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3.23 Electrical, Optical, and Magnetic Properties of Materials

Fall 2007

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Homework # 1, solution

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September 24, 2007

1 Linear operators, hermitian operators and more

1. What does it mean for an operator \hat{O} to be linear and hermitian?

solution:

linearity We say that an operator \hat{O} is linear when we have the following equality for any wavefunctions $\psi(\vec{r})$, $\phi(\vec{r})$ and any complex numbers α , β :

$$\hat{O}(\alpha\psi(\vec{r}) + \beta\phi(\vec{r})) = \alpha\hat{O}(\psi(\vec{r})) + \beta\hat{O}(\phi(\vec{r}))$$

hermiticity We say that operator \hat{O} is hermitian when we have the following equality for any wavefunctions $\psi(\vec{r})$, $\phi(\vec{r})$:

$$\langle \psi | \hat{O} \phi \rangle = \int \psi^*(\vec{r}) \hat{O}(\phi(\vec{r})) d^3\vec{r} = \int (\hat{O}(\psi(\vec{r})))^* \phi(\vec{r}) d^3\vec{r} = \langle \hat{O} \psi | \phi \rangle$$

2. Prove which of the following operators is linear, and which is hermitian:

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

solution:

linearity of x^2 , $\frac{d}{dx}$ and $\frac{1}{i} \frac{d}{d\phi}$ Let's call \hat{O} the following operator: $\frac{d}{dx}$. To check the linearity we must verify that: $\hat{O}(\alpha\psi(x) + \beta\phi(x)) = \alpha\hat{O}(\psi(x)) + \beta\hat{O}(\phi(x))$, which gives us $\frac{d}{dx}(\alpha\psi(x) + \beta\phi(x)) = \alpha\frac{d}{dx}(\psi(x)) + \beta\frac{d}{dx}(\phi(x))$. But this result is true because the derivative of a sum of functions is just the sum of the derivatives. If we multiply this equality by $\frac{1}{i}$, we can easily conclude that $\frac{1}{i} \frac{d}{d\phi}$ is also linear. The linearity of the x^2 operator is obvious: $x^2(\alpha\psi(x) + \beta\phi(x)) = \alpha x^2\psi(x) + \beta x^2\phi(x)$.

hermiticity of x^2 Let's now look at the property of hermiticity. We start with the x^2 operator. We first write down the $\langle \psi | \hat{x}^2 \phi \rangle$ integral, which is: $\int \psi^*(x) x^2 (\phi(x)) dx$. Then we move the x^2 term to the left and find $\int x^2 \psi^*(x) (\phi(x)) dx$. Now since x^2 is real we see that $(x^2\psi(x))^*$ is the same thing as $x^2\psi^*(x)$. We can then conclude that: $\langle \psi | \hat{x}^2 \phi \rangle = \int \psi^*(x) x^2 (\phi(x)) dx = \int (x^2\psi(x))^* \phi(x) dx$, and this last term is nothing but $\langle \hat{x}^2 \psi | \phi \rangle$, which proves that x^2 is hermitian.

non-hermiticity of $\frac{d}{dx}$ We will now focus on operator $\frac{d}{dx}$. Let's express the first integral: $\langle \psi | \frac{d}{dx} \phi \rangle = \int \psi^*(x) \frac{d}{dx}(\phi(x)) dx$. The "trick" is then to integrate by part. Using the integration by part formula: $\int_a^b \frac{du(x)}{dx} v(x) dx = [u(x)v(x)]_a^b - \int_a^b u(x) \frac{dv(x)}{dx} dx$, we find that $\langle \psi | \frac{d}{dx} \phi \rangle = [\psi^*(x)\phi(x)]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \frac{d\psi^*(x)}{dx} \phi(x) dx$. The first term on the right-hand side of the last equation is zero, because **if a wavefunction does not vanish at infinities, then this wavefunction can never be square integrable, i.e that the integral of its square modulus is a finite number**. Using this result, we can re-write $\langle \psi | \frac{d}{dx} \phi \rangle$ as $-\int_{-\infty}^{+\infty} \frac{d\psi^*(x)}{dx} \phi(x) dx$. The last step consists in realizing that $\frac{d\psi^*(x)}{dx} = (\frac{d\psi(x)}{dx})^*$, because $\frac{d}{dx}(\psi^*(x)) = \frac{d}{dx}(Re(\psi(x)) - i.Im(\psi(x))) = \frac{dRe(\psi(x))}{dx} - i.\frac{dIm(\psi(x))}{dx} = (\frac{dRe(\psi(x))}{dx} + i.\frac{dIm(\psi(x))}{dx})^* = (\frac{d\psi(x)}{dx})^*$. We are now in a position to conclude that $\frac{d}{dx}$ **is not** an hermitian operator, because we just showed that $\langle \psi | \frac{d}{dx} \phi \rangle = -\int_{-\infty}^{+\infty} \frac{d\psi^*(x)}{dx} \phi(x) dx = -\langle \frac{d}{dx} \psi | \phi \rangle$.

hermiticity of $\frac{1}{i} \frac{d}{dx}$ remark: *it seems that a lot of students got confused because of the choice of my variable ϕ that looks like a wavefunction. So i will use x instead of ϕ in my solution. Sorry for that!*

The first integral $\langle \psi | \frac{1}{i} \frac{d}{dx} \phi \rangle$ integrated by part gives us: $-\int_{-\infty}^{+\infty} \frac{1}{i} \frac{d\psi^*(x)}{dx} \phi(x) dx$. Moreover we have $\frac{d\psi^*(x)}{dx} = (\frac{d\psi(x)}{dx})^*$, so by knowing that $-\frac{1}{i} = (\frac{1}{i})^*$, we see that we actually end up with $\langle \psi | \frac{1}{i} \frac{d}{dx} \phi \rangle = -\int_{-\infty}^{+\infty} \frac{1}{i} (\frac{d\psi(x)}{dx})^* \phi(x) dx = \int_{-\infty}^{+\infty} (\frac{1}{i} \frac{d\psi(x)}{dx})^* \phi(x) dx$, which proves the hermiticity of $\frac{1}{i} \frac{d}{dx}$.

- 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 $[0, a]$.

solution:

We know from the lectures that the square modulus of the wavefunction gives us the probability to find a particle at a certain position \vec{r} in space. If this is so, then we must be certain to find the particle somewhere in space. The mathematical translation of this physical intuition is expressed through the **normalization condition**: $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$ (in this one dimensional case). Let's apply this normalization condition to our case of a particle in a one-dimensional well. We know that the wavefunction is zero outside the well, we can then conclude that the limits $\pm\infty$ in the integral can be reduced to 0 and a . Using this we find that the normalization leads us to:

$$\int_0^a |Ax(a-x)|^2 dx = 1$$

This equation gives us right away that: $|A| = \sqrt{\frac{30}{a^5}}$. We see that we found the modulus of A and not A itself. But this is a general feature of wavefunctions in quantum mechanics. Wavefunctions are defined **up to a global phase**. This means in particular that taking A as a real number equal to $\sqrt{\frac{30}{a^5}}$ is perfectly suitable!

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

solution:

By definition the expectation value of the position operator \hat{x} is given by (for a correctly **normalized** wavefunction):

$$\langle \psi | \hat{x} \psi \rangle = \langle \hat{x} \psi | \psi \rangle = \langle \psi | \hat{x} | \psi \rangle = \int \psi^*(x) x \psi(x) dx$$

Injecting the analytical expression of the wavefunction with the correct normalization constant, we find:

$$\begin{aligned} \langle \psi | \hat{x} | \psi \rangle &= \int_0^a (Ax(a-x))^* x Ax(a-x) dx = \int_0^a Ax(a-x)xAx(a-x) dx = \\ &= A^2 \frac{a^6}{60} = \frac{30}{a^5} \frac{a^6}{60} = \frac{a}{2} \end{aligned}$$

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

solution:

By definition, the expectation value of the kinetic energy is given by:

$$\langle \psi | \hat{T} | \psi \rangle = \int_0^a \psi^*(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi(x) dx$$

The second derivative of $\psi(x)$ gives us $-2A$, so we finally obtain that:

$$\langle \psi | \hat{T} | \psi \rangle = \frac{5\hbar^2}{ma^2}$$

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.

solution:

The stationary Schrodinger equation for one electron in a potential $V(\vec{r})$ is:

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r})$$

Now if the potential is zero, then the equation reduces to the following:

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r}) = E\psi(\vec{r})$$

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 functions.

solution:

If the analytical expression of ψ is the following: $\psi(x, y, z) = X(x)Y(y)Z(z)$ then the boundary conditions give us:

$$\psi(0, y, z) = \psi(L_x, y, z) = 0 \text{ gives } X(0)Y(y)Z(z) = 0 \text{ and } X(L_x)Y(y)Z(z) = 0 \\ \text{for any } y \text{ and } z$$

$$\psi(x, 0, z) = \psi(x, L_y, z) = 0 \text{ gives } X(x)Y(0)Z(z) = 0 \text{ and } X(x)Y(L_y)Z(z) = 0 \\ \text{for any } x \text{ and } z$$

$$\psi(x, y, 0) = \psi(x, y, w) = 0 \text{ gives } X(x)Y(y)Z(0) = 0 \text{ and } X(x)Y(y)Z(w) = 0 \\ \text{for any } x \text{ and } y$$

We can then conclude that we must have $X(0) = X(L_x) = 0$, $Y(0) = Y(L_y) = 0$ and $Z(0) = Z(w) = 0$. Those are the boundary conditions for our functions X , Y and Z .

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 functions 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.

solution:

Let's use the analytical expression $\psi(x, y, z) = X(x)Y(y)Z(z)$ and inject this expression in the Schrodinger equation. Deriving $\psi(x, y, z) = X(x)Y(y)Z(z)$ partially with respect to x (leaving y and z constant) gives us $\frac{\partial\psi(x,y,z)}{\partial x} = \frac{dX(x)}{dx}Y(y)Z(z)$, and the same kind of result is valid when deriving partially with respect to y and z . Using this result, we find that the Schrodinger equation can be written as:

$$-\frac{\hbar^2}{2m} \left(\frac{d^2 X(x)}{dx^2} Y(y) Z(z) + X(x) \frac{d^2 Y(y)}{dy^2} Z(z) + X(x) Y(y) \frac{d^2 Z(z)}{dz^2} \right) = EX(x)Y(y)Z(z)$$

Dividing the equation by $X(x)Y(y)Z(z)$ gives us:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{X} \frac{dX}{dx} + \frac{1}{Y} \frac{dY}{dy} + \frac{1}{Z} \frac{dZ}{dz} \right) = E$$

Now if we move the $\frac{1}{Y} \frac{dY}{dy}$ and $\frac{1}{Z} \frac{dZ}{dz}$ terms to the right-hand side of the equation, we see that:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{X} \frac{dX}{dx} \right) = E + \frac{\hbar^2}{2m} \left(\frac{1}{Y} \frac{dY}{dy} + \frac{1}{Z} \frac{dZ}{dz} \right)$$

The function on the left-hand side is **only a function of x**, whereas the right-hand side is **only a function of y and z**. Moreover this equation is true for **any** x, y and z. So the only way we can achieve this is by taking the two sides of this equation equal to a given constant E_x . We then end up with the following two equations:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{X} \frac{dX}{dx} \right) = E_x$$

$$E + \frac{\hbar^2}{2m} \left(\frac{1}{Y} \frac{dY}{dy} + \frac{1}{Z} \frac{dZ}{dz} \right) = E_x$$

Rearranging the second equation, we find:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{Y} \frac{dY}{dy} + \frac{1}{Z} \frac{dZ}{dz} \right) = E - E_x$$

Repeating the whole argument on this new two-dimensional Schrodinger-like equation, we can conclude that we must have a second constant E_y such that:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{Y} \frac{dY}{dy} \right) = E_y$$

and

$$-\frac{\hbar^2}{2m} \left(\frac{1}{Z} \frac{dZ}{dz} \right) = E - E_x - E_y$$

Calling E_z the constant on the right-hand side of the previous equation, we can finally write the 3 equations that we extracted from the full Schrodinger equation:

$$-\frac{\hbar^2}{2m} \left(\frac{1}{X} \frac{dX}{dx} \right) = E_x$$

$$-\frac{\hbar^2}{2m} \left(\frac{1}{Y} \frac{dY}{dy} \right) = E_y$$

$$-\frac{\hbar^2}{2m} \left(\frac{1}{Z} \frac{dZ}{dz} \right) = E_z$$

We also have $E = E_x + E_y + E_z$.

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) $\psi_{n_x, n_y, n_z}(x, y, z)$.

solution:

The boundary conditions found in question 2) were $X(0) = X(L_x) = 0$, $Y(0) = Y(L_y) = 0$ and $Z(0) = Z(w) = 0$. Using the analytical expressions given above for the X , Y and Z functions, we find that:

- First, using $X(0) = 0$, $Y(0) = 0$ and $Z(0) = 0$, we easily conclude that $B_x = B_y = B_z = 0$
- Second, using $X(L_x) = 0$, $Y(L_y) = 0$ and $Z(w) = 0$ we conclude that $A_x \sin(k_x L_x) = A_y \sin(k_y L_y) = A_z \sin(k_z w) = 0$

In this second conclusion, we realize that we cannot take the constants A_x , A_y and A_z to be zero, otherwise the X , Y and Z functions would be zero everywhere and the wavefunction itself would be zero everywhere. We must then have $\sin(k_x L_x) = 0$, $\sin(k_y L_y) = 0$ and $\sin(k_z w) = 0$. But since the sin function is only zero when the argument of the function is an integer multiple of π , we find that there must exist a set of three integer numbers (n_x, n_y, n_z) such that:

$$k_x L_x = n_x \pi, \quad k_y L_y = n_y \pi \quad \text{and} \quad k_z w = n_z \pi$$

Finally we use the relationship between k and E ($E = \frac{\hbar^2 k^2}{2m}$) to give the allowed eigenenergies:

$$E(n_x, n_y, n_z) = E_x + E_y + E_z = \frac{\hbar^2}{2m} \left(\frac{n_x^2 \pi^2}{L_x^2} + \frac{n_y^2 \pi^2}{L_y^2} + \frac{n_z^2 \pi^2}{w^2} \right)$$

The corresponding eigenfunctions are:

$$\psi_{n_x, n_y, n_z}(x, y, z) = A_x A_y A_z \sin(n_x \pi \frac{x}{L_x}) \sin(n_y \pi \frac{y}{L_y}) \sin(n_z \pi \frac{z}{w})$$

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:

$$\int_0^{L_x} \int_0^{L_y} \int_0^w \psi_{n_x, n_y, n_z}^*(x, y, z) \psi_{n_x, n_y, n_z}(x, y, z) dx dy dz = 1$$

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

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

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

solution:

Using the shorthand notation A_{n_x, n_y, n_z} for the constants $A_x A_y A_z$, we can rewrite the eigenfunctions as:

$$\psi_{n_x, n_y, n_z}(x, y, z) = A_{n_x, n_y, n_z} \sin(n_x \pi \frac{x}{L_x}) \sin(n_y \pi \frac{y}{L_y}) \sin(n_z \pi \frac{z}{w})$$

Now we inject this expression in the normalization condition and find:

$$\int_0^{L_x} \int_0^{L_y} \int_0^w |A_{n_x, n_y, n_z}|^2 \sin^2(n_x \pi \frac{x}{L_x}) \sin^2(n_y \pi \frac{y}{L_y}) \sin^2(n_z \pi \frac{z}{w}) dx dy dz = 1$$

This 3 dimensional integral can be separated in a product of three one dimensional integrals. The one dimensional integral over the x coordinate is:

$$\int_0^{L_x} \sin^2(n_x \pi \frac{x}{L_x}) dx$$

To integrate this integral, we use the following well-known trigonometric equality: $\sin^2(u) = \frac{1 - \cos(2u)}{2}$ and the fact that $\int \cos(u) du = \sin(u)$. Hence we have:

$$\int_0^{L_x} \sin^2(n_x \pi \frac{x}{L_x}) dx = \frac{L_x}{2} - \frac{1}{2} [\sin(2n_x \pi) - \sin(0)]$$

Now since n_x is an integer, $\sin(2n_x \pi)$ is zero and so is $\sin(0)$. In the end, the one dimensional integrals reduce to:

$$\int_0^{L_x} \sin^2(n_x \pi \frac{x}{L_x}) dx = \frac{L_x}{2}$$

$$\int_0^{L_y} \sin^2(n_y \pi \frac{y}{L_y}) dy = \frac{L_y}{2}$$

$$\int_0^w \sin^2(n_z \pi \frac{z}{w}) dz = \frac{w}{2}$$

And we easily conclude that:

$$|A_{n_x, n_y, n_z}| = \sqrt{\frac{8}{L_x L_y w}}$$

As in the case of question 3)a) of exercise 1, we see that an eigenfunction is defined up to a global phase, so we can choose A_{n_x, n_y, n_z} to be real and equal to $\sqrt{\frac{8}{L_x L_y w}}$.

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:

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

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 $\Delta E_z = E(0, 0, n_z + 1) - E(0, 0, n_z)$.

solution:

We use the formula for the einergy eigenvalues to find:

$$\Delta E_x = E(n_x + 1, 0, 0) - E(n_x, 0, 0) = \frac{\hbar^2 \pi^2}{2m L_x^2} ((n_x + 1)^2 - n_x^2) = \frac{\hbar^2 \pi^2}{2m L_x^2} (2n_x + 1)$$

$$\Delta E_x = \frac{\hbar^2 \pi^2}{2mL_y^2} (2n_y + 1)$$

$$\Delta E_z = \frac{\hbar^2 \pi^2}{2mw^2} (2n_z + 1)$$

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

solution:

From question 1), we easily conclude that:

$$\frac{\Delta E_z}{\Delta E_x} = \left(\frac{L_x}{w}\right)^2 \left(\frac{2n_z+1}{2n_x+1}\right)$$

$$\frac{\Delta E_z}{\Delta E_y} = \left(\frac{L_y}{w}\right)^2 \left(\frac{2n_z+1}{2n_y+1}\right)$$

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 $w \sim 10\text{nm}$ and $L_x = L_y \sim 1\mu\text{m}$, 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).

solution:

From the ratios found in question 2), and knowing that $\frac{2n_z+1}{2n_x+1}$ and $\frac{2n_z+1}{2n_y+1}$ are **of order unity**, we conclude that:

$$\frac{\Delta E_z}{\Delta E_x} = \frac{\Delta E_z}{\Delta E_y} \sim \left(\frac{L_x}{w}\right)^2$$

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?

solution:

From question 3), we see that the level spacing in the z direction are of order $\left(\frac{L_x}{w}\right)^2$ greater than in directions x and y. The levels are much closer in energy in the x and y directions than in the z direction, so a quantum particle will "feel" this difference, and the motion in the z direction will be quantized. A small thermal energy will be sufficient to have the quantum particle jump from one energy state to the next in the x and y directions, so we can safely describe the energy states as forming a quasi-continuum in the x and y directions.

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 characterized 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 $m^* = 0.067m$, where m is the mass of the electron in vacuum ($m = 9.109 \times 10^{-31}\text{kg}$). 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)?

solution:

We find that:

$$\Delta E_z = E(0, 0, 2) - E(0, 0, 1) = 3 \frac{\hbar^2 \pi^2}{2mw^2}$$

Plugging in the values for m and w , we end up with:

$$\Delta E_z = E(0, 0, 2) - E(0, 0, 1) \approx 2.7 * 10^{-20} \text{J which is about } 0.17 \text{ eV}$$

The corresponding temperature T is $T \approx \frac{0.17 \text{eV}}{k_B} \approx 1950 \text{K}$! So we would need to heat the device up to temperatures close to 1900K to start seeing higher energy levels in the z direction to be populated. We can safely say that the motion of electrons in this device operating at 300K is "frozen" in the z direction, and that we are dealing with a 2D electron gas (if dimensions in x and y directions are much bigger than in the z direction).