

* BAND THEORY OF SOLIDS {3rd chp}

Brillouin zone = Wigner-Seitz cell in the reciprocal space

→ FREE ELECTRON THEORY

↳ no potential energy

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

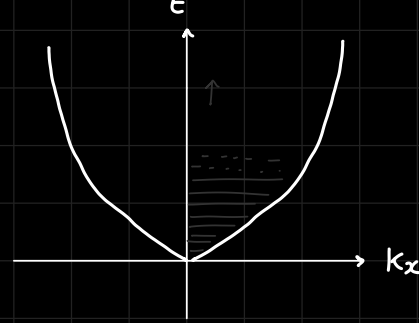
free e- are plane waves : $\psi = Ae^{\pm ikx}$

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

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

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

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.

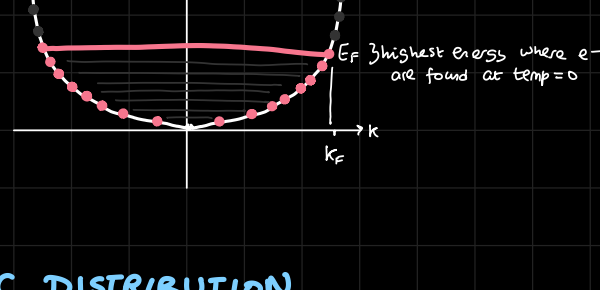
phase velocity: velocity of individual
particles like e-

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 $\rightarrow \infty$, the ΔE (energy band gap)
tends to $\rightarrow 0$.

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



FERMI-DIRAC DISTRIBUTION

the probability that a particle has energy (E) \downarrow

$$f(E) = \frac{1}{1 + e^{\left(\frac{E-E_F}{k_B T}\right)}}$$

distribution of electron's energies



k_B : Boltzmann constant

T: temperature

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- \rightarrow 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

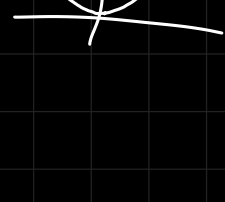
FERMI SURFACE

2d

FERMI SPHERE

3d

→



$$\rightarrow k_F = \frac{\sqrt{2mE_F}}{\hbar}$$

↓
k-space

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

$$f(E) = \frac{1}{1 + e^{\left(\frac{E+V-E_F}{k_B T}\right)}}$$

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

$$f(E) = \frac{1}{1 + e^{\left[\frac{E-E_F}{k_B T}\right]}}$$

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

$$\frac{E-E_F}{k_B T} = -\infty$$

so, $e^{(-\infty)} = 0$

$$\text{and } f(E) = 1$$

but at $E > E_F$,

$$\text{we have } e^{(+\infty)} = e^{\infty}$$

$$\text{and so, } f(E) = 0$$