EE201/MSE207 Lecture 13

Solids (free electron gas)

Simplest model : non-interacting electrons (no Coulomb interaction, no exchange correlation)

Idea: electrons occupy energy states from the lowest energy up (fermions)
At zero temperature, the highest occupied energy is called Fermi energy.

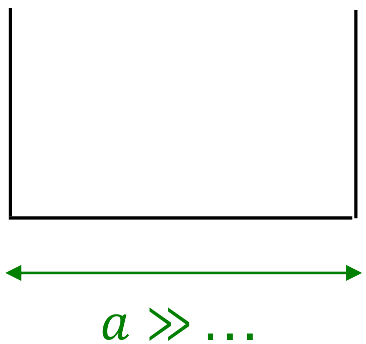
So, we need to count available states. Assume many electrons, so that even though states are discrete, we always consider "thick slices" in energy, and are interested only in density of states.

Density of states (DOS): number of available states per unit of energy (eV).

DOS does not depend on temperature (except due to change of material parameters), while Fermi level depends on temperature.

Goal for today: find DOS and Fermi energy (at $T = 0$) for quantum wires (1D), quantum wells (2D), and solids (3D)

Quantum wire: large 1D well (not in textbook)

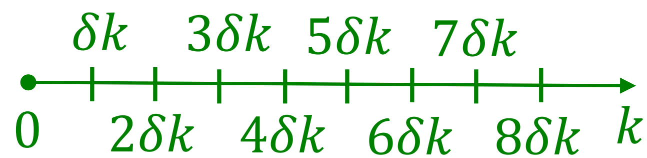


$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad (n \gg 1,\ a \text{ is large})$$

$$\psi_n(x) = \sqrt{2/a}\,\sin\left(\frac{n\pi}{a}\,x\right) = \sqrt{2/a}\,\sin(k_n x)$$

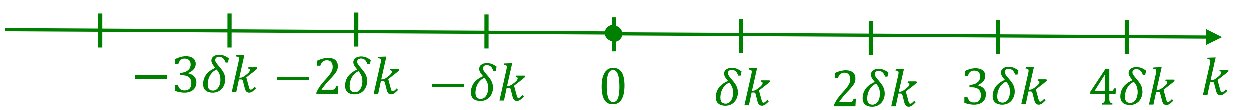
$$k_n = \frac{n\pi}{a}$$

One state per $\delta k = \dfrac{\pi}{a}$

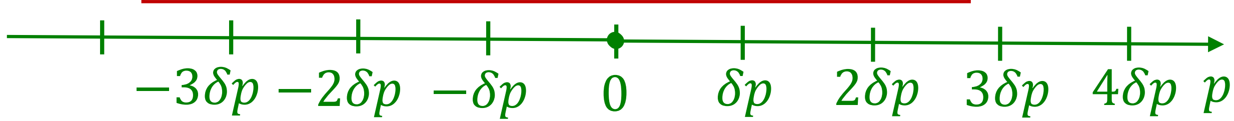


However, it is more convenient to use both positive and negative k
(physically corresponds to two directions of momentum)

Then one state per $\delta k = \dfrac{2\pi}{a}$



Equivalently, one state per $\delta p = \hbar\,\delta k = \dfrac{2\pi\hbar}{a}$



Quantum wire (cont.)

Rule: one state (quantum level) per $\delta p = \dfrac{2\pi\hbar}{a}$

So, number of states $\boxed{\Delta N = \dfrac{\Delta p\, a}{2\pi\hbar}}$ $\quad \dfrac{\text{length in space} \times \text{length in } p \text{ space}}{2\pi\hbar}$

Density of states $D(E) \equiv \dfrac{\Delta N}{\Delta E}$ (usually measured in 1/eV)

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \implies \Delta E = \frac{2n\,\pi^2\hbar^2}{2ma^2}\Delta n \implies \frac{\Delta n}{\Delta E} = \frac{ma^2}{n\pi^2\hbar^2} = \frac{a}{\pi\hbar}\sqrt{\frac{m}{2E}}$$

$$\boxed{D(E) = \frac{a}{\pi\hbar}\sqrt{\frac{m}{2E}}}\quad \boxed{\times 2\ \text{(spin)}}\qquad D(E) \propto \frac{1}{\sqrt{E}}$$

(absent for high magnetic field)

decreases with energy

Fermi energy We have $N \gg 1$ electrons, what is the maximum occupied energy?

$$E_F = \frac{(N/2)^2\pi^2\hbar^2}{2ma^2} = \boxed{\frac{\pi^2\hbar^2}{8m}\left(\frac{N}{a}\right)^2}$$

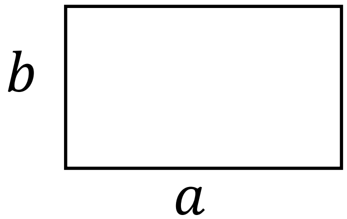
spin (absent for high B-field)

$\dfrac{N}{a}$: (linear) density of electrons

E_F is usually measured in eV (sometimes in Kelvin)

Quantum well, 2D electron gas, 2DEG (large 2D well)

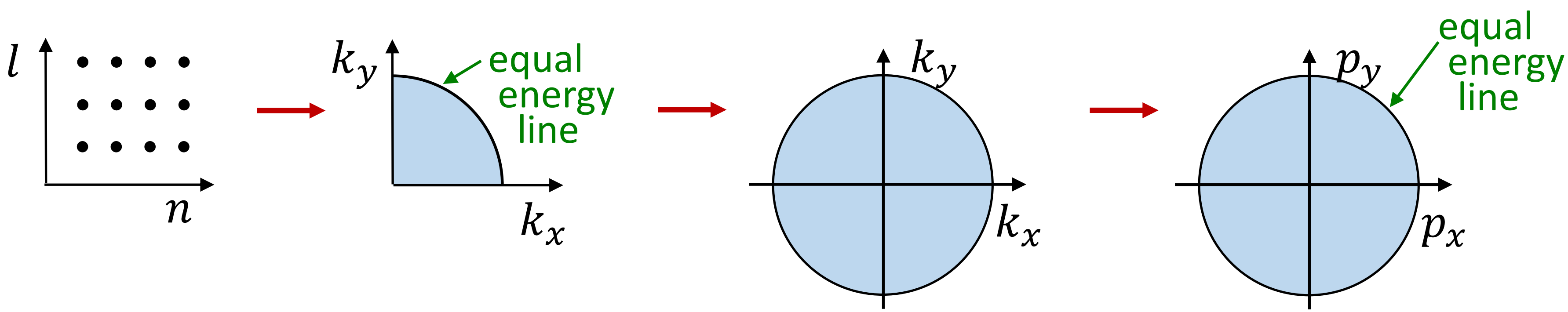
(not in textbook)



$$E_{n,l} = \frac{\pi^2\hbar^2}{2m}\left(\frac{n^2}{a^2} + \frac{l^2}{b^2}\right) \qquad n, l \gg 1$$

$$\psi(x,y) = \sqrt{2/a}\,\sin\Big(\underbrace{\frac{n\pi}{a}}_{k_x} x\Big)\sqrt{2/b}\,\sin\Big(\underbrace{\frac{l\pi}{b}}_{k_y} y\Big)$$

$$\Longrightarrow \quad E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2)$$



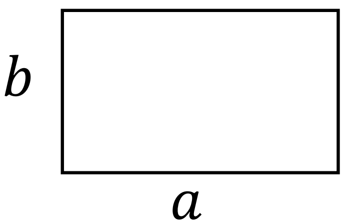
Again the rule

$$\Delta N = \frac{(\Delta p_x\, a)(\Delta p_y\, b)}{(2\pi\hbar)^2}$$

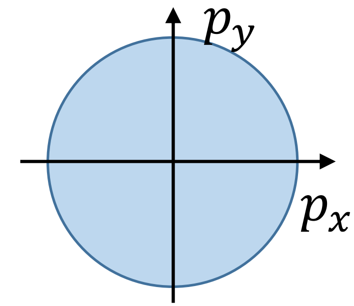
$$\frac{\text{area in space} \times \text{area in } p \text{ space}}{(2\pi\hbar)^2}$$

(so far no spin)

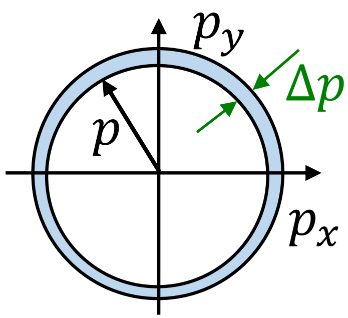
2D electron gas (cont.)



$$\Delta N = \frac{(\Delta p_x\, a)(\Delta p_y\, b)}{(2\pi\hbar)^2}$$



Density of states



$$E = \frac{p_x^2 + p_y^2}{2m} = \frac{p^2}{2m} \qquad \Delta E = \frac{2p\Delta p}{2m} = \frac{p\Delta p}{m}$$

$$\Delta N = \frac{ab\; 2\pi p\; \Delta p}{(2\pi\hbar)^2} \qquad D(E) = \frac{\Delta N}{\Delta E} = \frac{ab\; m}{2\pi\hbar^2}$$

$A = ab$ (area)

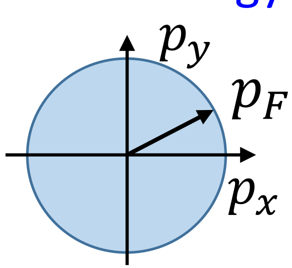
$$\frac{D(E)}{A} = \frac{m}{2\pi\hbar^2}$$

$\times\, 2$ (spin)

(absent for high magnetic field)

$D(E)$ does not depend on energy E

Fermi energy



$$N = \frac{A\,\pi p_F^2}{(2\pi\hbar)^2} \times 2(\text{spin}) = \frac{A p_F^2}{2\pi\hbar^2}$$

$$E_F = \frac{p_F^2}{2m} = \frac{\pi\hbar^2}{m}\,\frac{N}{A}$$

2D density in space

(twice larger E_F in high B-field)

Example

2DEG in GaAs, $n = \frac{N}{A} = 10^{12}\,\frac{1}{\mathrm{cm}^2}$. Find Fermi energy.

$m_{\mathrm{eff}} = 0.067\,m_0$

$$E_F = \frac{\pi\hbar^2}{m}\,n = \frac{\pi(1.05\cdot 10^{-34}\mathrm{Js})^2}{0.067\cdot 9.1\cdot 10^{-31}\mathrm{kg}}\cdot 10^{16}\,\frac{1}{\mathrm{m}^2} =$$

$$= 5.68\cdot 10^{-21}\mathrm{J} = 35\ \mathrm{meV} = 410\ \mathrm{K}$$

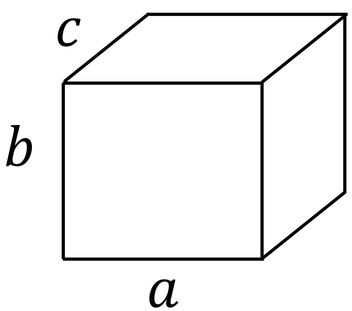
$\mathrm{eV} = 1.6\cdot 10^{-19}\ \mathrm{J}$

$k_B = 1.38\cdot 10^{-23}\,\frac{\mathrm{J}}{\mathrm{K}}$

Large 3D well: theory of metals

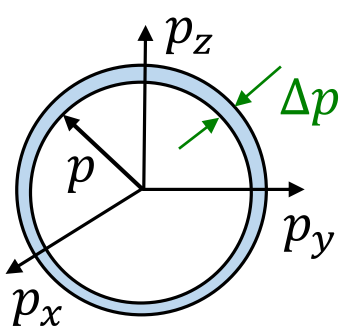
(slightly different in textbook)

$V = abc$



Same rule

$$\Delta N = \frac{(\Delta p_x\, a)(\Delta p_y\, b)(\Delta p_z\, c)}{(2\pi\hbar)^3} = \frac{V\, \Delta p_x \Delta p_y \Delta p_z}{(2\pi\hbar)^3}$$



Density of states $\quad D(E) = \dfrac{\Delta N}{\Delta E}$

$$\Delta N = \frac{V\, 4\pi p^2 \Delta p}{(2\pi\hbar)^3} \qquad \Delta E = \Delta\left(\frac{p^2}{2m}\right) = \frac{p}{m}\,\Delta p$$

$$\frac{\Delta N}{\Delta E} = \frac{V\, 4\pi p m}{(2\pi\hbar)^3} = \frac{V\, m\sqrt{2mE}}{2\pi^2\hbar^3} = \frac{V\, m^{3/2}\sqrt{E}}{\sqrt{2}\,\pi^2\hbar^3}$$

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

$\times\, 2$ (spin)

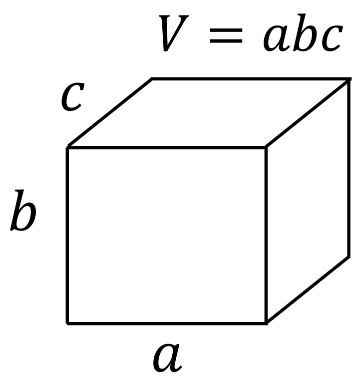
3D: $D(E) \propto \sqrt{E}$

2D: $D(E) \propto E^0$

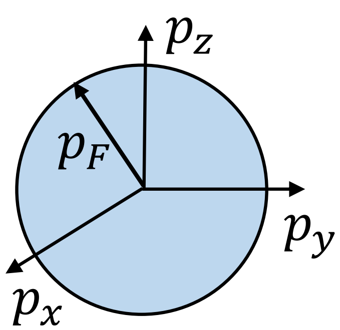
1D: $D(E) \propto 1/\sqrt{E}$

Some people call $D(E)/V$ density of states

Theory of metals (cont.)



$$\Delta N = \frac{V\,\Delta p_x \Delta p_y \Delta p_z}{(2\pi\hbar)^3}$$



Fermi energy

$$N = \frac{V\,\frac{4}{3}\pi p_F^3}{(2\pi\hbar)^3} \cdot 2(\text{spin}) = \frac{V\,p_F^3}{3\pi^2\hbar^3}$$

$$p_F = \hbar\left(3\pi^2\frac{N}{V}\right)^{1/3} \qquad k_F = \frac{p_F}{\hbar} = \left(3\pi^2\frac{N}{V}\right)^{1/3}$$

$$E_F = \frac{p_F^2}{2m} = \frac{\hbar^2}{2m}\left(3\pi^2\frac{N}{V}\right)^{2/3}$$

Example 1

Copper (Cu) mass density $\rho = 8.96 \frac{\mathrm{g}}{\mathrm{cm}^3}$ atomic mass $M = 63.5 \frac{\mathrm{g}}{\mathrm{mole}}$

Find E_F

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3}$$

$$\frac{N}{V} = 1 \cdot \frac{\mathrm{atoms}}{\mathrm{m}^3} = \rho \frac{N_A}{M} = 8.96 \cdot 10^3 \frac{\mathrm{kg}}{\mathrm{m}^3} \frac{6.02 \cdot 10^{23}\ 1/\mathrm{mole}}{63.5 \cdot 10^{-3}\ \mathrm{kg/mole}} = 8.5 \cdot 10^{28} \frac{1}{\mathrm{m}^3}$$

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3} = \frac{(1.05 \cdot 10^{-34})^2}{2 * 9.1 \cdot 10^{-31}} (3 \cdot 3.14^2 \cdot 8.5 \cdot 10^{28})^{2/3} =$$

$$= 1.1 \cdot 10^{-18}\mathrm{J} = 7.0\ \mathrm{eV} = 8.1 \cdot 10^4 \mathrm{K}$$

$\mathrm{eV} = 1.6 \cdot 10^{-19}\ \mathrm{J}$

$k_B = 1.38 \cdot 10^{-23} \frac{\mathrm{J}}{\mathrm{K}}$

$T_F \gg 300$ K ! degenerate electron gas

Fermi velocity $v_F = \sqrt{\frac{2E_F}{m}} = 1.6 \cdot 10^6 \frac{\mathrm{m}}{\mathrm{s}}$ (very high but still nonrelativistic)

Example 2

GaAs (bulk), doping of $10^{18}\,\frac{1}{\mathrm{cm}^3}$ $\quad m_{\mathrm{eff}} = 0.067\, m_0$

Find E_F

$$E_F = \frac{\hbar^2}{2m}\left(3\pi^2\frac{N}{V}\right)^{2/3} = \frac{(1.05\ \cdot 10^{-34})^2}{2 * 0.067 \cdot 9.1 \cdot 10^{-31}}(3\pi^2 \cdot 10^{24})^{2/3} =$$

$$= 8.65 \cdot 10^{-21}\mathrm{J} = 54\ \mathrm{meV} = 630\ \mathrm{K}$$

still > 300 K, behaves almost as a metal (degenerate semiconductor)

However, if doping of $10^{17}\mathrm{cm}^{-3}$, then only 140 K.