pi\hbar, \qquad\qquad n = 1, 2, 3, \cdots$$

$$\int_0^a \sqrt{2m\left(E+\frac{Ze^2}{r}\right)}dr = n\pi\hbar$$

Using the change of variable $x = a/r$, we have

$$\int_0^a \sqrt{2m\left(E+\frac{Ze^2}{r}\right)}dr = \sqrt{-2mE}\int_0^a \sqrt{\frac{a}{r}-1}dr = a\sqrt{-2mE}\int_0^1 \sqrt{\frac{1}{x}-1}dx$$
$$= \frac{\pi}{2}a\sqrt{-2mE} = -\pi Ze^2\sqrt{-\frac{m}{2E}}$$

In deriving this relation, we have used the integral $\int_0^1 \sqrt{1/x-1}dx = \pi/2$; this can be easily obtained by the application of the residue theorem.

$$E_n = -\frac{mZ^2e^4}{2\hbar^2}\frac{1}{n^2} = -\frac{Z^2e^2}{2a_\circ}\frac{1}{n^2}$$

where, $a_\circ = \hbar^2/(me^2)$ is the Bohr radius. This is the correct (Bohr) expression for the energy

Chapter 3

Time Dependent Perturbation Theory

SOLVED PROBLEMS

Problem: 3.1- A system in an unperturbed state n is suddenly subjected to a constant perturbation $H'(r)$ which exists during time $0 \to t$. Find the probability for transition from state n to state k and show that it varies simple harmonically with angular frequency $\frac{(E_k - E_n)}{2\hbar}$ and amplitude $\frac{4|H'_{kn}|^2}{(E_k - E_n)^2}$.

Solution

We know that

$$P_{nk}^{(t)} = \left| \frac{1}{i\hbar} \int_0^t < \psi_k | V(t') \psi_n | > e^{i\omega_{kn} t'} dt' \right|^2 \qquad \because V(t') = H'(r)$$

So, $P_{nk}^{(t)} = \left| \frac{1}{i\hbar} \int_0^t H'_{kn}(r) \exp(i\omega_{kn} t') \, dt' \right|^2$. When the perturbation is constant in time, $H'_{kn}(r)$ can be taken outside the integral. Hence,

$$P_{nk}(t) = \left| \frac{H'_{kn}(r)}{i\hbar} \int_0^t \exp\left(i\omega_{kn}t'\right) dt' \right|^2$$

$$= \left| -\frac{H'_{kn}}{\hbar\omega_{kn}} \left[\exp\left(i\omega_{kn}t\right) - 1\right] \right|^2 \qquad \because e^{i\omega_{kn}t} = e^{i\omega_{kn}\frac{t}{2}} \cdot e^{i\omega_{kn}}$$

$$= \left| -\frac{H'_{kn}}{\hbar\omega_{kn}} \exp\left(i\omega_{kn}{}^{t}/_{2}\right) \left[\exp\left(-i\omega_{kn}{}^{t}/_{2}\right) - \exp\left(i\omega_{kn}{}^{t}/_{2}\right)\right] \right|^2$$

$$= \left| -\frac{2iH'_{kn}}{\hbar\omega_{kn}} \exp\left(i\omega_{kn}{}^{t}/_{2}\right) \sin\left(\omega_{kn}{}^{t}/_{2}\right) \right|^2 \qquad \because e^{i\theta} - e^{-i\theta} = 2i\sin\theta$$

$$P_{nk}(t) = \left| \frac{4}{\hbar^2} \frac{\left|H'_{kn}\right|^2}{\omega_{kn}^2} \sin^2\left(\omega_{kn}{}^{t}/_{2}\right) \right|^2$$

Which is the probability for transition from state n to state k. From the above expression it is obvious that the probability varies simple harmonically with angular frequency $\frac{\omega_{kn}}{2} = \frac{(E_k - E_n)}{2\hbar}$. The amplitude of vibration is $\frac{4|H'_{kn}|^2}{\hbar^2\omega_{kn}^2} = \frac{4|H'_{kn}|^2}{(E_k - E_n)^2}$.

Problem: 3.2- Spontaneous emission exceeds stimulated emission in the visible region, whereas reverse the situation in the microwave region.

Solution

Visible region Wavelength $\approx 5000A^{\circ}$. So, Rate of spontaneous emission / Rate of stimulated emission $= e^{\frac{hv}{kT}} - 1$.

$$\frac{hv}{kT} = \frac{hc}{\lambda kT}$$

$$= \frac{\left(6.63\times10^{-34}Js\right)\left(3\times10^{8}ms^{-1}\right)}{\left(5000\times10^{-10}m\right)\left(1.38\times10^{-23}JK^{-1}\right)300K}$$

$$= 96.03$$

The rate of spontaneous emission $= (e^{96.03} - 1)\times$ rate of stimulated emission

$= 4.073\times$ rate of stimulated emission

Microwave region: Wavelength $\cong$ 1cm. Therefore,

$$\frac{hv}{kT} = \frac{hc}{\lambda kT}$$

$$= \frac{\left(6.63\times10^{-34}Js\right)\left(3\times10^{8}ms^{-1}\right)}{\left(0.01m\right)\left(1.38\times10^{-23}JK^{-1}\right)300K} = 0.004$$

The rate of spontaneous emission $= (e^{0.004} - 1) \times$ rate of stimulated emission

$= 0.004\times$ rate of stimulated emission.

Problem: 3.3- Prove the following:

I: If the source temperature is 1000K, in the optical region $\left(\lambda = 5000\mathring{A}\right)$, the emission is predominantly due to spontaneous transitions.

II: If the source temperature is 300K, in the microwave region $(\lambda = 1cm)$, the emission is predominantly due to stimulated transitions. The Boltzmann constant is $1.38 \times 10^{-23} JK^{-1}$.

Solution

Spontaneous emission rate/Stimulated emission rate $= \exp\left(\frac{hv}{kT}\right) - 1$

I: In the optical region $(\lambda = 5000 \times 10^{10}\text{m})$, $T = 1000K$

$$\begin{aligned} v &= \frac{c}{\lambda} = \frac{3 \times 10^8}{5000 \times 10^{-10}} = 6 \times 10^{14} Hz \\ \frac{hv}{kT} &= \frac{6.63 \times 10^{-34} \times 6 \times 10^{14}}{1.38 \times 10^{-23} \times 1000} = 28.8 \\ \exp(28.8) - 1 &= 3.22 \times 10^{12} \end{aligned}$$

Thus, the spontaneous emission is predominant.

II. In the microwave region $(\lambda = 0.01\text{m})$, $T = 300K$

$$\begin{aligned} v &= \frac{c}{\lambda} = \frac{3 \times 10^8}{10^{-2}} = 3 \times 10^{10} Hz \\ \frac{hv}{kT} &= \frac{6.63 \times 10^{-34} \times 3 \times 10^{10}}{1.38 \times 10^{-23} \times 300} = 4.8 \times 10^{-3} \\ \exp\left(4.8 \times 10^{-3}\right) - 1 &= 0.0048. \end{aligned}$$

Therefore, the stimulated emission is predominant.

Problem: 3.4- The time varying Hamiltonian $H'(t)$ induces transitions between states $|j\rangle$ and $|k\rangle$. Using time-dependent perturbation theory, show that the probability for a transition from state $|j\rangle$ to state $|k\rangle$ is the same as the probability for a transition from state $|k\rangle$ to state $|j\rangle$.

Solution

The probability for transition from state $|j\rangle$ to state $|k\rangle$ at time t is $P_{jk}(t)$ The relation is

$$P_{jk}(t) = \left|\frac{1}{i\hbar}\int_0^t \langle k|H'|j\rangle \exp(i\omega_{kj}t')\,dt'\right|^2$$

So the equation becomes

$$P_{jk}(t) = \left|\frac{1}{i\hbar}\int_0^t H'_{kj}(t') \exp(i\omega_{kj}t')\,dt'\right|^2$$

The probability for transition from state $|k\rangle$ to state $|j\rangle$ at time t is given by

$$P_{kj}(t) = \left|\frac{1}{i\hbar}\int_0^t \langle j|H'|k\rangle \exp(i\omega_{jk}t')\,dt'\right|^2$$

Since H' is Hermitian, $\langle k|H'|j\rangle = \langle j|H'|k\rangle$. Also, it follows that $\omega_{kj} = \frac{E_k - E_j}{\hbar} = -\omega_{jk}$. As the integrant of the second integral is the complex conjugate of that of the first one, we have

$$P_{kj}(t) = P_{jk}(t)$$

Problem: 3.5- A quantum mechanical system is initially in the ground state $|0\rangle$. At t=0, a perturbation of the form $H'(t) = H_\circ e^{-\alpha t}$, where α is a constant, is applied. Show that the probability that the system is in state $|1\rangle$ after long time is $P_{01} = \frac{|\langle 0|H_\circ|1\rangle|^2}{\hbar^2\left(\alpha^2+\omega_{10}^2\right)}$, $\omega_{10} = \frac{E_1 - E_0}{\hbar}$.

Solution

In the first order perturbation, the transition probability is given by equation,

$$P_{01}(t) = \left| \frac{1}{i\hbar} \int_0^t H'_{10}(t) \exp(i\omega_{10} t')\, dt' \right|^2$$

where,

$$H'_{10}(t) = \langle 1 | H'(t') | 0 \rangle \quad \text{and} \quad \omega_{10} = \frac{E_1 - E_0}{\hbar}$$

Substituting the value of $H'(t)$ and allowing $t \to \infty$, we get

$$\begin{aligned} P_{01}(t) &= \left| \frac{1}{i\hbar} \int_0^\infty \exp(i\omega_{10} t)\, e^{-\alpha t} \langle 1 | H_\circ | 0 \rangle\, dt \right|^2 \\ &= \left| \frac{1}{i\hbar} \int_0^\infty \exp(i\omega_{10} - \alpha)\, t \langle 1 | H_\circ | 0 \rangle\, dt \right|^2 \end{aligned}$$

$$\begin{aligned} P_{01}(t) &= \left| \frac{\langle 1 | H_\circ | 0 \rangle}{i\hbar} \left| \frac{\exp[-(\alpha - i\omega_{10})\, t]}{-(\alpha - i\omega_{10})} \right|_0^\infty \right|^2 \\ &= \left| \frac{\langle 1 | H_\circ | 0 \rangle}{i\hbar} \frac{1}{\alpha - i\omega_{10}} \right|^2 \end{aligned}$$

The probability for a transmission from state $|0>$ to a state $|1>$ after a long time is

$$= \frac{|\langle 0 | H_\circ | 1 \rangle|^2}{\hbar^2 (\alpha^2 + \omega_{10}^2)}$$

$\because H_\circ$ is Hermiteian

So

$$\langle 1 | H_\circ | 0 \rangle = \langle 0 | H_\circ | 1 \rangle$$

and

$$\begin{aligned} (\alpha - i\omega_{10})^2 &= (\alpha - i\omega_{10})(\alpha + i\omega_{10}) \\ &= \alpha^2 + i\omega_{10}^2 \end{aligned}$$

Chapter 4

Scattering Theory

SOLVED PROBLEMS

Problem: 4.1- A beam of particles is incident normally on a thin metal foil of thickness t. if $N_\circ$is the number of nuclei per unit volume of the foil, show that the fraction of incident particles scattered in the direction $(\theta, \phi)$is $D(\theta)N_\circ t d\Omega$, where $d\Omega$ is the small solid angle in the direction (θ, ϕ).

Solution

We know that, the differential scattering cross-section is

$$D(\theta) = \frac{dN/d\Omega}{J_{in}}$$

Where dN is the number scattered into solid angle $d\Omega$ in the direction (θ, ϕ) per unit time and $J_{in}$is the incident flux. Hence,

$$dN = D(\theta) J_{in} d\Omega$$

This is the number scattered per unit time by a single nucleus. The number of nuclei in a volume $At = N_\circ At$. The number scattered by $N_\circ At$ nuclei $= D(\theta) J_{in} d\Omega N_\circ At$. Thus, Number of particles striking an area A per second $= J_{in}A$. Fraction scattered in the direction (θ, ϕ) is

$$=\frac{D(\theta)J_{in}d\Omega N_{\circ}At}{J_{\text{in}}A}$$
$$=D(\theta)N_{\circ}td\Omega = \ N_{\circ}td\sigma$$

Problem: 4.2- In the theory of scattering by a fixed potential, the asymptotic form of the wave function is

$$\psi \xrightarrow[r\to\infty]{} A\left[e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right]$$

Obtain the formula for scattering cross-section in terms of the scattering amplitude $f(\theta)$.

Solution

The probability current density $J(r,t)$ is given by

$$J(r,t) = \frac{i\hbar}{2m}\left(\psi\nabla\psi^* - \psi^*\nabla\psi\right)$$

If $J(r,t)$ is calculated with the given wave function, we get interference terms between the incident and scattered wave. In the experimental arrangements, these do not appear. Hence we calculate the incident and scattered probability current densities J_{in} and J_{sc} separately. The value of J_{in} due to $Ae^{ikz}$is

$$J_{in} =\frac{i\hbar}{2m}\left[|A|^2(-ik) - |A|^2(ik)\right]$$
$$J_{in} =\frac{\hbar k|A|^2}{m}$$

The scattered probability current density due to $Af(\theta)\frac{e^{ikr}}{r}$

$$J_{sc} =\frac{i\hbar}{2m}|A|^2|f(\theta)|^2\left[-\frac{ik}{r^2} - \frac{1}{r^3} - \frac{ik}{r^2} + \frac{1}{r^3}\right]$$
$$J_{sc} =\frac{\hbar k}{m}|A|^2|f(\theta)|^2\frac{1}{r^2}$$

The differential scattering cross-section $D(\theta)$.

$$\begin{aligned} D(\theta) =& \frac{J_{sc}}{J_{in}} \frac{dA}{d\Omega} \\ =& \frac{\left(\frac{\hbar k}{m}\right) |A|^2 |f(\theta)|^2 \cdot \frac{1}{r^2} \cdot r^2 d\Omega}{\frac{\hbar k}{m} |A|^2 d\Omega} \\ D(\theta) =& |f(\theta)|^2 \end{aligned}$$

Problem: 4.3- Using Born approximation, calculate the differential and total cross-sections for scattering of a particle of mass $m$by the $\delta-$function potential $V(r) = g\delta(r), g =$constant.

Solution

The scattering amplitude

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int \exp(iq.r') V(r') d^3\tau'$$

Where $q = k - k'$and $q = 2k \sin\frac{\theta}{2}$. Here, $k$and $k'$are respectively, the wave vectors of the incident and scattered waves. Substituting the value of $V(r)$, we get

$$f(\theta) = -\frac{mg}{2\pi\hbar^2} \int \exp(iq.r') \delta(r') d^3\tau' \qquad \because \delta(n) = \begin{cases} 1 \text{ for } n=0 \\ 0 \text{ other wise} \end{cases}$$

Using the definition of $\delta-$function, we get

$$f(\theta) = -\frac{mg}{2\pi\hbar^2}$$

The differential scattering cross-section is

$$D(\theta) = |f(\theta)|^2 = \frac{m^2 g^2}{4\pi^2\hbar^4}$$

Since the distribution is isotropic, the total cross-section is given by

$$\sigma = 4\pi D(\theta) = \frac{m^2 g^2}{\pi\hbar^4}$$

Problem: 4.4- Write the asymptotic form of the wave function in the case of scattering by a fixed potential and explain. Also, what is Born approximation?

Solution

The general asymptotic solution is

$$\psi \xrightarrow[r\to\infty]{} A\left[e^{ikz} + f\left(\theta\right)\frac{e^{ikr}}{r}\right] \tag{4.1}$$

Where A is a constant. In this, the part e^{ikz}represents the incident plane wave along the $z-$axis. The wave vector k is given by

$$k^2 = \frac{2mE}{\hbar^2},$$

Where E is the energy. The second term of equation (i) represents the spherically diverging scattered wave. The amplitude factor $f\left(\theta\right)$ is called the scattering amplitude. If the potential $V(\vec{r})$ is weak enough, it will distort only slightly the incident plane wave.

Problem: 4.5- What is the formula for the first Born approximation for scattering amplitude $f\left(\theta\right)$? Under what condition is the Born approximation valid?

Solution

In the first Born approximation, the scattering amplitude

$$f(\theta) = -\frac{2m}{\hbar^2 q}\int_0^\infty sin(qr^{'})V(r^{'})r'dr'$$

Where $q\hbar$ is the momentum transfer from the incident particle to the scattering potential and

$$|q| = 2|k|sin\frac{\theta}{2}$$

With angle θ being the scattering angle, $V\left(r\right)$the potential, and m the mass. Moreover, the Born approximation is valid for weak scattering potentials and large incident energies.

Chapter 5

Relativistic Quantum Mechanics

SOLVED PROBLEMS

Problem: 5.1- Write Dirac's equation for a free particle. Find the probability density and the probability current density in Dirac's formalism.

Solution

Dirac's equation for a free particle is

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = -ic\hbar\alpha.\nabla\Psi + \beta m_\circ c^2\Psi \tag{5.1}$$

Here, α and β are 4×4 matrices and $\Psi\,(r,t)$ is a four-column vector. The Hermitian conjugate of above equation is

$$i\hbar\frac{\partial}{\partial t}\Psi^*(r,t) = +ic\hbar\alpha.\nabla\Psi^* + \beta m_\circ c^2\Psi^* \tag{5.2}$$

Multiplying Eq(5.1) by $\Psi^\dagger$ on left, Eq(5.2) by Ψ on right, and subtracting one from the other, we get

$$i\hbar\left(\Psi^\dagger\frac{\partial\Psi}{\partial t} - \frac{\partial\Psi^\dagger}{\partial t}\Psi\right) = -ic\hbar\left(\Psi^\dagger\alpha.\nabla\Psi + \nabla\Psi^\dagger.\alpha\Psi\right)$$

$$\frac{\partial}{\partial t}\left(\Psi^\dagger\Psi\right) + \nabla.\left(c\Psi^\dagger\alpha\Psi\right) = 0$$

$$\frac{\partial}{\partial t}\rho_r(r,t) + \nabla.J_r(r,t) = 0 \tag{5.3}$$

Where,

$$J_r(r,t) = c\Psi^\dagger \alpha \Psi \quad ; \quad \rho_r(r,t) = \Psi^\dagger \Psi$$

Eq(5.3) is the continuity equation and the equation $\rho_r(r,t)$ and $J_r(r,t)$ are the probability density and probability current density, respectively.

Problem: 5.2- For a Dirac particle moving in a central potential, show that the orbital angular momentum is not a constant of motion.

Solution

In the Heisenberg picture, the time rate of change of the $L = r \times P$ is given by

$$i\hbar \frac{dL}{dt} = [L, H]$$

Its x-component is

$$\begin{aligned} i\hbar \frac{d}{dt} L_x &= [L_x, H] = \left[yp_z - zp_y, c\alpha.P + \beta m_o c^2\right] \\ &= [yp_z, c\alpha.P] + [yp_z, \beta m_o c^2] - [zp_y, c\alpha.P] - [zp_y, \beta m_o c^2] \end{aligned}$$

Since α and β commute with r and p,

$$\begin{aligned} i\hbar \frac{d}{dt} L_x &= [yp_z, c\alpha_y.p_y] - [zp_y, c\alpha_z p_z] \\ i\hbar \frac{d}{dt} L_x &= c\alpha_y [y, p_y] p_z - c\alpha_z [z, p_z] p_y \qquad \because \quad [y, P_y] = i\hbar \ ; \ [P_x, P_y] = 0 \\ &= c\alpha_y i\hbar p_z - c\alpha_z i\hbar p_y \\ &= ci\hbar(p_z \alpha_y - p_y \alpha_z) \ \neq \ 0 \end{aligned}$$

Which shows that $L_x$is not a constant of motion. Similar relations hold good for $L_y$and L_z components. Hence the orbital angular momentum L is not a constant of motion.

Problem: 5.3- If one wants to write the relativistic energy E of a free particle as

$$\frac{E^2}{c^2} = (\alpha.P + \beta m_2 c)^2,$$

Show that $\alpha' s$ and $\beta' s$ have to be matrices and establish that they are non-singular and Hermitian.

Solution

The relativistic energy (E) of a free particle is given by

$$E^2 = c^2P^2 + m_o^2c^4 = c^2\left(P^2 + m_o^2c^2\right)$$

When E^2/c^2 is written as given in the problem,

$$\begin{aligned}
\frac{E^2}{c^2} &= P^2 + m_o^2c^2 = (\alpha.P + \beta m_o c)^2 \\
&= (\alpha.P)^2 + (\beta m_o c)^2 + \alpha.P\beta m_o c + \beta m_o c\alpha.P \\
&= \alpha_x^2p_x^2 + \alpha_y^2p_y^2 + \alpha_z^2p_z^2 \qquad \because (a+b+c)^2 = a^2+b^2+c^2+ab+ \\
&\qquad ba+bc+cb+ca+ac \\
&\quad + \beta^2m_o^2c^2 + (\alpha_x\alpha_y + \alpha_y\alpha_x)\,p_xp_y + (\alpha_x\alpha_z + \alpha_z\alpha_x)\,p_xp_z \\
&\quad + (\alpha_y\alpha_z + \alpha_z\alpha_y)\,p_yp_z + (\alpha_x\beta + \beta\alpha_x)\,m_ocp_x \\
&\quad + (\alpha_y\beta + \beta\alpha_y)\,m_ocp_y + (\alpha_z\beta + \beta\alpha_z)\,m_ocp_z
\end{aligned}$$

For this equation to be valid, it is necessary that

$$\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1, \{\alpha_x, \alpha_y\} = 0, \{\alpha_y, \alpha_z\} = 0$$

$$\{\alpha_z, \alpha_x\} = 0, \{\alpha_x, \beta\} = 0, \{\alpha_y, \beta\} = 0, \{\alpha_z, \beta\} = 0$$

It is obvious that the $\alpha' s$ and $\beta' s$ can not be ordinary numbers. The anti-commuting nature of the $\alpha' s$ and $\beta' s$ suggests that they have to be matrices. Since the square of these matrices are unit matrices, they are non-singular. As the $\alpha' s$ and $\beta' s$ determine the Hamiltonian, they must be Hermitian.

Problem: 5.4- show that the given matrix is not a constant of motion.

$$\sigma' = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}$$

Solution

The equation of motion of σ' in the Heisenberg picture is

$$i\hbar \frac{d\sigma'}{dt} = [\sigma', H]$$

Hence for σ' to be a constant of motion, ${\sigma'}_x$, ${\sigma'}_y$ and ${\sigma'}_z$ should commute with the Hamiltonian. Thus,

$$\begin{aligned} i\hbar \frac{d\sigma'}{dt} &= [{\sigma'}_x, H] = \left[{\sigma_x}', c\alpha.P + \beta m_o c^2\right] \\ &= [\sigma'_x, c\alpha \cdot P] + [\sigma'_x, \beta m_o c^2] \end{aligned}$$

Since ${\sigma'}_x$ commutes with β,

$$i\hbar \frac{d\sigma'}{dt} = [{\sigma'}_x, c\alpha_x p_x] + [{\sigma'}_x, c\alpha_y p_y] + [{\sigma'}_x, c\alpha_z p_z]$$

Since,

$$[{\sigma'}_x, \alpha_x] = 0, [{\sigma'}_x, \alpha_y] = 2i\alpha_z, [{\sigma'}_x, \alpha_z] = -2i\alpha_y$$

$$i\hbar \frac{d\sigma'}{dt} = [{\sigma'}_x, H] = 2ic(\alpha_z p_y - \alpha_y p_z) \neq 0$$

Hence the result.

Problem: 5.5- Show that Dirac's Hamiltonian for a free particle commutes with the operator $\sigma.P$, where P is the momentum operator and σ is the Pauli spin operator in the space of four component spinors.

Solution

Dirac's Hamiltonian for a free particle is

$$H = c\,(\alpha.P) + \beta m_o c^2$$

where,

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \quad ; \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

$$\alpha.P = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} . \ P = \begin{pmatrix} 0 & \sigma.P \\ \sigma.P & 0 \end{pmatrix}$$

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

$$[\sigma.P, H] = \left[\sigma.P, c\alpha.P + \beta m_o c^2\right] = [\sigma{\cdot}P, c\alpha{\cdot}P]+[\sigma{\cdot}P, \beta m_\circ]c^2 = c\,[\sigma.P, \alpha \cdot P]+[\sigma.P, \beta]\, m_\circ c^2$$

$$= c\left[\begin{pmatrix} \sigma.P & 0 \\ 0 & \sigma.P \end{pmatrix}, \begin{pmatrix} 0 & \sigma.P \\ \sigma.P & 0 \end{pmatrix}\right] + m_\circ c^2 \left[\begin{pmatrix} \sigma.P & 0 \\ 0 & \sigma.P \end{pmatrix}, \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\right]$$

$$= 0 + 0 = 0$$

Hence the result.

Chapter 6

Application to Quantum Mechanics

SOLVED PROBLEMS

Problem: 6.1- A sample of certain element is placed in a 0.300 T magnetic field and suitably excited. How far apart are the Zeeman components of 450 nm spectral line of this element ?

Solution

The separation of the Zeeman component is

$$\Delta\nu = \frac{eB}{4\pi m}$$

Since, $\nu = c/\lambda, d\nu = -cd\lambda/\lambda^2$, and so, disregarding the minus sign,

$$\begin{aligned} \Delta\lambda &= \frac{\lambda^2 \Delta\nu}{c} = \frac{eB\lambda^2}{4\pi mc} \\ &= \frac{1.60 \times 10^{-19} \times 0.300 \times (4.50 \times 10^{-7})^2}{4\pi 9.11 \times 10^{-31} \times 3.00 \times 10^8} = 2.83 \times 10^{-12} \text{ m} = 0.00283\text{m} \end{aligned}$$

Problem: 6.2- Compute the change in wavelength of the $2p \to 1s$ photon when a hydrogen atom is placed in a magnetic field of $2.00T$.

Solution

The energy of the photon from $n = 2$ to $n = 1$ is $E = -13.6eV\left(\frac{1}{2^2} - \frac{1}{1^2}\right) = 10.2eV$, and its wavelength is $\lambda = hc/E = (1240eV.nm)/(10.2eV) = 122nm$. The energy change ΔE of the levels is

$$\begin{aligned}\Delta E = \mu_B B =&(9.27 \times 10^{-24} J/T)(2.00T)\\ =&18.5 \times 10^{-24} J = 11.6 \times 10^{-5} eV\end{aligned}$$

We know that

$$\begin{aligned}\Delta\lambda =&\frac{\lambda^2}{hc}\Delta E\\ =&\frac{(122nm)^2}{1240eV.nm}11.6 \times 10^{-5} eV\\ =&0.00139nm\end{aligned}$$

Even for fairly large magnetic field of $2T$, the change on wavelength is very small, but it is easily measureable using an optical spectrometer.

Problem: 6.3- A collection of hydrogen atoms is placed in a magnetic field of $3.50T$. Ignoring the effects of electron spin, find the wavelengths of the three normal Zeeman components of the $3d$ to $2p$ transition.

Solution

In the absence of a magnetic field, the $3d$ to $2p$ energy difference is

$$E = (-13.6057eV)\left(\frac{1}{3^2} - \frac{1}{2^2}\right) = 1.88968eV$$

and the wavelength is

$$\begin{aligned}\lambda =&\frac{hc}{E}\\ =&\frac{1239.842eN.nm}{1.88968eV}\\ =&656.112nm\end{aligned}$$

The magnetic field gives a change in wavelength of

$$\begin{aligned}\Delta\lambda =& \frac{\lambda^2}{hc}\Delta E \\ =& \frac{(656.112nm)^2}{1239.842eV.nm}(5.79\times 10^{-5}eV/T)(3.50T) \\ =& 0.0703nm\end{aligned}$$

The wavelengths of the three normal Zeeman components are then $656.112nm$, $656.112nm + 0.070nm = 656.182nm$, and $656.112nm - 0.070nm = 656.042nm$.

Problem: 6.4- In a normal Zeeman effect experiment using a magnetic field of a stregth $0.3T$, find the splitting between the components of a $660nm$ spectral line.

Solution

Given that

$$\begin{aligned}B =& 0.3T \\ \lambda =& 660nm\end{aligned}$$

We know that

$$\begin{aligned}\Delta\lambda =& \frac{eB\lambda^2}{4\pi mc} \\ =& \frac{1.6\times 10^{-19}\times 0.3\times (660\times 10^{-9})^2}{4\times 3.14\times 9.1\times 10^{-31}\times 10^8} \\ =& 6.08\times 10^{-12}m \;=\; 6pm\end{aligned}$$

Problem: 6.5- Calculate the wavelengths of the components of the first line of the Lyman series, taking the fine structure of the 2p level into account.

Solution

The energy of the 2p to 1s Lyman transition is

$$E = (-13.6057eV)\left(\frac{1}{2^2} - \frac{1}{1^2}\right) = 10.20428eV$$

and its wavelength (in the absence of fine structure) is

$$\begin{aligned}\lambda =&\frac{hc}{E}\\ =&\frac{1239.842eN.nm}{10.20428eV}\\ =&121.5022nm\end{aligned}$$

With the fine structure energy splitting of $4.5 \times 10^{-5}eV$, the wavelength splitting is

$$\begin{aligned}\Delta\lambda =&\frac{\lambda^2}{hc}\Delta E\\ =&\frac{(121.5nm)^2}{1240eV.nm}(4.5 \times 10^{-5}eV)\\ =&0.00054nm\end{aligned}$$

The fine structure splits one level up by $0.5\Delta E$ and the other down by the same amount, so the wavelengths are

$$\lambda + \frac{1}{2}\Delta\lambda = 121.5024nm$$

and

$$\lambda - \frac{1}{2}\Delta\lambda = 121.5019nm$$


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