* BAND THEORY OF SOLIDS {3rd chp}

Brillouin zone ≡ Wigner-Seitz cell in the reciprocal space

→ FREE ELECTRON THEORY

↳ no potential energy

$$E\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$ — from Schrodinger's wave eqn

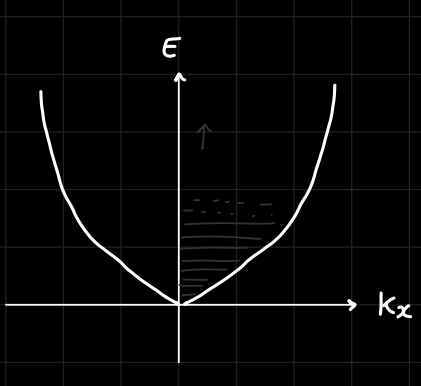
free e⁻ are plane waves : $\psi = Ae^{\pm ikx}$

→ momentum : $i\hbar\frac{\partial\psi}{\partial x} = \pm\hbar k\psi$

→ Energy : $\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{\hbar^2k^2}{2m}\psi$

→ Grp velocity : $\frac{\partial\omega}{\partial k} = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{\hbar k}{m}$

very closely packed energy bands if container of e⁻ is very large, we can conclude that the energy band graph looks continuous.



wave packets: superposition of different waves of separate electrons

group velocity: velocity of a whole group e⁻ / wave packets.

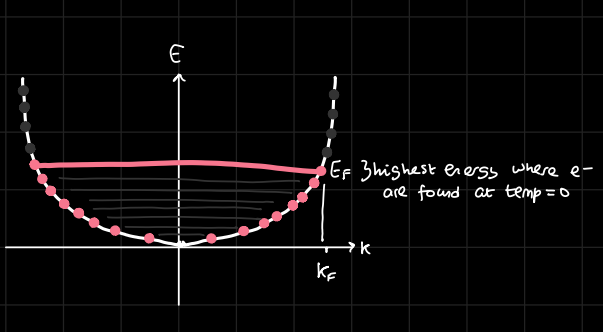
phase velocity: velocity of individual particles like e⁻

properties like conductivity, temperature etc. can be figured out using this free e⁻ theory but this theory is incomplete on its own without the crystal nature.

→ FERMI-SURFACE

We have seen in the "particle in a box" problem, that energy levels are discretized. But as the width approaches → ∞, the ΔE (energy band gap) tends to → 0.

$\frac{\hbar^2k^2}{2m} = E_F$ → fermi-level



FERMI-DIRAC DISTRIBUTION

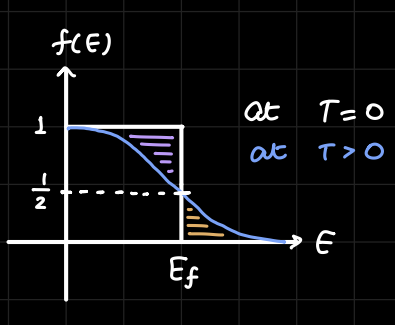
the probability that a particle has energy (E) ↓

$$f(E) = \frac{1}{1 + e^{\left(\frac{E-E_f}{k_bT}\right)}}$$

k_b: Boltzman constant

T: temperature

distribution of electron's energies



At T=0,

E_f is the highest energy where we can find a valence electron with energy = E

When we increase the temperature, the valence electrons move to higher energy levels

↳ valence e⁻ → conduction e⁻

▨ : The e⁻ occupy this space

▨ : Holes occupy this space which was earlier occupied by electrons

In case of **METAL**, the gap between the new energy band (conduction) and E_F (fermi level) is very small.

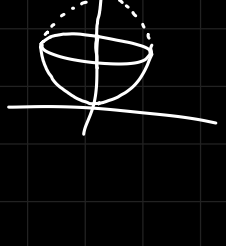
↳ # of free e⁻ for metals is very high

In 12th, we were taught that there was an overlap between the conduction band and valence band but the idea was that they were indistinguishable

In case of **SEMICONDUCTOR**, the gap is high and hence conduction e⁻ and valence e⁻ can be distinguished easily. ↓

Same case for insulators as well

FERMI LINE	1d
FERMI SURFACE	2d
FERMI SPHERE	3d →



→ k_F (k-space) $= \frac{\sqrt{2mE_F}}{\hbar}$

we have discussed fermi energy at equilibrium, i.e. at V=0 but generally,

$$f(E) = \frac{1}{1 + e^{\frac{(E+V-E_f)}{k_bT}}}$$

we can find the # of e⁻ at a particular energy level using this fermi-energy formula and hence we can find out the current

$$f(E) = \frac{1}{1 + e^{\left[\frac{E-E_f}{k_bT}\right]}}$$

at T = 0 and for $E < E_f$,

$\frac{E-E_f}{k_bT} = -\infty$

so, $e^{\wedge(\cdots)} = 0$

and $f(E) = 1$

but at $E > E_f$,

we have $e^{\wedge(\cdots)} = e^{\infty}$

and so, $f(E) = 0$