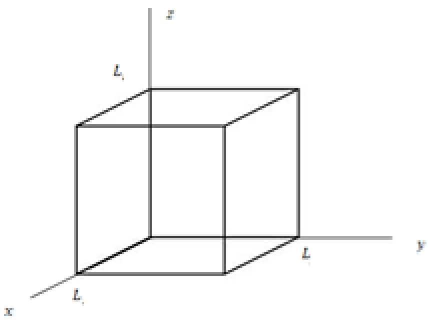
PH102, 2014W, Lecture Notes: February 4, Tues, Class 9

What counts as quantum gases?

Let's consider a system of N particles in a 3-D box where the energy of each particle is defined by three quantum numbers (n_x, n_y, n_z).



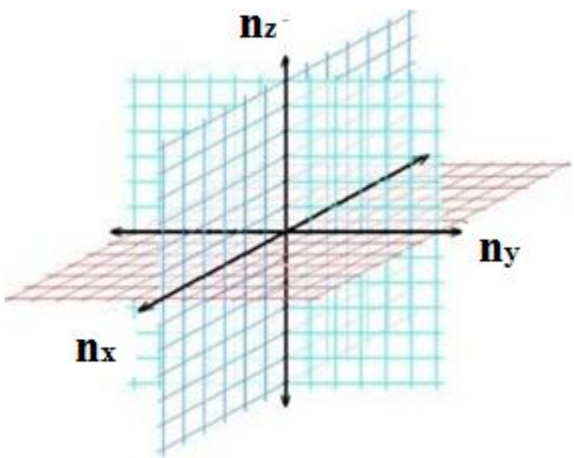
The 3D Box

$$U(\vec{x}) = \begin{cases} 0 & 0 < x, y, z < L, \\ \infty & otherwise \end{cases}$$

$$\psi\,(x, y, z) = A\ \sin\frac{n_x \pi x}{L} \sin\frac{n_y \pi y}{L} \sin\frac{n_z \pi z}{L}$$

$$E_{(n_x, n_y, n_z)} = (n_x^2 + n_y^2 + n_z^2)\frac{\pi^2\hbar^2}{2mL^2}$$

Note that E is dependent upon three quantum number coordinates n_x, n_y, n_z which can be put into 3 dimensional Cartesian coordinates as shown below:



In that space we can define

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

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

$$n = \sqrt{\frac{2mL^2}{\pi^2\hbar^2}}\sqrt{E}$$

Density of states: how many states are available between E and E+dE and n_x, n_y, n_z *are greater than* 0

$$D(E) = \frac{No. of\ states\ at\ E + dE - No. of\ states\ at\ E}{dE} = \frac{1}{8}(4\pi n^2)\frac{dn}{dE} =$$

$$= \frac{\pi n^2}{2}\sqrt{\frac{2mL^2}{\pi^2\hbar^2}}\left(\frac{1}{2}\right)\frac{1}{\sqrt{E}} = \sqrt{\frac{2mL^2}{\pi^2\hbar^2}}\left(\frac{\pi}{4}\right)\frac{2mL^2}{\pi^2\hbar^2}\sqrt{E} = \frac{m^{3/2}}{\pi^3\hbar^3\sqrt{2}}\sqrt{E}\ L^3 = \frac{m^{3/2}V}{\pi^3\hbar^3\sqrt{2}}\sqrt{E}$$

Considering spin of the particle in the system then D(E) will increase by $(2s+1)$

$$D(E) = (2s+1)\frac{m^{3/2}V}{\pi^3\hbar^3\sqrt{2}}\sqrt{E}$$

Calculate the total number of particles

$$N = \int_0^\infty \mathcal{N}(E)D(E)dE = \frac{m^{3/2}V}{\pi^3\hbar^3\sqrt{2}}\int_0^\infty \frac{\sqrt{E}}{Be^{E/k_BT} \mp 1}dE =$$

$$\bar{E} = \frac{\int_0^\infty E\mathcal{N}(E)D(E)dE}{\int_0^\infty \mathcal{N}(E)D(E)dE} = \frac{\int_0^\infty \frac{E^{\frac{3}{2}}}{Be^{\frac{E}{k_BT}} \mp 1}dE}{\int_0^\infty \frac{\sqrt{E}}{Be^{\frac{E}{k_BT}} \mp 1}dE}$$

$$= \frac{3}{2}k_BT\left[1 \mp \frac{\pi^3\hbar^3\sqrt{2}}{(2s+1)(2\pi mk_BT)^{3/2}}(\frac{N}{V})^1 + \cdots\right]$$

For classical limit, the second term in the expression should be very small:

$$\frac{\pi^3\hbar^3\sqrt{2}}{(2s+1)(2\pi mk_BT)^{3/2}}(\frac{N}{V})^1 \sim \frac{\hbar^3}{(mk_BT)^{3/2}}(\frac{N}{V})^1 \ll 1$$

Example 1: Estimate whether molecules in the air should be treated as classical particles.

From the ideal gas law $PV = Nk_BT \rightarrow \frac{N}{V} = \frac{P}{k_BT}$

$\frac{\hbar^3}{(mk_BT)^{3/2}}(\frac{N}{V})^1 = \frac{\hbar^3}{(mk_BT)^{3/2}}\frac{P}{k_BT} \cong 9 \text{ x } 10^{-9}$ very small! → Classical treatment fits

At T=0, when all fermions fill up the energy levels up to the **Fermi energy**:

$$N = \int_0^{E_F} \mathcal{N}(E)D(E)dE = \int_0^{E_F}(2s+1)\frac{m^{3/2}V}{\pi^3\hbar^3\sqrt{2}}\sqrt{E}\ dE = (2s+1)\frac{m^{\frac{3}{2}}V}{\pi^3\hbar^3\sqrt{2}}(\frac{2}{3}E_F^{\frac{3}{2}})$$

$$E_F = \frac{\pi^2\hbar^2}{m}\left[\frac{3}{(2s+1)\pi\sqrt{2}}\frac{N}{V}\right]^{2/3}$$

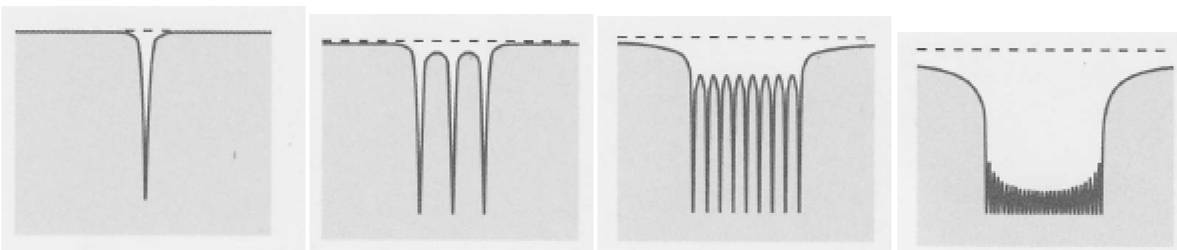
Example 2: Calculate Fermi Energy for Silver:

- Atomic Number for Silver is 79 and mass number 107.9 x 1.66 x $10^{-27}kg$
- Density of silver = 10.5 x $10^3 kg/m^3$
- $5d^1 6s^1$ and one valence electron per atom contributes to the quantum gas model
- So, $density = \frac{mass}{volume} = \frac{N\ atoms \text{ x } mass\ per\ atom}{volume\ (V)}$
- $\frac{N}{V} = \frac{density}{mass\ per\ atom} = \frac{0.5 \text{ x } 10^3 kg/m^3}{107.9 \text{ x } 1.66 \text{ x } 10^{-27}kg} = 5.86 \text{ x } 10^{28} m^{-3}$
- $E_F = \frac{\pi^2\hbar^2}{m}\left[\frac{3}{(2s+1)\pi\sqrt{2}}\frac{N}{V}\right]^{2/3}$=5.5 eV
- Compare this with k_BT at room temperature (300K) = 0.026eV

- Therefore, $\frac{E_F}{k_B T} >> 1$ at room temperature, electrons in Silver should be considered using Fermi-Dirac statistics. To electrons in a metal, room temperature is very cold. Much higher temperature is needed for electrons in a metal to spread around like classical particles.

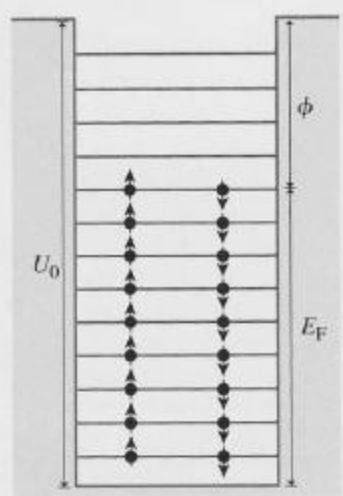
Example 3: Fermion Gas Treatment: Conduction Electron Energy Levels

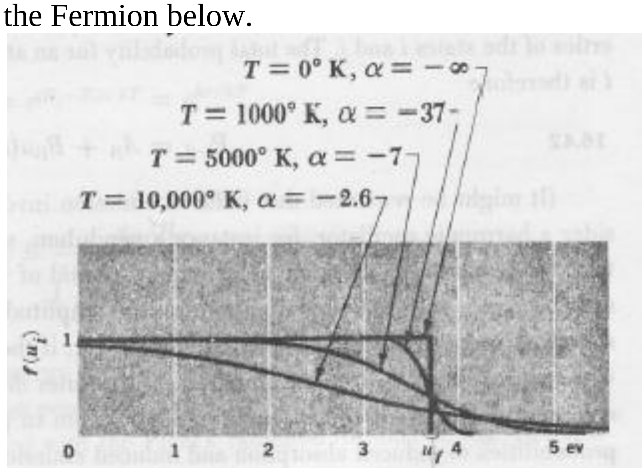
- Electrons in the conduction band can be treated as a system of free moving electrons confined in a finite potential well created by ions in the metal. See below for how ions in an one dimensional lattice can create a potential that resembles the finite potential well studied earlier in the course.



- According to the Exclusion Principle, no two electrons occupy the same quantum state, resulting in stacking up the energy levels with two electrons per energy level as shown in the diagram on the right. The Fermi Energy is shown as where the Energy level that the valence electron(s) occupy. Not all electrons participate in conduction. Only a few electrons at the top level can gain energy See the occupation index for the Fermion below.

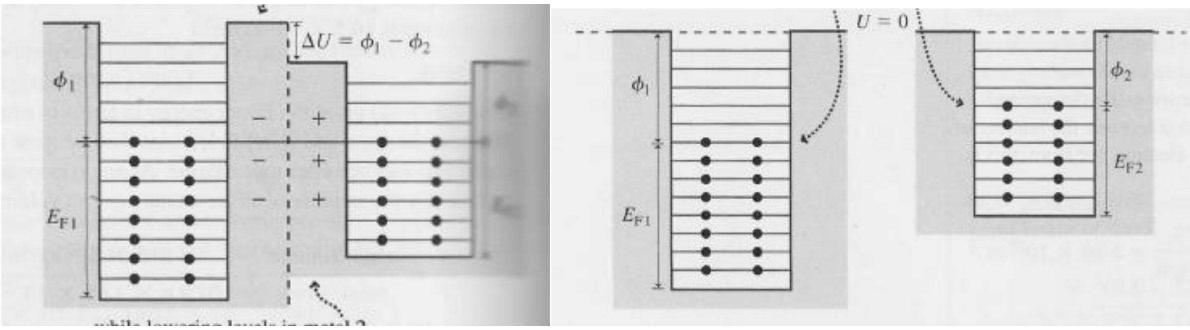
Figure 9.17 Electron energies in a "cold" metal.





- The work function ϕ represents the minimum amount of energy needed to free an electron from the metal. $\phi = U_0 - E_F$.
- A potential (called contact potential) can be created when two metals with different work functions are joined. When they are separate, each metal has a neutral charge distribution. When they are in contact, electrons in the higher energy level of metal 2 transfer to metal

1, thus raising electron energy levels in metal 1 and lowering electron energy levels in metal 2. As a result, metal 1 is negatively charged by gaining electrons and metal 2 is positively charged by losing electrons to metal 1. The flow of electrons stops when Fermi Energies of the two metals become the same. Therefore, the energy difference is created: $\Delta U = \phi_1 - \phi_2$, resulting in potential difference $V_1 - V_2 = \frac{\phi_1 - \phi_2}{-e} = (\phi_2 - \phi_1)/e$



Example 4: Boson Gas and Bose-Einstein Condensation

- He_4 has two electrons and two protons. At the ground state, both electrons of He_4 are in the 1S state with opposite spins. Therefore, the total spin number is zero. At low temperatures, He_4 follow the Bose-Einstein statistics.
- SuperFluid behavior can be observed at 2.2K where its viscosity becomes negligible and thermal conductivity becomes perfect. At that temperature, liquid He can spill through the small molecular level cracks and can creep over the edge of the container. See the video clip such as http://www.youtube.com/watch?v=2Z6UJbwxBZI