3.23 Electrical, Optical, and Magnetic Properties of Materials
Fall 2007

Homework # 1

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<u>**Homework is due on Wednesday September 19th, 5pm**</u>

1 Linear operators, hermitian operators and more

1. What does it mean for an operator $\hat{O}$ to be linear and hermitian?
2. Prove which of the following operators is linear, and which is hermitian:

$$\frac{d}{dx},\ \frac{1}{i}\frac{d}{d\phi},\ x^2$$

3. Let's consider a particle of mass m trapped in a one dimensional well of length a. The wavefunction of the particle is given by $\psi(x) = Ax(a - x)$. The wavefunction is **zero outside the well**.

   a) Find a value for A such that the wavefunction is normalized over the interval $[0, a]$.

   b) Calculate the expectation value of the position x of the particle in the well.

   c) What is the expectation value of the kinetic energy of the particle in the well?

2 The 2D electron gas

2D electron gases are observed at the interface between a semiconductor and a metal. One of the easiest model used to describe the main properties of the 2D electron gas is to consider **non-interacting free** electrons. In this model, we consider that the Coulomb repulsion between electrons is zero and that they do not feel any forces inside the box. This problem is concerned with the proper derivation of the eigenfunctions and the energy eigenvalues of a free electron in a 2D geometry.

2.1 General solution for the 3D case

Let's consider a box of dimensions L_x and L_y in respectively the x and y directions, and w in the z direction. An electron is enclosed in this box and cannot escape from it, but the electron is free to move inside it. This means that the potential energy of the electron is zero inside the box and infinite outside it.

Since the electron cannot escape, then the electron's wavefunction has to vanish on the sides of the box. So we will write that:

$$\psi(0, y, z) = \psi(L_x, y, z) = 0 \text{ for the x direction}$$

$$\psi(x, 0, z) = \psi(x, L_y, z) = 0 \text{ for the y direction}$$

$$\psi(x, y, 0) = \psi(x, y, w) = 0 \text{ for the z direction}$$

Those constitute the **boundary conditions** for our problem.

1) Write down the Schrodinger equation for an electron moving inside the box.

Now we will make the *ansatz* that you have seen in class and use the method of separation of variables to solve the Schrodinger equation. The wavefunction can be written as: $\psi(x, y, z) = X(x)Y(y)Z(z)$.

2) Translate the boundary conditions for ψ in the x, y and z directions in boundary conditions for respectively the X, Y and Z fonctions.

3) By using the *ansatz* for the wavefunction ψ, write the left hand side of the Schrodinger equation as a sum of 3 terms that are respectively fonctions of x, y and z only. The right hand side is reduced to a constant E.

4) The only mathematical solution for the Schrodinger equation expressed in question 3) is that each term of the equation is equal to a constant and that those constants add up to E. Let's call E_x, E_y and E_z those constants. Write down the 3 separate equations for the X, Y and Z functions.

The general solution for those three equations should be:

- $X(x) = A_x \sin(k_x x) + B_x \cos(k_x x)$ with $k_x = \sqrt{\frac{2mE_x}{\hbar^2}}$
- $Y(y) = A_y \sin(k_y y) + B_y \cos(k_y y)$ with $k_y = \sqrt{\frac{2mE_y}{\hbar^2}}$
- $Z(z) = A_z \sin(k_z z) + B_z \cos(k_z z)$ with $k_z = \sqrt{\frac{2mE_z}{\hbar^2}}$

5) Use the boundary conditions found in question 2) to find the allowed values for E_x, E_y and E_z in terms of integers n_x, n_y and n_z. Find which constants in the set $(A_x, A_y, A_z, B_x, B_y, B_z)$ are zero and simplify the general solutions for X, Y and Z. Finally write down the allowed total energies (the eigenenergies) $E(n_x, n_y, n_z)$ and the associated allowed wavefunctions (the eigenfunctions) $\psi_{n_x,n_y,n_z}(x, y, z)$.

At this stage we see that we still have some unknowns in the problem, namely the normalization constants in front of the eigenfunctions. Let's denote by A_{n_x,n_y,n_z} the constants in front of $\psi_{n_x,n_y,n_z}(x, y, z)$. We know from physical intuition that the probability of finding the electron inside the box is 1. So for any eigenfunction, we must have:

$$\int_0^{L_x} \int_0^{L_y} \int_0^{w} \psi^*_{n_x,n_y,n_z}(x, y, z)\psi_{n_x,n_y,n_z}(x, y, z)dxdydz = 1$$

This is the **normalization condition** for the eigenfunctions.

6) Using the analytical expressions for the eigenfunctions obtained in question 5), prove that:

$$A_{n_x,n_y,n_z} = \sqrt{\frac{8}{L_x L_y w}} = \sqrt{\frac{8}{V}}, \text{ where } V \text{ is the volume of the box}$$

2.2 When can we talk about a 2D gas?

Now that we have solved our problem mathematically, let's have a closer look at the energy eigenvalues:

$$E(n_x, n_y, n_z) = \frac{\hbar^2\pi^2}{2m}(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{w^2}) = \frac{h^2}{8m}(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{w^2})$$

1) What is the energy difference ΔE_x between state $E(n_x+1, 0, 0)$ and state $E(n_x, 0, 0)$? In the same way, calculate $\Delta E_y = E(0, n_y+1, 0) - E(0, n_y, 0)$ and $\Delta E_z = E(0, 0, n_z+1) - E(0, 0, n_z)$.

2) Calculate the ratios $\frac{\Delta E_z}{\Delta E_x}$ and $\frac{\Delta E_z}{\Delta E_y}$.

3) Now imagine that the box is very elongated in the x and y directions, i.e L_x and L_y are macroscopic, and very thin in the z direction. To make things clearer, let's take $w \sim 10$nm and $L_x = L_y \sim 1\mu$m, which are typical dimensions in semiconductor/metal junctions. In real devices the ratios $\frac{2n_z+1}{2n_x+1}$ and $\frac{2n_z+1}{2n_y+1}$ are **of order unity**. Knowing this, give a typical value for the ratios calculated in question 2).

4) From the numerical result of question 3), what can you deduce in terms of level spacings in x and y directions compared to the level spacing in the z direction? In which direction(s) of space can you consider that the allowed energy states form a quasi-continuum and in which direction(s) the allowed energy levels are quite well separated?

When talking about real devices (that are always 3-dimensional), we can speak of a 2D gas of electrons when the motion of each electron is "frozen" in one direction (let's call it the z direction) and not in the two others (x and y). By "frozen", we mean that the energy difference between the energy states caracterized by $n_z = 1$ and $n_z = 2$ is bigger than any typical thermal energy $k_B T$.

5) Calculate the energy difference $\Delta E_z = E(0, 0, 2) - E(0, 0, 1)$ in a GaAs device for which the width w is 10nm and the mass of the electron is $m^* = 0.067$m, where m is the mass of the electron in vacuum (m= $9.109 * 10^{-31}$kg). What is the temperature T corresponding to this energy difference, i.e such that $k_B T = \Delta E_z$? Is the motion of the electron in the z direction "frozen" for this system when operated at room temperature (300K)?