Phys 570

Lecture #2

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EFFECT OF TEMPERATURE ON THE FERMI-DIRAC DISTRIBUTION

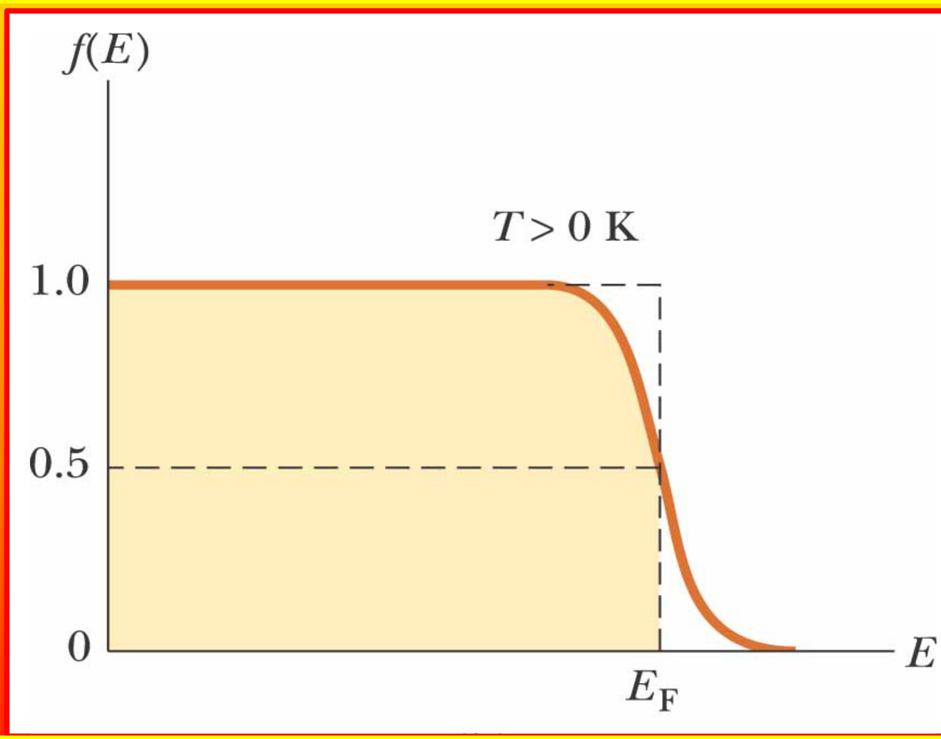
- *The ground state is the state of the N electron system at absolute zero*. What happens as the temperature is increased? The solution is given by the Fermi-Dirac distribution function.
- The kinetic energy of the electron gas increases as the temperature is increased: some energy levels are occupied which were vacant at absolute zero, and some levels are vacant which were occupied at absolute zero .The **Fermi-Dirac distribution gives the probability that an orbital at energy ε** will be occupied in an ideal electron gas in thermal equilibrium.

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1} \qquad (5)$$

μ is a function of the temperature; it is to be chosen in such a way that the total number of particles = *N. At absolute zero* $\mu = \varepsilon_F$

EFFECT OF TEMPERATURE ON THE FERMI-DIRAC DISTRIBUTION

because in the limit *T* → *0 the function f(ε) changes discontinuously from the value 1 (filled) to* the value 0 (empty) at $\varepsilon = \varepsilon_F = \mu$. *At all temperatures f(ε) is equal to ½ when ε = μ,* for then the denominator of (5) has the value 2.

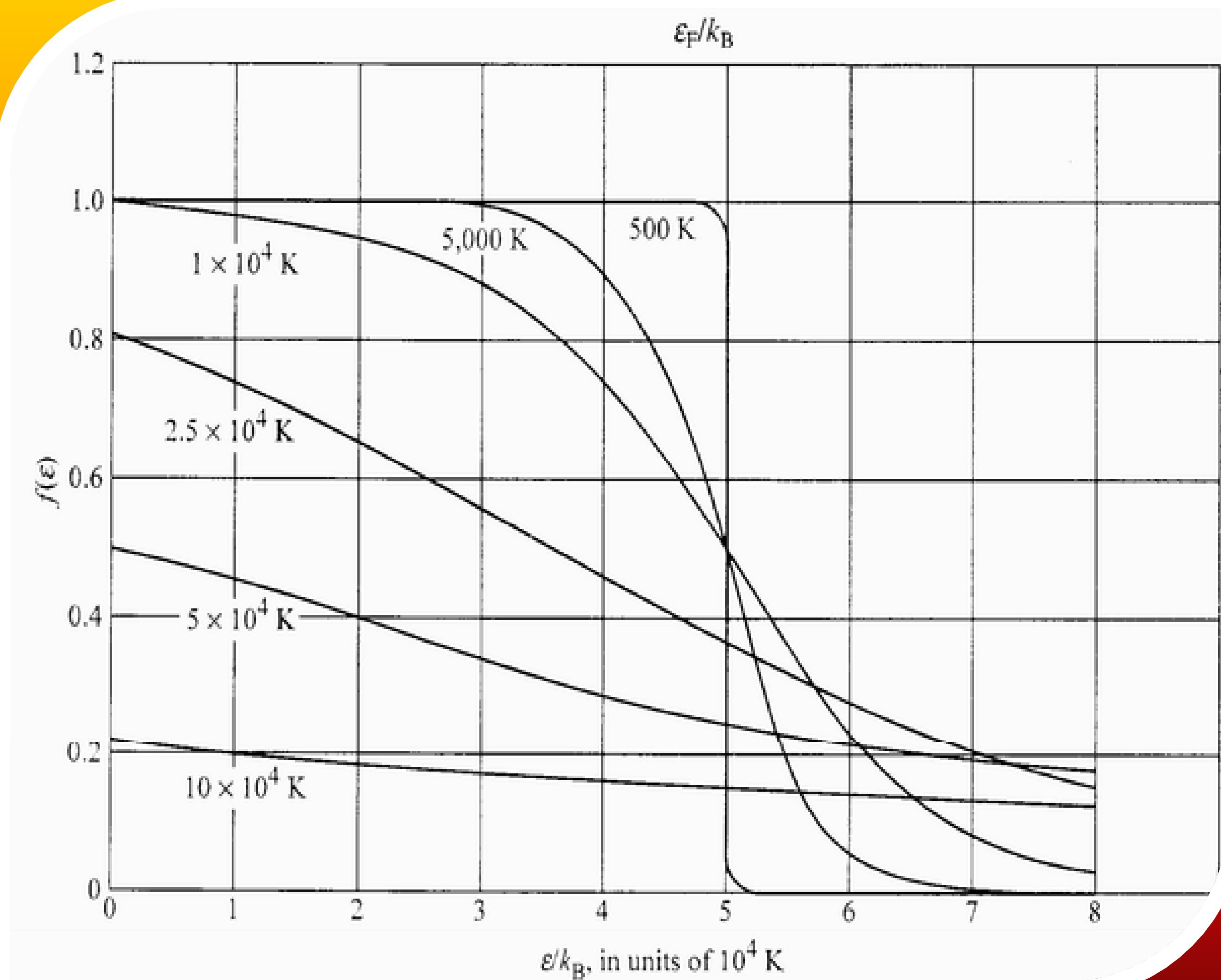


f(ε) = 1 (means full)
f(ε) = 0 (means vacant)

At very low temp. f(ε) becomes similar to Boltzmann or Maxwell Distribution.

EFFECT OF TEMPERATURE ON THE FERMI-DIRAC DISTRIBUTION

f(ε) at the various temperatures, for *$T_\varepsilon = \varepsilon_F/K_BT$ = 50,000 K. The total number of particles* is constant, independent of temperature.

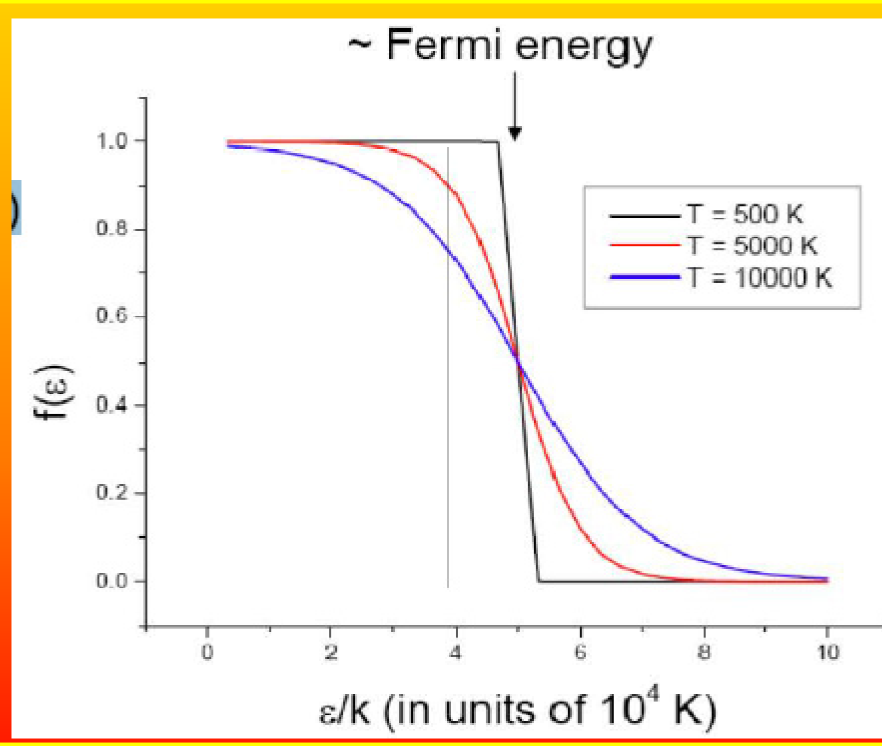


FERMI-DIRAC DISTRIBUTION

This is what the $f(\varepsilon)$ looks like at different Temperatures

- As T → 0 K, it becomes a step function
- Note that the lower energy levels are usually filled first, and as temperature increases;

no of electrons at higher energy levels increases.



Fermi energy changes as the temperature changes because it is defined as: $\mu = F_{n+1} - F_n$ (n= no. of particles, electrons)

Where F is the Helmholtz Free Energy: F=U-TS

U: System energy, S: Entropy (Increases as T increase)

Chapter 6: Free Electron Fermi Gas

Different DISTRIBUTION Systems

Distribution System	Notes	
Maxwell-Boltzmann distribution	•identical particles •distinguishable •wave function : not overlap	$f(\varepsilon) = Ae^{-\varepsilon/k_B T}$
Bose-Einstein distribution	•Identical particles •indistinguishable •wave function : overlap •spin quantum number = 0,1,2, …	$f(\varepsilon) = \frac{1}{e^{\alpha}e^{\varepsilon/k_B T} - 1}$
Fermi-Dirac distribution	•Identical particles •indistinguishable •wave function: overlap •spin quantum number = 1/2,3/2,5/2 ….	$f(\varepsilon) = \frac{1}{e^{\alpha}e^{\varepsilon/k_B T} + 1}$

FREE ELECTRON GAS IN THREE DIMENSIONS

We just need to extend our results for 1-D.

$$\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{dx^2}+\frac{\partial^2}{dy^2}+\frac{\partial^2}{dz^2}\right)\psi_k(r)=\varepsilon_k\psi_k(r) \qquad (6)$$

for a cube of length L we have:

$$\psi_n(r)=A\sin\left(\frac{\pi n_x x}{L}\right)\sin\left(\frac{\pi n_y y}{L}\right)\sin\left(\frac{\pi n_z z}{L}\right) \qquad (7)$$

n_x, ny, n_z are all positive intigers.

ψ is periodic in x, y, z with period L. Thus:

$$\psi(x+L,y,z)=\psi(x,y,z) \qquad (8)$$

$$\psi(x,y+L,z)=\psi(x,y,z), \quad \psi(x,y,z+L)=\psi(x,y,z)$$

FREE ELECTRON GAS IN THREE DIMENSIONS

Wave functions satisfying the free particle Schrodinger equation and the periodicity condition are of the form of a traveling plane

$$\psi_k(r) = e^{ik.r} \qquad (9)$$

$$\text{with: } k_x, k_y, k_z = 0;\ \pm\frac{2\pi}{L};\ \pm\frac{4\pi}{L};\ ...... \qquad (10)$$

Any component of k of the form *2nπ/L will satisfy the periodicity* condition over a length L, where *n is a positive or negative integer.* these values of k_x satisfy (8), for:

$$e^{ik_x(x+L)} = e^{i\frac{2n\pi}{L}(x+L)} = e^{i\frac{2n\pi}{L}x}.e^{i2n\pi} = e^{i\frac{2n\pi}{L}x} = e^{ik_x x} \qquad (11)$$

Differentiate (9) twice then put it back in Eq. (6):

$$\varepsilon_k = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}(k_x^2 + k_x^2 + k_x^2) \qquad (12)$$

The energy at the surface of the sphere is the Fermi energy:

$$\varepsilon_F = \frac{\hbar^2}{2m} k_F^2 \qquad (14)$$

We can calculate the total No. of states inside Fermi Sphere from dividing the total Fermi sphere volume on the volume of one state

Volume of one state: $\left(\frac{2\pi}{L}\right)^3$

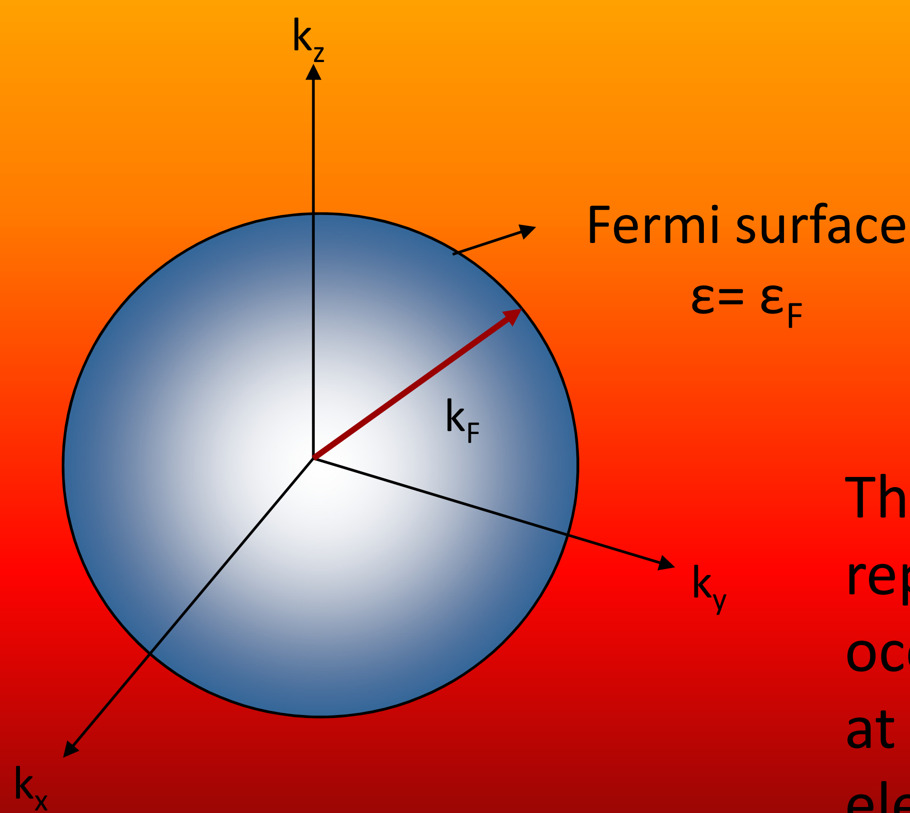
Total volume of Fermi Sphere: $\frac{4}{3}\pi k_F^3$

$$\therefore\ N = 2.\frac{4}{3}\pi k_F^3 \Big/ \left(\frac{2\pi}{L}\right)^3 = \frac{V}{3\pi^2} k_F^3 \quad \text{(Total No. of states)} \qquad (15)$$

$$\Rightarrow\ k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} \qquad (16)$$

Hencem k_F depends only on particle concentration

The occupied states are inside the Fermi sphere in *k*-space as shown below; the radius is Fermi wave number k_F



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

The surface of the Fermi sphere represents the boundary between occupied & unoccupied k states at absolute zero for the free electron gas.

Calculated values of $\mathbf{k_F}$, $\mathbf{v_F}$ and $\mathbf{E_F}$ are given in Table 1 for selected metals.

Table 1 Calculated free electron Fermi surface parameters for metals at room temperature (Except for Na, K, Rb, Cs at 5 K and Li at 78 K)

Valency	Metal	Electron concentration, in cm^{-3}	Radius[a] parameter r_s	Fermi wavevector, in cm^{-1}	Fermi velocity, in $cm\ s^{-1}$	Fermi energy, in eV	Fermi temperature $T_F = \epsilon_F/k_B$, in deg K
1	Li	4.70×10^{22}	3.25	1.11×10^{8}	1.29×10^{8}	4.72	5.48×10^{4}
	Na	2.65	3.93	0.92	1.07	3.23	3.75
	K	1.40	4.86	0.75	0.86	2.12	2.46
	Rb	1.15	5.20	0.70	0.81	1.85	2.15
	Cs	0.91	5.63	0.64	0.75	1.58	1.83
	Cu	8.45	2.67	1.36	1.57	7.00	8.12
	Ag	5.85	3.02	1.20	1.39	5.48	6.36
	Au	5.90	3.01	1.20	1.39	5.51	6.39
2	Be	24.2	1.88	1.93	2.23	14.14	16.41
	Mg	8.60	2.65	1.37	1.58	7.13	8.27
	Ca	4.60	3.27	1.11	1.28	4.68	5.43
	Sr	3.56	3.56	1.02	1.18	3.95	4.58
	Ba	3.20	3.69	0.98	1.13	3.65	4.24
	Zn	13.10	2.31	1.57	1.82	9.39	10.90
	Cd	9.28	2.59	1.40	1.62	7.46	8.66
3	Al	18.06	2.07	1.75	2.02	11.63	13.49
	Ga	15.30	2.19	1.65	1.91	10.35	12.01
	In	11.49	2.41	1.50	1.74	8.60	9.98
4	Pb	13.20	2.30	1.57	1.82	9.37	10.87
	Sn(*w*)	14.48	2.23	1.62	1.88	10.03	11.64

[a] The dimensionless radius parameter is defined as $r_s = r_0/a_H$, where a_H is the first Bohr radius and r_0 is the radius of a sphere that contains one electron.

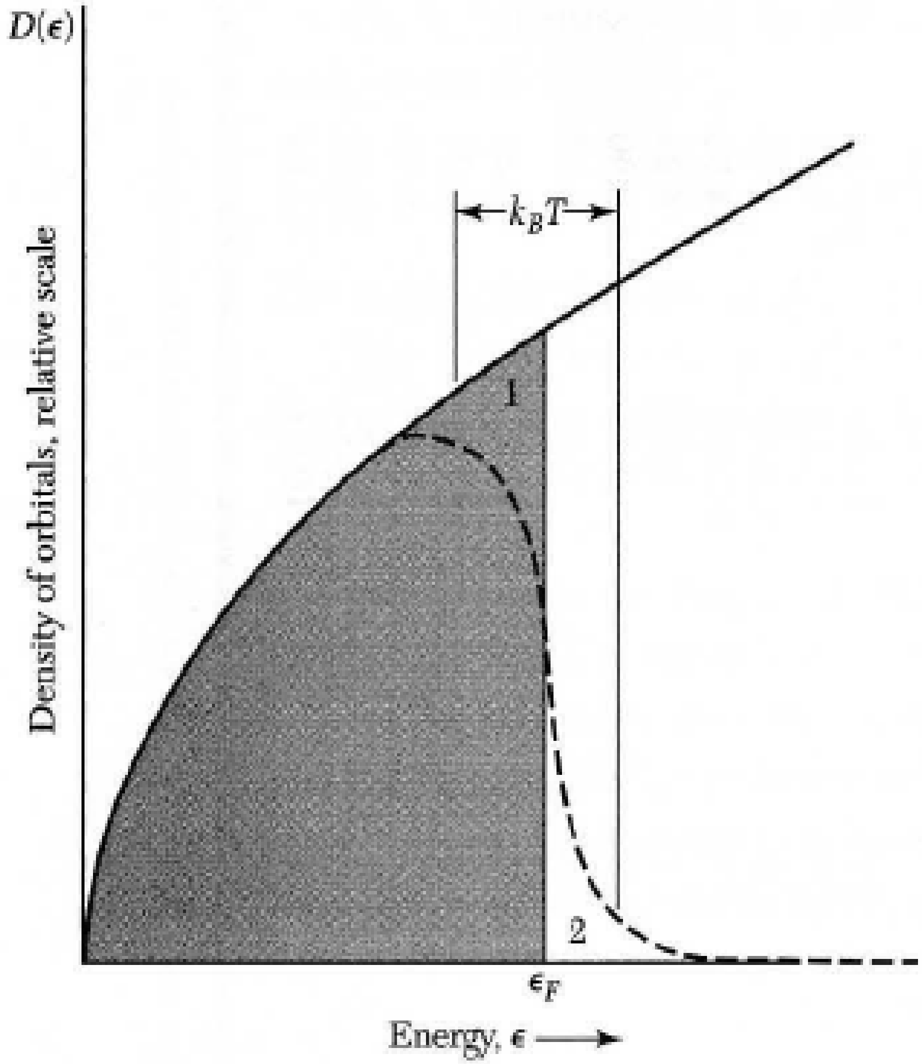


Figure 5 Density of single-particle states as a function of energy, for a free electron gas in three dimensions. The dashed curve represents the density $f(\epsilon, T)D(\epsilon)$ of filled orbitals at a finite temperature, but such that k_BT is small in comparison with ϵ_F. The shaded area represents the filled orbitals at absolute zero. The average energy is increased when the temperature is increased from 0 to T, for electrons are thermally excited from region 1 to region 2.

The number of orbitals per unit energy range: D(ϵ) = density of states.

$$N = \frac{V}{3\pi^2}\left(\frac{2m\varepsilon}{\hbar^2}\right)^{3/2} \qquad (19)$$

This leads to:

$$D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{V}{2\pi^2}.\left(\frac{2m}{\hbar^2}\right)^{3/2}.\varepsilon^{1/2} \quad (20)$$

Equation (19):

$$\ln N = \frac{3}{2}\ln\varepsilon + const\ .$$

Hence:

$$\frac{dN}{N} = \frac{3}{2}.\frac{d\varepsilon}{\varepsilon} \Rightarrow D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{3N}{2\varepsilon} \quad (21)$$

Within a factor of the order of unity, the number of orbitals per unit energy range at the Fermi energy is the total number of conduction electrons divided by the Fermi energy.