Lecture9

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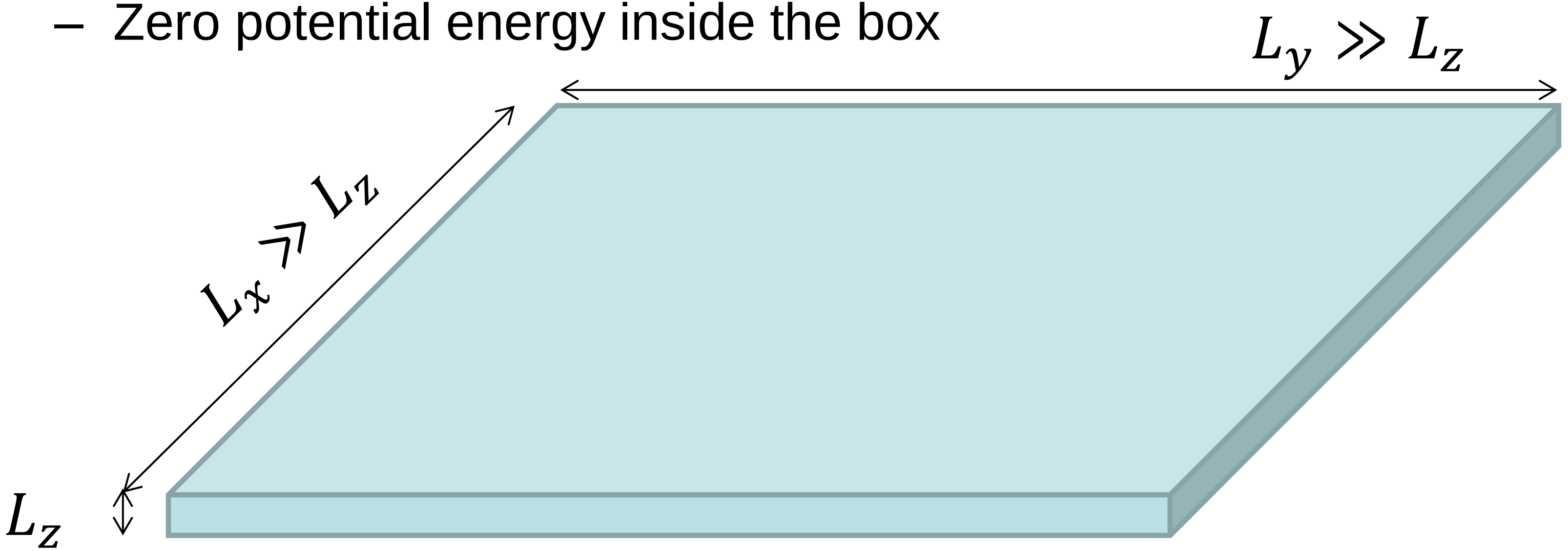
Thin and wide box

- Consider a thin and wide box. (3D infinite potential well)
  - Length along the confinement direction, L_z
  - At all six surfaces, the wavefunction vanishes.
  - Zero potential energy inside the box



Eigen-energy?

- Hamiltonian operator

$$H = -\frac{\hbar^2}{2m_{xx}}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_{yy}}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_{zz}}\frac{\partial^2}{\partial z^2}$$

  - We can find the following solution:

$$\psi_{l,m,n}(x,y,z) = A_{l,m,n}\sin\left(\frac{l\pi}{L_x}x\right)\sin\left(\frac{m\pi}{L_y}y\right)\sin\left(\frac{n\pi}{L_z}z\right)$$

  - Of course, the eigen-energy is given by

$$E_{l,m,n} = \frac{\hbar^2}{2m_{xx}}\frac{l^2\pi^2}{L_x^2} + \frac{\hbar^2}{2m_{yy}}\frac{m^2\pi^2}{L_y^2} + \frac{\hbar^2}{2m_{zz}}\frac{n^2\pi^2}{L_z^2}$$

Fermi-Dirac distribution

- Let us assume that there is a state whose eigen-energy is $E_{l,m,n}$.
  - Still, the Fermi level is located at 0 eV.
  - Then, the Fermi-Dirac distribution is given by

$$f_{FD} = \frac{1}{1 + \exp\left(\frac{E_{l,m,n}}{k_B T}\right)}$$

Total number?

- Number of electrons at a certain state
  - For a state with (l, m, n), the number of electrons is $2 \times f_{FD}\left(E_{l,m,n}\right)$. The factor of 2 is due to the spin degeneracy.
- There are many states.
  - The total number is given by

$$2 \times \sum_{l=1}^{\infty} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} f_{FD}\left(E_{l,m,n}\right)$$

MATLAB example (1)

- Let us consider $L_x = L_y = 100\ \mathrm{nm}$ and $L_z = 5\ \mathrm{nm}$.
  - In practical sense, L_z is reasonable. L_x and L_y are somewhat large.
  - Also, assume that $m_{xx} = m_{yy} = 0.19\, m_0$ and $m_{zz} = 0.91\, m_0$.
  - First, define some constants.

```
h = 6.626176e-34; % Planck constant, J s
hbar = h / (2*pi); % Reduced Planck constant, J s
q = 1.602192e-19; % Elementary charge, C
m0 = 9.109534e-31; % Electron rest mass, kg
k_B = 1.380662e-23; % Boltzmann constant, J/K
T = 300.0; % Temperature, K
```

MATLAB example (2)

- What is the number?
  - Set the box size and the masses.

```
Lx = 100e-9; Ly = 100e-9; Lz = 5e-9; % Lenghs, m
mxx = 0.19; myy = 0.19; mzz = 0.91; % Masses, m0
```

  - Calcultate the total number. How large is it?

```
lmax = 50; mmax = 50; nmax = 50;
totalNumber = 0;
for l=1:lmax
   for m=1:mmax
      for n=1:nmax
         E = (hbar*pi)^2/2/m0*(1/mxx*(l/Lx)^2 + 1/myy*(m/Ly)^2 + 1/mzz*(n/Lz)^2);
         totalNumber = totalNumber + 2/(1+exp(E/(k_B*T)));
      end
   end
end
```

Subband

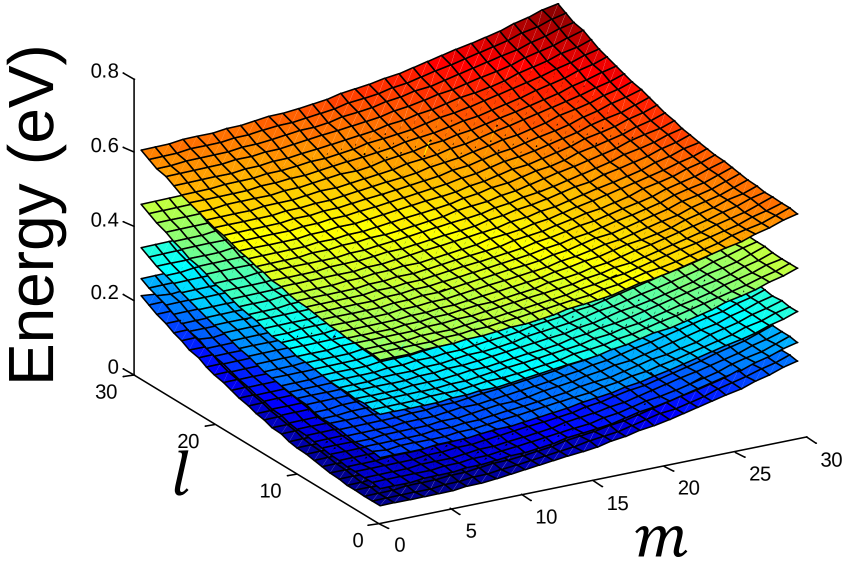
- Consider a 3D box.
  - The eigen-energy is given by

$$E_{l,m,n} = \frac{\hbar^2}{2m_{xx}} \frac{\pi^2}{L_x^2} l^2 + \frac{\hbar^2}{2m_{yy}} \frac{\pi^2}{L_y^2} m^2 + \frac{\hbar^2}{2m_{zz}} \frac{\pi^2}{L_z^2} n^2$$

  - We assume that $L_z \ll L_x$ and $L_z \ll L_y$.
  - Then, we have $\frac{\hbar^2}{2m_{zz}} \frac{\pi^2}{L_z^2} \gg \frac{\hbar^2}{2m_{xx}} \frac{\pi^2}{L_x^2}$ and $\frac{\hbar^2}{2m_{zz}} \frac{\pi^2}{L_z^2} \gg \frac{\hbar^2}{2m_{yy}} \frac{\pi^2}{L_y^2}$.
  - Change in n introduces big difference in $E_{l,m,n}$.
  - Different n values correspond to different “subbands.”

On (l, m) plane

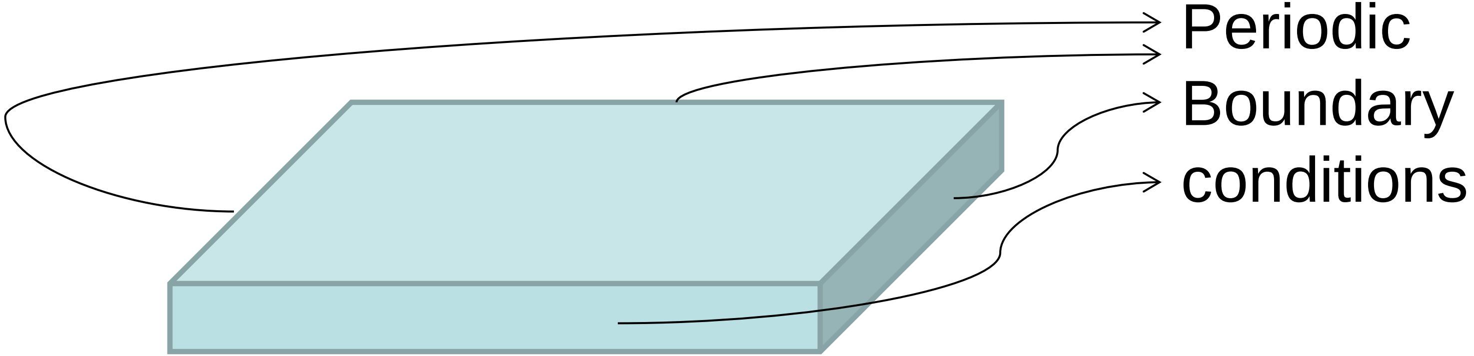
- For given n values, draw $E_{l,m,n}$.




```
(Defining some constants. Copy-and-paste.)
lmax = 30;
mmax = 30;
E = zeros(lmax,mmax);
for n = 1:5;
  for l = 1:lmax
    for m = 1:mmax
      E(l,m) = (hbar*pi)^2/2/m0*(1/mxx*(l/Lx)^2 + 1/myy*(m/Ly)^2 + 1/mzz*(n/Lz)^2);
    end
  end
  surface(E/q);
  hold on;
end
```

For a given subband with n

- It is treated as if
  - Quantum confinement along the z direction only.
  - No quantum confinement along other directions.
  - Periodic boundary conditions are applied to those boundaries.



Periodic boundary condition

- Consider the y direction.
  - A sub-problem

$$-\frac{\hbar^2}{2m_{yy}}\frac{\partial^2}{\partial y^2}\psi_y(y) = E_y\psi_y(y)$$

  - Its periodic boundary condition, $\psi_y(0) = \psi_y(L_y)$.
  - With a quantized $k_y = \frac{2\pi}{L_y}m$ (m is the integer.)

$$\psi_y(y) = A_y \exp(ik_y y)$$

  - When k_y is increased by $\frac{2\pi}{L_y}$, a new state can be found.

Total number, revisited (1)

- Previously, we calculated it.
  - In this time, a slightly different approach

$$2\sum_{l=1}^{\infty}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} f_{FD}(E_{l,m,n}) = 2\sum_{n=1}^{\infty}(\#\text{of electrons for the } n\text{th subband})$$

  - Also, summations are converted into integrals.

$$\sum_{l=1}^{\infty}\sum_{m=1}^{\infty} f_{FD}(E_{l,m,n}) = \frac{L_x}{2\pi}\int_{-\infty}^{\infty} dk_x \frac{L_y}{2\pi}\int_{-\infty}^{\infty} dk_y\, f_{FD}\left(\frac{\hbar^2 k_x^2}{2m_{xx}} + \frac{\hbar^2 k_y^2}{2m_{yy}} + E_{z,n}\right)$$

$$= \frac{L_x L_y}{(2\pi)^2}\int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y\, f_{FD}\left(\frac{\hbar^2 k_x^2}{2m_{xx}} + \frac{\hbar^2 k_y^2}{2m_{yy}} + E_{z,n}\right)$$

Total number, revisited (2)

- Further simplification?
  - When $m_{xx} = m_{yy}$, we have the following relation:

$$\frac{L_x L_y}{(2\pi)^2} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y\, f_{FD}\left(\frac{\hbar^2 k_x^2}{2m_{xx}} + \frac{\hbar^2 k_y^2}{2m_{yy}} + E_{z,n}\right) = \frac{L_x L_y}{(2\pi)^2} \int_{0}^{\infty} dk \int_{0}^{2\pi} d\theta\, k f_{FD}\left(\frac{\hbar^2 k^2}{2m_{xx}} + E_{z,n}\right)$$

$$= \frac{L_x L_y}{(2\pi)^2} (2\pi) \int_{0}^{\infty} dk\, k f_{FD}\left(\frac{\hbar^2 k^2}{2m_{xx}} + E_{z,n}\right) = \frac{L_x L_y}{(2\pi)^2} (2\pi) \int_{0}^{\infty} dE_{xy} \frac{m_{xx}}{\hbar^2} f_{FD}\left(E_{xy} + E_{z,n}\right)$$

  - Great! But for general cases?

Review

- 2DEG (Two-dimensional electron gas)
  - Its wavefunction can be written as

$$\psi_{k_x,k_y,n}(x,y,z) = A_{k_x,k_y,n} e^{+ik_x x} e^{+ik_y y} \psi_{z,n}(z)$$

  - Its eigenenergy can be written as

$$E_{k_x,k_y,n} = \frac{\hbar^2 k_x^2}{2m_{xx}} + \frac{\hbar^2 k_y^2}{2m_{yy}} + E_{z,n}$$

- Number of electrons for a subband (per spin)

$$\frac{L_x L_y}{(2\pi)^2} \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y \, f_{FD}\left(\frac{\hbar^2 k_x^2}{2m_{xx}} + \frac{\hbar^2 k_y^2}{2m_{yy}} + E_{z,n}\right)$$

In general, $m_{xx} \neq m_{yy}$

- How to simplify the integral
  - By introducing $k'_x = \sqrt{\frac{m_d}{m_{xx}}} k_x$ and $k'_y = \sqrt{\frac{m_d}{m_{yy}}} k_y$, we have

$$\frac{\hbar^2 k_x^2}{2m_{xx}} + \frac{\hbar^2 k_y^2}{2m_{yy}} = \frac{\hbar^2}{2m_d} k'^2$$

  - Also, $dk_x = \sqrt{\frac{m_{xx}}{m_d}} dk'_x$ and $dk_y = \sqrt{\frac{m_{yy}}{m_d}} dk'_y$
- Number of electrons for a subband (per spin)

$$\frac{L_x L_y}{(2\pi)^2} \frac{\sqrt{m_{xx} m_{yy}}}{m_d} \int_{-\infty}^{\infty} dk'_x \int_{-\infty}^{\infty} dk'_y \, f_{FD}\left(\frac{\hbar^2 k'^2}{2m_d} + E_{z,n}\right)$$

Let us say $m_d = \sqrt{m_{xx} m_{yy}}$

- Then,

$$\frac{L_x L_y}{(2\pi)^2} \int_{-\infty}^{\infty} dk'_x \int_{-\infty}^{\infty} dk'_y \, f_{FD}\left(\frac{\hbar^2 k'^2}{2m_d} + E_{z,n}\right)$$

$$= \frac{L_x L_y}{(2\pi)^2} (2\pi) \int_0^{\infty} dk' k' f_{FD}\left(\frac{\hbar^2 k'^2}{2m_d} + E_{z,n}\right)$$

  – By setting $E_{xy} = \frac{\hbar^2}{2m_d} k'^2$, we find that $k' dk' = dE_{xy} \frac{m_d}{\hbar^2}$. The number of electron becomes

$$\frac{L_x L_y}{(2\pi)^2} (2\pi) \frac{m_d}{\hbar^2} \int_0^{\infty} dE_{xy} f_{FD}(E_{xy} + E_{z,n})$$

Fermi-Dirac integral

- The Fermi-Dirac integral of order 0
  - By setting $e_{xy} = \frac{E_{xy}}{k_B T}$, we find that

$$\int_0^\infty dE_{xy} f_{FD}\left(E_{xy} + E_{z,n}\right) = k_B T \int_0^\infty de_{xy} \frac{1}{1 + \exp\left(e_{xy} - \frac{-E_{z,n}}{k_B T}\right)}$$

$$= k_B T \mathcal{F}_0\left(\frac{-E_{z,n}}{k_B T}\right) = k_B T \ln\left(1 + \exp\left(\frac{-E_{z,n}}{k_B T}\right)\right)$$

$$\mathcal{F}_0(\eta) \equiv \int_0^\infty \frac{dx}{1 + \exp(x - \eta)} = \ln(1 + e^\eta)$$

Summary

- Number of electrons for a subband (per spin)

$$\frac{L_x L_y}{(2\pi)^2}(2\pi)\frac{m_d}{\hbar^2}k_B T \ln\left(1+\exp\left(\frac{-E_{z,n}}{k_B T}\right)\right)$$

  – Recall that $m_d = \sqrt{m_{xx}m_{yy}}$.

- Total number of electrons

$$2\sum_{n=1}^{\infty}\frac{L_x L_y}{(2\pi)^2}(2\pi)\frac{m_d}{\hbar^2}k_B T \ln\left(1+\exp\left(\frac{-E_{z,n}}{k_B T}\right)\right)$$

MATLAB example

- $L_x = L_y = 100\ \mathrm{nm}$ and $L_z = 5\ \mathrm{nm}$.
  - In practical sense

```
(Defining some constants. Copy-and-paste.)
Lx = 100e-9; Ly = 100e-9; Lz = 5e-9; % Lenghs, m
mxx = 0.19; myy = 0.19; mzz = 0.91; % Masses, m0
nmax = 50;
coef = 2*Lx*Ly/(2*pi)*sqrt(mxx*myy)*m0/(hbar^2)*(k_B*T);
totalNumber = 0;
for n=1:nmax
  Ez = (hbar^2)/(2*mzz*m0)*(pi*n/Lz)^2;
  subbandNumber = coef*log(1+exp(-Ez/(k_B*T)));
  totalNumber = totalNumber + subbandNumber;
end
```

How to find $n(x, y, z)$

- The total number is known. But, how can we find $n(x, y, z)$?
  - Each state, $\psi_{k_x,k_y,n}(x, y, z)$, contributes $\left|\psi_{k_x,k_y,n}(x, y, z)\right|^2$.
  - Recall that the wavefunction can be written as

$$\psi_{k_x,k_y,n}(x, y, z) = A_{k_x,k_y,n} e^{+ik_x x} e^{+ik_y y} \psi_{z,n}(z)$$

  - Then, $\left|\psi_{k_x,k_y,n}(x, y, z)\right|^2 = \left|A_{k_x,k_y,n}\right|^2 \left|\psi_{z,n}(z)\right|^2$
  - Integration of $\left|\psi_{k_x,k_y,n}(x, y, z)\right|^2$ over the box should give unity.

$$L_x L_y \left|A_{k_x,k_y,n}\right|^2 \int_0^{L_z} dz \left|\psi_{z,n}(z)\right|^2 = 1$$

Normalization of $\psi_{z,n}(z)$

- If $\psi_{z,n}(z)$ is normalized in the 1D structure,
  - We have the following condition:

$$\left|A_{k_x,k_y,n}\right|^2 = \frac{1}{L_x L_y}$$

  - Therefore, each state contributes

$$\left|\psi_{k_x,k_y,n}(x,y,z)\right|^2 = \frac{1}{L_x L_y}\left|\psi_{z,n}(z)\right|^2$$

  - Note that every state in a subband has the same electron density. (In general, it does not hold.)

1D infinite potential well

- When $\psi_{z,n}(z) = A_{z,n} \sin\left(\frac{n\pi}{L_z} z\right)$,
  - The value of $A_{z,n}$ is $\sqrt{\frac{2}{L_z}}$.
  - Therefore, when fully occupied, a state in the n-th subband contributes an electron density of (per spin)
  $$\frac{2}{L_x L_y L_z} \sin^2\left(\frac{n\pi}{L_z} z\right)$$
  - Finally, the electron density can be obtained by considering all subbands.

MATLAB example (1)

- Preparing some constants (the same as before)

```
h = 6.626176e-34; % Planck constant, J s
hbar = h / (2*pi); % Reduced Planck constant, J s
q = 1.602192e-19; % Elementary charge, C
m0 = 9.109534e-31; % Electron rest mass, kg
k_B = 1.380662e-23; % Boltzmann constant, J/K
T = 300.0; % Temperature, K
Lx = 100e-9; Ly = 100e-9; Lz = 5e-9; % Lenghs, m
mxx = 0.19; myy = 0.19; mzz = 0.91; % Masses, m0
nmax = 10;
coef = 2*Lx*Ly/(2*pi)*sqrt(mxx*myy)*m0/(hbar^2)*(k_B*T);
```

MATLAB example (2)

- Calculation of `elec`

```
totalNumber = 0;
Nz = 51;
z = transpose([0:Nz-1])*Lz/(Nz-1);
elec = zeros(Nz,1); % Electron density, /m^3
for n=1:nmax
  Ez = (hbar^2)/(2*mzz*m0)*(pi*n/Lz)^2;
  subbandNumber = coef*log(1+exp(-Ez/(k_B*T)));
  totalNumber = totalNumber + subbandNumber;
  elec = elec + 2/(Lx*Ly*Lz)*(sin(n*pi*z/Lz).^2)*subbandNumber;
end
plot(z/1e-9,elec/1e6)
```