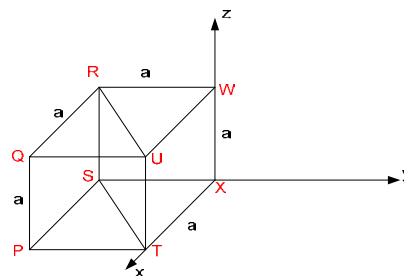


Assignment : Crystallography

1. Find Miller indices for the planes RWXS, UWXT and PSXT.



2. Prove that the relation between the reciprocal translation vector \vec{G}_{hkl} and the normal distance d_{hkl} to the plane (hkl) of real crystals is:

$$d_{hkl} = \frac{2\pi n}{|\vec{G}_{hkl}|}$$

3. Obtain the reciprocal primitive translation vectors of the real simple cubic lattice.
4. Obtain the reciprocal primitive translation vectors of the real FCC cubic lattice.
5. Obtain the reciprocal primitive translation vectors of the real BCC cubic lattice.

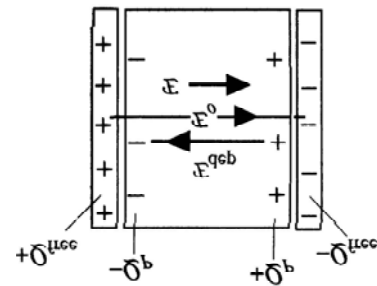
Assignment : Dielectric Materials

1. Polarization. Consider a parallel-plate capacitor with free-space between the plates. The capacitor has been charged to a voltage V_o with Q_o . The battery has been suddenly removed and then a dielectric slab of relative permittivity ϵ_r is inserted to fit between the plates. Assume an isotropic and linear dielectric medium.

- Find the electric field E_p due to the surface bounded polarization charges in terms of the polarization P .
- Find the relation between the polarization P and the net electric field E inside the medium

a -

$$\begin{aligned} \therefore E &= E_o - E_{dep} = \frac{E_o}{\epsilon_r} \\ E_{dep} &= E_o - E \\ E_{dep} &= E \left(\frac{E_o}{E} - 1 \right) = E(\epsilon_r - 1) \end{aligned}$$



b - $Q = Q_o + Q_p$

Q : total charges after inserting the slab

Q_o : charges before insertion of the slab

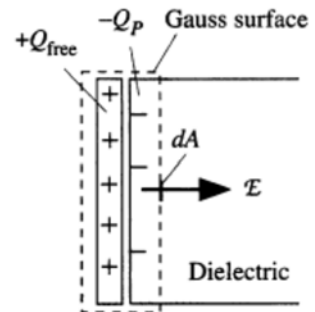
Q_p : charges due to the polarization of the dielectric slab, bound charges

$$Q_o = \epsilon_o EA$$

$$Q = \epsilon_r Q_o, \text{ and } Q_p = PA$$

$$\epsilon_r \epsilon_o E_p A = \epsilon_o EA + PA \quad \therefore P = \epsilon_o (\epsilon_r - 1) E$$

$$\text{or } E = \frac{P}{\epsilon_o (\epsilon_r - 1)}$$



2. Relative Permittivity and Polarizability. Given N number of dipoles per unit volume, show that the relative permittivity (ϵ_r) and the total polarizability (α) are related by $\epsilon_r = 1 + N\alpha/\epsilon_o$.

$$\bar{P} = N\bar{p}_{av} = \epsilon_o (\epsilon_r - 1) \bar{E}$$

$$\bar{p}_{av} = \alpha \bar{E}$$

$$\therefore \epsilon_r = 1 + N\alpha/\epsilon_0$$

3. Electronic Polarization. Consider a neutral atom be placed in a static electric field. Assume that the nucleus is surrounded by a cloud of Z electrons each with mass m_e and charge e . Prove that the AC electronic polarizability α_e can be written as

$$\alpha_e(\omega) = \frac{Ze^2 m_e}{m_e(\omega_e^2 - \omega^2)}$$

where ω_e is electronic polarization resonance frequency

Let E be sinusoidally varying with exponential representation $E = E_0 e^{j\omega t}$. Then,

$$\frac{d^2 x}{dt^2} + \omega_e^2 x = \left(\frac{e}{m_e}\right) E_0 e^{j\omega t}$$

Assume the solution be in the form $x = x_0 e^{j\omega t}$, then by substituting in the equation we get,

$$-\omega^2 x_0 + \omega_e^2 x_0 = \left(\frac{e}{m_e}\right) E_0$$

Thus, the displacement amplitude $x_0(\omega) = \frac{eE_0}{m_e} \frac{1}{\omega_e^2 - \omega^2}$

The ac electronic polarizability $\alpha_e(\omega) = \frac{p_e(\omega)}{E(\omega)}$.

$$\therefore \alpha_e(\omega) = \frac{(Ze)x_0(\omega)e^{j\omega t}}{E_0 e^{j\omega t}} = \frac{(Ze)^2}{Zm_e} \frac{1}{\omega_e^2 - \omega^2}$$

4. Relative Permittivity. Assume there are $N=2 \times 10^{27}$ atoms per unit volume with $Z=2$ and they are placed in a static field of $E=160$ V/m. Let the electronic resonance frequency for each atom be $\omega_e=55.9 \times 10^{15}$ rad/s. Calculate the static relative permittivity ϵ_r and the polarization vector P .

$$\alpha_e = \frac{(Ze)^2}{(Zm_e)\omega_e^2} = \frac{(2 \times 1.6 \times 10^{-19})^2}{2 \times 9.1 \times 10^{-31} \times (55.9 \times 10^{15})^2} = 1.8 \times 10^{-41} \text{ Fm}^2$$

$$\epsilon_r = 1 + \frac{N\alpha}{\epsilon_0} = 1 + \frac{2 \times 10^{27} \times 1.8 \times 10^{-41}}{8.85 \times 10^{-12}} = 1.00407$$

$$P = \alpha_e E = 1.8 \times 10^{-41} \times 160 = 2.8 \times 10^{-39} \text{ Cm}$$

5. **Electronic Polarizability.** The electronic polarizability of the Ar atom is 1.7×10^{-40} F m^2 . What is the static dielectric constant of solid Ar if its density is 1.8 g cm^{-3} ?

$$\epsilon_r = 1 + \frac{N\alpha}{\epsilon_0} = 1 + \frac{\frac{1.8 \times 10^6}{39.95} \times 6.02 \times 10^{23} \times 1.7 \times 10^{-40}}{8.85 \times 10^{-12}} = 1 + 052 = 1.52$$

Assignment : Magnetic Materials

1. Find the magnetic flux density B within a magnetic material that corresponds to the maximum magnetization M where the density $n=8.2 \times 10^{28}$ atoms/ m^3 and each atom has a dipole moment of $m=5 \times 10^{-27}$ A.m². Let the material permeability $\mu=3.77 \times 10^{-5}$. [533 μ T]

$$B = B_0 + \mu_0 M$$

$$\mu_r = \frac{B}{B_0}$$

$$B = \frac{B}{\mu_r} + \mu_0 M$$

$$B \left(1 - \frac{1}{\mu_r}\right) = \mu_0 M$$

$$\therefore B = \frac{\mu_r}{\mu_r - 1} (\mu_0 M)$$

$$\mu_r = \frac{\mu}{\mu_0} = \frac{3.77 \times 10^{-5}}{4\pi \times 10^{-7}} \approx 30$$

$$M = (8.2 \times 10^{28}) \times (5 \times 10^{-27}) = 410$$

$$\therefore B = \frac{30}{30-1} \times 4 \times \pi \times 10^{-7} \times 410 \approx 533 \mu T$$

2. A coil of 200 turns is wound uniformly over a non-magnetic material having a mean circumference of 600 mm. If the current through the coil is 4 A, calculate (a) the magnetic field strength, (b) the flux density, and (c) the stored energy in the non-magnetic medium. [1333 A/m, 1675 μ T, 1.116 J]

a - Ampere's law: $H = \frac{NI}{l} = \frac{200 \times 4}{0.6} \approx 1333$ A/m

b - $B_0 = \mu_0 \times H = 4\pi \times 10^{-7} \times 1333 \approx 1675$ μ T

c - $W_{vol} = \frac{1}{2} BH = \frac{1}{2} \times 1333 \times 1675 \times 10^{-6} \approx 1.116$ J

3. Assume that an electron is describing a circular orbit of radius a about a positively charged nucleus.

a. Show that the equivalent orbital dipole moment is $\frac{ea^2\omega}{2}$, where ω is the electron's angular velocity.

b. By equating the Coulomb and centrifugal forces, show that ω is $(4\pi\epsilon_0 m_e a^3 / e^2)^{-1/2}$, where m_e is the electron mass.

c. Find the values of the angular velocity and the orbital magnetic moment for a hydrogen atom, where $a=6 \times 10^{-11}$ m; let $B=0.5$ T.

$$a - m_o = I \times A = \frac{e\omega_o}{2\pi} \times \pi a^2 = \frac{e\omega_o a^2}{2}$$

$$b - F_a = F_c$$

$$\frac{e^2}{4\pi\epsilon_o a^2} = m_e \omega_o^2 a$$

$$\omega_o = \sqrt{\frac{e^2}{4\pi\epsilon_o m_e a^3}}$$

$$c - \omega_o = \sqrt{\frac{(1.6 \times 10^{-19})^2}{4\pi \times 8.85 \times 10^{-12} \times 9.1 \times 10^{-31} \times (6 \times 10^{-11})^3}} \approx 1.17 \times 10^{14} \text{ rad/sec}$$

$$m_{orb} = \frac{1.6 \times 10^{-19} \times 1.17 \times 10^{14} \times (6 \times 10^{-11})^2}{2} \approx 3.37 \times 10^{-26} \text{ Am}$$

If a magnetic field B_o of 0.5 T is now applied:

$$\omega \approx -\frac{eB_o}{2m_e} + \omega_o$$

$$\omega = -\frac{1.6 \times 10^{-19} \times 0.5}{2 \times 9.1 \times 10^{-31}} + 1.17 \times 10^{14} = 4.4 \times 10^{10} + 1.17 \times 10^{14} \approx 1.170044 \times 10^{14}$$

$$m = \frac{e\omega a^2}{2} = \frac{\omega}{\omega_o} \times m_o = \frac{1.170044}{1.17} \times 3.37 \times 10^{-26} \text{ Am}$$

4. The hydrogen atom described in the previous problem is subjected to a magnetic field having the same direction as that of the atom. Show that forces caused by B result in a decrease of the angular velocity by $eB/(2m_e)$ and a decrease in the orbital moment by $\frac{e^2 a^2 B}{4m_e}$.

Equating the forces, we get

$$F_c + F_m = F_a$$

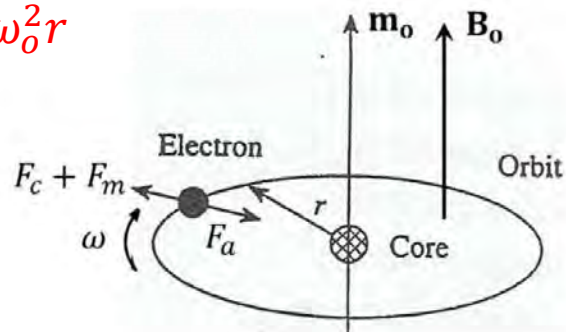
$$m_e \omega^2 r + e\omega r B_o = m_e \omega_o^2 r$$

Solving the equation

$$\omega = -\frac{eB_o}{2m_e} + \frac{1}{2} \sqrt{\left(\frac{eB_o}{m_e}\right)^2 + 4\omega_o^2}$$

For the case of $\frac{eB_o}{m_e} \ll \omega_o$

$$\therefore \omega = -\frac{eB_o}{2m_e} + \omega_o$$



$$\Delta\omega = \omega - \omega_0 = -\frac{eB_0}{2m_e}$$

The new magnetic moment

$$m = \frac{e\omega a^2}{2} a_n$$

$$\therefore \Delta m = m - m_0$$

$$= \frac{ea^2}{2} (\omega - \omega_0) a_n$$

$$= -\frac{e^2 a^2 B_0}{4m_e}$$

5. Consider bismuth with $\chi_m = -16.6 \times 10^{-5}$ and aluminum with $\chi_m = 2.3 \times 10^{-5}$. Suppose that we subject each sample to an applied magnetic field B_0 of 1 T applied in $+x$ direction. What are the magnetization M and the equivalent magnetic field $\mu_0 M$ in each sample? Which is paramagnetic and which is diamagnetic?

$$M = \chi_m H$$

- a- bismuth with $\chi_m = -16.6 \times 10^{-5}$, χ_m is negative, it is a diamagnetic material

$$\mu_r = \chi_m + 1$$

$$M = \chi_m \frac{B_0}{\mu_r \mu_0} = \chi_m \frac{B_0}{(\chi_m + 1) \mu_0}$$

$$= -16.6 \times 10^{-5} \frac{1}{(-16.66 \times 10^{-5} + 1) \times 4\pi \times 10^{-7}}$$

$$\approx -1.33 \times 10^2 \text{ A/m} \quad \text{in the negative x-direction.}$$

$$B = \mu_0 M = \frac{\chi_m B_0}{1 + \chi_m} \approx 16.66 \times 10^{-5} \text{ T}$$

- b- aluminum with $\chi_m = 2.3 \times 10^{-5}$, χ_m is positive, it is a paramagnetic material

$$\mu_r = \chi_m + 1$$

$$M = \chi_m \frac{B_0}{\mu_r \mu_0} = \chi_m \frac{B_0}{(\chi_m + 1) \mu_0} = 2.3 \times 10^{-5} \frac{1}{(2.3 \times 10^{-5} + 1) \times 4\pi \times 10^{-7}}$$

$$\approx 18.3 \text{ A/m} \quad \text{in the positive x-direction.}$$

$$B = \mu_0 M = \frac{\chi_m B_0}{1 + \chi_m} \approx 2.3 \times 10^{-5} \text{ T}$$

6. Compute the magnetic susceptibility due to diamagnetism in a solid with an atomic density of $10^{29}/\text{m}^3$. Each atom has 10

orbiting electrons. Assume a small magnetic induction of 0.1 T is applied and the average radius of the orbit is 0.1 nm, find the change in the magnetic moment for a single electron.

$$B = \mu_0 \mu_r H = \mu_0 \mu_r \frac{N(10I_e)}{2\pi a}$$

Assignment #1

1- We have postulated that the quantum mechanical wave functions satisfy certain mathematical conditions of good behavior. Examine the following functions for this good behavior, pointing out why some of them do not qualify.

a - $\psi(x) = x$ for $x \geq 0$
 $= 0$ elsewhere

b - $\psi(x) = x^2$

c - $\psi(x) = e^{-x^2}$

d - $\psi(x) = e^{-x}$

a - $\psi(x) = x$ $x \geq 0$
 does not qualify

1- not continuous up to 1st derivative

2- not finite, hence

3- not square integrable.

b - $\psi(x) = x^2$

1- not finite, hence

2- not square integrable

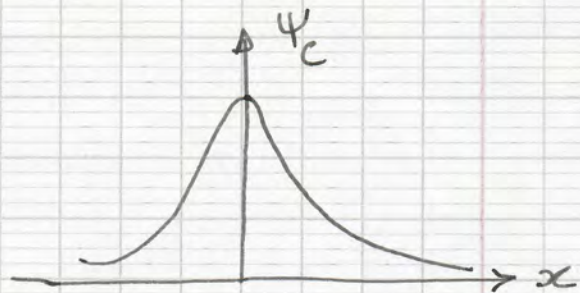
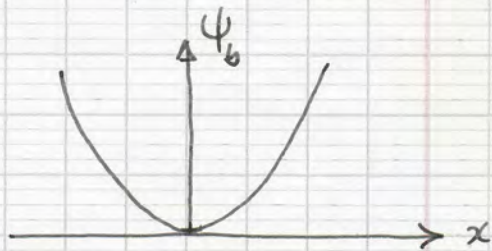
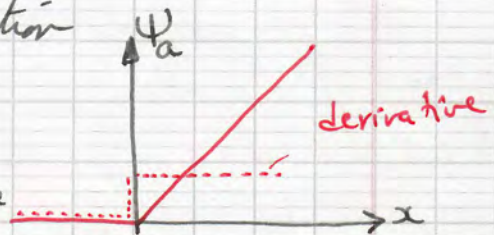
c - $\psi(x) = e^{-x^2}$
 Good Candidate

d - $\psi(x) = e^{-x}$

- not finite, hence

- not square integrable.

Solution



2- Consider two operators \underline{O}_1 and \underline{O}_2 defined by the following operations

$$\underline{O}_1 \psi(x) = \psi(x) + x$$

$$\underline{O}_2 \psi(x) = \frac{d\psi(x)}{dx} + 2\psi(x)$$

Check for the linearity of \underline{O}_1 and \underline{O}_2 .

Solution

$$\begin{aligned} \underline{O}_1 [\psi_1(x) + \psi_2(x)] &= \psi_1(x) + \psi_2(x) + x \\ &\neq \underline{O}_1 \psi_1(x) + \underline{O}_1 \psi_2(x) \end{aligned}$$

Because $\underline{O}_1 \psi_1(x) = \psi_1(x) + x$

$$\underline{O}_1 \psi_2(x) = \psi_2(x) + x$$

$$\therefore \underline{O}_1 \psi_1(x) + \underline{O}_1 \psi_2(x) = \psi_1(x) + \psi_2(x) + 2x$$

On the other hand;

$$\underline{O}_2 [\psi_1(x) + \psi_2(x)] = \frac{d[\psi_1(x) + \psi_2(x)]}{dx} + 2[\psi_1(x) + \psi_2(x)]$$

$$= \frac{d\psi_1(x)}{dx} + 2\psi_1(x) + \frac{d\psi_2(x)}{dx} + 2\psi_2(x)$$

$$= \underline{O}_2 \psi_1(x) + \underline{O}_2 \psi_2(x)$$

Thus \underline{O}_2 is linear.

3- Test the following operators for linearity:

a- $\underline{O}_1 \psi(x) = x^2 \psi(x)$

b- $\underline{O}_2 \psi(x) = e^{\psi(x)}$

c- $\underline{O}_3 \psi(x) = \psi^*(x)$

d- $\underline{O}_4 \psi(x) = x^2 \frac{d\psi}{dx}$

Solution

a- $\underline{O}_1 [\psi_1(x) + \psi_2(x)] = x^2 [\psi_1(x) + \psi_2(x)]$

$= x^2 \psi_1(x) + x^2 \psi_2(x)$

$= \underline{O}_1 \psi_1(x) + \underline{O}_1 \psi_2(x)$ Linear

b- $\underline{O}_2 [\psi_1(x) + \psi_2(x)] = e^{\psi_1(x) + \psi_2(x)} = e^{\psi_1(x)} \cdot e^{\psi_2(x)}$

$\neq \underline{O}_2 \psi_1(x) + \underline{O}_2 \psi_2(x)$ Nonlinear

c- $\underline{O}_3 [\psi_1(x) + \psi_2(x)] = [\psi_1(x) + \psi_2(x)]^* = \psi_1^*(x) + \psi_2^*(x)$

$= \underline{O}_3 \psi_1(x) + \underline{O}_3 \psi_2(x)$ Linear

d- $\underline{O}_4 [\psi_1(x) + \psi_2(x)] = x^2 \left[\frac{d\psi_1}{dx} + \frac{d\psi_2}{dx} \right]$

$= x^2 \frac{d\psi_1}{dx} + x^2 \frac{d\psi_2}{dx}$

$= \underline{O}_4 \psi_1(x) + \underline{O}_4 \psi_2(x)$ Linear

4. Evaluate the following commutators by operating on a wave function

a - $[x, \frac{d}{dx}]$

b - $[x^2, \frac{d}{dx}]$

Solution

$$\begin{aligned} \text{a - } [x, \frac{d}{dx}] \psi &= x \frac{d}{dx} \psi - \frac{d}{dx} x \psi \\ &= x \frac{d\psi}{dx} - x \frac{d\psi}{dx} - \psi = -\psi \end{aligned}$$

$$\therefore [x, \frac{d}{dx}] = -1$$

$$\begin{aligned} \text{b - } [x^2, \frac{d}{dx}] \psi &= x^2 \frac{d}{dx} \psi - \frac{d}{dx} x^2 \psi \\ &= x^2 \frac{d\psi}{dx} - x^2 \frac{d\psi}{dx} - 2x \psi \\ &= -2x \psi \end{aligned}$$

$$\therefore [x^2, \frac{d}{dx}] = -2x$$

5- Prove that the position operator \underline{x} and the linear momentum operator $\underline{p} = (-j\hbar \frac{d}{dx})$ do not commute, and find their commutator.

Solution

$$[\underline{x}, \underline{p}]\psi = (\underline{x}\underline{p} - \underline{p}\underline{x})\psi$$

$$\underline{x}\underline{p}\psi = x \cdot -j\hbar \frac{d\psi}{dx} = -j\hbar x \frac{\partial \psi}{\partial x}$$

$$\underline{p}\underline{x}\psi = -j\hbar \frac{d}{dx}(x\psi) = -j\hbar (x \frac{d\psi}{dx} + \psi)$$

$$(\underline{x}\underline{p} - \underline{p}\underline{x})\psi = j\hbar \psi$$

$$\therefore [\underline{x}, \underline{p}] \neq 0$$

therefore \underline{x} & \underline{p} do not commute.

6. A certain system is described by the Hamiltonian operator:

$$H = \frac{-d^2}{dx^2} + x^2$$

Show that $\psi = Ax e^{-\frac{x^2}{2}}$ is an eigenfunction of H and determine the eigenvalue.

Solution
for ψ to be an eigenfunction.

$$H\psi = \lambda\psi$$

$$H\psi = \left(\frac{-d^2}{dx^2} + x^2 \right) Ax e^{-\frac{x^2}{2}}$$

$$\frac{d}{dx} Ax e^{-\frac{x^2}{2}} = A[-x^2 + 1] e^{-\frac{x^2}{2}}$$

$$\frac{d^2}{dx^2} Ax e^{-\frac{x^2}{2}} = A[(1-x^2)(-x) + (-2x)] e^{-\frac{x^2}{2}}$$

$$= A[x^3 - 3x] e^{-\frac{x^2}{2}}$$

$$H\psi = A[3x - x^3] e^{-\frac{x^2}{2}} + Ax^3 e^{-\frac{x^2}{2}}$$

$$= 3Ax e^{-\frac{x^2}{2}} = 3\psi$$

$\therefore \psi$ is an eigenfunction

with $\lambda = 3$ eigenvalue.

Solid-state
Electronics

7- A particle in a one-dimensional box of length a is in the ground state. Calculate the probability of finding the particle in the interval $\Delta x = 0.01a$ at the point $x = a/2$.

Solution

The normalized wave function in the ground state, $n=1$ is given as:

$$\Psi_1 = \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} e^{-j \frac{E_1}{\hbar} t}$$

Thus the required probability is given as:

$$\int_{\frac{a}{2} - \frac{\Delta x}{2}}^{\frac{a}{2} + \frac{\Delta x}{2}} |\Psi_1|^2 dx$$

However $\sin \Delta x$ is small, we can approximate the integral as:

$$\begin{aligned} |\Psi_1(x = \frac{a}{2})|^2 \cdot \Delta x &= \frac{2}{a} \cdot \sin^2 \frac{\pi}{2} \cdot (0.01a) \\ &= 0.02 = 2\% \end{aligned}$$

8- A one-dimensional impenetrable box of length a contains an electron that suffers a small perturbation and emits a photon of frequency $\nu = \frac{3E_1}{h}$, where E_1 is the energy of the ground state. Would it be correct to conclude that the initial state of the electron is the $n=2$ box state. Why or why not?

Solution

If we assumed the electron to be in the $n=2$ box state, its energy would be four times that of the ground state since $E_n = n^2 E_1$

for $n=2$ $E_2 = 4E_1$

If the electron is perturbed and goes down to the ground state, a photon of frequency proportional to the difference of $E_2 - E_1$ would be emitted.

$$\nu_{\text{emitted}} = \frac{E_2 - E_1}{h} = \frac{4E_1 - E_1}{h} = \frac{3E_1}{h}$$

So, yes it would be correct!!

- 9- Consider an electron in a one dimensional box with impenetrable walls of width 10^8 cm.
- Calculate three lowest allowed values of energy
 - the frequency of light that would cause the electron to jump from the ground to the third excited energy level.
 - When the electron deexcites, what are the frequencies of the emitted photons
 - Plot the probability distribution for all three states and comment on where the electron is most likely to be found.

Solution

$$a - E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} = n^2 \frac{\hbar^2}{8ma^2} = n^2 E_0 ; E_0 = 37.7 \text{ eV}$$

$$E_1 = E_0, E_2 = 4E_0, E_3 = 9E_0$$

$$b - h\nu = E_3 - E_1 = 8E_0$$

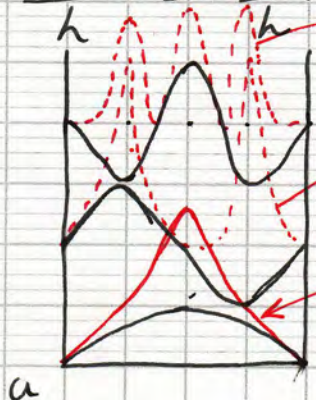
$$\therefore \nu = \frac{8E_0}{h}$$

$$c - \nu_{21} = \frac{E_2 - E_1}{h} = \frac{3E_0}{h}$$

$$\nu_{31} = \frac{E_3 - E_1}{h} = \frac{8E_0}{h}$$

$$\nu_{32} = \frac{E_3 - E_2}{h} = \frac{5E_0}{h}$$

d.



$n=3; \frac{a}{4}, \frac{a}{2}, \frac{3a}{4}$

$n=2; \frac{a}{4} \text{ and } \frac{3a}{4}$

$n=1; \frac{a}{2}$

10- Find the probable current density (probability current) for the plane wave $e^{j(kx - \omega t)}$

Solution

$$J_x = \frac{-j\hbar}{2m} \left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right]$$

$$\frac{d\psi}{dx} = jk\psi$$

$$\frac{d\psi^*}{dx} = -jk\psi^*$$

$$J(x,t) = \frac{-j\hbar}{2m} \left[+jk\psi\psi^* + jk\psi\psi^* \right]$$

$$= \frac{\hbar k}{2m} = \frac{p}{m} = v$$

Assignment #2

- 1- Derive an expression for the flux, current density, of free particles moving along the x-direction. First, start by writing down the continuity equation which is a conservation law, expressing the fact that a change in the particle density in a region of space is compensated for by a net change in flux into that region. Then write down the time-dependent Schrödinger wave equation for free particles. Eventually, by way of analogy you get the expression of the current density or flux.

Solution

Continuity equation.

$$\frac{\partial \rho}{\partial t} = - \frac{\partial J}{\partial x}$$

$$\frac{\partial (e \cdot P)}{\partial t} = - \frac{\partial J}{\partial x}$$

$$\frac{\partial P}{\partial t} + \frac{\partial J}{\partial x} = 0$$

J here is the number of particles / unit area / sec

or in the most general form

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

P : is the probability density function = $\Psi^* \Psi$

$$P = \Psi^* \Psi$$

Schrödinger Wave equation for a free particle is written as

$$H \Psi = i \hbar \frac{\partial \Psi}{\partial t}$$

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x) \quad \text{for free particles } V(x)=0$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = j\hbar \frac{\partial \psi}{\partial t} \quad \rightarrow (1)$$

Taking the complex conjugate

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} = -j\hbar \frac{\partial \psi^*}{\partial t} \quad \rightarrow (2)$$

Differentiating the probability P with respect to t yields:

$$\frac{\partial P}{\partial t} = \psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \quad (3)$$

Substituting now from (1) and (2) into (3)

$$\frac{\partial P}{\partial t} = \frac{1}{j\hbar} \left[\psi^* \left(-\frac{\hbar^2}{2m} \right) \frac{\partial^2 \psi}{\partial x^2} + \left(+\frac{\hbar^2}{2m} \right) \psi \frac{\partial^2 \psi^*}{\partial x^2} \right]$$

$$= \frac{j\hbar}{2m} \left[-\psi \frac{\partial^2 \psi^*}{\partial x^2} + \psi^* \frac{\partial^2 \psi}{\partial x^2} \right]$$

$$= \frac{j\hbar}{2m} \frac{\partial}{\partial x} \left[-\psi \frac{\partial \psi^*}{\partial x} + \psi^* \frac{\partial \psi}{\partial x} \right]$$

$$\therefore \frac{\partial P}{\partial t} + \frac{\hbar}{2jm} \frac{\partial}{\partial x} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right] = 0$$

By analogy to the continuity equation

$$\therefore J_x = \frac{\hbar}{2jm} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$$

2- The wavefunction for a particle is given by:

$$\psi(x) = A e^{jkx} + B e^{-jkx}$$

what flux does this represent.

Solution

$A e^{jkx}$ represents a wave going in the positive x -direction \equiv incident or travelling wave.

$B e^{-jkx}$ represents a wave going in the negative x -direction, reflected or backward wave

3. What is the flux associated with a particle described by the eigenfunction:

$$\psi(x) = u(x) e^{jkx}$$

where $u(x)$ is a real function.

Solution

$$J = \frac{\hbar}{2jm} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$$

$$\psi^* \frac{\partial \psi}{\partial x} = u(x) e^{-jkx} \left[u jk e^{jkx} + \frac{\partial u}{\partial x} e^{jkx} \right]$$

$$= jku^2 + u \frac{\partial u}{\partial x}$$

$$\psi \frac{\partial \psi^*}{\partial x} = u e^{jkx} \left[u (-jk) e^{-jkx} + \frac{\partial u}{\partial x} e^{-jkx} \right]$$

$$= -jku^2 + u \frac{\partial u}{\partial x}$$

$$J_x = \frac{\hbar}{2jm} \left[jku^2 + u \frac{\partial u}{\partial x} - (-jku^2 + u \frac{\partial u}{\partial x}) \right]$$

$$= \frac{\hbar}{2jm} \cdot 2jku^2 = \frac{\hbar k}{m} u^2(x)$$

4. Show that the flux, the particle current density J , may be written as:

$$J = \frac{1}{2m} [\psi^* \underline{p} \psi + (\psi^* \underline{p} \psi)^*]$$

where \underline{p} is the linear momentum operator.

Solution

J may be regarded as $p \psi$

current density $\rightarrow J = (e \cdot \underset{\substack{\uparrow \\ \text{probability}}}{p}} \cdot \underset{\substack{\leftarrow \text{momentum}}}{\frac{p}{m}} \text{ or } \frac{\langle p \rangle}{m}$

flux $J = \frac{1}{m} \psi^* \underline{p} \psi$

Since J has to be real

$$J = \frac{1}{2m} [\psi^* \underline{p} \psi + (\psi^* \underline{p} \psi)^*]$$

\Downarrow

$$\begin{aligned} \text{or } J_x &= \frac{\hbar}{2im} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right] \\ &= \frac{1}{2m} \left[\psi^* (-i\hbar \frac{\partial}{\partial x}) \psi - \psi (i\hbar \frac{\partial}{\partial x}) \psi^* \right] \\ &= \frac{1}{2m} \left[\psi^* \underline{p} \psi + \psi \underline{p}^* \psi^* \right] \\ &= \frac{1}{2m} \left[\psi^* \underline{p} \psi + (\psi^* \underline{p} \psi)^* \right] \end{aligned}$$

Region II

$$\frac{d^2 \psi_2}{dx^2} - \frac{2m}{\hbar^2} (V_0 - E) \psi_2 = 0$$

$$\psi_2 = C e^{\beta x} + D e^{-\beta x}$$

$$\beta = \sqrt{\frac{2m}{\hbar^2} (V_0 - E)}$$

ψ_2 has to be finite so $C = 0$

$$\psi_2 = D e^{-\beta x}$$

Boundary conditions at $x=0$

$$\psi_1(0) = \psi_2(0)$$

$$A + B = D \quad \text{--- (1)}$$

$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$$

$$j\alpha(A - B) = -\beta D$$

$$A - B = \frac{-\beta D}{j\alpha} \quad \text{--- (2)}$$

add (1) + (2)

$$\therefore 2A = D \left(1 - \frac{\beta}{j\alpha}\right)$$

$$\therefore D = \frac{2j\alpha A}{j\alpha - \beta}$$

Back into (1)

$$\begin{aligned} B &= D - A \\ &= A \left(\frac{2j\alpha}{j\alpha - \beta} - 1 \right) \\ &= A \frac{j\alpha + \beta}{j\alpha - \beta} \end{aligned}$$

$$\therefore \psi_1 = A \left(\overset{\substack{\uparrow \\ \text{incident}}}{e^{j\alpha x}} + \frac{j\alpha + \beta}{j\alpha - \beta} \overset{\substack{\leftarrow \\ \text{reflected}}}{e^{-j\alpha x}} \right)$$

$$\psi_2 = \frac{2j\alpha A}{j\alpha - \beta} \overset{\substack{\uparrow \\ \text{transmitted.}}}{e^{-\beta x}}$$

1- Transmission Coefficient T :

$$T = \frac{J_t}{J_i}$$

$$\begin{aligned} J_i &= \frac{-jk}{2m} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) \\ &= \frac{-jk}{2m} \left[A^* e^{-j\alpha x} \cdot j\alpha A e^{j\alpha x} - A e^{j\alpha x} \cdot (-j\alpha A^* e^{-j\alpha x}) \right] \\ &= \frac{-jk |A|^2}{2m} (j\alpha + j\alpha) = \frac{2k\alpha |A|^2}{2m} = \frac{\alpha k |A|^2}{m} \end{aligned}$$

$$\begin{aligned} J_t &= \frac{-jk}{2m} \left[D^* e^{-\beta x} (-D\beta e^{-\beta x}) - D e^{-\beta x} (-D^*\beta) e^{-\beta x} \right] \\ &= \frac{-jk |D|^2}{2m} [-e^{-2\beta x} + e^{-2\beta x}] = 0 \end{aligned}$$

Assignment # 3

1- Derive an expression for the density of available energy states of a particle trapped inside a three dimensional potential well and obeys Fermi-Dirac Statistics.

Solution

As before:

$$E_n = \frac{h^2}{8ma^2} n^2$$

where $n^2 = n_x^2 + n_y^2 + n_z^2$.

$$n_x = 1, 2, 3, \dots, \infty$$

$$n_y = 1, 2, 3, \dots, \infty$$

$$n_z = 1, 2, 3, \dots, \infty$$

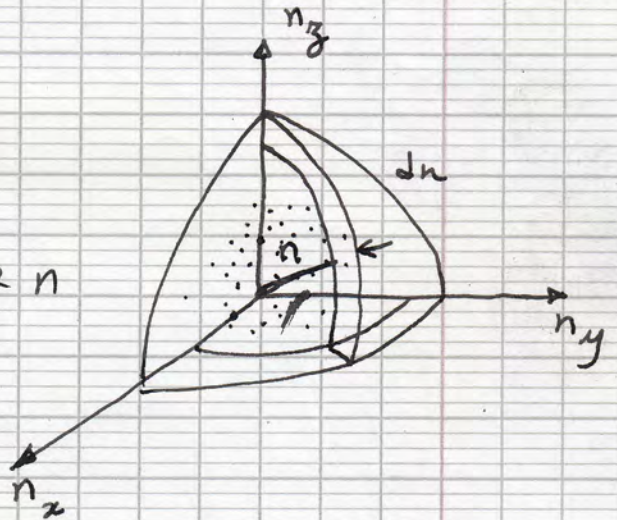
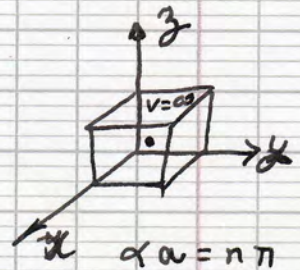
$$dS(n) = \frac{1}{8} (4\pi n^2 dn)$$

Note that positive and negative n gives the same energy.

Now, we need to convert this number of states into a function of the energy E rather than n .

$$E = \frac{h^2}{8ma^2} n^2$$

$$dE = \frac{h^2}{4ma^2} dn$$



$$\therefore dn = \frac{4ma^2}{h^2 n} dE$$

$$dS(E) = \frac{1}{8} \left(4\pi n^2 \cdot \frac{4ma^2}{h^2 n} \right) dE$$

$$= \frac{1}{8} \left(\frac{16\pi n ma^2}{h^2} \right) dE$$

$$= \frac{2\pi ma^2}{h^2} \cdot \sqrt{\frac{8ma^2 E}{h^2}} dE$$

$$= \frac{4\sqrt{2}\pi ma^3}{h^3} \sqrt{E} dE$$

Fermi Dirac statistics \Rightarrow i.e. particles which obey the Pauli Exclusion principle; we then multiply by 2.

$$d g_{FD}(E) = \frac{8\sqrt{2}\pi m a^3}{h^3} \sqrt{E} dE$$

where we also divided by a^3 to get the number of states per unit volume.

21B
per unit volume 21

2. Find the total number of electrons obeying Fermi-Dirac statistics at 0°K , from which deduce an expression for the Fermi energy E_f .

Solution

$$\begin{aligned}n &= \int_0^\infty dg_{\text{F.D.}} P_{\text{FD}} \\&= \int_0^{E_f} \frac{8\sqrt{2} m^{3/2}}{h^3} \sqrt{E} dE \\&= \frac{8\sqrt{2} \pi m^{3/2}}{h^3} \frac{2}{3} E_f^{3/2} \\&= \frac{16\sqrt{2}}{3} \frac{\pi m^{3/2}}{h^3} E_f^{3/2}\end{aligned}$$

Hence

$$\begin{aligned}E_f &= \left(\frac{3nh^3}{16\sqrt{2}\pi m^{3/2}} \right)^{2/3} = \left(\frac{3n}{16\sqrt{2}\pi} \right)^{2/3} \left(\frac{h^3}{m^{3/2}} \right)^{2/3} \\&= \left(\frac{3n}{\pi} \right)^{2/3} \left(\frac{1}{8 \cdot 2^{3/2}} \right)^{2/3} \frac{h^2}{m} \\&= \left(\frac{3n}{\pi} \right)^{2/3} \frac{h^2}{8m}\end{aligned}$$

3- Find the average energy of electrons obeying Fermi-Dirac statistics inside solids at 0°K .

Solution

$$\langle E \rangle = \frac{\int_0^\infty E dg_{FD} P_{FD}}{\int_0^\infty dg_{FD} P_{FD}}$$

at $T = 0^\circ\text{K}$ $P_{FD} = 1$ for $E \sim 0 \rightarrow E_f$

$$\begin{aligned} \therefore \langle E \rangle &= \frac{\int_0^{E_f} \frac{8\sqrt{2}\pi m^{3/2}}{h^3} E^{3/2} dE}{\int_0^{E_f} \frac{8\sqrt{2}\pi m^{3/2}}{h^3} E^{1/2} dE} \\ &= \frac{\frac{2}{5} E_f^{5/2}}{\frac{2}{3} E_f^{3/2}} \end{aligned}$$

$$\langle E \rangle = \frac{3}{5} E_f$$

4- Prove that the average energy of an electron inside a metal at 0°K is equal to three fifths of the Fermi level. Find the average energy of an electron at 0°K inside silver if it is a monovalent and its gram molecular volume is 10.28 cm^3 . Given that:

$$\begin{aligned} \text{Avogadro's number} & N_A = 6.023 \times 10^{23} \text{ mole}^{-1} \\ \text{Plack's constant} & h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s} \end{aligned}$$

Solution

In problem (3), we had proved that $\langle E \rangle = \frac{3}{5} E_f$

E_f from problem (2) is :

$$E_f = \left(\frac{3n}{\pi} \right)^{2/3} \frac{h^2}{8m}$$

where n = number of particles per unit volume.

a molecular volume 10.28 cm^3 contains 6.023×10^{23} atoms, each containing one electron.

$$n = \frac{6.023 \times 10^{23}}{10.28 \times 10^{-6} \times 1} = 5.86 \times 10^{28} \text{ electrons/volume}$$

$$\begin{aligned} \therefore E_f &= \left(\frac{3 \times 5.86 \times 10^{28}}{\pi} \right)^{2/3} \frac{(6.626 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31}} \frac{1}{1.6 \times 10^{-19}} \\ &= 5.5 \text{ eV} \end{aligned}$$

$$\therefore E_{av} = \frac{3}{5} \times 5.5 = 3.3 \text{ eV}$$

5- If the E-K diagram of the conduction band is approximated by:

$$E = Ak^2 + B$$

Find the effective mass.

Solution

$$m^* = \frac{\hbar^2}{d^2E/dk^2}$$

$$\frac{dE}{dk} = 2Ak$$

$$\frac{d^2E}{dk^2} = 2A$$

$$\therefore m^* = \frac{\hbar^2}{2A}$$