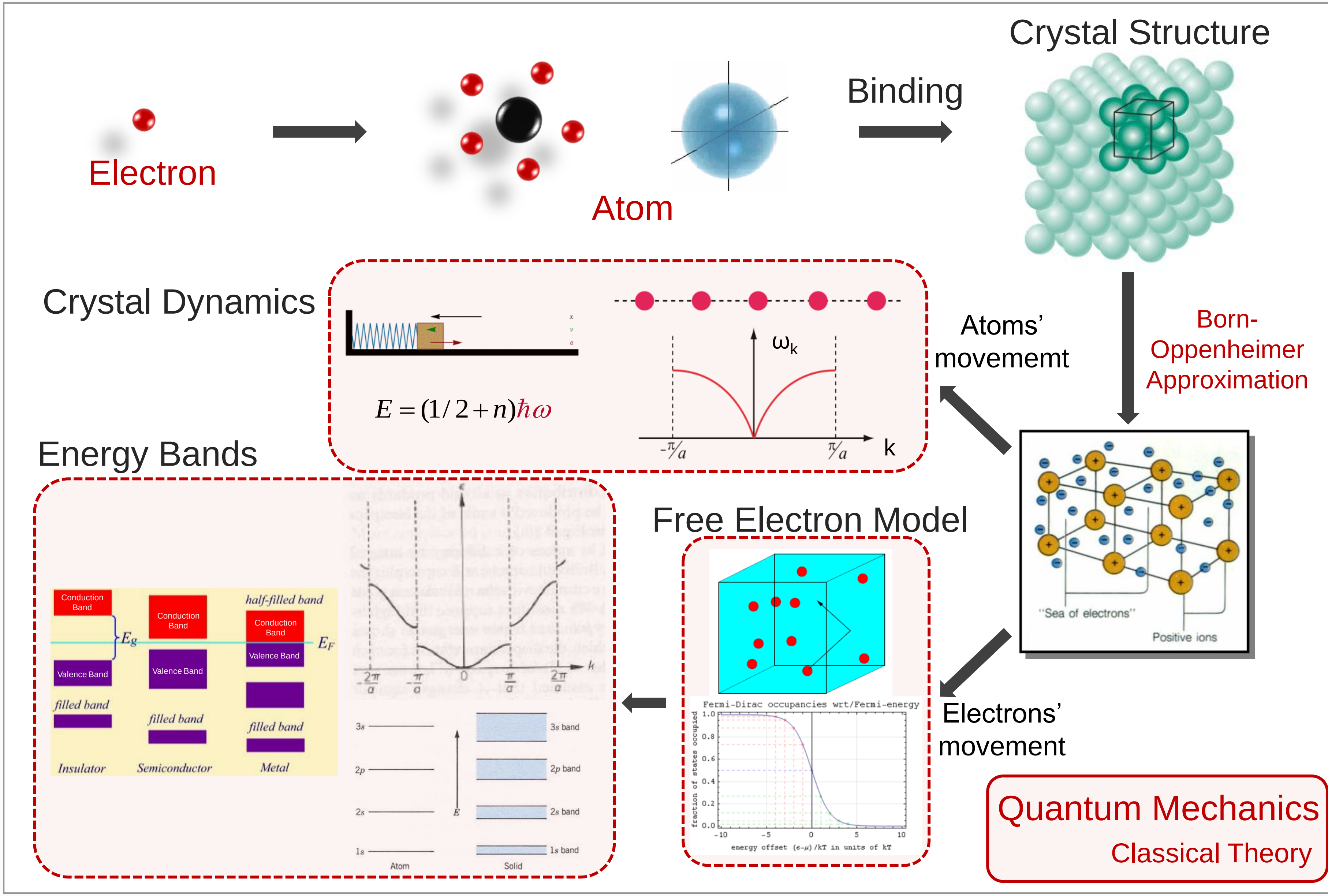
Chapter 3

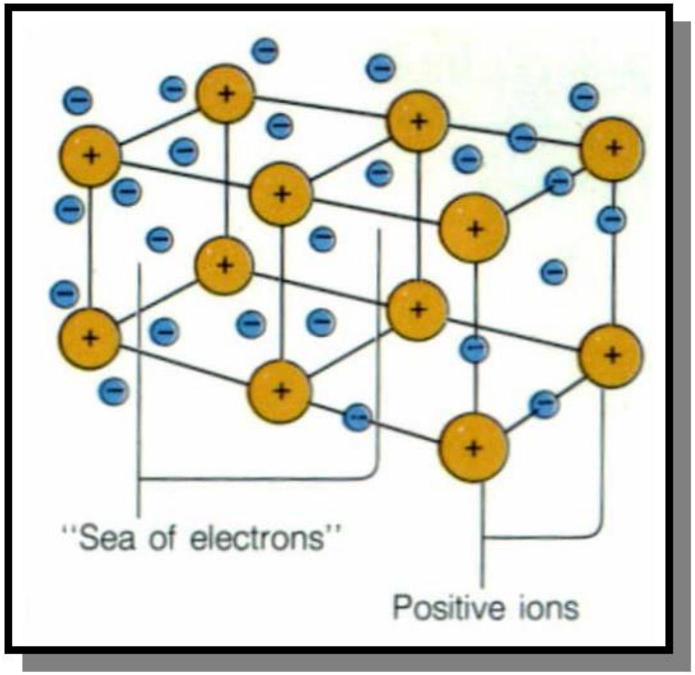
Free electrons in solids

Today’s lecture

Profile



· Introduction



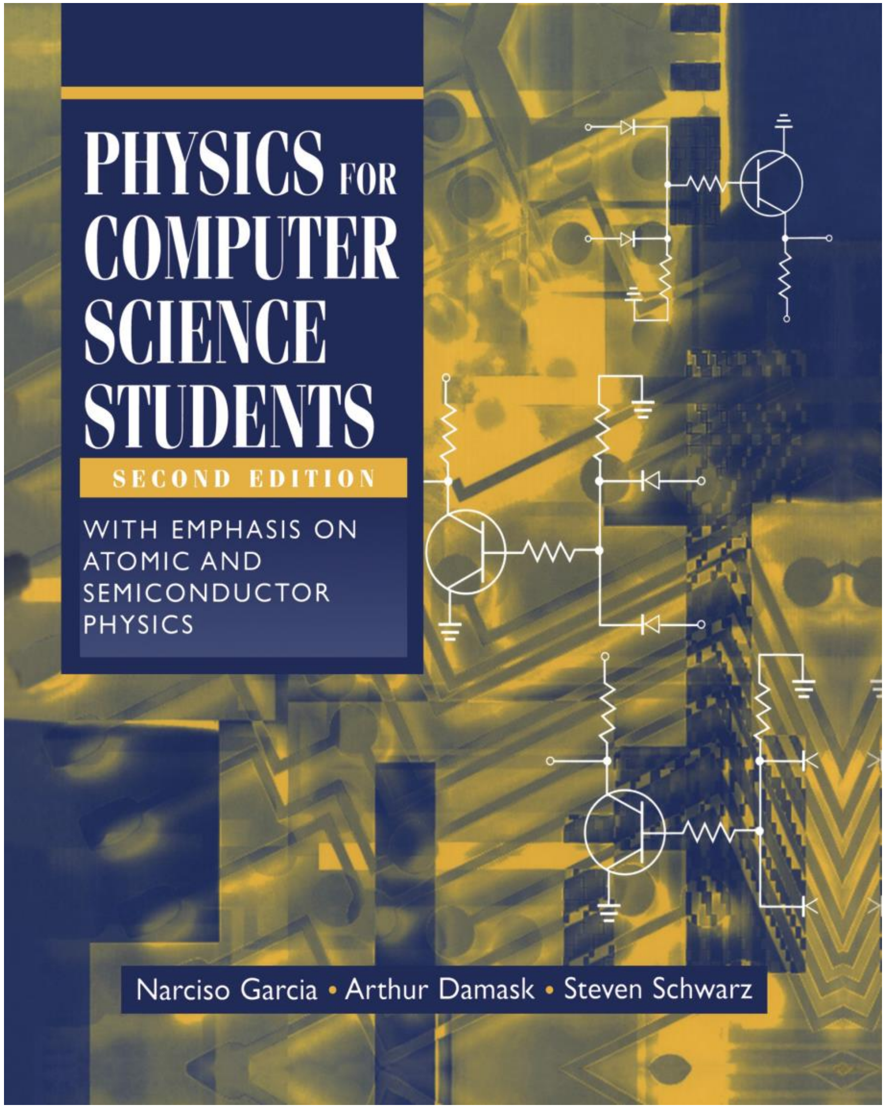
Crystal dynamics

Electron theory

Free electron theory → Energy band theory

Acknowledgement:

《**Physics for computer science students: with emphasis on atomic and semiconductor physics**》



Chapter 3 Free electrons in solids

3.1 Free electron model

3.1.1 Drude Model

- Classical Free Electron Model

3.1.2 Sommerfeld Model

- Quantum Mechanical Free Electron Model

3.2 Heat capacity of free electron gas

3.3 Transport properties of conductive electrons

· Introduction

Drude Classical Free Electron Model

- Independent electron approximation
- Free electron approximation
- Collision assumption
- Relaxation time approximation

Sommerfeld Quantum Mechanical Free Electron Model

- Independent electron approximation
- Free electron approximation
- No collision
- Quantum statistics: Fermi-Dirac Distribution

Energy band theory

Free Electron Model
+
Periodical potential field

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3.4 Electron emission and contacting voltage

Ohm's Law

$$U = IR \qquad J = \sigma\varepsilon$$

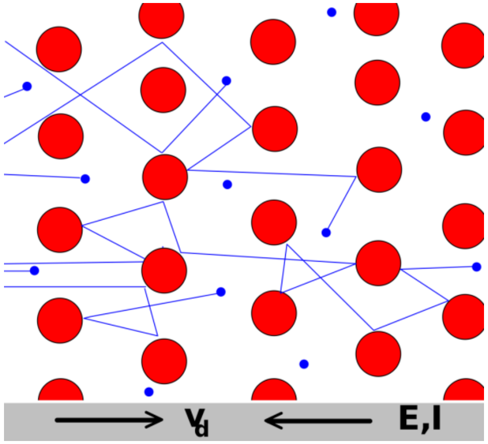
J: Current density

ε: Electric field intensity

σ: Conductivity

$$\sigma = \frac{1}{\rho}$$ **ρ: Resistivity**

Paul Karl Ludwig Drude



Drude Model electrons

The Drude model of electrical conduction was proposed in 1900 by Paul Drude to explain the transport properties of electrons in materials (especially metals). The model, which is an application of kinetic theory, assumes that the microscopic behavior of electrons in a solid may be treated classically and looks much like a pinball machine, with a sea of constantly jittering electrons bouncing and re-bouncing off heavier, relatively immobile positive ions.

Assumption of the electron gas:

(1) Independent electron approximation

No electrostatic interaction and collision among free electrons

(2) Free electron approximation

No electrostatic interaction between free electrons and ions

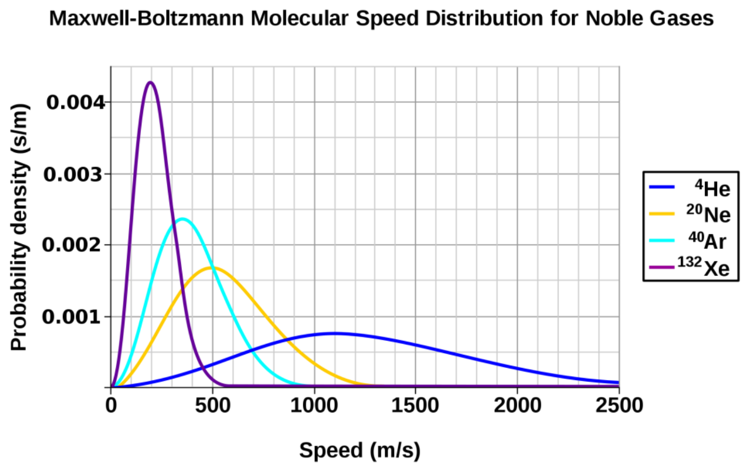
Free electron gas

(3) Collision assumption

Velocity of electrons after collision with ions only concerns with temperature, but not the velocity before collision

(4) Relaxation time approximation

Relaxation time τ is independent with the position and velocity of electrons

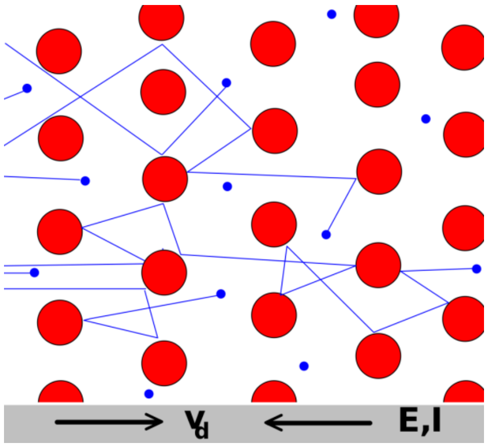


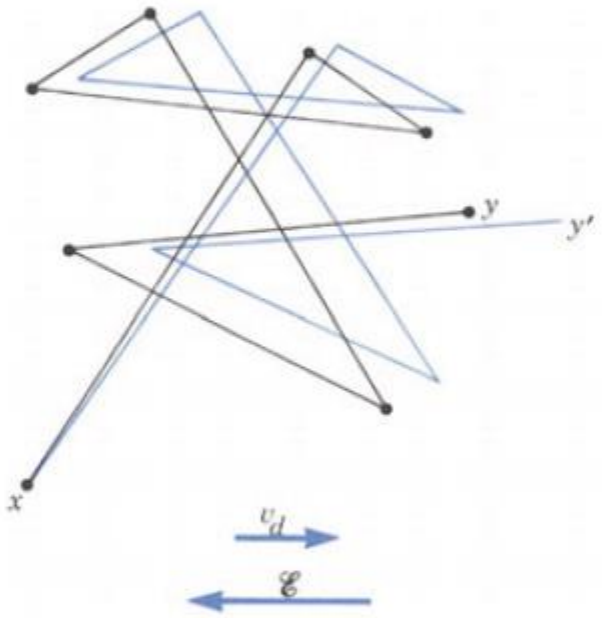
Without electric field, free e- moves randomly

At room temperature, $v_{RMS} = \left(3k_B T/m\right)^{1/2} = 1.2\times10^5\,\mathrm{m\cdot sec^{-1}}(\sim 120\,\mathrm{km\cdot sec^{-1}})$

No net current

With electric field, things are different

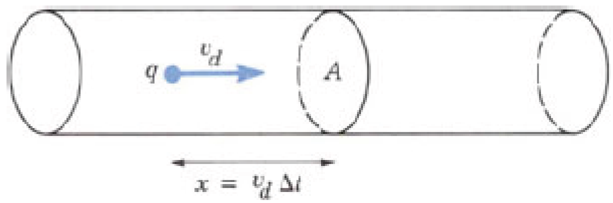




v_d : drift velocity (漂移速度) , $v_d \ll v_{RMS}$ (a net movement)

$$J = \sigma\varepsilon\,?$$

Current density: the electric quantity per unit area of cross section per second



$$J = \frac{n(-e)(\mathbf{v_d}\Delta t)\cdot A}{\Delta t \cdot A} = -ne\mathbf{v_d} \quad \textbf{vs} \quad J = \sigma\varepsilon$$

v_d must be proportional to electric field intensity

τ: average time between collision

$$\mathbf{v_d} = \mathbf{v}_0 + \mathbf{a}t = \frac{F}{m}t = -\frac{e\varepsilon}{m}\tau \quad (F = ma = e\varepsilon) \quad (\text{suppose } v_0=0)$$

$$J = -ne\mathbf{v_d} = -ne\cdot -\frac{e\varepsilon}{m}\tau = \sigma\varepsilon \qquad \sigma = \frac{ne^2}{m}\tau$$

Prove: τ independent of ε

$$\tau = mean\ \ free\ path / v$$

mean free path :
average distance traveled between collisions

$$v = v_{RMS} + v_d \approx v_{RMS} \quad (v_d \ll v_{RMS})$$

$$\tau = mean\ \ free\ path / v_{RMS}$$ **τ independent of ε**

(1) Specific Heat

Equipartition theorem of energy: in thermal equilibrium, energy is shared equally among all of its various forms. For example, the average kinetic energy per degree of freedom in the translational motion of a molecule should equal that of its rotational motions.

$$\bar{\varepsilon} = \frac{1}{2}(t + r + 2s)k_B T$$

t, r, s: free degree of translation, rotation and vibration

For solids,

t=0, r=0, s=3

$$\bar{\varepsilon} = \frac{1}{2}(t + r + 2s)k_B T = 3k_B T$$

Total energy of 1mol solid state matter

$$E = N\bar{\varepsilon} = 3Nk_B T$$

$$C_v^{mol} = \frac{\partial E}{\partial T} = 3Nk_B = 3R$$

Dulong-Petit Law

For monoatomic gas (electron gas)

t=3, r=s=0

$$\bar{\varepsilon} = \frac{1}{2}(t + r + 2s)k_B T = \frac{3}{2}k_B T$$

Total energy of 1mol monoatomic gas (electron gas)

$$E = N\bar{\varepsilon} = \frac{3}{2}Nk_B T$$

$$C_v^{mol} = \frac{\partial E}{\partial T} = \frac{3}{2}Nk_B = \frac{3}{2}R$$

(1) Specific Heat

From Drude Model: $C_v^{mol}(\,from\, e^-) = 3/2\,R$

Experimentally: $C_v^{mol}(\,from\, e^-) = 10^{-4}\,RT = 0.03R$ (If T=300K)

Classical FEM: all free electrons contribute to heat capacity.
Disaster! Heat capacity is much less than predicted. Free e- gives such a small contribution to C_v (free e- have poor ability to absorb heat)

(2) Temperature dependence of σ

From Drude Model: $\sigma = \dfrac{ne^2}{m}\tau$ **τ is temperature dependent**

Experimentally: $\sigma \propto T^{-1}$

Still important!

Summary of Drude Theory

- Based on kinetic theory of gases.

- Successes
  - Ohm's Law.
  - Wiedemann-Franz ratio comes out close to right for most materials
  - Many other transport properties predicted correctly

- Failures
  - Specific Heat of electrons
  - Temperature dependence of σ
  - Wiedemann-Franz ratio
  - The Seebeck/Peltier coefficient come out wrong by a factor of 100.

- Despite the shortcomings of Drude theory, it nonetheless was the only theory of metallic conductivity for a quarter of a century (until the Sommerfeld theory improved it), and it remains quite useful today.

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Drude
Classical Free Electron
Model

Independent electron approximation
Free electron approximation
Collision assumption
Relaxation time approximation

Sommerfeld
Quantum Mechanical
Free Electron Model

Independent electron approximation
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No collision
Quantum statistics: Fermi-Dirac Distribution

Energy band theory

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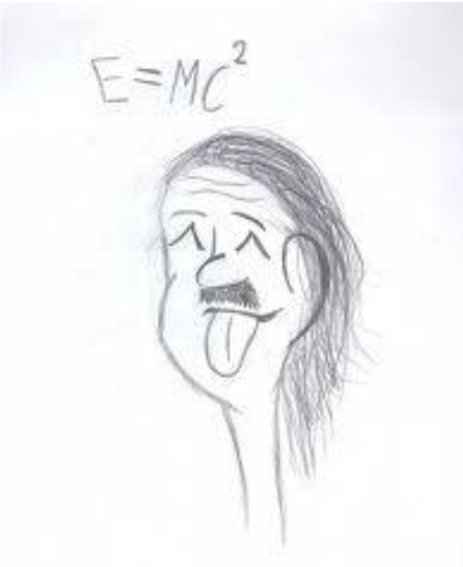


Find the characteristics of motion of the free electrons by quantum mechanics

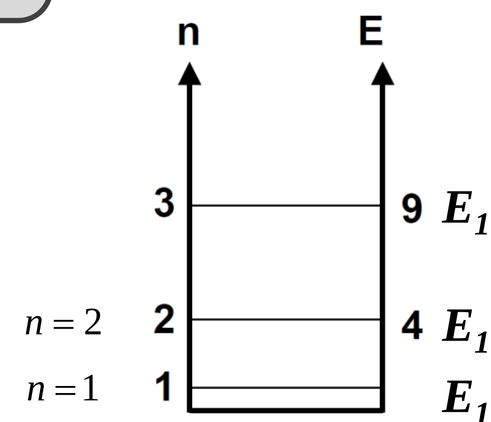
Quantized Energy

How the energy levels are occupied by free electrons

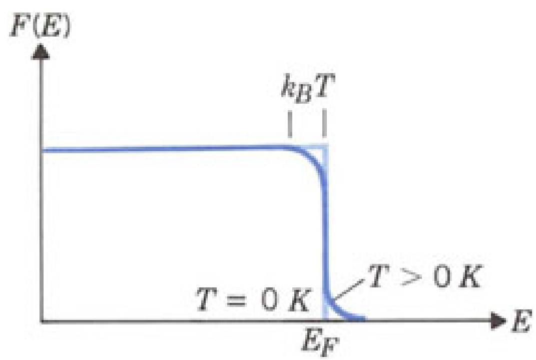
Fermi-Dirac distribution

Find Fermi energy E_F

Find the electron number near the E_F



CFE model predicts → C_V = 3/2 R
experiments show → $C_V = 10^{-4}$ RT



Find the characteristics of motion of the free electrons by quantum mechanics → Schrodinger Equation

Quantized Energy

How the energy levels are occupied by free electrons

0K

>0K

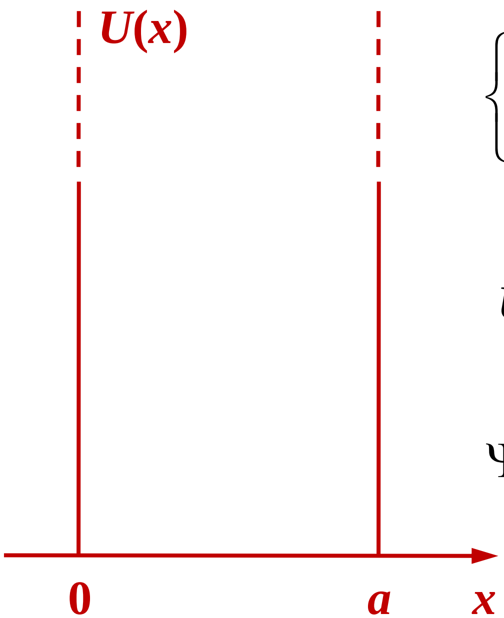
Fermi-Dirac distribution

Find Fermi energy E_F ← k distribution

Find the electron number near the E_F ← Density of state

Infinite Potential Well

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+U(x)\right)\psi(x)=E\psi(x)$$



$$\begin{cases} U(x)=0, & 0<x<a \\ U(x)=\infty, & x>a, x<0 \end{cases}$$

$$U(x,t) \text{——} U(x)$$

$$\Psi(x,t)=\psi(x)e^{-iEt/\hbar}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$$

$$\frac{d^2\psi}{dx^2}+\frac{2mE}{\hbar^2}\psi=0$$

$$k=\frac{\sqrt{2mE}}{\hbar}$$

$$\frac{d^2\psi}{dx^2}+k^2\psi=0$$

$$\psi=A\sin kx+B\cos kx$$

$$E=\frac{(\hbar k)^2}{2m}$$

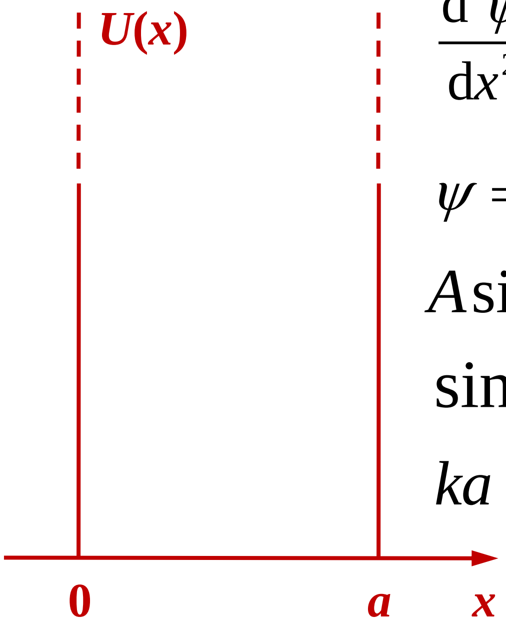
$$\psi(x)=0, \quad x>a, x<0$$

$$\psi(0)=B\cos 0=B=0$$

$$\psi(a)=A\sin ka+B\cos ka=0$$

$$B=0$$

$$A\sin ka=0$$



$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi = A\sin kx + B\cos kx$$

$$A\sin ka = 0$$

$$\sin ka = 0$$

$$ka = n\pi \qquad k = n\frac{\pi}{a}$$

$$n = 1, 2, 3, \ldots$$

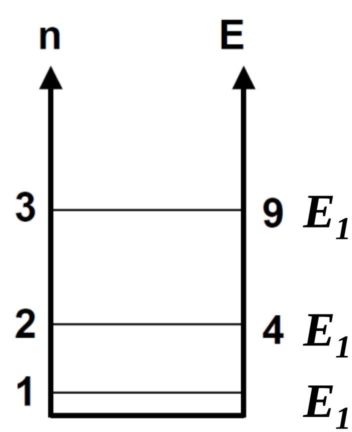
$$\psi(x) = A\sin\frac{n\pi}{a}x \qquad 0 \le x \le a$$

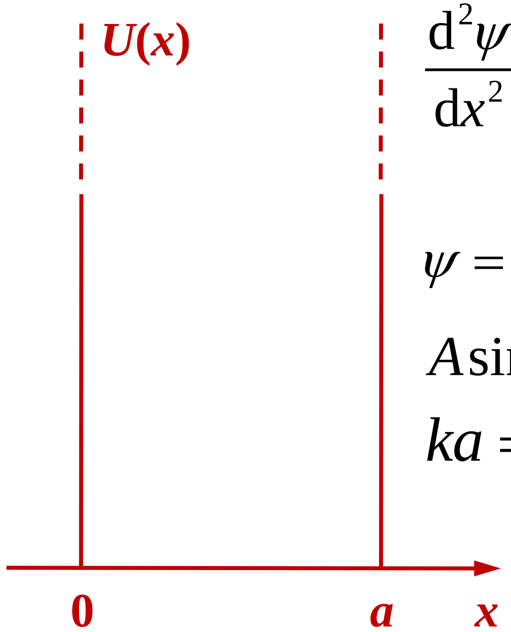
$$\int_0^a |\psi|^2 dx = 1 \qquad A = \sqrt{\frac{2}{a}}$$

$$\psi(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$$

$$|\psi_n|^2 = \frac{2}{a}\sin^2\frac{n\pi}{a}x$$

$$n = 1, 2, 3, \ldots$$





$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi = A\sin kx + B\cos kx$$

$$A\sin ka = 0$$

$$ka = n\pi \qquad n = 1, 2, 3, \dots$$

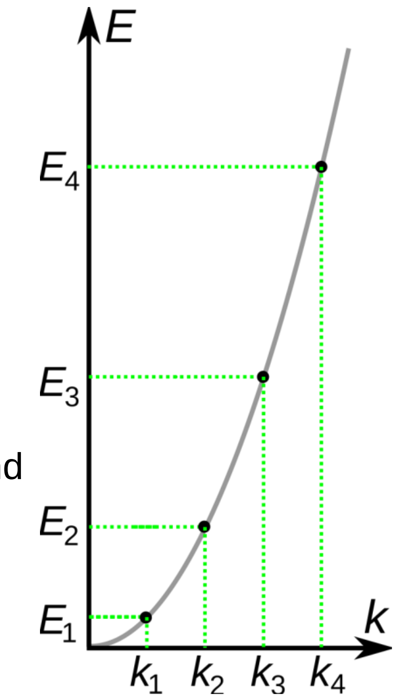
$$k = n\frac{\pi}{a}$$

$$E = \frac{(\hbar k)^2}{2m}$$

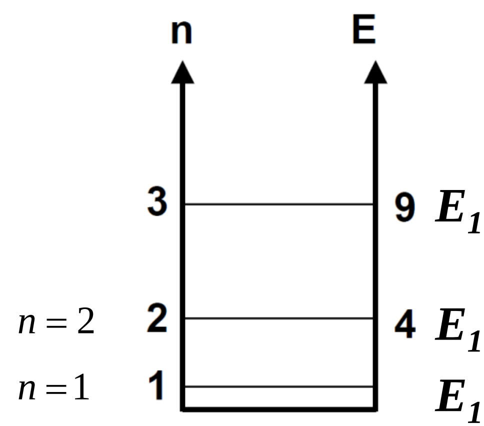
$$E = E_n = \frac{\pi^2\hbar^2}{2ma^2}n^2$$

$$n = 1, 2, 3, \dots$$

$m\downarrow$, $a\downarrow$, $\Delta E\uparrow$, quantum effect strengthen $\rightarrow$ nano-material



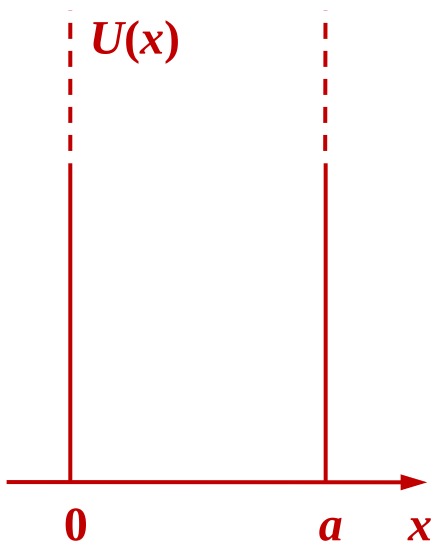
The energy of a particle in a box (black circles) and a free particle (grey line) both depend upon wavenumber.



$$E_2 = \frac{2\pi^2\hbar^2}{ma^2}$$

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

1D Infinite Potential Well

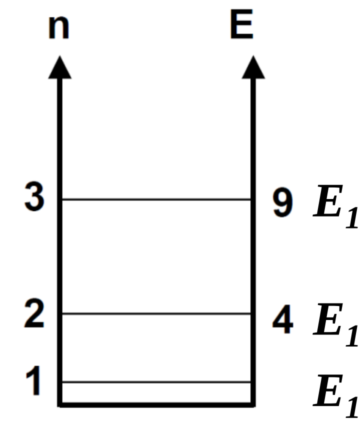


$$\begin{cases} U(x) = 0, & 0 < x < a \\ U(x) = \infty, & x > a, x < 0 \end{cases}$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

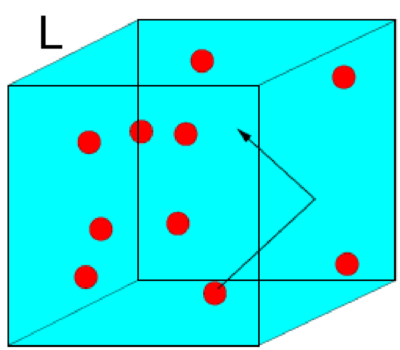
$$\psi(x) = \sqrt{\frac{2}{a}}\sin kx$$

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



$$E = E_n = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2\hbar^2}{2ma^2}n^2 \qquad n = 1, 2, 3, \ldots$$

3D Infinite Potential Well



$$\begin{cases} U = 0 & 0 \le x, y, z \le L \\ U = \infty & x, y, z > L, x, y, z < 0 \end{cases}$$

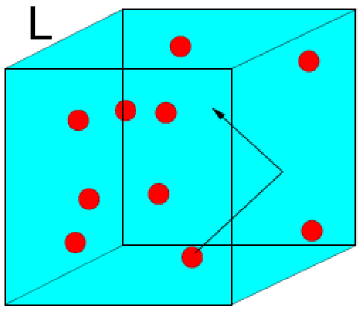
$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right)\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x, y, z) = E\psi(x, y, z)$$

$$\psi(x, y, z) = \psi(x)\psi(y)\psi(z)$$

Drude Model - Classical FEM | **Sommerfeld Model - Quantum Mechanical FEM**

· **Potential Well** · F-D Distribution · Fermi Energy · Density of State · e^- number near E_F · e^- gas Energy



$$\begin{cases} U = 0 & 0 \le x, y, z \le L \\ U = \infty & x, y, z > L, x, y, z < 0 \end{cases}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x, y, z) = E\psi(x, y, z)$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x)\psi(y)\psi(z) = E\psi(x)\psi(y)\psi(z)$$

$$\left(\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{\psi(y)}\frac{\partial^2\psi(y)}{\partial y^2} + \frac{1}{\psi(z)}\frac{\partial^2\psi(z)}{\partial z^2}\right) + \frac{2m}{\hbar^2}E = 0$$

$$E = \frac{\hbar^2 k^2}{2m}$$

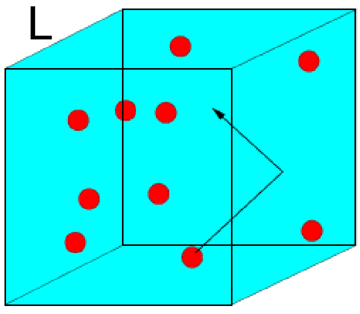
$$\vec{k} = k_x\vec{i} + k_y\vec{j} + k_z\vec{l}$$

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

$$\left(\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + \frac{1}{\psi(y)}\frac{\partial^2\psi(y)}{\partial y^2} + \frac{1}{\psi(z)}\frac{\partial^2\psi(z)}{\partial z^2}\right) + (k_x{}^2 + k_y{}^2 + k_z{}^2) = 0$$

$$\begin{cases} \dfrac{1}{\psi(x)}\dfrac{\partial^2\psi(x)}{\partial x^2} = -k_x^2 \\ \dfrac{1}{\psi(y)}\dfrac{\partial^2\psi(y)}{\partial y^2} = -k_y^2 \\ \dfrac{1}{\psi(z)}\dfrac{\partial^2\psi(z)}{\partial z^2} = -k_z^2 \end{cases}$$

$$\begin{cases} \dfrac{\partial^2\psi(x)}{\partial x^2} + k_x^2\psi(x) = 0 \\ \dfrac{\partial^2\psi(y)}{\partial y^2} + k_y^2\psi(y) = 0 \\ \dfrac{\partial^2\psi(z)}{\partial z^2} + k_z^2\psi(z) = 0 \end{cases}$$



$$x=0,\psi(x)=0;\ x=L,\psi(x)=0$$
$$y=0,\psi(y)=0;\ y=L,\psi(y)=0$$
$$z=0,\psi(z)=0;\ z=L,\psi(z)=0$$

$$\psi(x,y,z)=\psi(x)\psi(y)\psi(z)$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z)=E\psi(x,y,z)$$

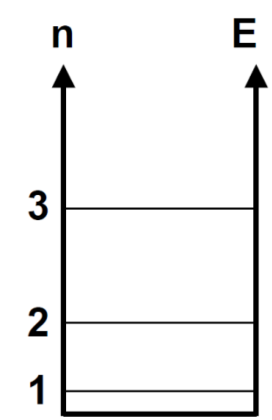
$$\frac{\partial^2\psi(x)}{\partial x^2}+k_x^2\psi(x)=0$$
$$\frac{\partial^2\psi(y)}{\partial y^2}+k_y^2\psi(y)=0$$
$$\frac{\partial^2\psi(z)}{\partial z^2}+k_z^2\psi(z)=0$$

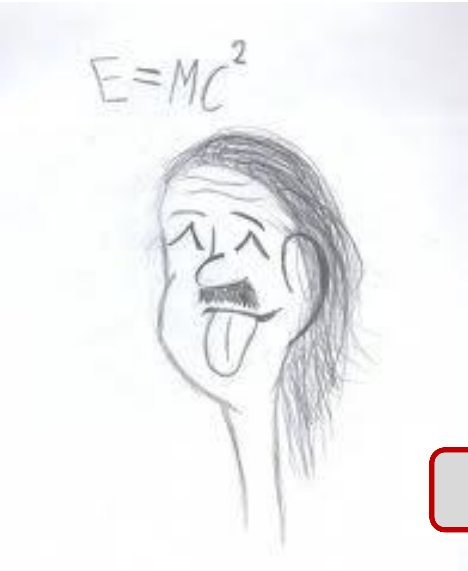
Boundary condition ⇒

$$\psi(x)=A_x\sin k_x x \qquad k_x=\frac{n_x\pi}{L} \qquad n_x=1,2,3,\ldots$$
$$\psi(y)=A_y\sin k_y y \qquad k_y=\frac{n_y\pi}{L} \qquad n_y=1,2,3,\ldots$$
$$\psi(z)=A_z\sin k_z z \qquad k_z=\frac{n_z\pi}{L} \qquad n_z=1,2,3,\ldots$$

$$E=\frac{\hbar^2k^2}{2m}=\frac{\hbar^2}{2m}(k_x{}^2+k_y{}^2+k_z{}^2)=\frac{\pi^2\hbar^2}{2mL^2}(n_x{}^2+n_y{}^2+n_z{}^2)$$

$$n_x,n_y,n_z=1,2,3,\ldots$$





Find the characteristics of motion of the free electrons

Quantized Energy

0K

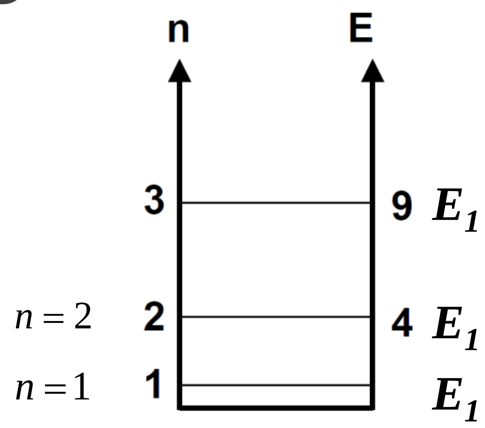
>0K

How the energy levels are occupied by free electrons

Fermi-Dirac distribution

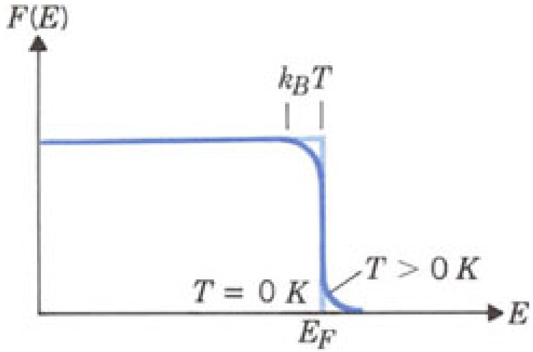
Find Fermi energy E_F

Find the electron number near the E_F

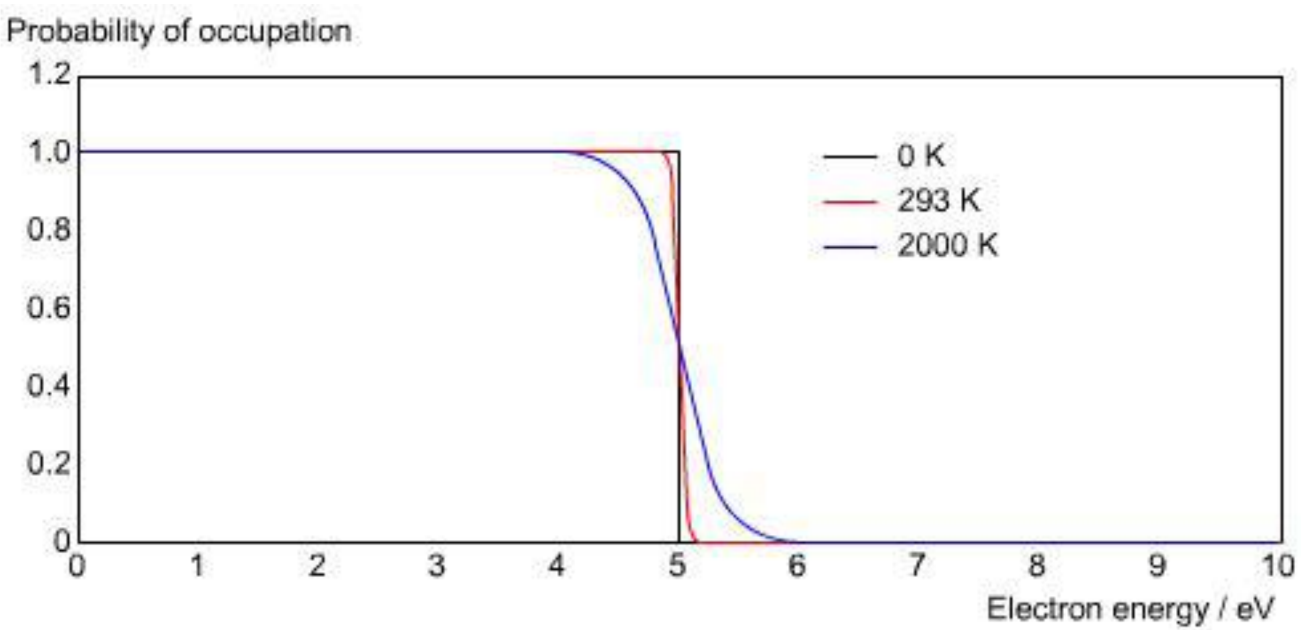


CFE model predicts → $C_v = 3/2\ R$

experiments show → $C_v = 10^{-4}\ RT$



Fermi-Dirac Distribution



Fermi-Dirac distribution for several temperatures

$$F_l = \frac{\alpha_l}{\omega_l} = \frac{1}{e^{(\alpha+\beta E_l)}+1} = \frac{1}{e^{(E_l-\mu)/k_B T}+1} = \frac{1}{e^{(E-E_F)/k_B T}+1}$$

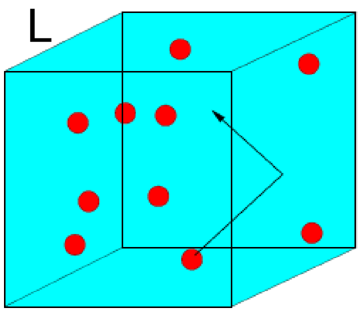
Occupancy Condition at T=0K

- Classical theory

Pauli's Exclusion Principle

Occupancy Condition at T=0K

- Quantum mechanically



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

$$= E_0(n_x^2 + n_y^2 + n_z^2)$$

$$E_0 = \frac{\pi^2 \hbar^2}{2mL^2}$$

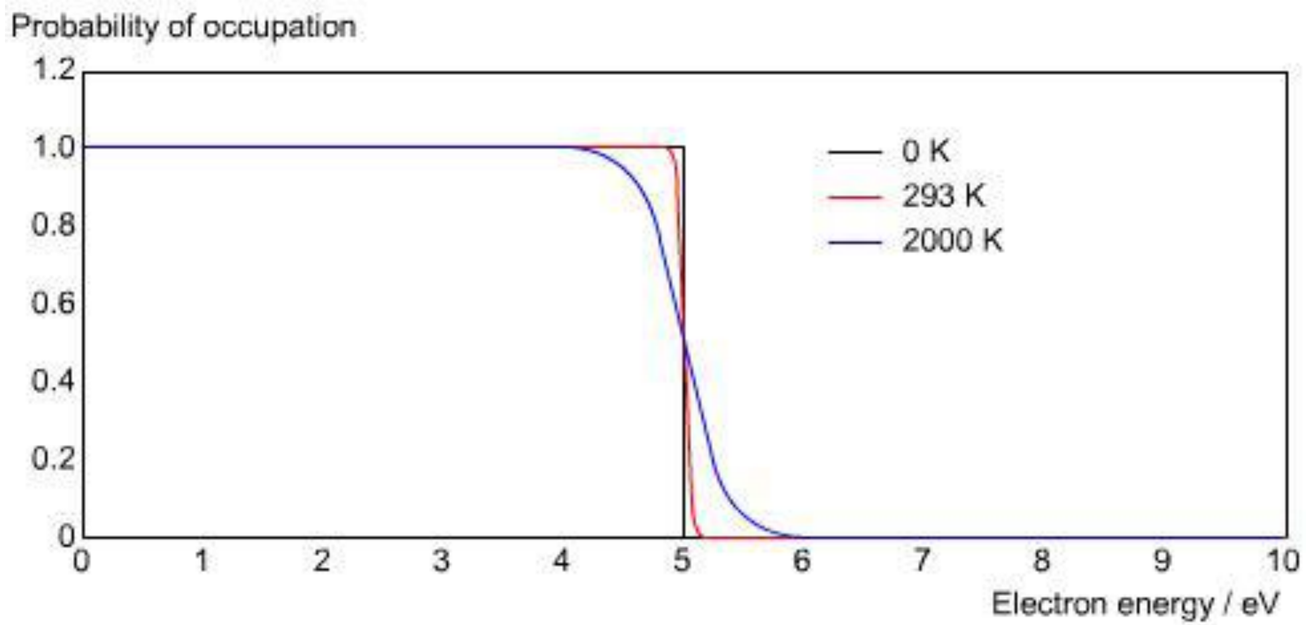
$$n_x, n_y, n_z = 1, 2, 3, \ldots$$

Occupancy Condition at T=0K

- Quantum mechanically

★★★The Fermi energy： the highest energy a fermion can take at absolute zero temperature.

Fermi-Dirac Distribution



Fermi-Dirac distribution for several temperatures

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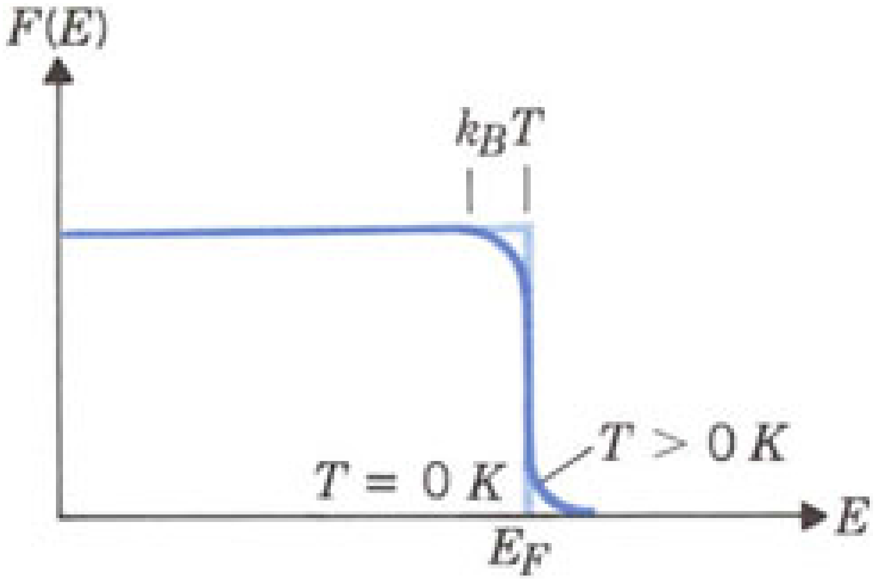
Occupancy Condition at T>0K

- Quantum mechanically

$$F(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1}$$

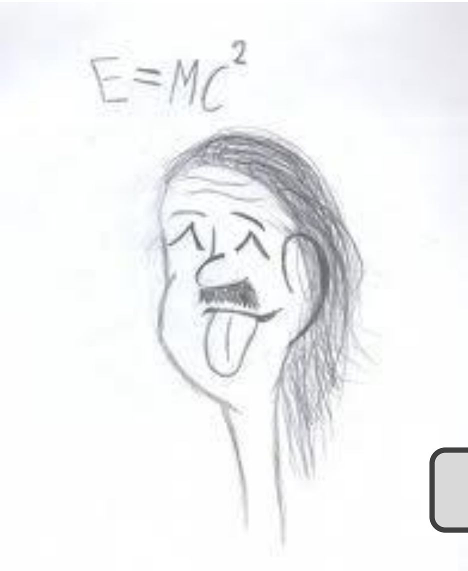


Occupancy Condition at T=0K and T>0K

- Quantum mechanically

Explain → { **CFE model predicts → C_V = 3/2 R**
experiments show → C_V = 10^{-4} RT

1. Fermi Energy value?
2. e^- number near E_F ?



Find the characteristics of motion of the free electrons

Quantized Energy

0K

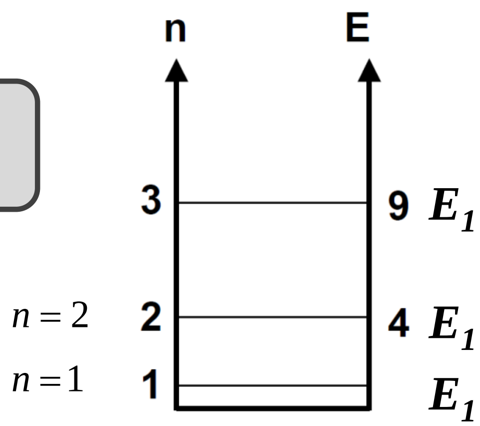
>0K

How the energy levels are occupied by free electrons

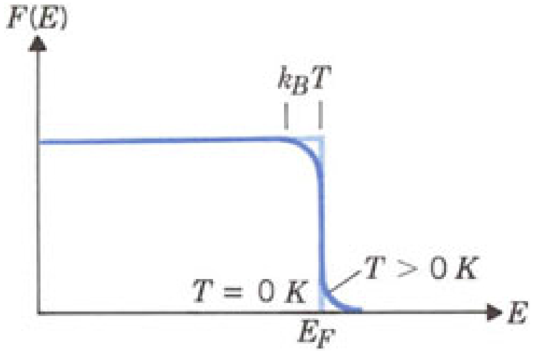
Fermi-Dirac distribution

Find Fermi energy E_F ← k distribution

Find the electron number near the E_F ← Density of state



- CFE model predicts → $C_v = 3/2\ R$
- experiments show → $C_v = 10^{-4}\ RT$



Calculation of Fermi Energy (E_F) at T=0K

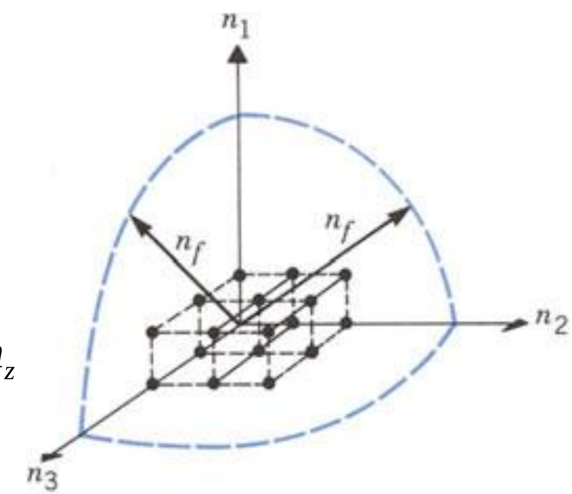
$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}(k_x{}^2 + k_y{}^2 + k_z{}^2)$$

$$\vec{k} = k_x \vec{i} + k_y \vec{j} + k_z \vec{l}$$

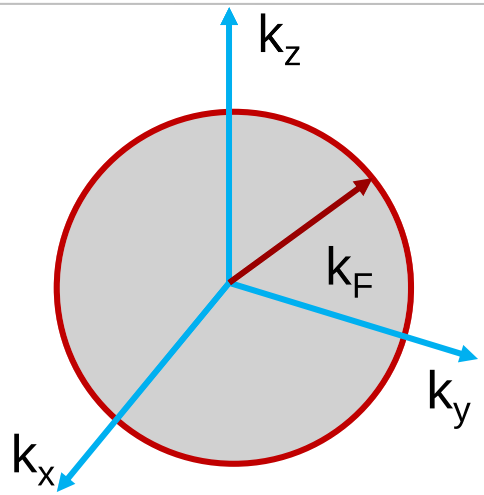
$$k_x = \frac{\pi}{L} n_x, \quad k_y = \frac{\pi}{L} n_y, \quad k_z = \frac{\pi}{L} n_z$$

$$E = (n_x{}^2 + n_y{}^2 + n_z{}^2) E_0 = n^2 E_0$$

$$E_0 = \frac{\pi^2 \hbar^2}{2mL^2} \qquad n_x, n_y, n_z = 1, 2, 3, \ldots$$



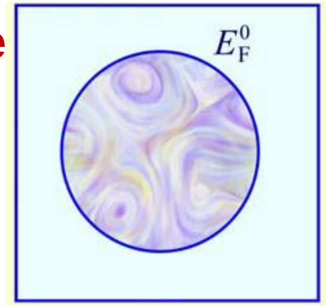
States on the same sphere are degenerate states



Fermi wave vector k_F

$$E_F = \frac{(\hbar k_F)^2}{2m}$$

Fermi sphere



The radius of the Fermi sphere is called the **Fermi wave vector *k_F***

At T=0K,
Inside Fermi sphere, all orbits are occupied;
Outside Fermi sphere, all orbits are empty.

Calculation of Fermi Energy (E_F) at T=0K

$$E_F = \frac{(\hbar k_F)^2}{2m}$$

$$\underbrace{\rho(k)\cdot V_{\text{Fermi sphere}}}_{V_F} = N(k) \quad (number\ \ of\ \ k)$$

$\Updownarrow$ Each k $\Leftrightarrow$ 2 electrons

number of electrons

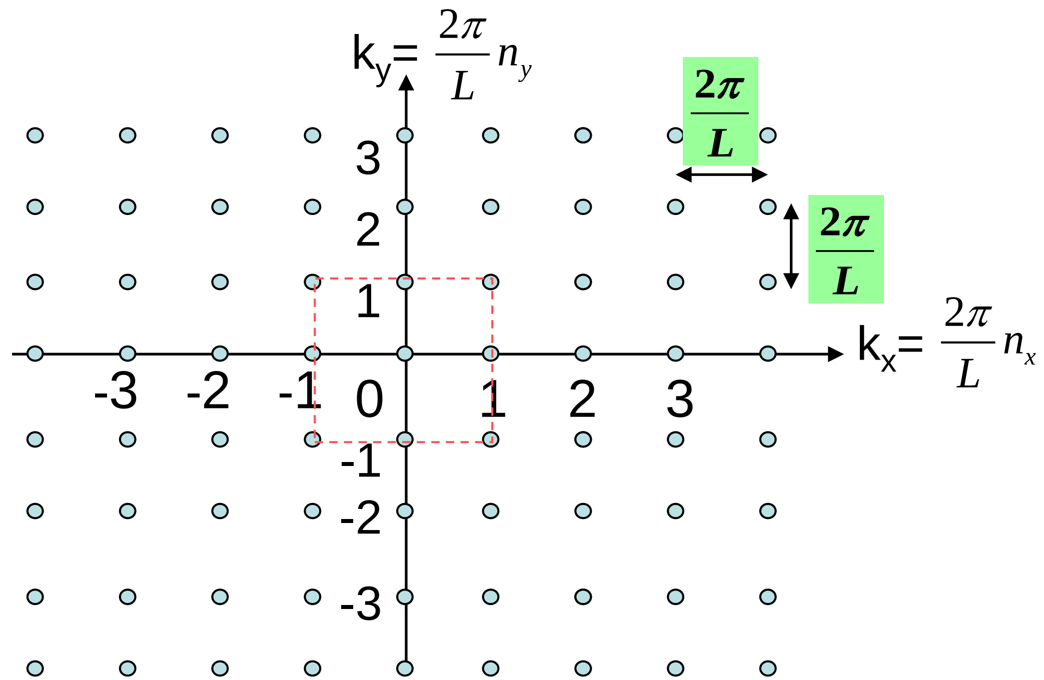
Distribution density of k : ρ(k)

$$k_x = \frac{2\pi}{L} n_x, \quad k_y = \frac{2\pi}{L} n_y, \quad k_z = \frac{2\pi}{L} n_z$$

2D

$$s_k = \frac{2\pi}{L}\cdot\frac{2\pi}{L} = \frac{(2\pi)^2}{S}$$

$$\rho(k) = \frac{1}{s_k} = \frac{S}{4\pi^2}$$



3D

$$v_k = \frac{2\pi}{L}\cdot\frac{2\pi}{L}\cdot\frac{2\pi}{L} = \frac{(2\pi)^3}{V}$$

$$\rho(k) = \frac{1}{v_k} = \frac{V}{8\pi^3}$$

Calculation of Fermi Energy (E_F) at T=0K

$$\rho(k) = \frac{V}{8\pi^3} \longrightarrow E_F = \frac{(\hbar k_F)^2}{2m}$$

Number of k

$$V_F \cdot \rho(k) = \left(\frac{4\pi k_F^3}{3}\right)\left(\frac{V}{8\pi^3}\right) = \frac{k_F^3}{6\pi^2}V$$

Number of e^- $\quad N = 2 \cdot \frac{k_F^3}{6\pi^2}V$

Density of e^- $\quad n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$

$$k_F = (3\pi^2 n)^{1/3}$$

$$E_F^0 = \frac{(\hbar k_F)^2}{2m} = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

$E_F^0 = 5.84*10^{-38} n^{2/3}$ J

E.g.

The valance electron density n=N/V is
1.402×10^{28} m^{-3}

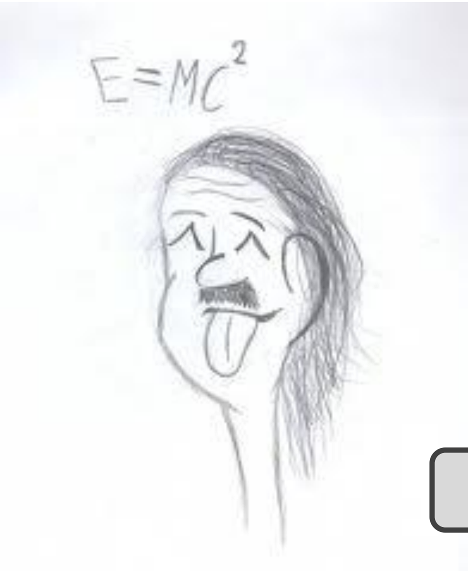
Fermi-energy E_F: $\quad E_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} = 2.12eV$

Comparison:
For a conductor of a=4cm

$$E_1 = 2.3\times10^{-41}\text{eV}$$

Fermi wave vector k_F: $\quad k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = 0.746\,\mathring{A}^{-1}$

Fermi temperature T_F: $\quad T_F = \frac{E_F}{k_B} = 2.46\times10^4 K$



Find the characteristics of motion of the free electrons

Quantized Energy

How the energy levels are occupied by free electrons

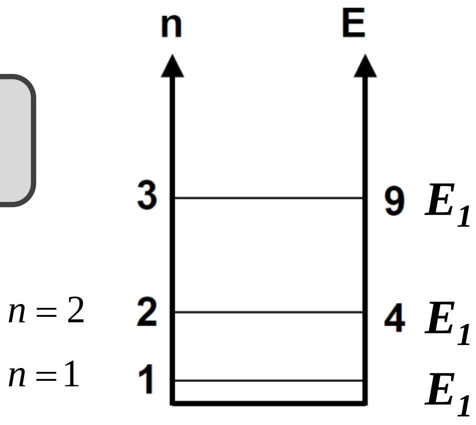
0K

>0K

Fermi-Dirac distribution

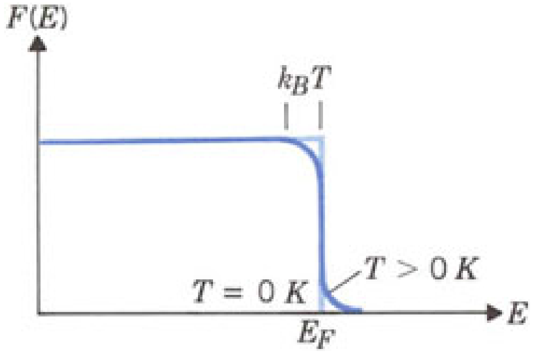
Find Fermi energy E_F ← k distribution

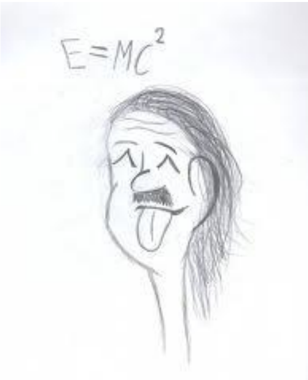
Find the electron number near the E_F ← Density of state



CFE model predicts → $C_v = 3/2\ R$

experiments show → $C_v = 10^{-4}\ RT$





Find the characteristics of motion of the free electrons by quantum mechanics → Schrodinger Equation

Quantized Energy

How the energy levels are occupied by free electrons

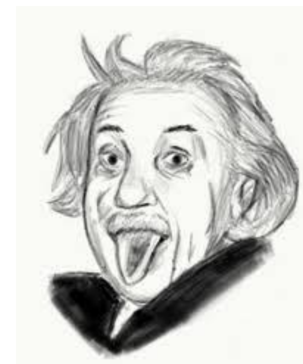
Fermi-Dirac distribution

Find Fermi energy E_F ← k distribution

Find the electron number near the E_F ← Density of state

电子气能量 ← Find the electron number near the E_F

$$C_V^e = \frac{\partial E}{\partial T}$$



Density of state (DOS)

DOS: the number of electronic energy states (orbits) per unit energy. --- g(E)

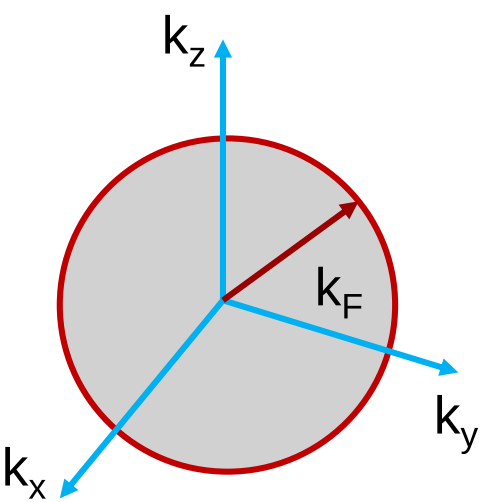
$$g(E) = \frac{\mathrm{d}Z}{\mathrm{d}E}$$

Remember: In crystal dynamics, the density of states g(ω) is defined as the number of oscillators (or k) per unit frequency interval.

Each k state represents two possible electron states: one for spin up, the other for spin down, thus the total number of electronic states in a sphere of diameter k is :

$$Z(E) = 2 \cdot \rho(\boldsymbol{k}) \cdot \frac{4}{3}\pi k^3 = 2 \cdot \frac{V}{8\pi^3} \cdot \frac{4}{3}\pi k^3 = \frac{Vk^3}{3\pi^2}$$

Density of state (DOS)



$$g(E) = \frac{\mathrm{d}Z}{\mathrm{d}E} = \frac{\mathrm{d}Z}{\mathrm{d}k} \cdot \frac{\mathrm{d}k}{\mathrm{d}E}$$

$$g(E) = \frac{\mathrm{d}Z}{\mathrm{d}k} \cdot \frac{\mathrm{d}k}{\mathrm{d}E} = \frac{V}{2\pi^2} \cdot \left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot E^{1/2}$$

$$g(E) = C \cdot E^{1/2}$$

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

$$\frac{\mathrm{d}Z}{\mathrm{d}k} = \frac{Vk^2}{\pi^2}$$

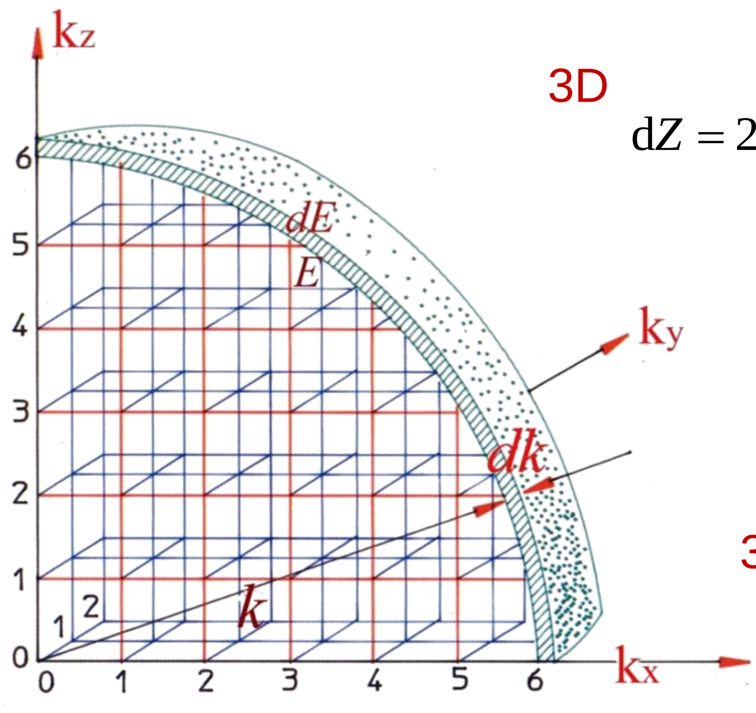
$$E = \frac{\hbar^2 k^2}{2m}$$

$$\frac{\mathrm{d}E}{\mathrm{d}k} = \frac{\hbar^2 k}{m}$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\frac{\mathrm{d}k}{\mathrm{d}E} = \sqrt{\frac{m}{2}}\frac{E^{-1/2}}{\hbar}$$

Another Way to Calculate DOS



For a free electron gas in 3D, the density of states for free electrons increases with the increase of energy E.

3D

$$dZ = 2\cdot\rho(k)\cdot 4\pi k^2\cdot dk = 2\cdot\frac{V}{(2\pi)^3}\cdot 4\pi\cdot\frac{2mE}{\hbar^2}\cdot\sqrt{\frac{m}{2}}\frac{E^{-1/2}}{\hbar}\cdot dE$$

$$g(E) = \frac{dZ}{dE} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

$$g(E) = C\cdot E^{1/2} \qquad C = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}$$

3D

$$dZ = 2\cdot\rho(k)\cdot 4\pi k^2\cdot dk = 2\cdot\frac{V}{8\pi^3}\cdot 4\pi k^2\cdot dk = \frac{Vk^2}{\pi^2}dk$$

$$g(E) = \frac{dZ}{dE} = \frac{Vk^2}{\pi^2}\frac{dk}{dE} = \frac{Vk^2}{\pi^2}\frac{m}{\hbar^2 k} = \frac{mVk}{\pi^2\hbar^2} = \frac{mV}{\pi^2\hbar^2}\sqrt{\frac{2mE}{\hbar^2}}$$

1D

$$dZ = 2\cdot\rho(k)\cdot 2\cdot dk = 4\frac{L}{2\pi}dk$$

$$g(E) = \frac{dZ}{dE} = \frac{2L}{\pi}\frac{dk}{dE} = \frac{2L}{\pi}\frac{m}{\hbar^2 k} = \frac{2L}{\pi}\frac{m}{\hbar^2\sqrt{\frac{2mE}{\hbar^2}}}$$

$$g(E) = C\cdot E^{-1/2}$$

2D

$$dZ = 2\cdot\rho(k)\cdot 2\pi k\cdot dk = 4\pi k\frac{S}{4\pi^2}dk$$

$$g(E) = \frac{dZ}{dE} = \frac{kS}{\pi}\frac{dk}{dE} = \frac{kS}{\pi}\frac{m}{\hbar^2 k} = \frac{mS}{\pi\hbar^2}$$

g(E) has no relationship with E or k

Situation of Orbits Occupied by Electrons

DOS $g(E)$: the number of electronic energy states (orbits) per unit energy.
$f(E)$: probability that an electronic energy state be occupied.

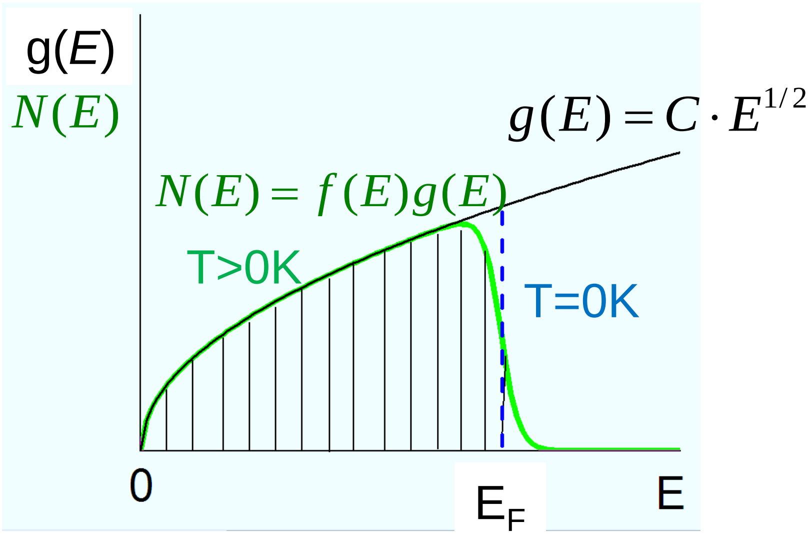
Define ***N(E)*** as Electron energy distribution function

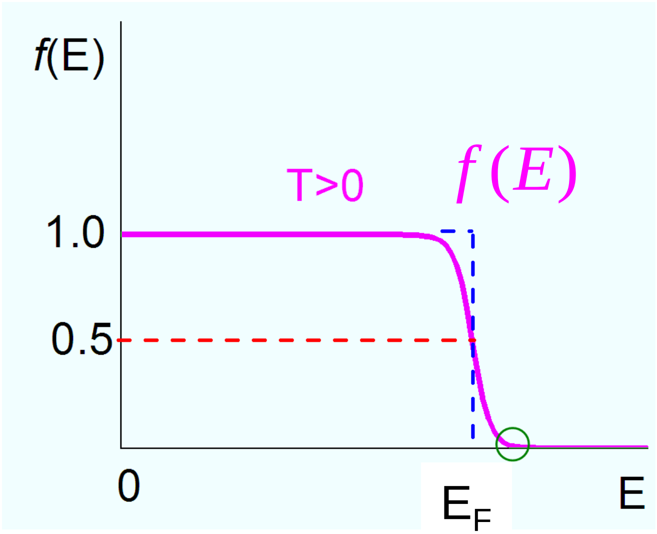
$N(E)\mathrm{d}E$ = number of e^- with energies between E and $E+\mathrm{d}E$

$g(E)f(E)\mathrm{d}E$=number of e- with energies between E and $E+\mathrm{d}E$

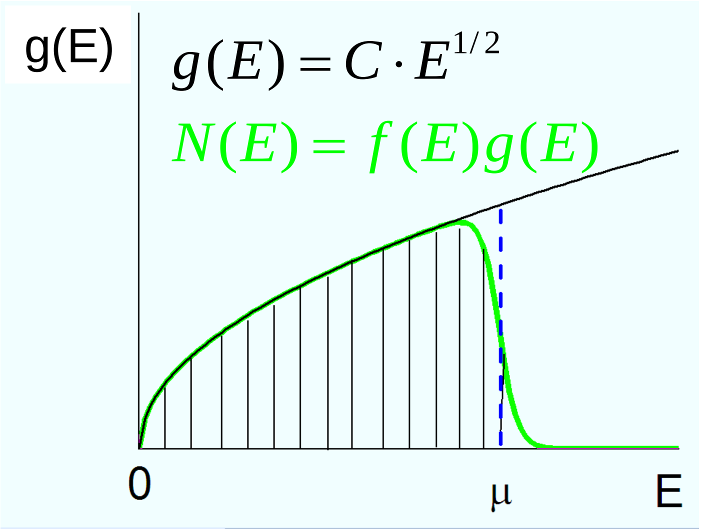
$$N(E) = g(E)\,f(E)$$

Total number of e^- $N = \int_0^\infty g(E)\,f(E)\mathrm{d}E$





Another method of getting Fermi energy



Total number of e⁻ $\quad N = \int_0^\infty g(E) f(E) \mathrm{d}E$

$$g(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

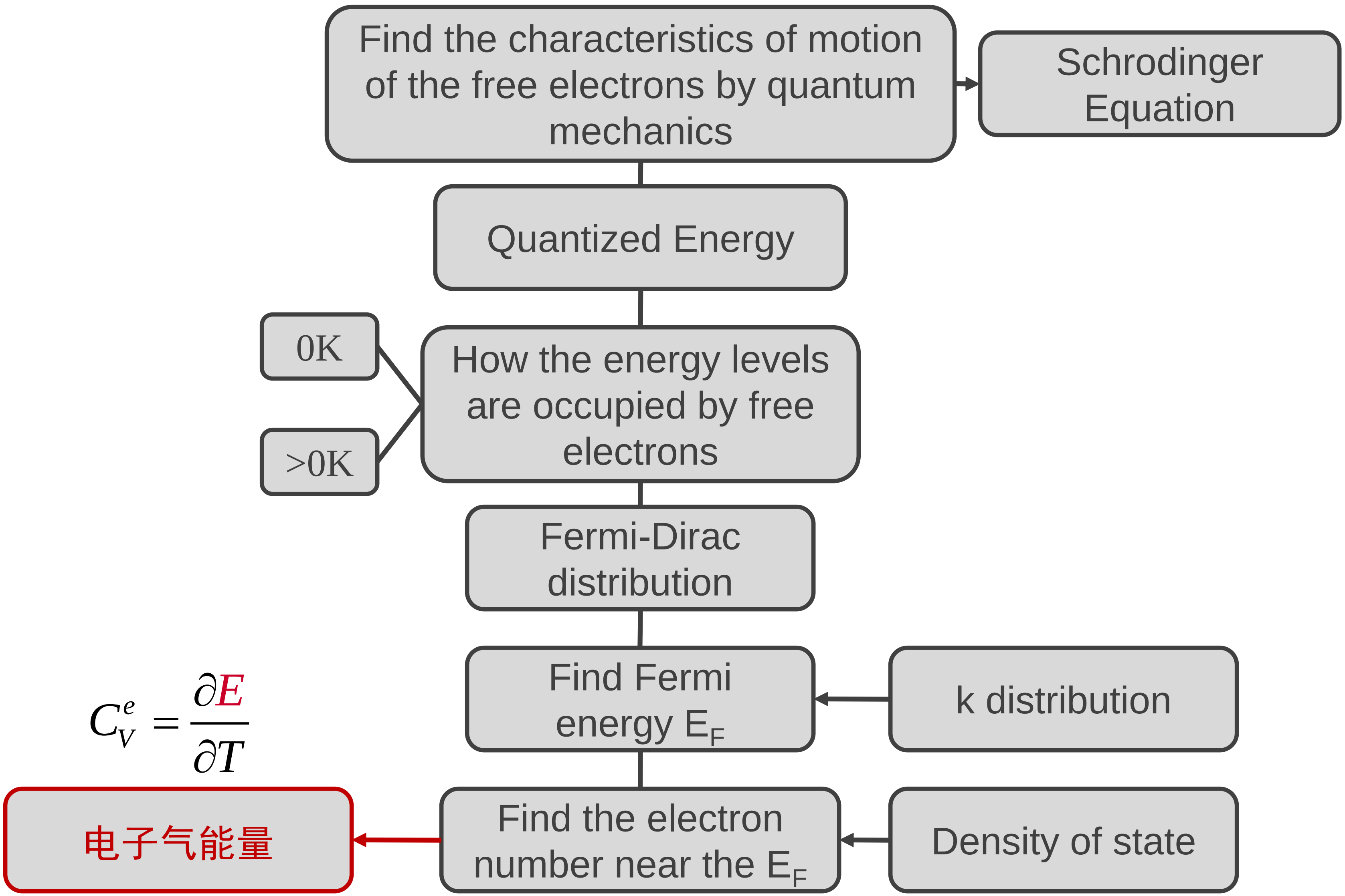
T=0K

$$N = \int_0^{E_F^0} f(E) g(E) \mathrm{d}E = \int_0^{E_F^0} \frac{V}{2\pi^2\hbar^3}(2m)^{3/2} E^{1/2} \mathrm{d}E = \frac{V}{3\pi^2\hbar^3}(2mE_F^0)^{3/2}$$

$$\downarrow$$

$$E_F^0 = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{\frac{2}{3}} = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{\frac{2}{3}} \longrightarrow k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = \left(3\pi^2 n\right)^{1/3}$$

$$E_F = \frac{\hbar^2 k_F{}^2}{2m_e}$$


Find the characteristics of motion of the free electrons by quantum mechanics
Schrodinger Equation
Quantized Energy
0K
>0K
How the energy levels are occupied by free electrons
Fermi-Dirac distribution
Find Fermi energy E_F
k distribution
$C_V^e = \frac{\partial E}{\partial T}$
电子气能量
Find the electron number near the E_F
Density of state

Total energy for electron gas

T=0K

$$E_t = \int E\mathrm{d}N = \int E\cdot g(E)\cdot f(E)\cdot \mathrm{d}E$$

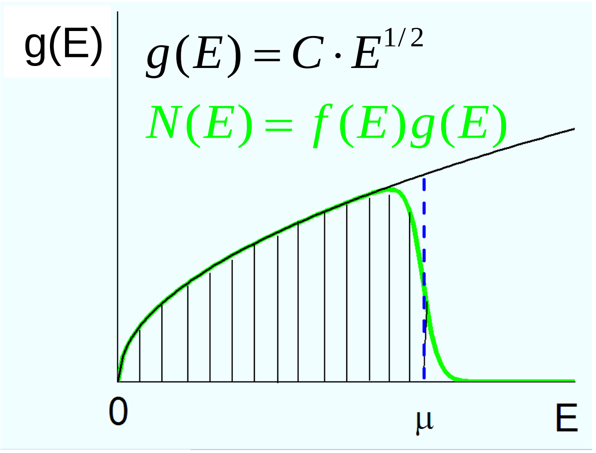
$$= \int_0^{E_F^0} C\cdot E^{1/2} E\mathrm{d}E = \int_0^{E_F^0} CE^{3/2}\mathrm{d}E = \frac{2C}{5}\left(E_F^0\right)^{5/2}$$

Average energy for free electrons

$$\overline{E} = \frac{\frac{2C}{5}\left(E_F^0\right)^{5/2}}{N} = \ldots = \frac{3}{5}E_F^0 \qquad E_t = \frac{3}{5}NE_F^0$$

At T=0K， the average energy of a free electron is 60% of the Femi energy.

Q: Is the result similar to that of classical theory?



$$N = \int_0^{\infty} g(E)f(E)\mathrm{d}E$$

$$= \int_0^{E_F^0} g(E)\mathrm{d}E$$

$$= \frac{V}{3\pi^2\hbar^3}(2mE_F^0)^{3/2}$$

$$E_F^0 = \frac{\hbar^2}{2m}\left(3\pi^2\frac{N}{V}\right)^{2/3}$$

$$C = \frac{V(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}$$

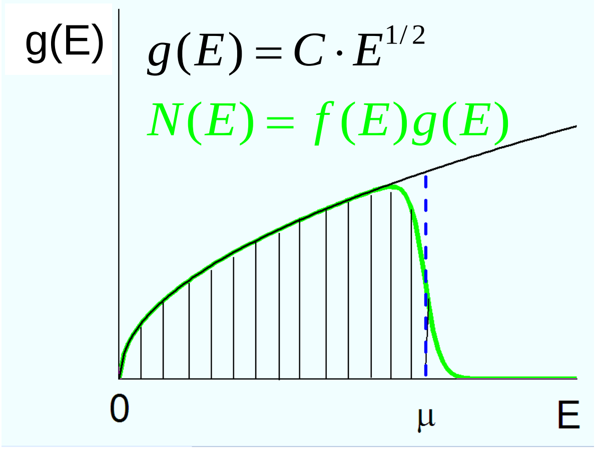
Total energy for electron gas

T>0K

$$E_t = \int E \cdot g(E) \cdot f(E) \mathrm{d}E$$

$$= C\int_0^{\infty} E^{3/2} \frac{1}{\mathrm{e}^{(E-E_F)/k_B T}+1} \mathrm{d}E$$

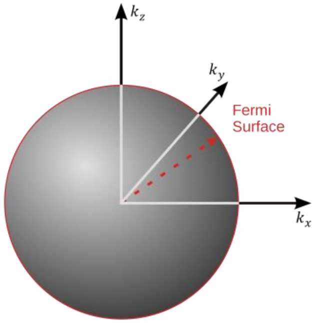
$$= \cdots = \frac{3}{5} N E_F^0 [1 + \frac{5}{12}\pi^2 (\frac{k_B T}{E_F^0})^2]$$



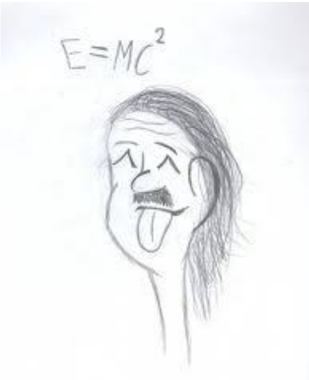
$$N = \int_0^{\infty} g(E) f(E) \mathrm{d}E$$

$$= \int_0^{\infty} \frac{1}{e^{(E-E_F)/k_B T}+1} g(E) \mathrm{d}E$$

Fermi energy



$$E_F = E_F^0 \left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{E_F^0}\right)^2\right] = E_F^0 \left[1 - \frac{\pi^2}{12}\left(\frac{T}{T_F}\right)^2\right] \approx E_F^0$$



Find the characteristics of motion of the free electrons by quantum mechanics → Schrodinger Equation

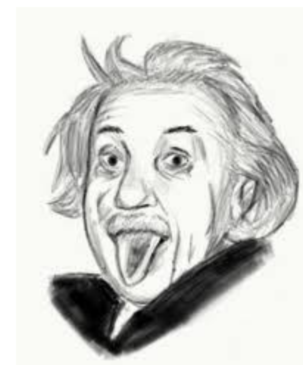
Quantized Energy

How the energy levels are occupied by free electrons (0K, >0K)

Fermi-Dirac distribution

Find Fermi energy E_F ← k distribution

电子气能量 ← Find the electron number near the E_F ← Density of state



Drude Model - Classical FEM	Sommerfeld Model - Quantum Mechanical FEM

· Potential Well · F-D Distribution · Fermi Energy · Density of State · e^- number near E_F · e^- gas Energy

A. Piccard, E. Henriot, P. Ehrenfest, E. Herzen, Th. De Donder, E. Schrödinger, J.E. Verschaffelt, W. Pauli, W. Heisenberg, R.H. Fowler, L. Brillouin;
B. P. Debye, M. Knudsen, W.L. Bragg, H.A. Kramers, P.A.M. Dirac, A.H. Compton, L. de Broglie, M. Born, N. Bohr;
I. Langmuir, M. Planck, M. Skłodowska-Curie, H.A. Lorentz, A. Einstein, P. Langevin, Ch. E. Guye, C.T.R. Wilson, O.W. Richardson

Drude Model - Classical FEM | Sommerfeld Model - Quantum Mechanical FEM

· Potential Well · F-D Distribution · Fermi Energy · Density of State · e^- number near E_F · e^- gas Energy

Photograph of the first conference in 1911 at the Hotel Metropole. Seated (L-R): W. Nernst, M. Brillouin, E. Solvay, H. Lorentz, E. Warburg, J. Perrin, W. Wien, M. Skłodowska-Curie, and H. Poincaré. Standing (L-R): R. Goldschmidt, M. Planck, H. Rubens, A. Sommerfeld, F. Lindemann, M. de Broglie, M. Knudsen, F. Hasenöhrl, G. Hostelet, E. Herzen, J.H. Jeans, E. Rutherford, H. Kamerlingh Onnes, A. Einstein and P. Langevin.

Arnold Johannes Wilhelm Sommerfeld

Arnold Sommerfeld (1868 - 1951), a German physicist who is one of the founders of the quantum mechanics

Doctoral students

Werner Heisenberg
Wolfgang Pauli
Peter Debye
Paul Sophus Epstein
Hans Bethe
Ernst Guillemin
Karl Bechert
Paul Peter Ewald
Herbert Fröhlich
Erwin Fues
Helmut Hönl
Ludwig Hopf
Walther Kossel
Adolf Kratzer
Alfred Landé
Otto Laporte
Wilhelm Lenz
Rudolf Peierls
Walter Rogowski
Rudolf Seeliger
Heinrich Welker
Gregor Wentzel

1935

Chapter 3 Free electrons in solids

3.1 Free electron model

3.1.1 Drude Model

- Classical Free Electron Model

3.1.2 Sommerfeld Model

- Quantum Mechanical Free Electron Model

3.2 Heat capacity of free electron gas

3.3 Transport properties of conductive electrons

3.4 Hall effect and thermal-electric effect