Phys 570
Theory of Solids

Physics & Astronomy Dept.
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Lecture #1

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Chapter 6: Free Electron Fermi Gas

Introduction

We can understand many physical properties of metals, and not only of the simple metals, in terms of the free electron model. ***According*** to this model, the valence electrons of the constituent atoms become conduction electrons and move about freely through the volume of the metal. The utility of the free electron model is greatest for properties that depend essentially on the kinetic properties of the conduction electrons.

The interpretation of metallic properties in terms of the motion of free electrons was developed long before the invention of quantum mechanics. ***The classical theory*** had several conspicuous successes, notably the derivation of the form of Ohm's law and the relation between the electrical and thermal conductivity.

The classical theory fails to explain the heat capacity and the magnetic susceptibility of the conduction electrons.

- **Classical Model:**
- Metal is an array of positive ions with electrons that are free to move through the ionic array
  - Electrons are treated as an ideal neutral gas, and their total energy depends on the temperature and applied field
  - In the absence of an electrical field, electrons move with randomly distributed thermal velocities
  - When an electric field is applied, electrons acquire a net drift velocity in the direction opposite to the field

- **Quantum Mech. Model:**
- Electrons are in a potential well with infinite barriers: They do not leave metal, but free to move inside
  - Electron energy levels are discrete (quantized) and well defined, so average energy of electron is not equal to $(3/2)k_B T$
  - Electrons occupy energy levels according to Pauli's exclusion principle
  - Electrons acquire additional energy when electric field is applied

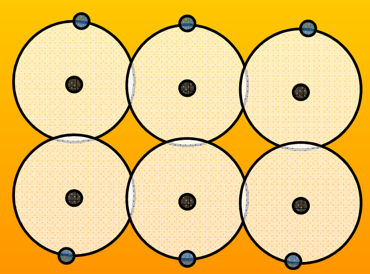
Chapter 6: Free Electron Fermi Gas

The model in Brief

- This model explains lots of properties in metals.
- It assumes free electrons in the so called conduction band:
- Example: Na^{11}: We have 11 electrons distributed as follows:
- $1s^2\ 2s^2\ 2p^6\ 3s^1$ ← Valance electron (loosely bound)
- Hence, there is a free electron/atom in the 3S state
- Or we have one electron/atom in the 3S conduction Band.
- For a crystal of *N* atoms: we have *N* conduction electrons and *N* +tive Ions.

- Classical Theory fails to explain for C_v (heat capacity) and χ_p (magnetic Suc.) for the full range of Temperature.
- What is Fermi Gas? : It is a collection of large No. of electrons that are free to move but subject to Pauli Exclusion Principle

Conduction electrons in Sodium



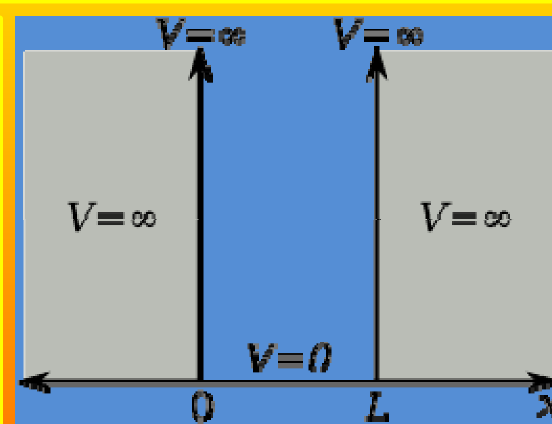
Na atoms in ***Na*** crystal overlap slightly. This leads to the fact that a valance electron is not attached to a particular ion, but belongs to all neighbouring ions at the same time.

- Accordingly; electrons can virtually move freely all over the crystal leading to conduction of electricity.

Chapter 6: Free Electron Fermi Gas

Energy Levels in 1-D

- Consider a free electron gas in one dimension, taking account of quantum theory and of the Pauli principle. An electron of mass m is confined to a length L by infinite harriers.



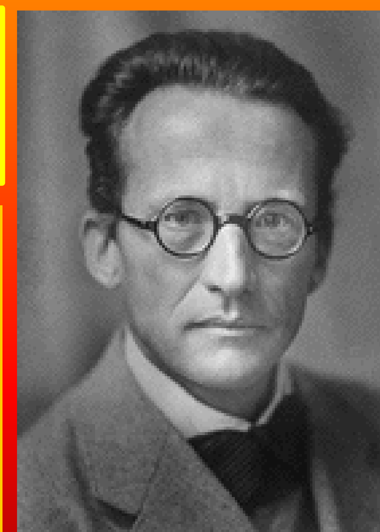
- We will have to use Schrödinger Wave Equation to solve the problem and find out energy levels.

$$H\psi_n = \varepsilon_n \psi_n$$

$$with: H = \frac{p^2}{2m} \qquad where: p = -i\hbar \frac{d}{dx}$$

$$\therefore H\psi_n = -\frac{\hbar^2}{2m}\frac{d_2\psi_n}{dx^2} = \varepsilon_n \psi_n \qquad (1)$$

ε_n is the energy of the electron in the nth. state (orbit).



E. Schrödinger

(1887-1961)

- Applying Boundary Conditions for the wave function:

$$\left.\begin{aligned}\psi_n(0) &= 0\\ \psi_n(L) &= 0\end{aligned}\right\}\ \psi \text{ at borders } = 0$$

$$\left.\begin{aligned}\psi_n &= A\sin\left(\frac{2\pi}{\lambda_n}x\right)\\ \text{or }\ \psi_n &= A\sin\left(\frac{n\pi}{L}x\right)\end{aligned}\right\}\text{satisfies the wave function at boundary} \qquad (2)$$

$$\Rightarrow\ \frac{d\psi_n}{dx} = A\frac{n\pi}{L}\cos\left(\frac{n\pi}{L}x\right)\ \ and\ \ \Rightarrow\ \frac{d_2\psi_n}{dx^2} = -A\left(\frac{n\pi}{L}\right)^2\sin\left(\frac{n\pi}{L}x\right)$$

$$\therefore\ -\frac{\hbar^2}{2m}(-A)\left(\frac{n\pi}{L}\right)^2\sin\left(\frac{n\pi}{L}x\right) = \varepsilon_n A\sin\left(\frac{n\pi}{L}x\right)$$

$$\therefore\ \varepsilon_n = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2} \qquad (3)$$

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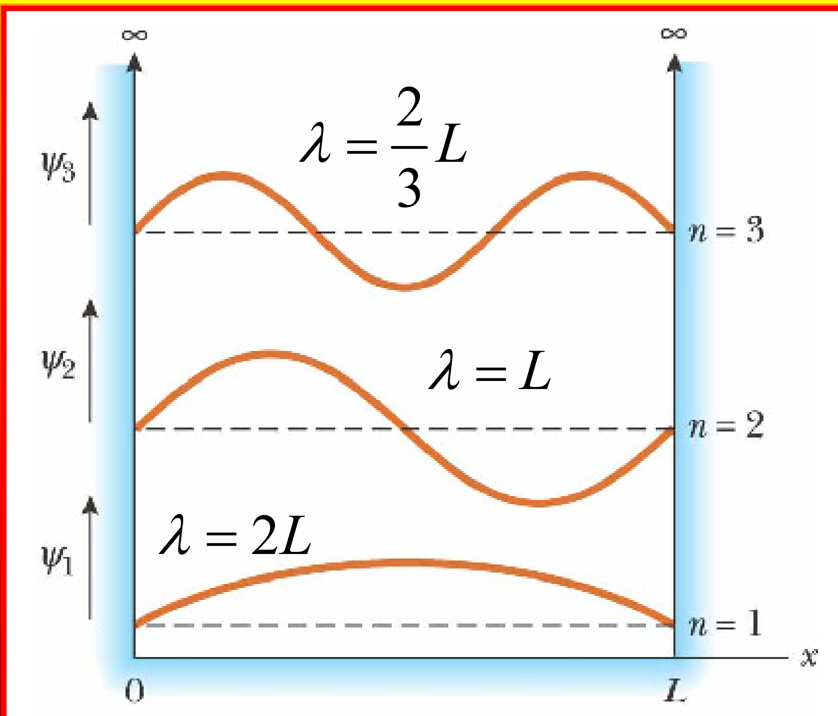
Energy Levels in 1-D

- Every state (n) can have two electrons; one at $m_s=+½$ and one at: $m_s=-½$.
- If state n has energy ε_n and a state m also has energy ε_n : We call this degeneracy.

- When we have many electrons, the energy levels are filled from the bottom to the top. The last filled level is the Fermi level and is denoted as: n_F
- Right: 1-D potential well. Energy of electron is shown for lowest 3 states (n=1,2, and 3)



Energy Levels in 1-D

Ref. Introductory Quantum Mechanics

- We can easily calculate the location of Fermi Level n_F for N-electron system (even No.): $2n_F = N$
- ➔ $n_F = N/2$
- Example: N = 6 electrons:
- n =1 has 2 electrons
- n =2 has 2 electrons
- n =3 has 2 electrons (n_F)
- ---
- Total: 6 electrons ➔ $n_F = 6/2 = 3$

let ε_F = Fermi Energy

ε_F is the energy of the n_F level. in Ground Sate for N electrons:

$$(3) \Rightarrow \varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{n_F \pi}{L}\right)^2 = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2L}\right)^2 \qquad (4)$$