Physics PY4118
Physics of Semiconductor Devices

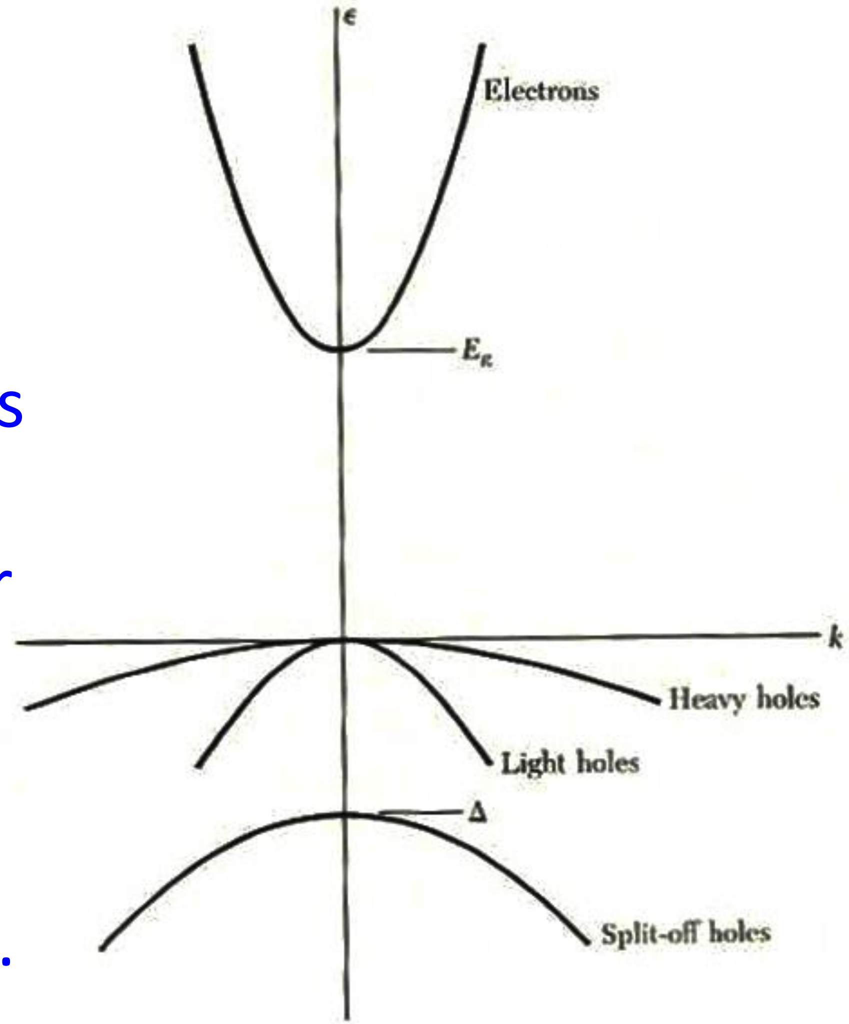
Band Filling

Semiconductor Bands

The lowest filled bands are filled with electrons that are bound near the atomic nucleus.

The electrons in the highest bands are used in co*valent* bonds. They are called *valence* electrons. Their bands are *valence bands*.

The next band, unpopulated at $0K$, is called the *conduction band*.



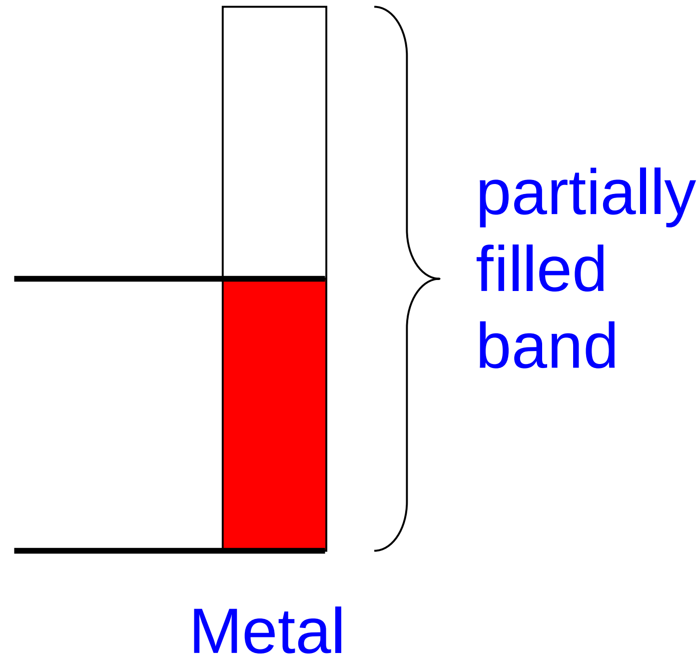
Fermi Level and Energy

- Pauli exclusion leads to electrons populating higher states rather than all sitting in the ground state
- Fermi statistics govern how electrons move into even higher states due to temperature

Fermi Level in Metals

Highest occupied energy level at T=0K

$$E = E_F$$



$$E = 0$$

Energy level at the bottom of the partially filled band

Pauli's Exclusion Principle at Work.

Fermi Level in Metals

Fermi Velocity: $$\frac{1}{2} m {v_F}^2 = E_F$$

Copper: $$E_F = 7eV \qquad v_F = 1.6 \times 10^6 \, m/\sec$$

RT: $$k_B T \cong 0.025eV$$ 1000°C: $$k_B T \cong 0.11eV$$

The amount of thermal energy is much less that the Fermi Energy!
Even at high Temperature.

Metals conduct very well even at very low T

The Occupation Probability (1)

- Or: “What is the probability that an available level will be populated?”

- A group of probability distribution functions have been derived using Statistical Mechanics.

- Other names are “Energy Distribution Functions”

The Occupation Probability (2)

- Maxwell - Boltzmann
  - Identical – no Pauli
  - distinguishable

$$P(E) = e^{-\frac{E-E_F}{k_B T}}$$

- Bose-Einstein
  - Identical – no Pauli
  - indistinguishable

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

- Fermi-Dirac
  - Identical - Pauli
  - indistinguishable

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

The Occupation Probability (3)

If: $e^{\frac{E-E_F}{k_BT}} >> 1$ Or: $E - E_F > k_BT$

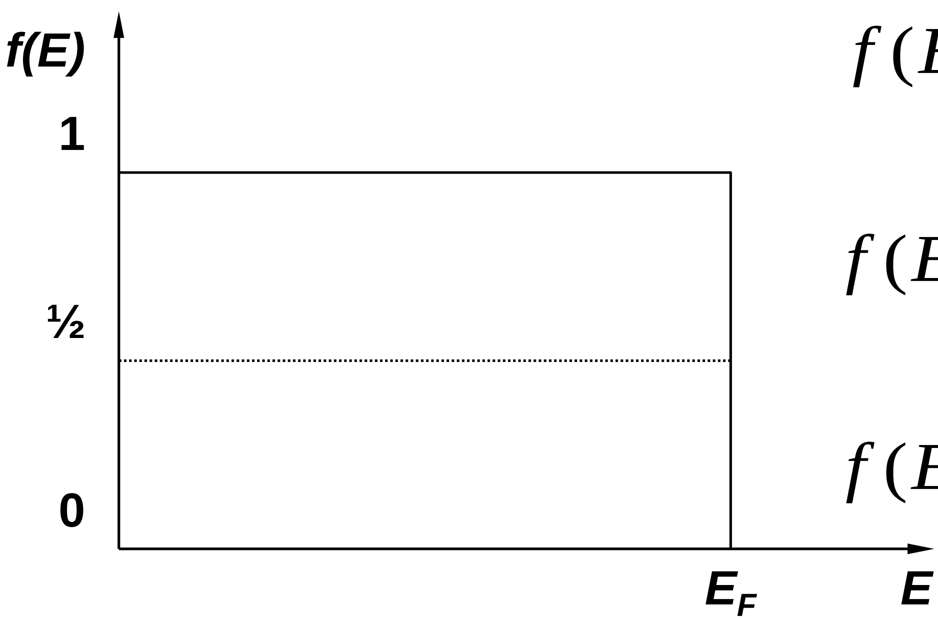
Remember, at RT: $k_BT = \frac{1}{40} eV$

$$f(E) = \frac{1}{e^{\frac{E-E_F}{k_BT}} + 1} \Rightarrow P(E) = e^{-\frac{E-E_F}{k_BT}}$$

Fermi - Dirac ➡ Maxwell - Boltzmann

The Fermi Function (1)

If T=$0K$, f(E) is a simple step function with an edge at E_F, i.e., all the states with energies below the fermi energy E_F, are completely occupied, and all the states with energies above E_F are completely vacant.

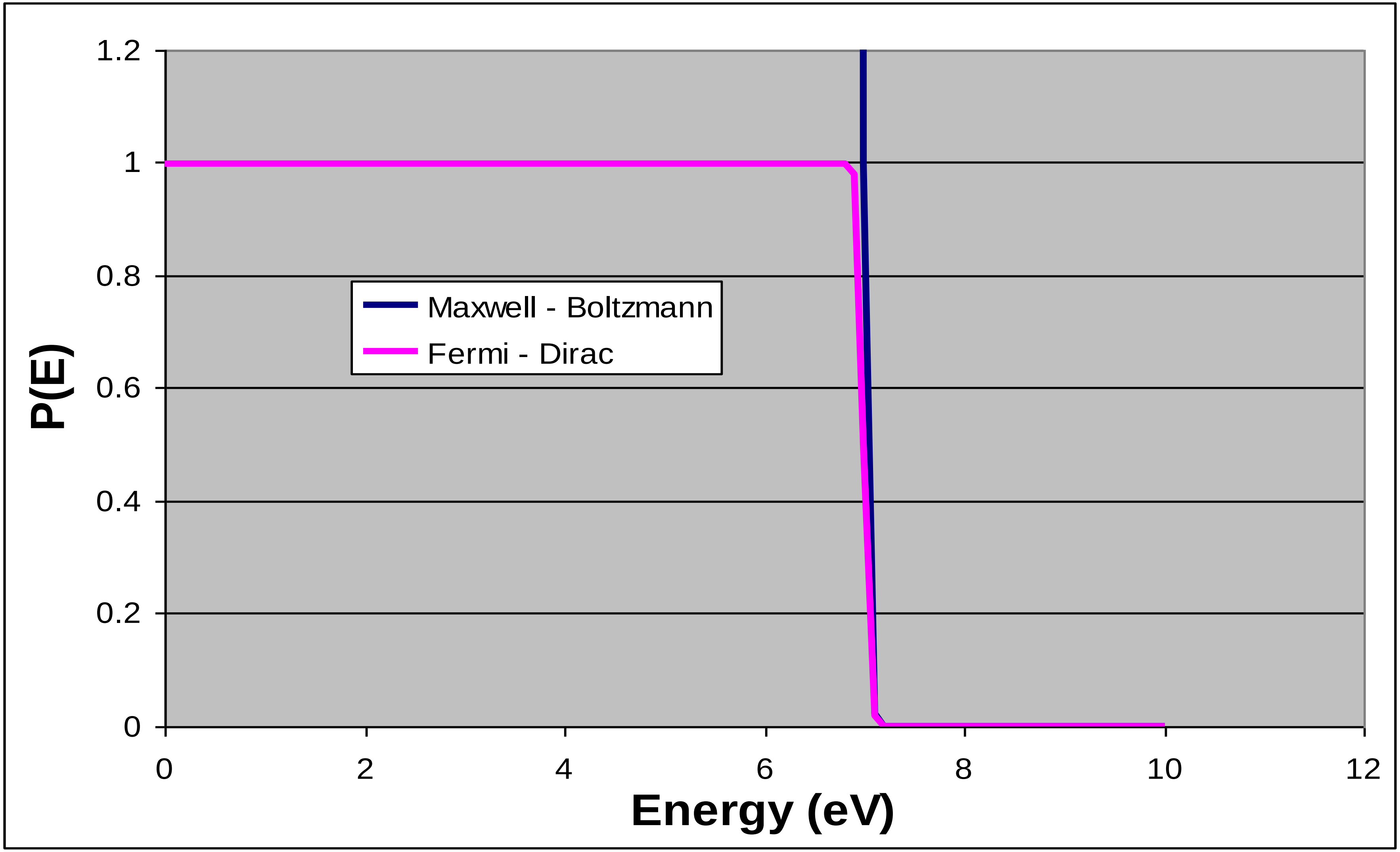


$$f(E<E_F,0)=\frac{1}{\exp[-\infty]+1}=\frac{1}{1}=1$$

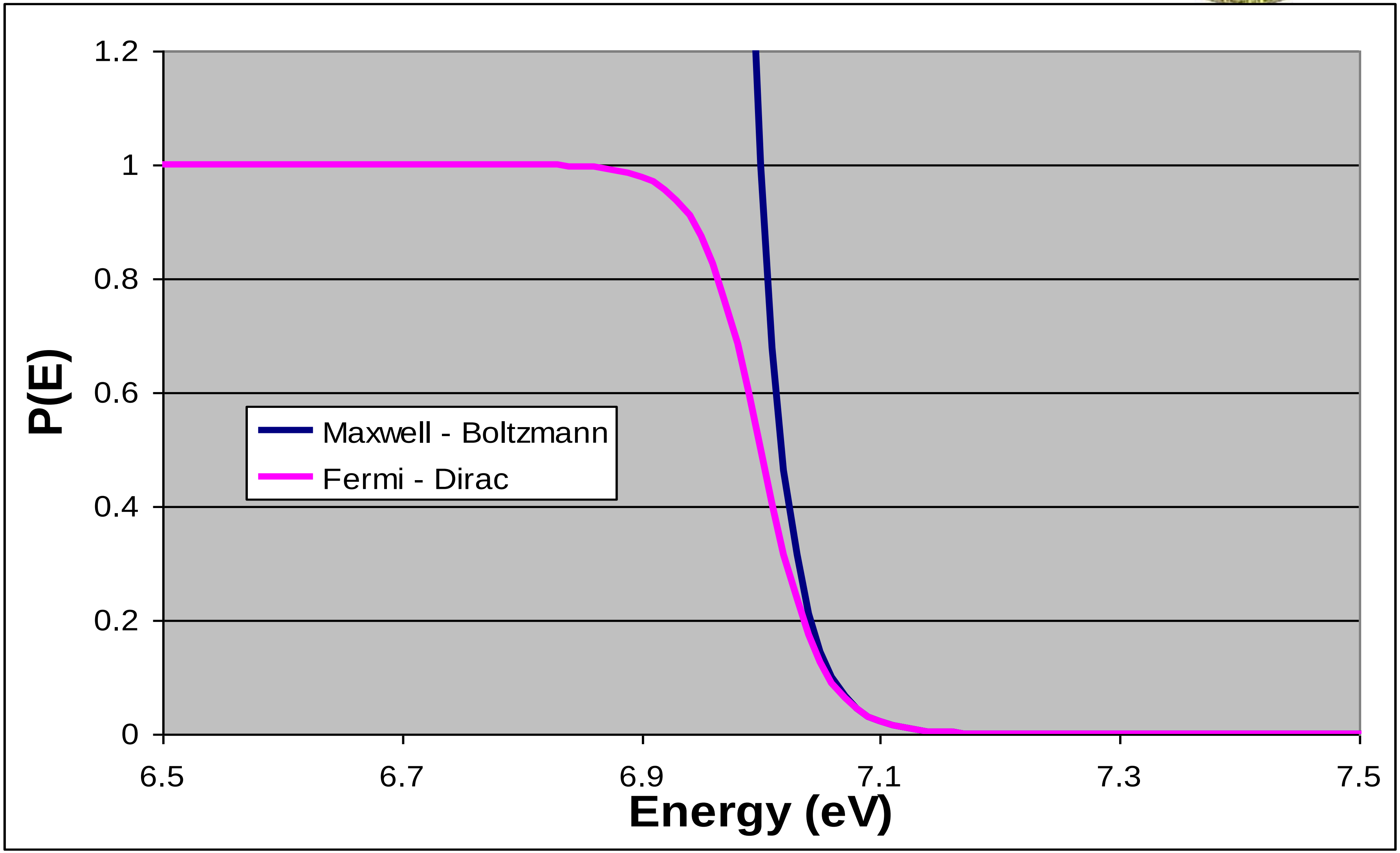
$$f(E>E_F,0)=\frac{1}{\exp[+\infty]+1}=\frac{1}{\infty}=0$$

$$f(E=E_F,0)=\frac{1}{\exp[0]+1}=\frac{1}{2}$$

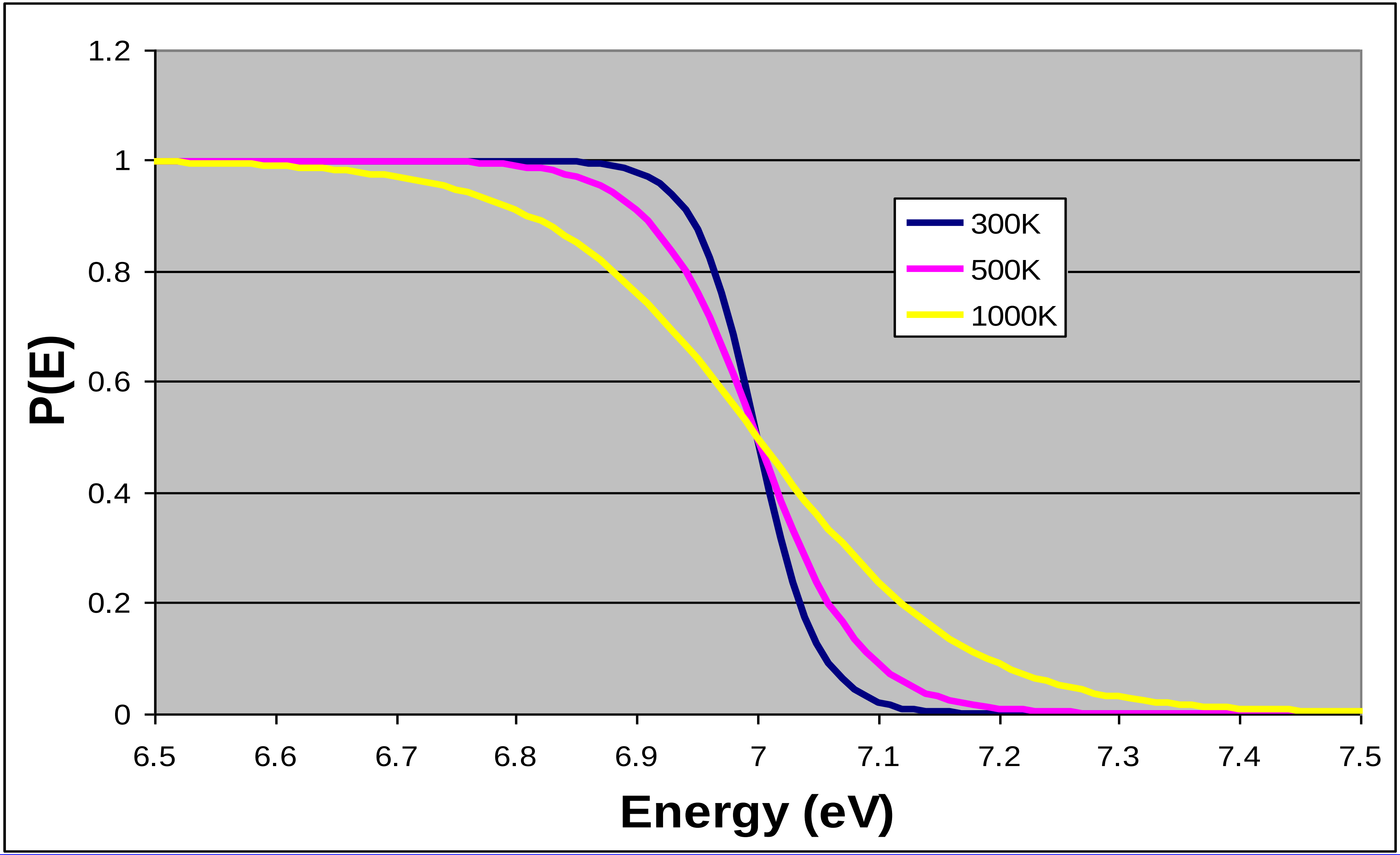
The Fermi Function (2)



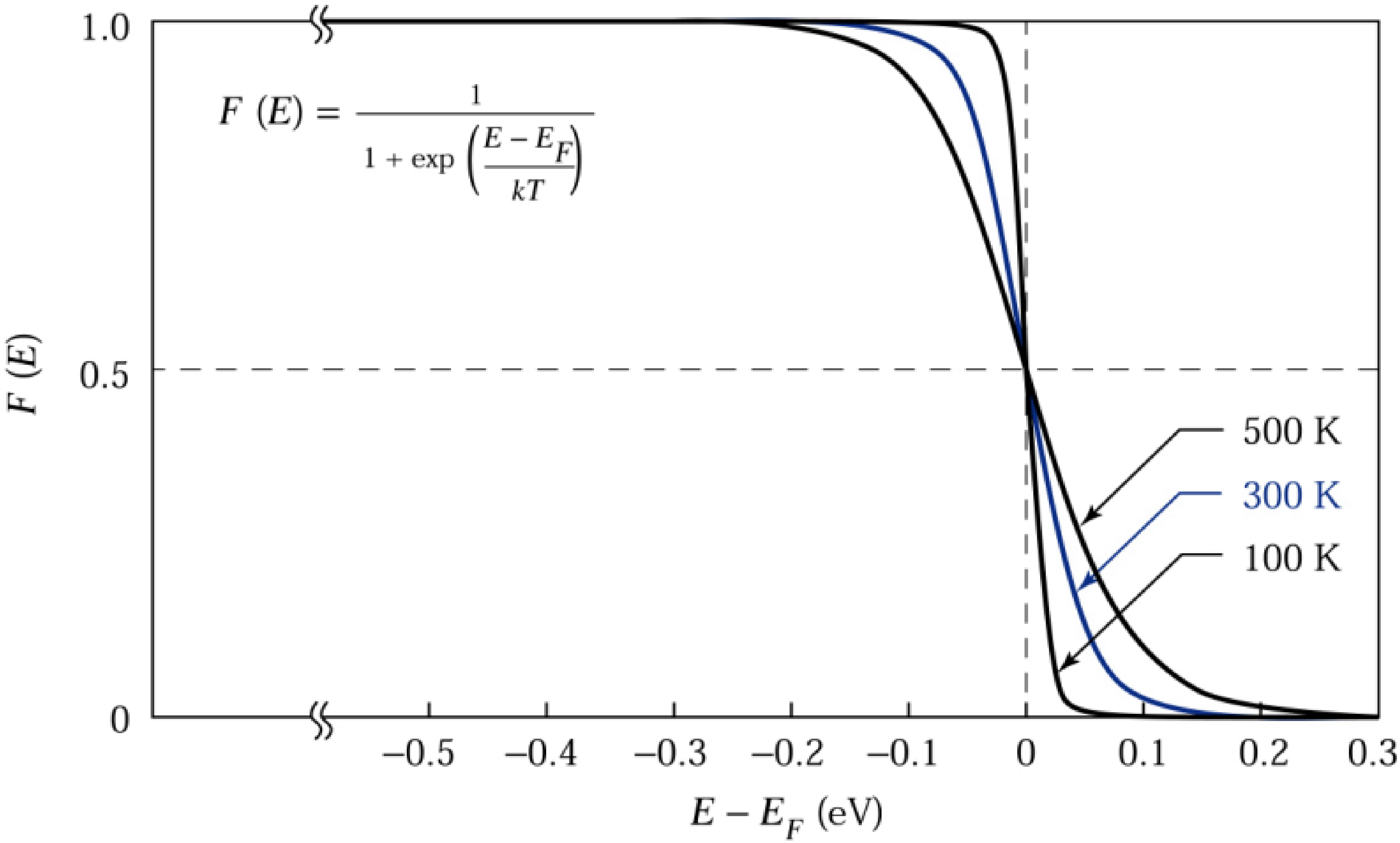
The Fermi Function (3)



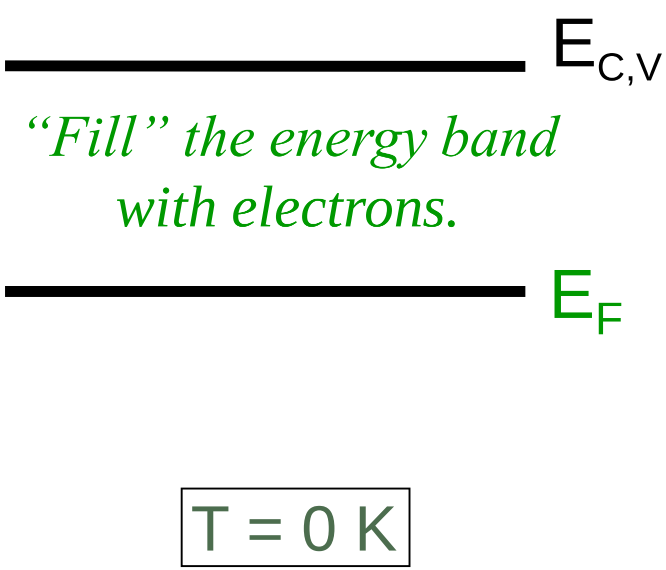
The Fermi Function (4)

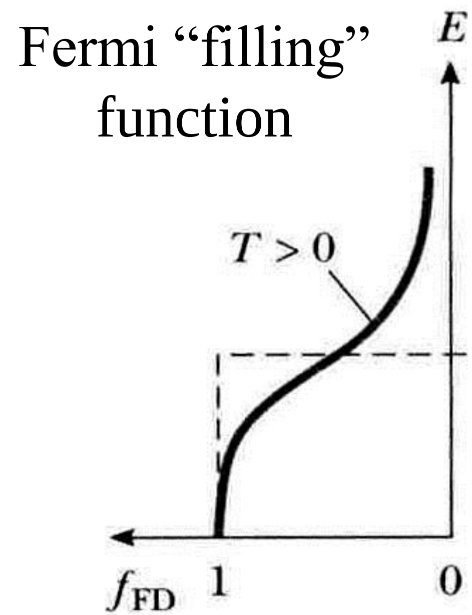


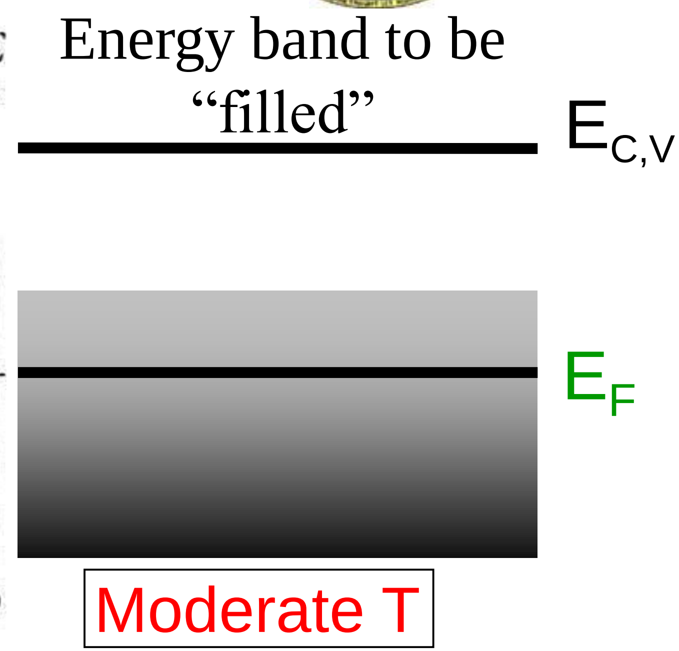
The Fermi Function (5)



Band Diagram: Metal

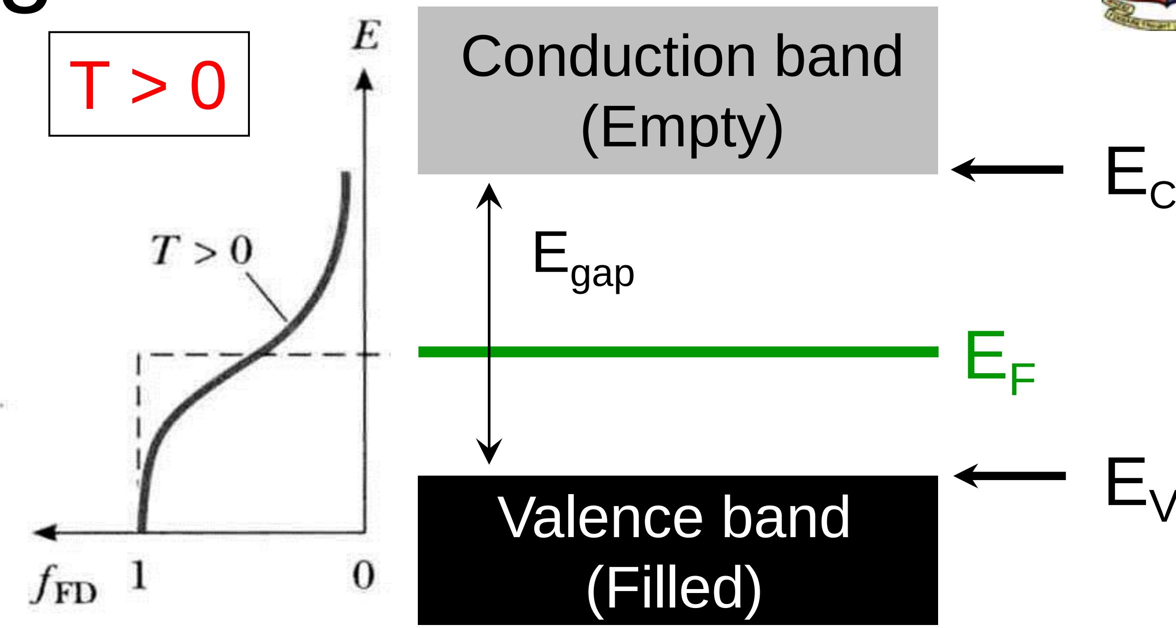






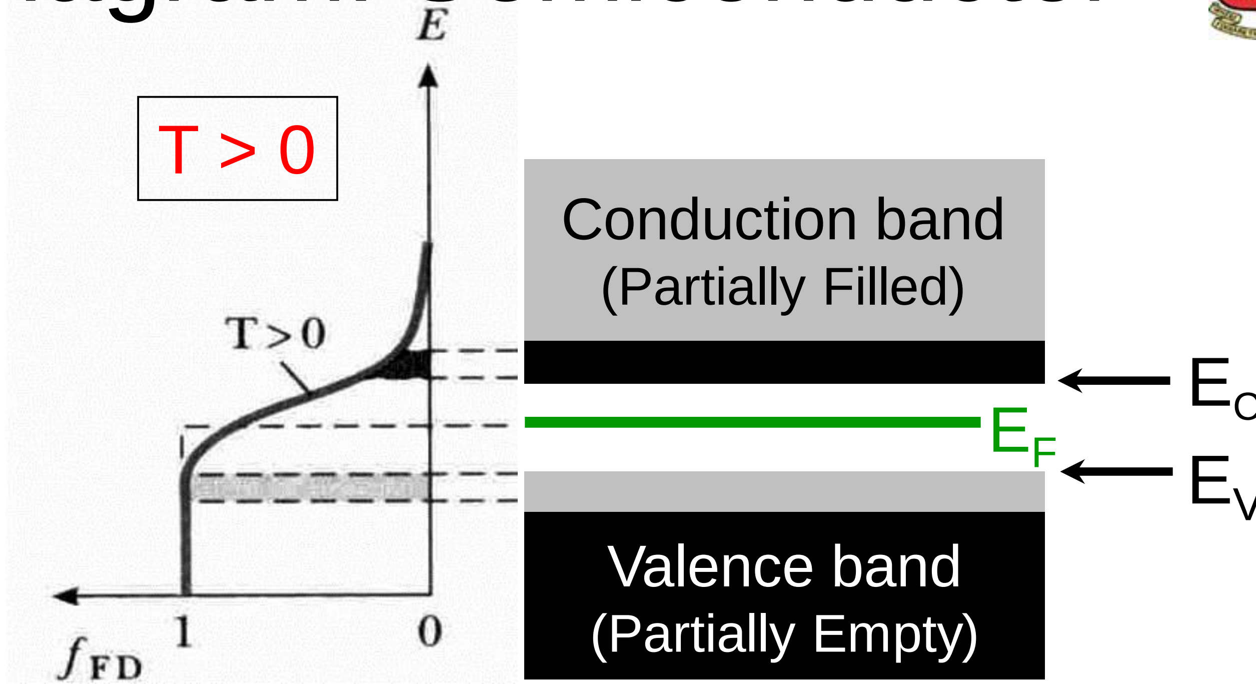
- At **T = 0**, energy levels below $\mathbf{E_F}$ are filled with electrons, while all levels above $\mathbf{E_F}$ are empty.
- Electrons are free to move into "empty" states of conduction band with only a small electric field E, leading to high electrical conductivity!
- At **T > 0**, electrons have a probability to be thermally "excited" from below the Fermi energy to above it.

Band Diagram: Insulator



- At **T = 0**, lower valence band is filled with electrons and upper conduction band is empty, leading to zero conductivity.
  - Fermi energy E_F is at midpoint of large energy gap (2-10 eV) between conduction and valence bands.
- At **T > 0**, electrons are NOT thermally "excited" from valence to conduction band, leading to zero conductivity.

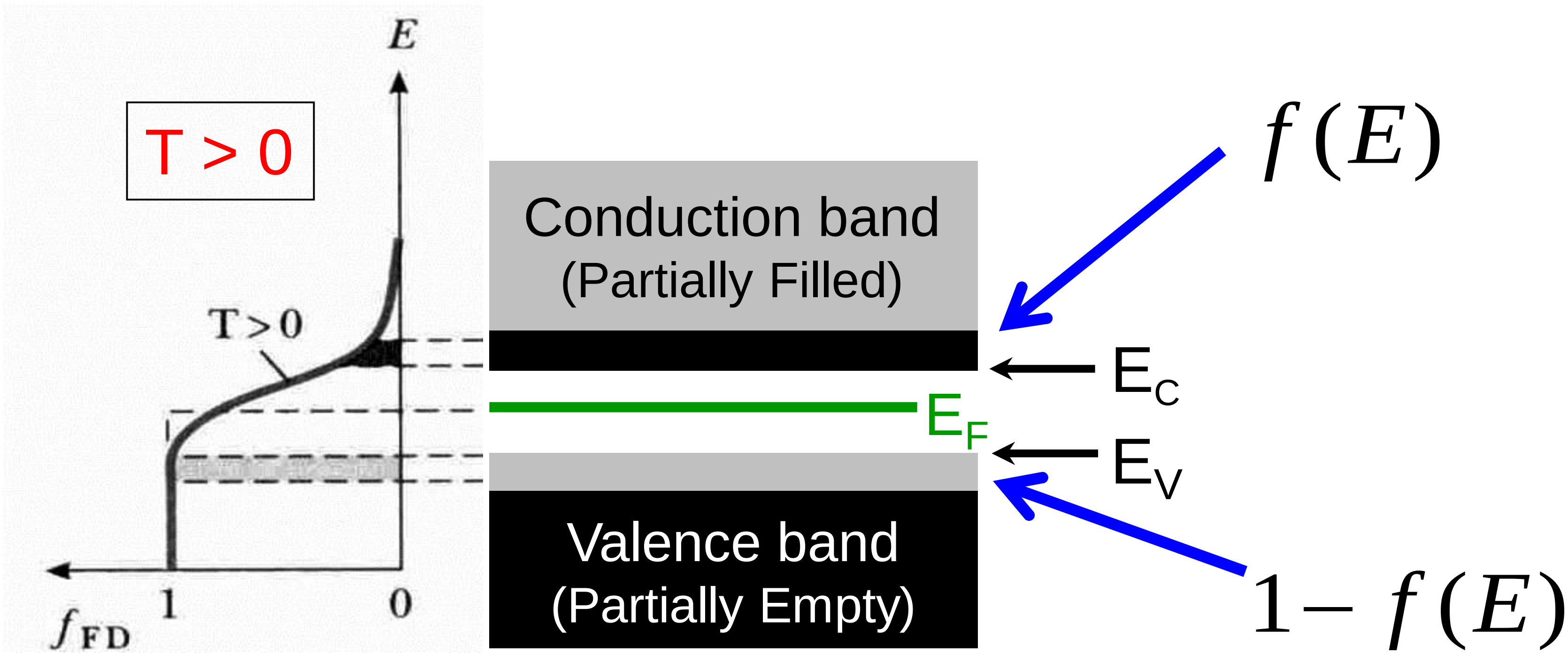
Band Diagram: Semiconductor



- At **T = 0**, valence band is filled with electrons and conduction band is empty, leading to zero conductivity.
- At **T > 0**, electrons thermally "excited" from valence to conduction band, leading to partially empty valence and partially filled conduction bands.

Thus: Semiconductor

Re-examine the Semiconductor



It is the absence of an electron that makes a hole

Symmetry of f(E)

$$f(E-E_F)=\frac{1}{e^{\frac{E-E_F}{k_BT}}+1}=\frac{1}{e^{\frac{\Delta E}{k_BT}}+1}$$

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

The function is symmetric around the Fermi energy.
That is: the distribution of electrons above the E_F
equals the distribution of holes below E_F

Examples

$$f(E) = \frac{N_x}{N_0} = \frac{1}{e^{\frac{E-E_F}{k_B T}} + 1}$$

	$E - E_F$ (eV)	f(E) T=290C	f(E) T=800C
	0.1	2×10^{-2}	2×10^{-1}
IR	0.5	2×10^{-9}	7×10^{-4}
Red	1	4×10^{-18}	5×10^{-7}
Blue	1.5	9×10^{-27}	4×10^{-10}
	5	1×10^{-87}	3×10^{-32}

Focus

- The Pauli exclusion principle leads to high energy electron states being filled even at low temperature.
- Fermi Dirac statistics provide the probability that available electron states will be populated.
- But how many electrons, and how many electron states are there?

Conduction Electrons in Metals?

How many are there?

Number of Conduction Electrons In Sample = Number of Atoms In Sample × Number of Valence electrons In Sample

n = Number of Conduction Electrons In Sample ÷ Sample Volume

Conduction Electrons?

How many are there?

$$\text{Number of Atoms In Sample} = \frac{\text{Material Density} \times \text{Sample Volume}}{\text{Molar Mass} \,/\, N_A}$$

$$N_A = \text{Avogadro's Number}$$
$$= 6.022 \times 10^{23} / mol$$

Number Density

$$n = \frac{\text{Material Density} \times \text{Number of Valence electrons In Sample} \times N_A}{\text{Molar Mass}}$$

Number Density

Copper

$$n = \frac{8.96\ \text{g/cm}^3 \times 1 \times N_A}{63.54\ \text{g}}$$

$$= 9 \times 10^{22} cm^{-3} = 9 \times 10^{28} m^{-3}$$

Number Density

Silicon

$$n = \frac{2.65\ \text{g/cm}^3 \times 0 \times N_A}{28.08\ \text{g}}$$

$$= 0\ m^{-3}$$

This calculation was for metals.

For semiconductors we need Fermi statistics

Focus

- We know the probability that a state is filled.
- We know the number of electrons available.
- How many electron states are there?

➡ Density of States

Infinite barrier 3D box (1)

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

Divide by: $\psi(x,y,z)=\psi_x(x)\psi_y(y)\psi_z(z)$

$$\Rightarrow\quad \frac{1}{\psi_x}\frac{d^2\psi_x}{dx^2}+\frac{1}{\psi_y}\frac{d^2\psi_y}{dy^2}+\frac{1}{\psi_z}\frac{d^2\psi_z}{dz^2}+k^2=0$$

$$k^2=k_x^2+k_y^2+k_z^2$$

$$\Rightarrow\quad \frac{1}{\psi_i}\frac{d^2\psi_i}{dx^2}+k_i^2=0 \qquad i=x,y,z$$

3x 1D solutions

Infinite barrier 3D box (2)

With a box of dimensions: A,B,C with a corner at (0,0,0)

$$\psi(x,y,z) = D\sin(k_x x)\sin(k_y y)\sin(k_z z)$$

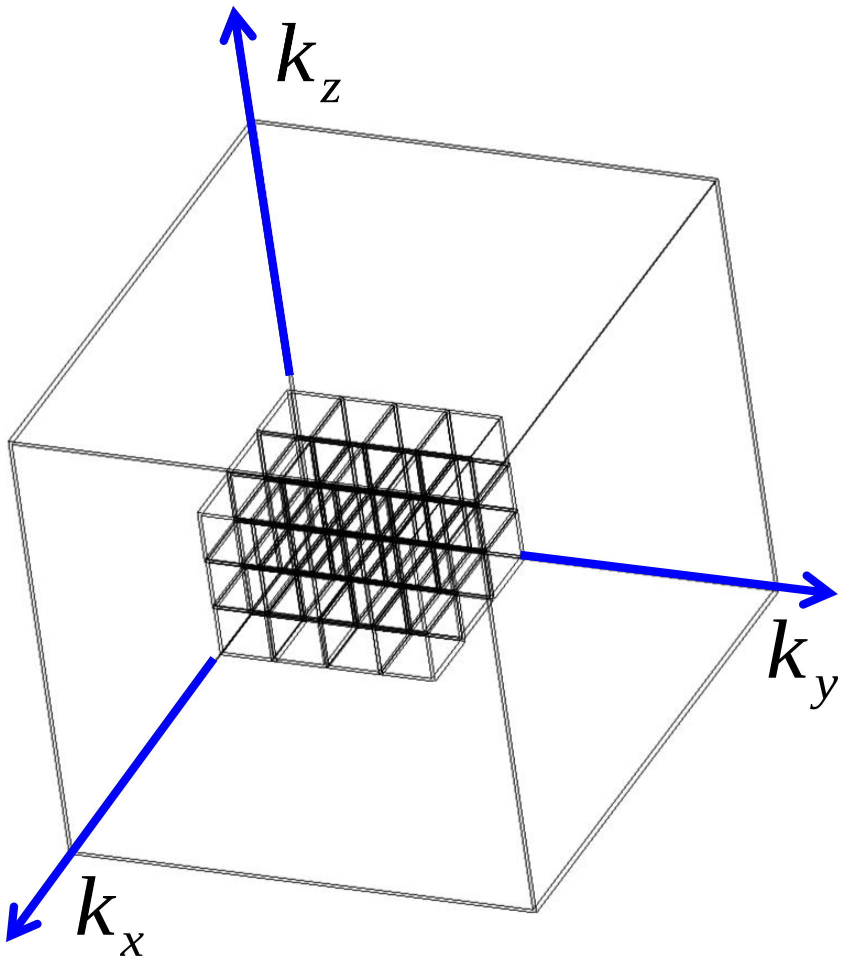
$$k_x = \frac{n_1\pi}{A} \qquad k_y = \frac{n_2\pi}{B} \qquad k_z = \frac{n_3\pi}{C}$$

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\pi^2}{2m}\left[\left(\frac{n_1}{A}\right)^2 + \left(\frac{n_2}{B}\right)^2 + \left(\frac{n_3}{C}\right)^2\right]$$

We are interested in the number of states with an energy less than the Fermi Energy:

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

Density of States (1)



The volume (in k-space) of one state is: $$V_k = \left(\frac{\pi}{A}\right)\left(\frac{\pi}{B}\right)\left(\frac{\pi}{C}\right) = \frac{\pi^3}{V}$$

The volume (in k-space) of the Fermi sphere is: $$V_F = \frac{4}{3}\pi k_F^3$$

BUT, we are only interested in the positive quadrant: $k_i > 0$

AND, there are 2 spin states

Density of States (2)

So, the number of filled states is:

spin 3D

$$N = 2 \times \left(\frac{1}{2}\right)^3 \frac{V_F}{V_k} = 2 \times \frac{1}{8}\frac{\frac{4}{3}\pi k_F^3}{\frac{\pi^3}{V}} = \frac{1}{3}\frac{k_F^3 V}{\pi^2}$$

Thus: $k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}}$

$$n = \frac{N}{V}$$

And: $E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} = \frac{\hbar^2 \left(3\pi^2 n\right)^{\frac{2}{3}}}{2m}$

Fermi Energy Revisited – Metal

$$E_F = \frac{\hbar^2 \left(3\pi^2 n\right)^{\frac{2}{3}}}{2m}$$

Copper: $n = 8.5 \times 10^{28} m^{-3}$

$E_F = 7eV$ As we have assumed

Note, that this calculation was only based on the properties of the material. Our previous assumption was not used.

Fermi Energy Semiconductor

$$E_F = \frac{\hbar^2 \left(3\pi^2 n\right)^{\frac{2}{3}}}{2m}$$

Silicon: $n = 0 \rightarrow 5\times 10^{21} m^{-3}$

$$E_F = 0 \rightarrow 1.1eV$$

Density of States (3)

Inverting we get the number density: $n = \frac{1}{3\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{\frac{3}{2}}$

And can then calculate the density of states: $\rho(E) = \frac{dn}{dE}$

$$\rho(E) = \frac{dn}{dE} = \frac{3}{2}\frac{1}{3\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{\frac{1}{2}}\frac{2m}{\hbar^2} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E}$$

For a semiconductor: $\rho(E) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E - E_C}$

Aside

We now have the tools we need to talk about semiconductors:

- Bands: limit the allowable k,E values
- Fermi statistics: provide the proportion of filled states
- Density of states provides the number of available states

Population of Bands

To actually predict the distribution of carriers in the band we need both Fermi statistics and the density of states:

Density of Occupied States

$$\rho_O(E)\Delta E = \rho(E)f(E)\Delta E = \frac{dn(E)}{dE}f(E)\Delta E$$

The number of carriers within ΔE

Copper @ 8eV:

$$f(E) = 5\times10^{-18}$$

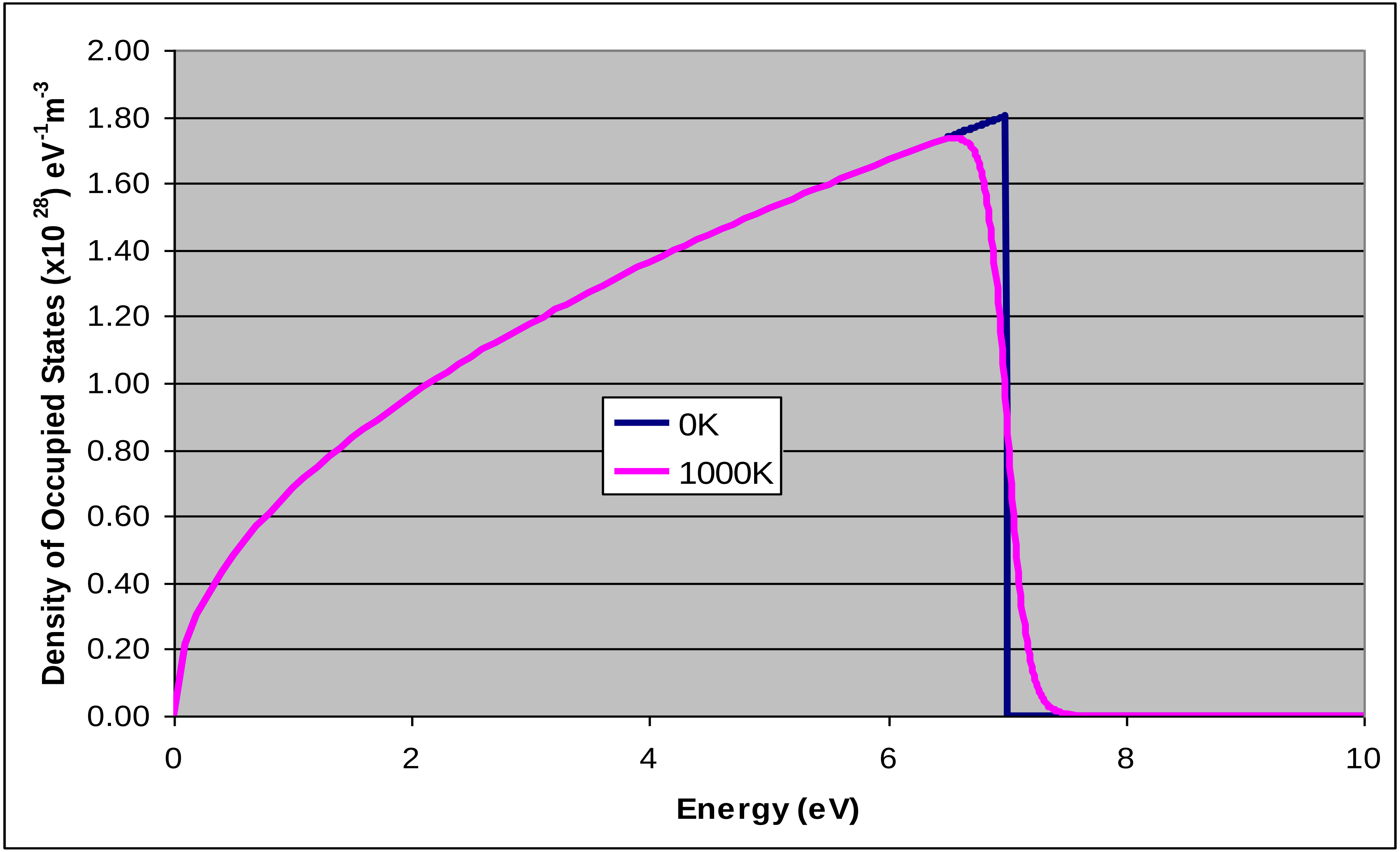
Fermi-Dirac Statistics

$$\rho(E) = 1.9\times10^{28}$$

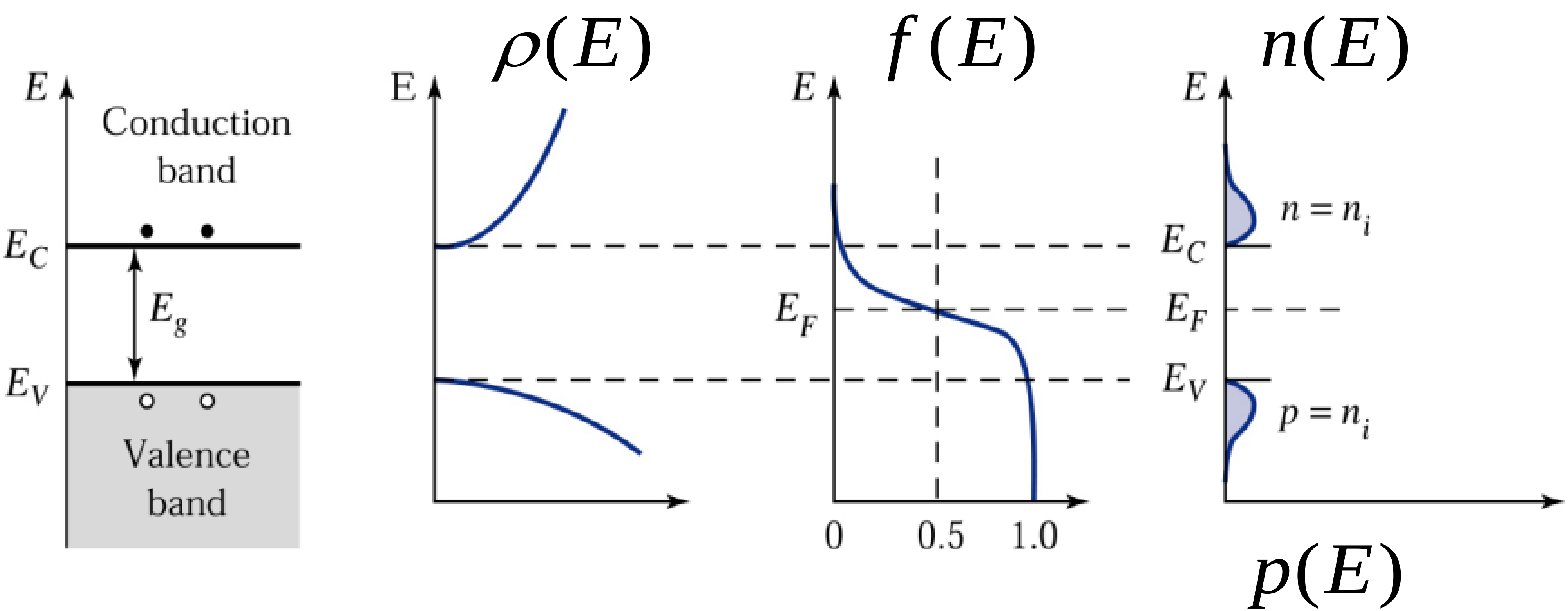
$$\rho_O(E) = 9.7\times10^{10}$$

Above the Fermi Level the number of occupied states Decreases exponentially.

Density of Occupied States



Density of Semiconductor States



Intrinsic Semiconductor