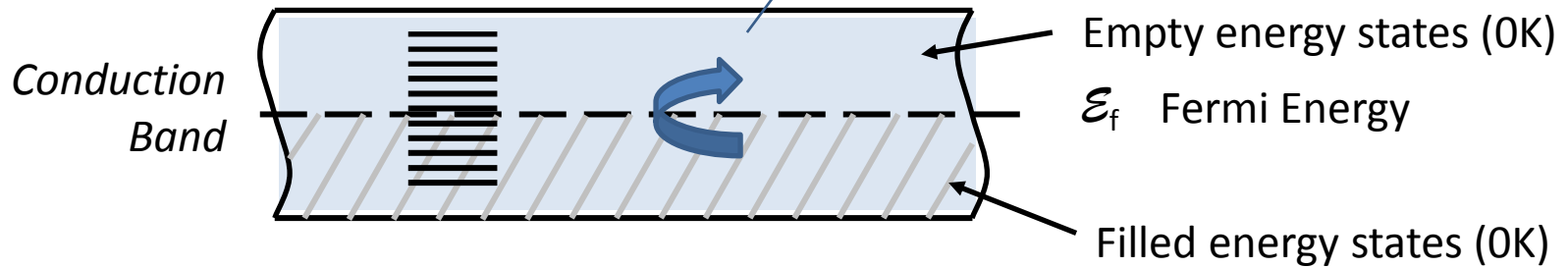# Chapter 2

Electrical Conduction in **Metals**
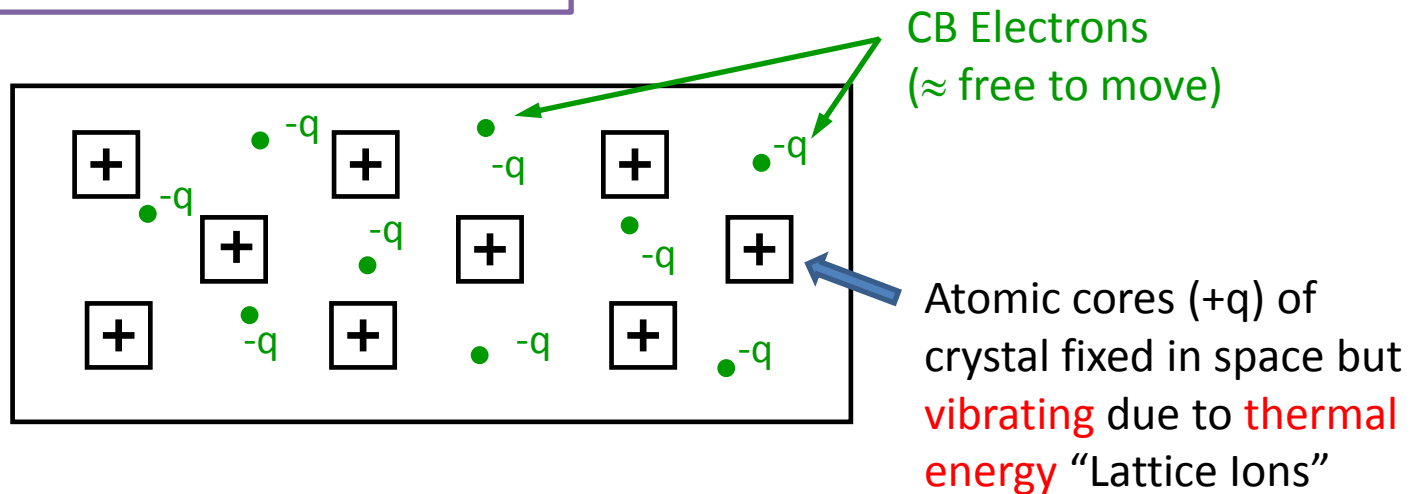
Reminder: Energy Band Structure in a METAL

- Metals are crystalline solids in which the outermost band (the "Conduction Band" or CB) is only partially filled at 0K

- These materials are good conductors of electricity although only electrons contribute to current flow, i.e. there are no holes involved

- The current density is given by $J = J_e = q\,n\,v_e$ at a given electric field E, where v_e is the response velocity

- We wish now to study the phenomenon of electrical conduction in a metal in more detail and in particular:

    (1) **to explore the relationship between v_e and E and**
    (2) **to investigate the variation of electron concentration with energy within the CB.**

Electrical Conduction in Metals

Energy Band Picture:

If T > 0, electrons can move to higher energy levels

Conduction Band

Empty energy states (0K)

$\mathcal{E}_f$ Fermi Energy

Filled energy states (0K)

Atomic/Crystal Picture (T>0K):

CB Electrons
($\approx$ free to move)

-q -q -q
-q -q -q
-q -q -q
-q -q -q

Atomic cores (+q) of crystal fixed in space but vibrating due to thermal energy "Lattice Ions"

The Drude Model for Current Flow in a Metal (1900)

- The atomic picture begins by noting that metals are made of atoms with just a few outermost electrons (typically 1 or 2).

- The atoms come together to form a crystal in which these outermost electrons are "shared" among all the lattice ions – "**sea of electrons**" model.

- In 1900, Paul Drude proposed a simple but effective model to explain electrical conduction in a metal at a time which preceded the development of Quantum Mechanics

- The model is classical and treats the crystal as a kind of complicated pinball machine in 3 dimensions, with "free" electrons (in the CB) continually bouncing off vibrating atomic cores and then heading off in random directions

Metals in Thermal Equilibrium

- The free electrons move rapidly around the crystal due to thermal energy but are subject to continuous collisions or "scattering events"

- Considered as a thermodynamic system, the electrons are normally in _thermal equilibrium_ with the crystal where the 'heat' stored in the material shows itself as a vibration of the atomic cores in the lattice – the more the metal is heated the more strongly the lattice ions vibrate

- If the material is at a temperature T, then from classical physics (the _equipartition of energy_ principle) the thermal energy of a particle is ½ kT for each degree of freedom. Here k is Boltzmann's constant - a basic constant of Nature.

- For movement in a 3D crystal, the total thermal energy of an electron is therefore: 3 x (½ kT).

Random Thermal Velocity of Electrons in Metals

- In this Course, we will always deal with Boltzmann's constant k in combination with T and the product kT will be called the "thermal energy". At room temperature (300K) is works out at 0.0259eV (or about 1/40th of an electronVolt)

    N.B.   Thermal Energy: kT = 0.0259 eV at T = 300K

- We can estimate the random thermal velocity (v_{th}) of the "free" or CB electrons by equating the (3D) thermal energy with the Kinetic Energy of an electron:

$$\mathcal{E} = \tfrac{1}{2} m\, v_{th}^2 = \tfrac{3}{2} kT$$

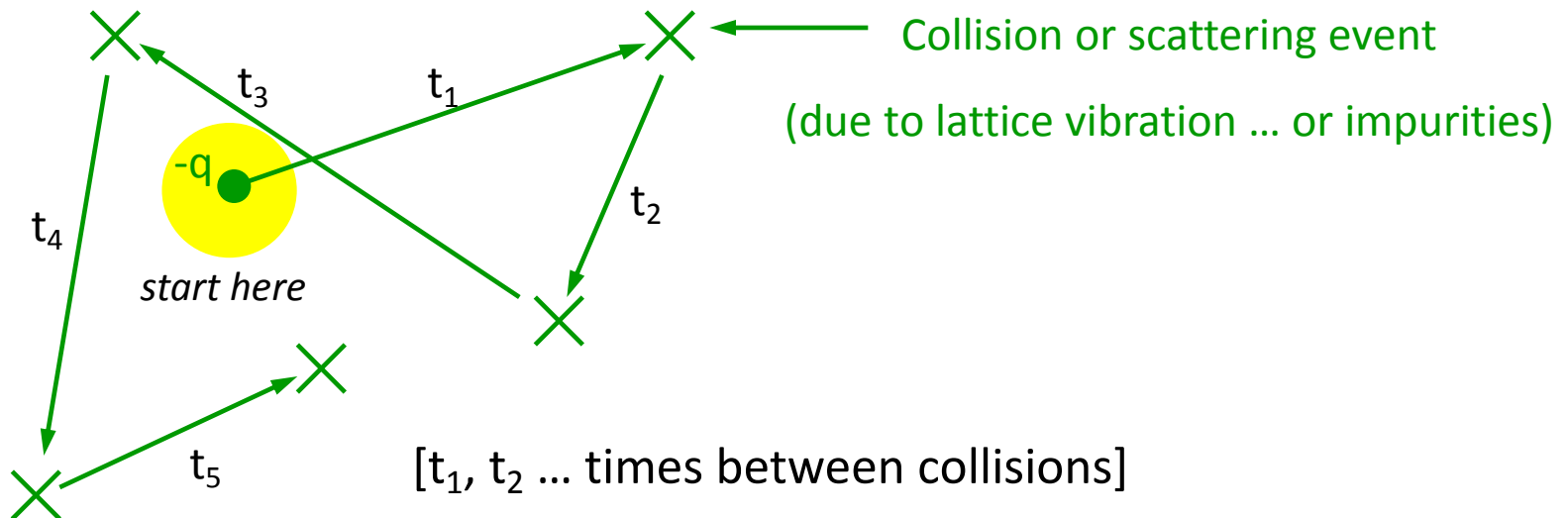- <u>Exercise</u>: prove that v_{th} = 1.7 x 10^7 cm/sec at 300K

Collisions and Scattering Events

- If we were to follow the path of an individual electron over time, it would be observed to experience a series of "collisions" or "scattering events" in the lattice.

  There are two main causes for these collisions:

1) Lattice Vibration: due to thermal energy in the solid. As T increases, lattice vibration increases scattering due to this source. This is increasingly significant at higher temperatures.

2) Crystal Impurities and Imperfections: Real crystals do not perfectly repeat in space and impurities also exist. The effects of these tend to be more important at lower temperatures.

Electron Motion in a Metal (No Voltage Applied)

Collision or scattering event

(due to lattice vibration ... or impurities)

t_3 t_1

-q

start here

t_4

t_2

t_5 [t_1, t_2 ... times between collisions]

CB electron undergoing random collision events in the lattice.
Notice: the electron on average does not move in any one direction.

The average of the times t_1, t_2, t_3 ... is called the mean free time between collisions ($\overline{\tau}$), and it is a very short interval in a metal, typically $\approx 10^{-14}$ sec.

Side Discussion: Electrical Noise

A snapshot at a given instant will show (statistically) that a slightly greater no. of electrons can move one direction rather than the other. This is the basic physical effect underlying the important phenomenon of <u>electrical noise</u>.

Resistor

$47k\Omega$

Tiny Open Circuit Voltage Exists

Volts
~1 μV

t
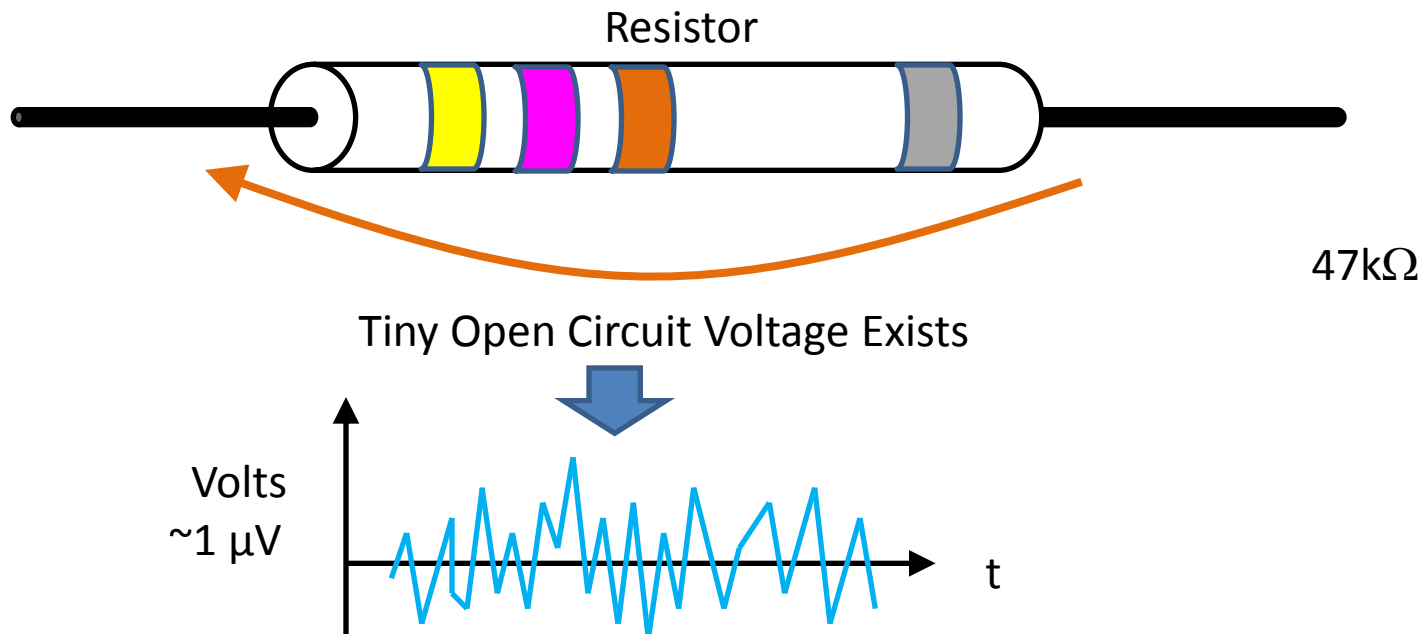
Electrical Noise

- The noise may also show up as a small disturbance on a steady or "DC" current since the current flow is a statistical phenomenon involving a large number of individual charged particles
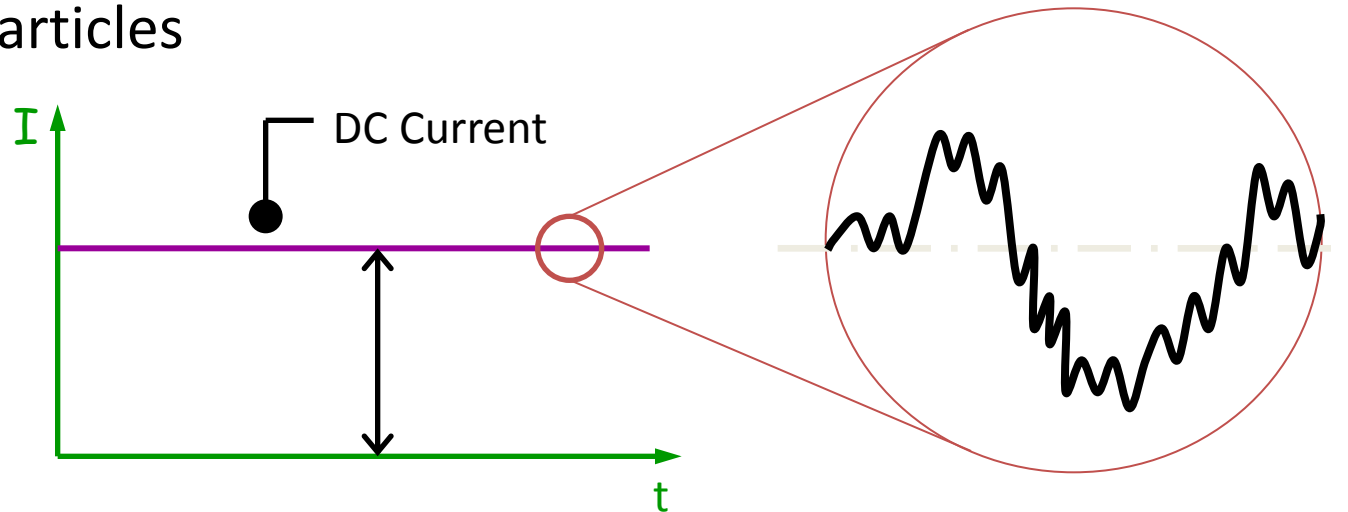
- This kind of noise is called thermal, Johnson or "white noise"
- Other kinds of electrical noise arise e.g. in transistors ("shot noise") or due to surfaces ("flicker noise"): more in SSE2

Conduction of Electric Current in Metals

- In thermal equilibrium, averaged over time, there is no net movement of free electron charge in any one direction.

- Now, apply a voltage (V) to the metal sample. This produces an electric field E. (V/m)

E

No E field

start here

-q

With E field:
note slightly
curved trajectory
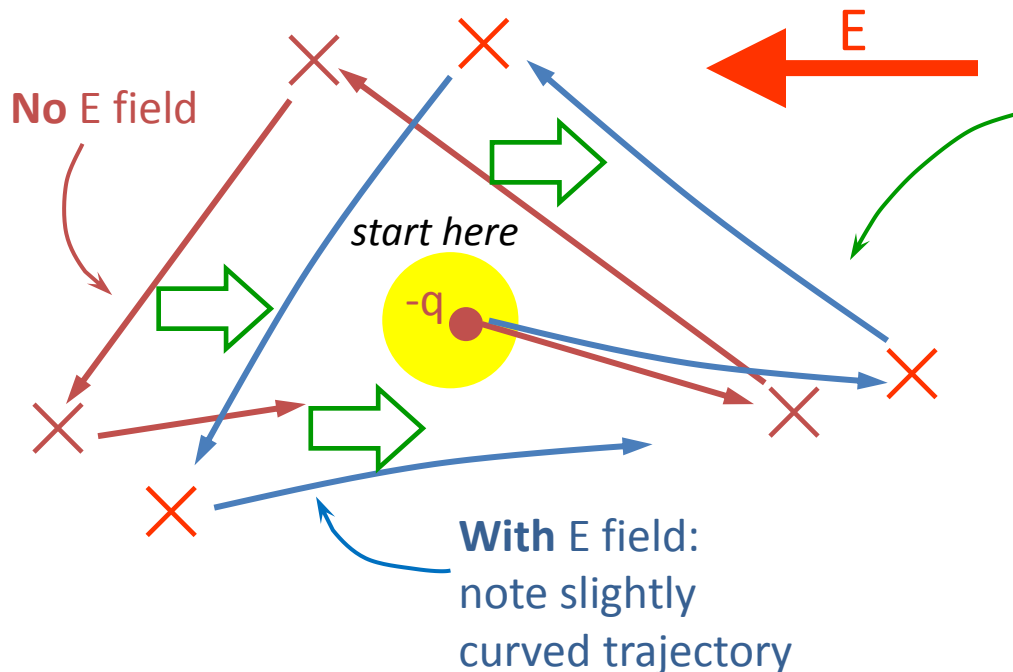
With the E field present, an electron acquires a cumulative displacement in direction (-E)

Between collisions :
Fast thermal velocity.

Over time :
A gradual displacement takes place along –E : **drift velocity**

Electrical Conduction in Metals

- We will denote the **electron drift velocity** in a metal by $v_e(t)$

- Ignoring signs for simplicity, then if an electric field E exists, Newton's Law gives:

$$F = m \cdot a = m \cdot \frac{dv_e(t)}{dt}$$

- Where "m" is the mass of the electron. We will propose that the force on the electron due to the electric field E (= q.E) is opposed by a "frictional" force due to the random collisions with the lattice:

$$\frac{m \cdot v_e}{\bar{\tau}}$$

- This effectively assumes that the momentum gained between collisions is on average randomised to zero. Then the dynamic equation of motion of the electron is given by:

$$m \cdot \frac{dv_e(t)}{dt} = q \cdot E - \frac{m \cdot v_e}{\bar{\tau}}$$

Solution to Dynamic Equation of Motion

- We are looking for a solution to the 1st Order Ordinary Differential Equation (ODE):

$$\frac{dv_e(t)}{dt} = \frac{q \cdot E}{m} - \frac{v_e}{\bar{\tau}}$$

- The **total solution** is the sum of the **steady-state solution** and the **transient solution**:

$$v_e(t) = v_e{}^{SS} + v_e{}^{TR}(t)$$

- The **_steady-state_** solution is (set time-derivative to zero):

$$0 = \frac{q \cdot E}{m} - \frac{v_e{}^{SS}}{\bar{\tau}}$$

$$\Rightarrow v_e{}^{SS} = \frac{q \cdot E \cdot \bar{\tau}}{m}$$

Solution to Dynamic Equation of Motion

- The *transient solution* is found from the unforced solution when E = 0:

$$\frac{d v_e{}^{TR}(t)}{dt} = -\frac{v_e{}^{TR}(t)}{\bar{\tau}}$$

- The solution to this equation is:
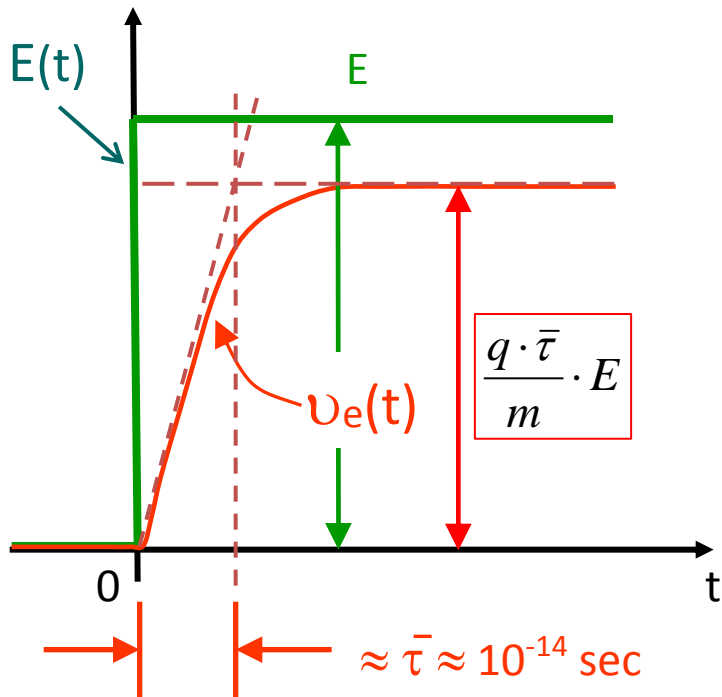
$$v_e{}^{TR}(t) = K \cdot e^{-\frac{t}{\bar{\tau}}}$$

- … where K is a constant. If we require $v_e(0) = 0$ then:

$$K = -\frac{q \cdot E \cdot \bar{\tau}}{m}$$

- The *total dynamic solution* is then easily obtained as:

$$v_e(t) = \frac{q \cdot E \cdot \bar{\tau}}{m} \cdot \left[1 - e^{-\frac{t}{\bar{\tau}}} \right]$$

Dynamic Solution

$$\frac{q \cdot \bar{\tau}}{m} \cdot E$$

$\approx \bar{\tau} \approx 10^{-14}$ sec

- The graph shows the dynamic response of electron current to an instantaneous step-change in electric field (at time t = 0)

- The response is very fast by normal electronic standards (less than 1 picosec ~THz+)[1]

- We will ignore the transient part of the response from now on (but be aware that it exists)

[1] Note: frequencies: 1MHz (1 MegaHertz) = 10^6 Hz;
1GHz (1 GigaHertz) = 1000MHz = 10^9 Hz
1THz (1 TeraHertz) = 1000GHz = 10^{12} Hz

Electron Mobility

- If we concentrate on the **steady-state response** we have:

$$v_e = \frac{q \cdot \bar{\tau}}{m} \cdot E$$

- This shows that the drift velocity is <u>linearly proportional</u> to the electric field. The constant of proportionality is defined as **the (electron) mobility μ_e**: (units: m^2/Volt-sec or: cm^2/Volt-sec)

- Note that a high value of mobility is generally desirable.

- Define:
$$\mu_e = \frac{q \cdot \bar{\tau}}{m}$$
the *electron mobility*

- Hence:
$$v_e = \mu_e \cdot E$$

Example 2.1

Conductivity/Resistivity of a Metal

- Substituting for the drift velocity into the formula for current density obtained earlier, we find:

$$J = q \cdot n \cdot v_e = \left(q \cdot n \cdot \mu_e \right) \cdot E$$

- This shows that a linear relationship also connects current density and electric field within a metal.

- The constant of proportionality is defined as the **electrical conductivity (σ)** of the metal:

$$\sigma = q \cdot n \cdot \mu_e \quad \Rightarrow \quad J = \sigma \cdot E$$

- This relationship between J and E is sometimes referred to as the **microscopic version of Ohm's Law**

- The reciprocal of the conductivity is the **resistivity ρ = (1/σ)**

From Microscopic to Macroscopic...

Example of a metal rod with an applied voltage V:
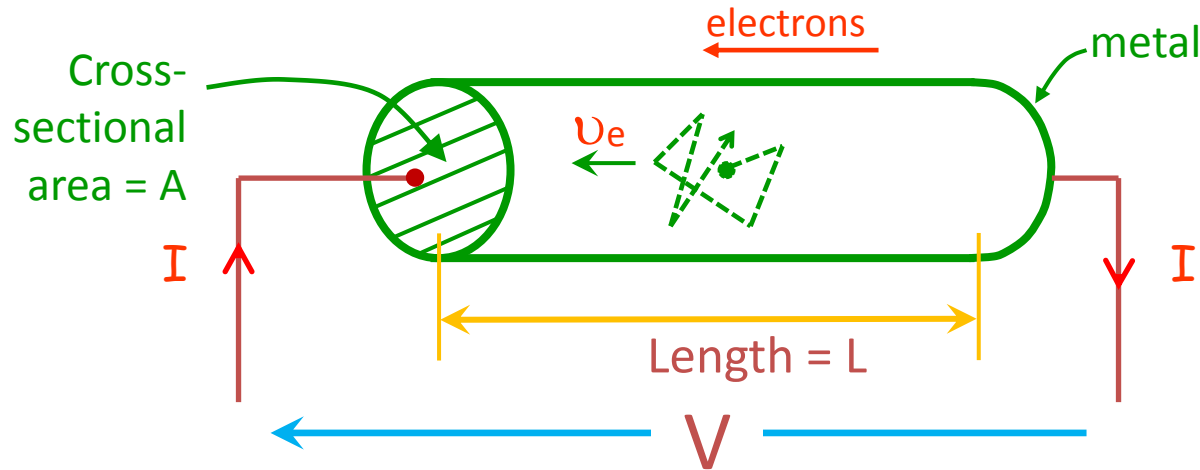
- We have three simple, known formulas connecting various quantities:

$$(1).\quad J = \frac{I}{A} \qquad (2).\quad E = \frac{V}{L} \qquad (3).\quad J = \sigma \cdot E$$

- Substituting (3) into (1) we find: $\qquad \sigma \cdot E = \frac{I}{A}$

"Ohm's Law"

- Now substitute for "E" using (2): $\sigma \cdot \left(\dfrac{V}{L}\right) = \dfrac{I}{A}$

- This can be re-arranged to give:

$$V = \left(\frac{L}{\sigma \cdot A}\right) \cdot I = \left(\frac{\rho \cdot L}{A}\right) \cdot I$$

- We define the quantity in brackets as the **Electrical Resistance "R"**, so that:

$$V = I \cdot R$$

- Where the resistance can be written as:

$$R = \left(\frac{\rho \cdot L}{A}\right)$$

Ohm's Law: "In a metallic conductor at a constant temperature, the current flowing is proportional to the voltage applied"

Temperature Dependence of Resistance

As the temperature increases in a metal, we may expect the lattice ions to vibrate more strongly, reducing the mean free time between collisions and therefore lowering the mobility. The overall concentration of CB electrons per unit volume in a metal is not expected to change much with temperature, and so the conductivity will decrease. The electrical resistance of a metallic sample will therefore be expected to increase with increasing temperature.

$$R = \frac{\rho \cdot l}{A} = \frac{l}{\sigma \cdot A}$$

Formula valid for any uniform cross-section

(ρ)

I

A

l
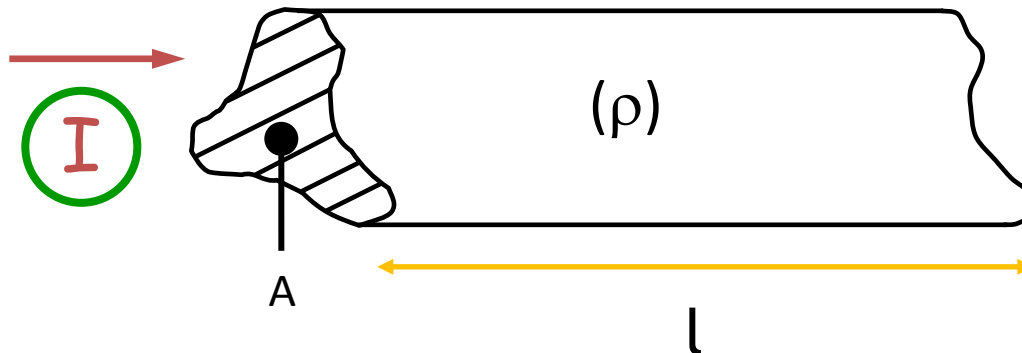
Resistivity vs. Resistance. Units

- Note that conductivity σ (or resistivity $\rho=1/\sigma$) are properties of a *material* or *substance*;
- On the other hand, Resistance R (or conductance G = 1/R) are properties of a particular *thing* or *object*.
- The unit of **resistance** is the **Ohm (Ω)** so that $1\Omega = 1V/1A$. The unit of **conductance** is the **Siemen (S)**. $1S = 1/\Omega = 1A/1V$.
- Other Units:
  - **Mobility:** $v_e = \mu_e \cdot E$ hence: (m/sec) $= \mu_e \cdot$ (Volt/m)
       so the units of mobility are   **m²/(Volt·sec)**
  - **Conductivity:** $J = \sigma \cdot E$ hence: (Amp/m²) $= \sigma \cdot$ (Volt/m)
       so the units of conductivity are   **(S/m)**
  - **Resistivity:** $J = E/\rho$ hence: (Amp/m²) = (Volt/m) $/\rho$
       so the units of resistivity are   **(Ω·m)**

$\boxed{\sigma \text{ has units of (S/m); } \rho \text{ has units of } (\Omega\text{-m})}$

Range of Electrical Conductivity in Nature
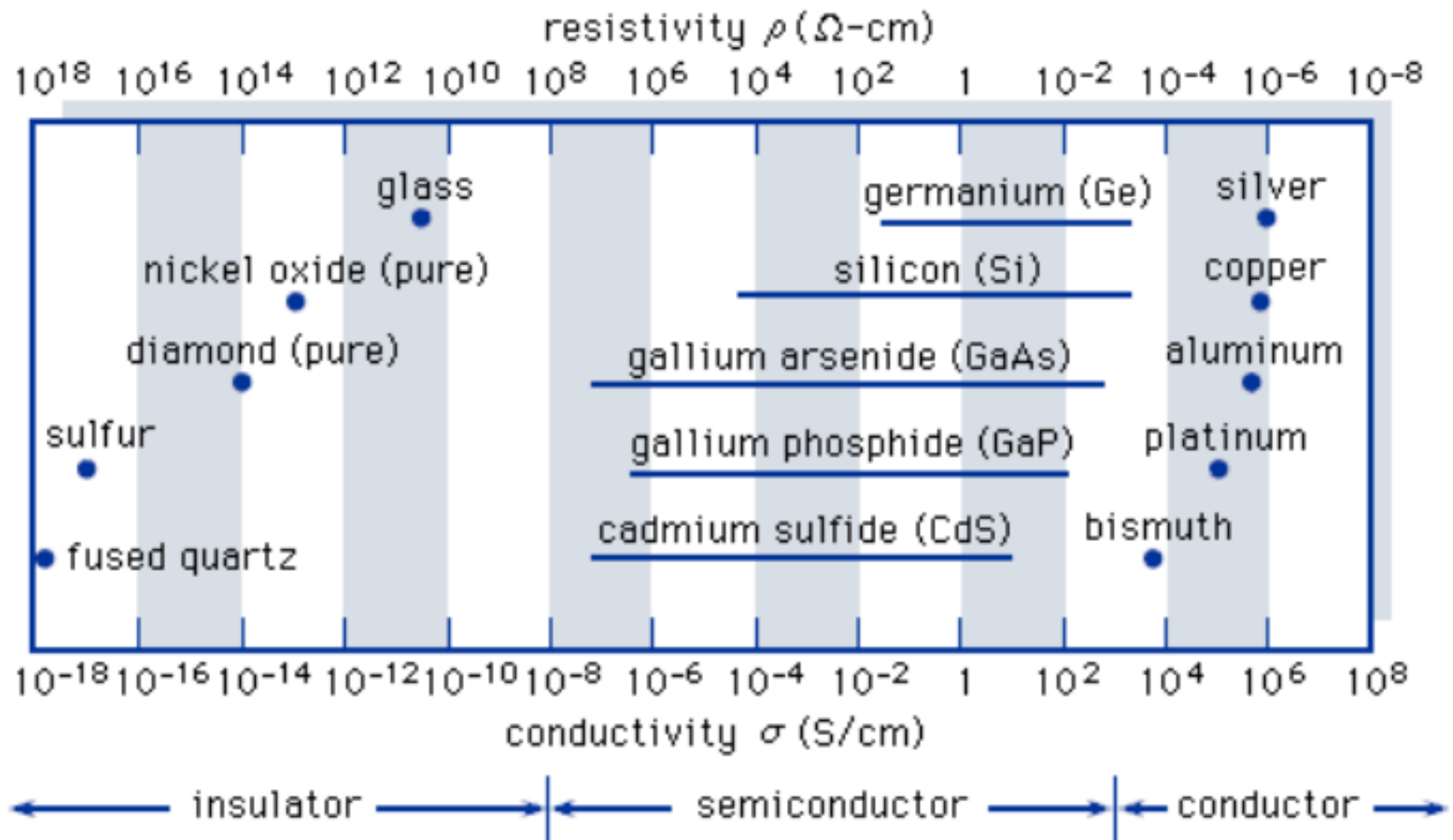
Example 2.2

Number Density of Electrons in the CB of a Metal

- Basic question to be addressed: how are the electrons that are located in the CB of a metal, distributed in terms of energy?
- We define: $N(\mathcal{E}).\Delta\mathcal{E}$ = number of C.B. electrons per unit volume with an energy in the range between $\mathcal{E}$ and $(\mathcal{E} + \Delta\mathcal{E})$
- If we can find an expression for $N(\mathcal{E})$ in terms of the energy $\mathcal{E}$, we will know this distribution.
- Note that in metals, the zero for the energy axis is customarily taken as at the bottom of the Conduction Band

Note orientation of axes!!

We want to find $N(\mathcal{E})$
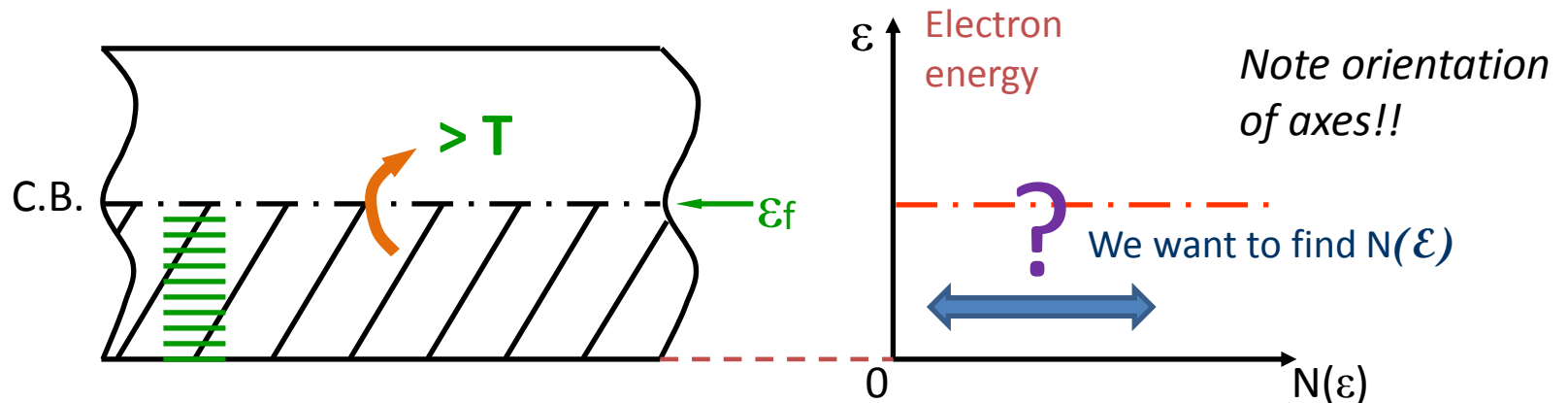
Relating N($\mathcal{E}$) to the Electron Concentration "n"

- The function N($\mathcal{E}$) is called the "*number density function*";

- By definition of the electron concentration "n" (= the number of free or CB electrons per unit volume), we have in general:

$$n = \int_0^\infty N(\varepsilon) \cdot d\varepsilon$$

… approximating the upper limit of the integral as infinity

- In the special case of T=0K, or absolute zero temperature, we have by definition of the Fermi energy or Fermi level, $\mathcal{E}_f$, that N($\mathcal{E}$) = 0, for all energy $\mathcal{E}$ > $\mathcal{E}_f$. Therefore the electron concentration integral at 0K becomes:

$$n = \int_0^{\varepsilon_f} N(\varepsilon) \cdot d\varepsilon$$

Number Density Function in a Metal

To find an expression for N($\mathcal{E}$) the "*number density function"* we define two new functions S($\mathcal{E}$) and f($\mathcal{E}$):

$$N(\varepsilon)\cdot \Delta\varepsilon \quad = \quad (S(\varepsilon)\cdot \Delta\varepsilon) \quad x \quad (f(\varepsilon))$$

"Number Density Function"   =   "Density of States Function"   x   "Probability of Occupation Function"

S($\mathcal{E}$)$\cdot \Delta\mathcal{E}$ = the Density of States Function which is the number of energy states per unit volume between $\mathcal{E}$, ($\mathcal{E}$ + $\Delta\mathcal{E}$)

f($\mathcal{E}$) = the Probability of Occupation Function which is the probability that a state at energy $\mathcal{E}$ will be occupied
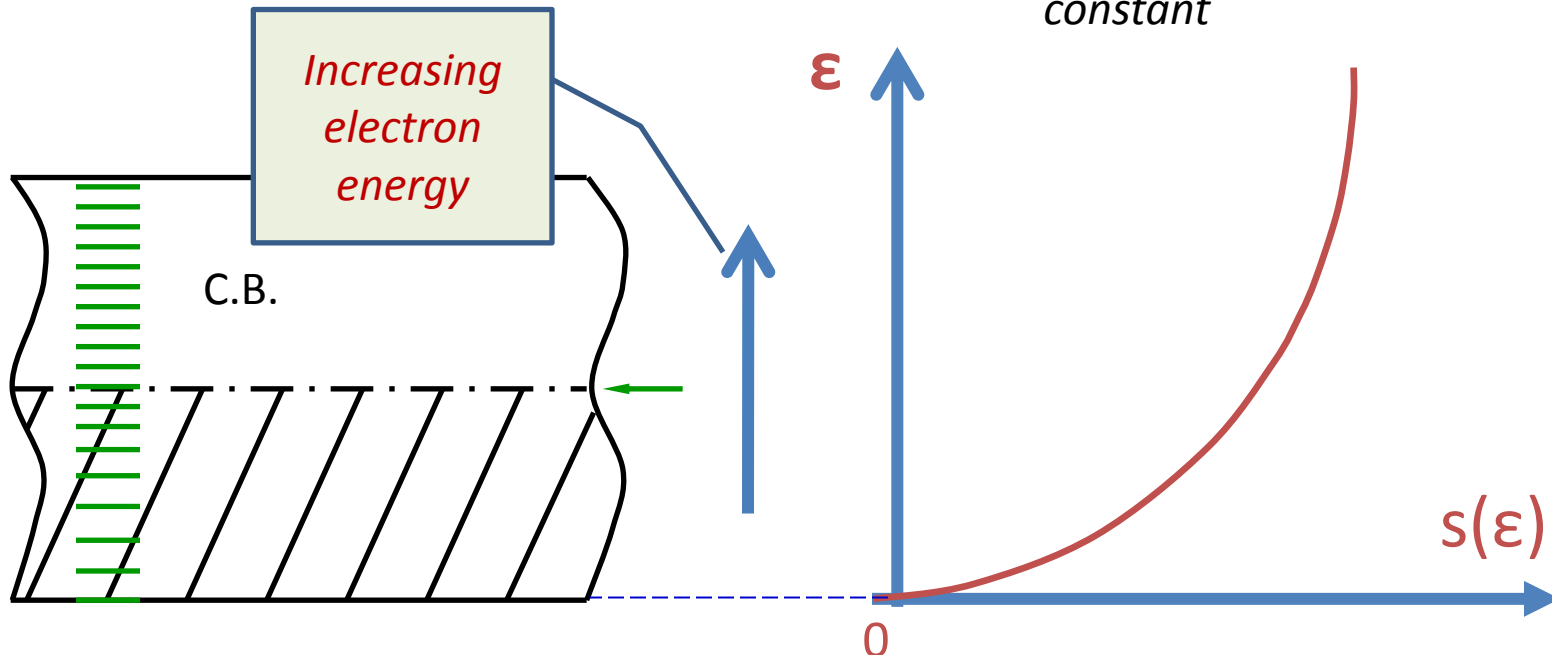
Density of States Function in CB

- Quantum mechanical analysis is required (see 3rd Year SSE). This shows that:

$$S(\varepsilon) = \left(\frac{8 \cdot \sqrt{2} \cdot \pi \cdot m^{3/2}}{h^3} \right) \cdot \sqrt{\varepsilon} = C \cdot \sqrt{\varepsilon}$$

No need to remember this formula!

constant

Increasing electron energy

C.B.

ε

s(ε)

0

http://britneyspears.ac/lasers.htm

The Probability of Occupation Function f($\mathcal{E}$)

- f($\mathcal{E}$) is defined as the probability that if a state exists at an energy $\mathcal{E}$, then that state will be occupied by an electron.

- This kind of analysis comes from Statistical Physics :

- For example, in the case ordinary molecules in a gas (which are <u>not</u> subject to the Pauli exclusion principle) it is found that the probability of a molecule having a particular energy ε is given by the *Maxwell-Boltzmann Distribution*:

$$f(\varepsilon) = \underbrace{K}_{const} \cdot e^{-\varepsilon/kT}$$

.

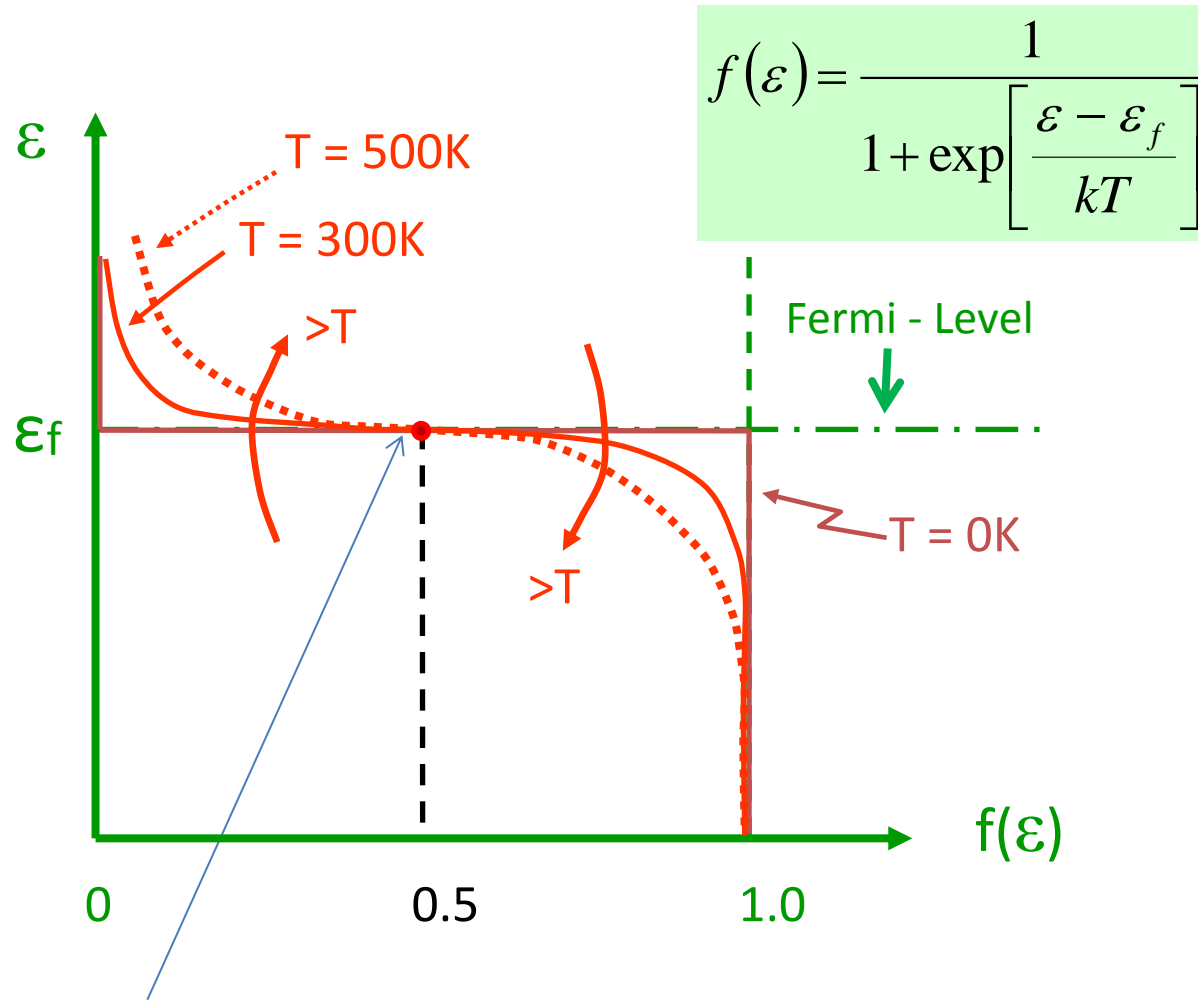# The Probability of Occupation Function f($\mathcal{E}$)

- In the case of electrons in the C.B. of a metal the Pauli Exclusion principle <u>does</u> apply and a different result then arises :

$$f(\varepsilon) = \frac{1}{1 + \exp\left[\dfrac{\varepsilon - \varepsilon_f}{kT}\right]}$$

The Fermi Dirac Distribution

- The Fermi-Dirac Distribution is said to apply to *fermions*.

- As the temperature T → 0K, then:

   whenever $\mathcal{E}$ < $\mathcal{E}_f$, f($\mathcal{E}$) → (1/(1+0)) = 1   while abruptly

   whenever $\mathcal{E}$ > $\mathcal{E}_f$, f($\mathcal{E}$) → (1/(1+∞)) = 0

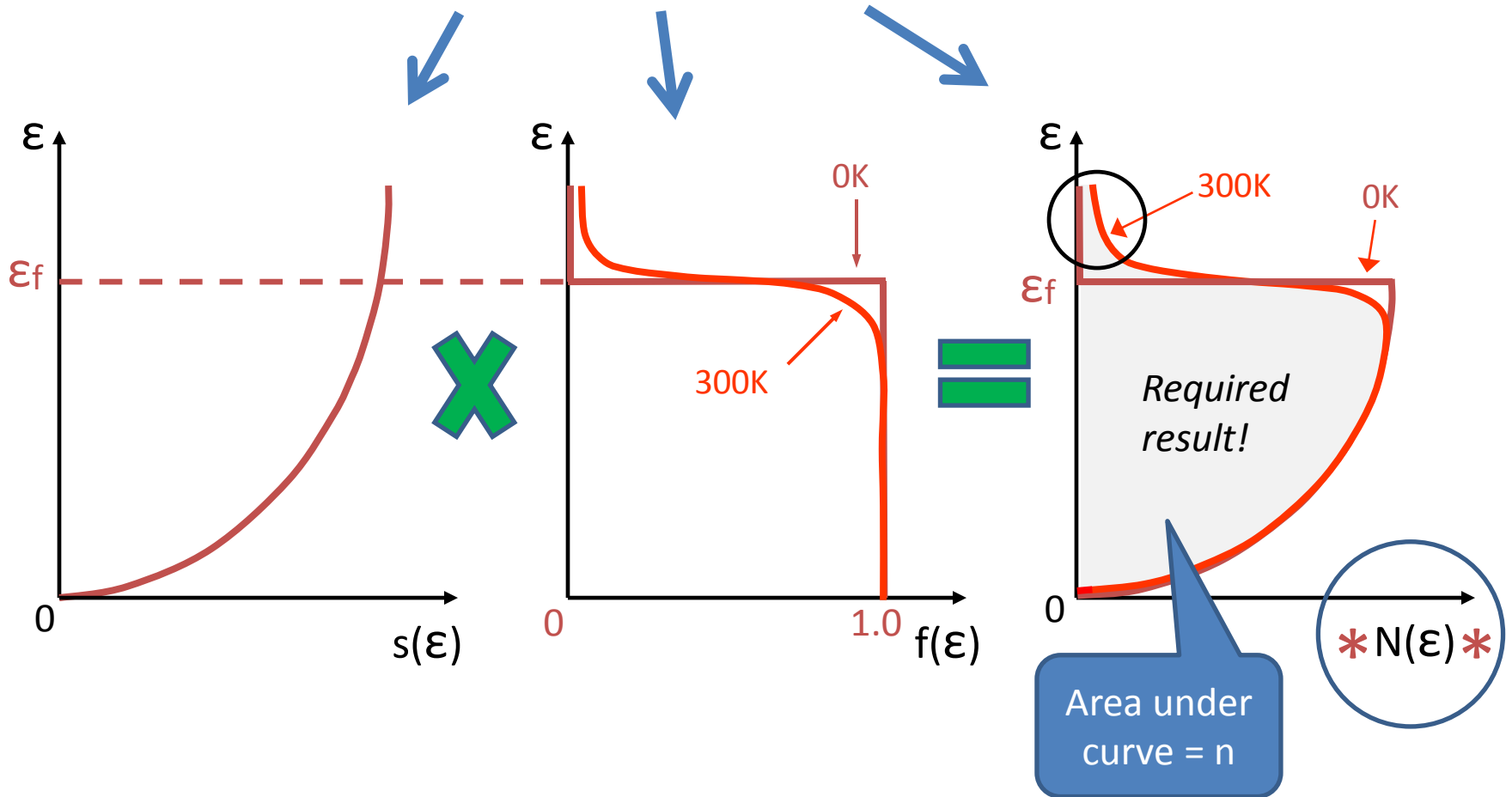- At higher temperatures, there is a smoother transition between 1 and 0.

The Probability of Occupation Function f(ε)

$$f(\varepsilon) = \frac{1}{1 + \exp\left[\dfrac{\varepsilon - \varepsilon_f}{kT}\right]}$$

T = 500K

T = 300K

>T

ε

εf

Fermi - Level

>T

T = 0K

f(ε)

0   0.5   1.0

N.B. For any T > 0K, whenever $\mathcal{E} = \mathcal{E}_f$ then f($\mathcal{E}$) = 0.5

CB Carrier Distribution Functions (Metal)

Now : find: $S(\mathcal{E})$ **x** $f(\mathcal{E})$ **=** $N(\mathcal{E})$

Area under curve = n

Electron Concentration in a Metal

- In principle, we can calculate the concentration of CB electrons (n) at any "T" using:

$$n = \int_0^\infty N(\varepsilon) \cdot d\varepsilon = \int_0^\infty S(\varepsilon) \cdot f(\varepsilon) \cdot d\varepsilon$$

$$= \int_0^\infty S(\varepsilon) \cdot f(\varepsilon) \cdot d\varepsilon = \int_0^\infty \left(\frac{8 \cdot \sqrt{2} \cdot \pi \cdot m^{3/2}}{h^3} \right) \cdot \left[\frac{\sqrt{\varepsilon} \cdot d\varepsilon}{1 - e^{[(\varepsilon - \varepsilon_f)/kT]}} \right]$$

- This integral cannot be solved analytically. However in the special case where T = 0K, the upper limit on the integral becomes $\mathcal{E}_f$ and we can replace f($\mathcal{E}$) with 1 in the range between 0 and $\mathcal{E}_f$. with the result that the integral can then be solved...

Concentration of Free Electrons in the CB of a Metal at 0K

Substitute for $S(\varepsilon)$:

$$n = \frac{8\sqrt{2}\pi \cdot m^{3/2}}{h^3} \cdot \int_0^{\varepsilon_f} \sqrt{\varepsilon} \cdot d\varepsilon \quad = \quad \frac{8\sqrt{2}\pi \cdot m^{3/2}}{h^3} \cdot \left(\frac{2}{3} \varepsilon^{3/2} \Big|_0^{\varepsilon_f} \right)$$

$$\Rightarrow \quad n \quad = \quad \frac{16\sqrt{2}\pi \cdot m^{3/2}}{3h^3} \cdot \varepsilon_f^{3/2}$$

No need to remember this formula!

This shows a direct relationship between Fermi level and CB electron concentration at 0K in a metal. If we know one of these quantities, then we can determine the other.

Worked Example

Example:

In a metal at 0K, what percentage of the total no. of free electrons have energies in the range $0.1\varepsilon_f$ to $0.2\varepsilon_f$?

Solution:

$$\text{Fraction} = \frac{(\text{no. of electrons in range } 0.1\varepsilon_f \text{ to } 0.2\varepsilon_f)}{(\text{total no. of C.B. electrons})}$$

$$= \frac{\int_{0.1\varepsilon_f}^{0.2\varepsilon_f} S(\varepsilon)d\varepsilon}{\int_{0}^{\varepsilon_f} S(\varepsilon)d\varepsilon}$$

Solution.. cont'd:

$$= \frac{\int_{0.1\varepsilon_f}^{0.2\varepsilon_f} S(\varepsilon)d\varepsilon}{\int_0^{\varepsilon_f} S(\varepsilon)d\varepsilon}$$

$$= \frac{\int_{0.1\varepsilon_f}^{0.2\varepsilon_f} const \cdot \sqrt{\varepsilon} \cdot d\varepsilon}{\int_0^{\varepsilon_f} const \cdot \sqrt{\varepsilon} \cdot d\varepsilon}$$

$$= \left[\frac{\left(\frac{2}{3} \cdot \varepsilon^{3/2} \right) \Big|_{0.1\varepsilon_f}^{0.2\varepsilon_f}}{\left(\frac{2}{3} \cdot \varepsilon^{3/2} \right) \Big|_{0.}^{\varepsilon_f}} \right]$$

$$= \left(\frac{0.2^{3/2} \cdot \varepsilon_f^{3/2} - 0.1^{3/2} \cdot \varepsilon_f^{3/2}}{\varepsilon_f^{3/2}} \right) = \left(0.2^{3/2} - 0.1^{3/2} \right) = 0.0578$$
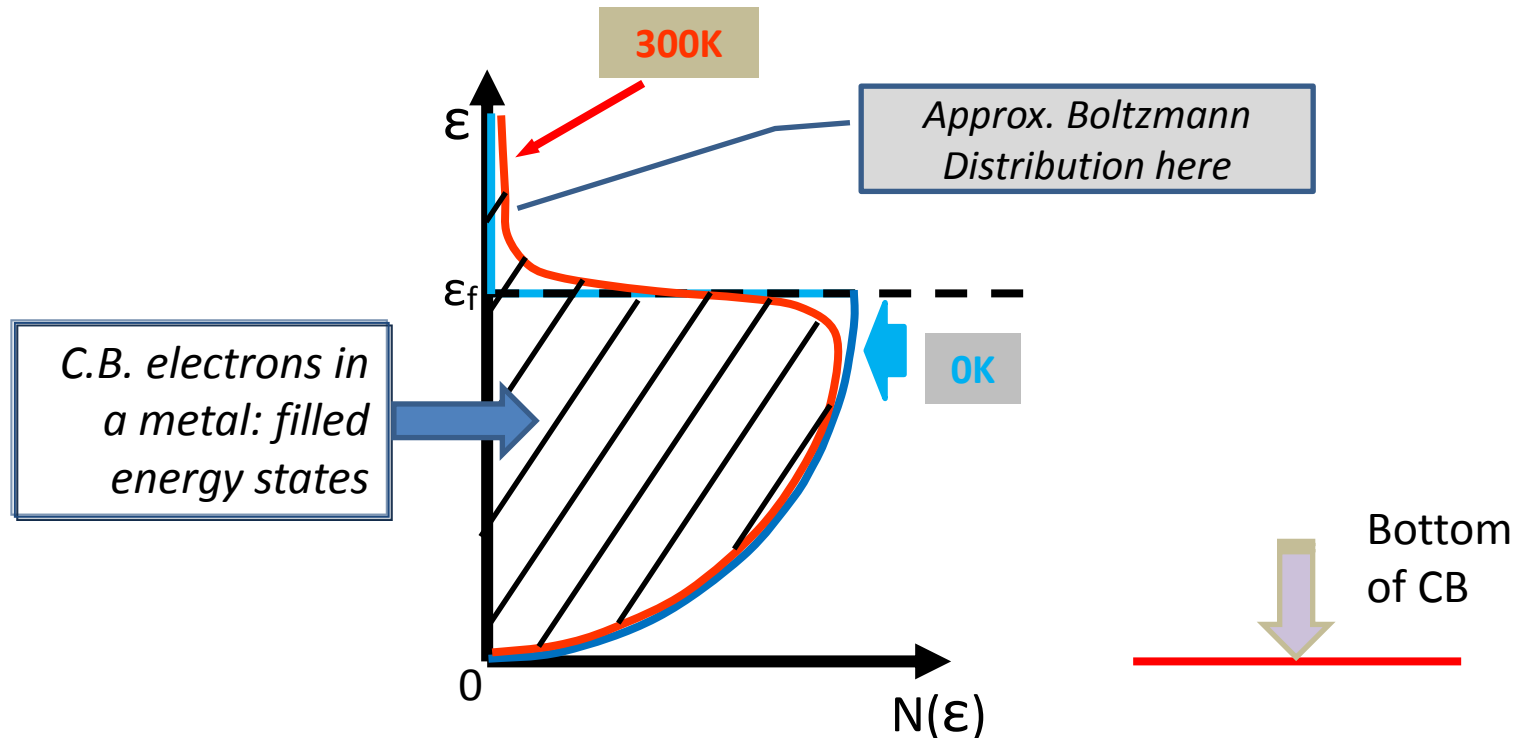
$$= \quad 5.78\%$$

EXAMPLE 2.3

CB Number Density Distribution in Metals

Note : For T > 0K, if $(\mathcal{E} - \mathcal{E}_f) \gg kT$, then:

$$f(\varepsilon) \approx e^{-(\varepsilon - \varepsilon_f)/kT} = const. \cdot e^{-\varepsilon/kT}$$

i.e. the Fermi-Dirac distribution tends to approximate to a Boltzmann distribution for energies several kT in excess of ε_f

Vacuum Level and Work Function

ε

VACUUM LEVEL

300K

$q\Phi_m$

ε_f

Thermionic Emission of electrons from the surface of a heated metal

0

N(ε)
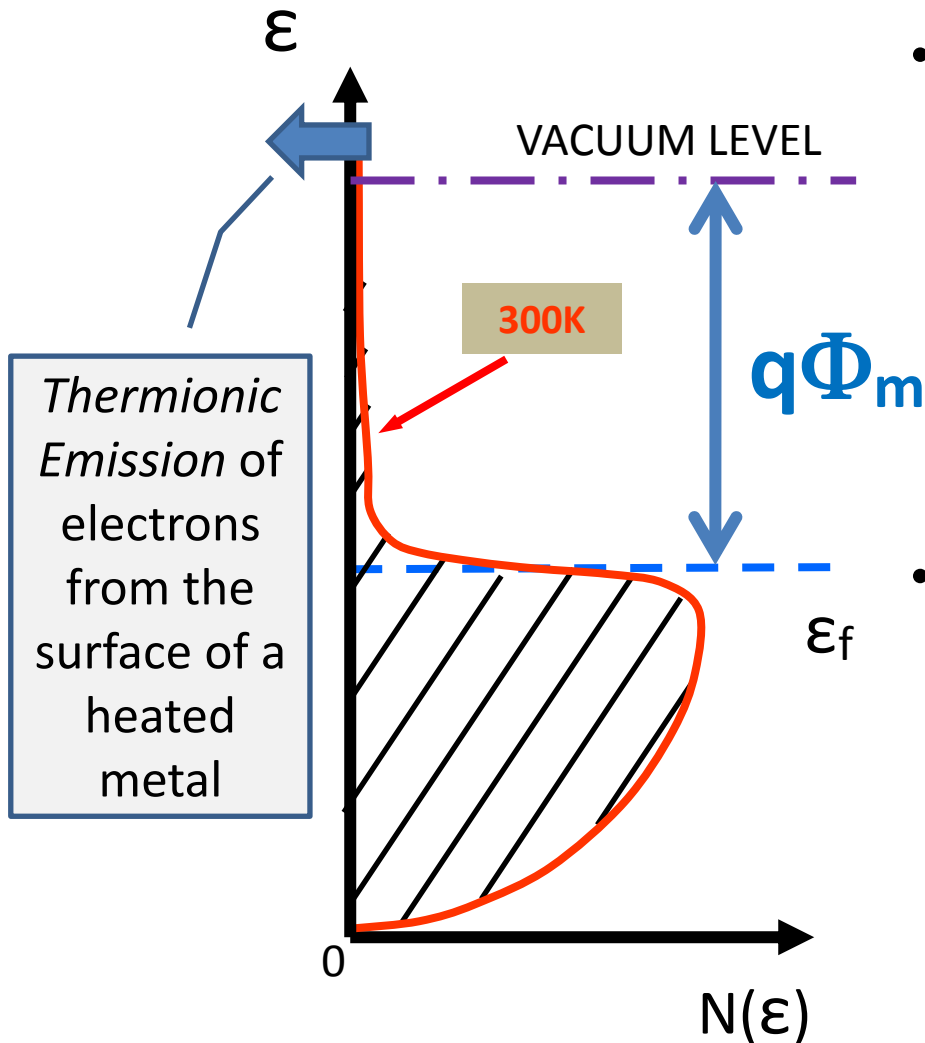
- With sufficient heat electrons can be "boiled off" or can escape from the metal: this is called "*thermionic emission*" and requires that their energy exceeds the "vacuum level". This was used in old vacuum tubes or "valves"

- The Work Function $q\Phi_m$ is an important parameter for a metal and is the energy required to move an electron from the Fermi level to the vacuum level (Normally this is measured in eV. Then Φ_m has the units of Volts)

Photons and Energy

- In 1900, while researching the theory of energy radiated by hot bodies, and trying to explain experimental results, Max Planck was led to the conclusion that light (or more generally electromagnetic radiation) could deliver energy only in small discrete units that become known as **photons**;

- The energy of each photon at a frequency "f" is given by:

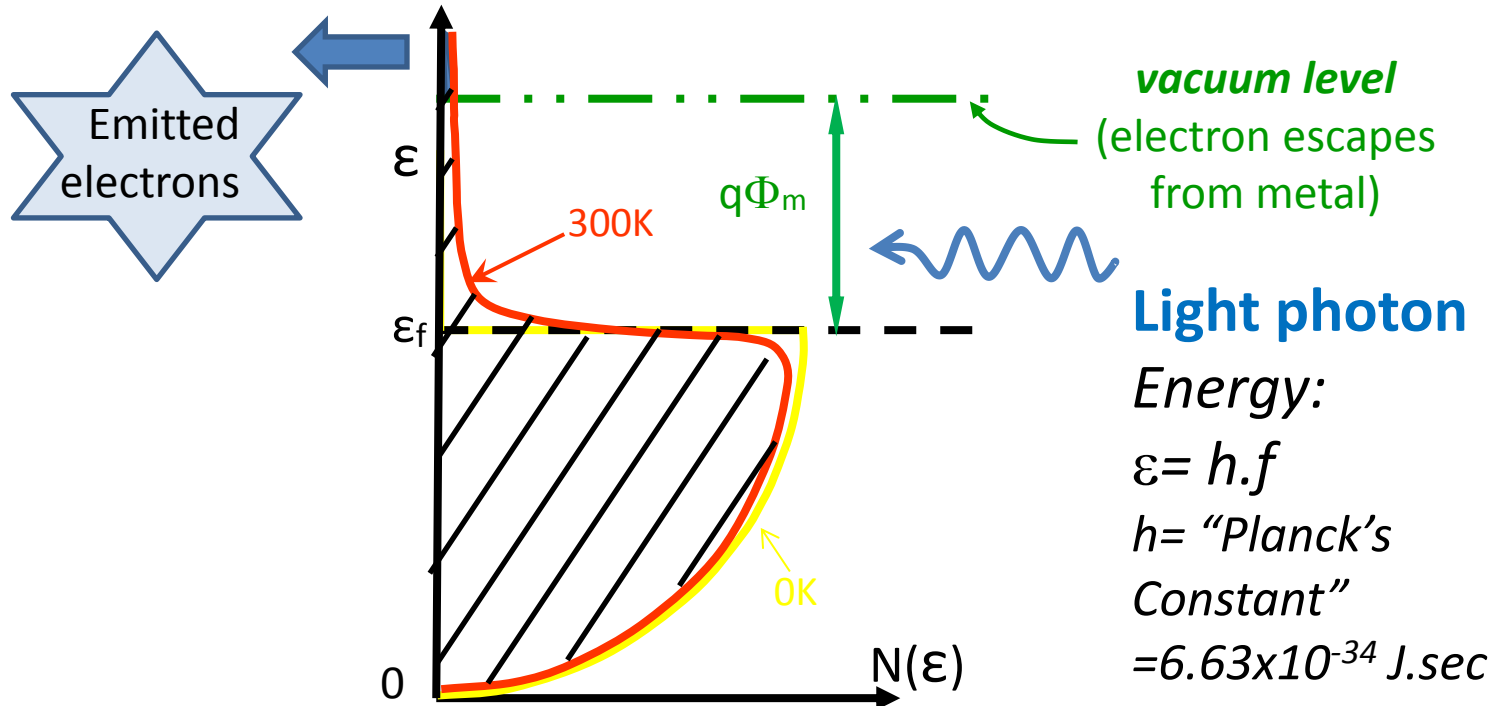$$\varepsilon = h \cdot f$$

... where h = 6.63×10^{-34} J-sec is Planck's Constant, a fundamental constant of Nature

The Photoelectric Effect

- In 1905, Einstein used Planck's ideas to explain experimental observations of the photoelectric effect whereby light can cause electrons to be emitted from a metal *only* above a certain frequency (f) and then the emitted electron energy depends only on the frequency of the light, not on its intensity. This is consistent with:

$$KE = \tfrac{1}{2} \cdot m \cdot v^2 = \varepsilon - q \cdot \Phi_m = h \cdot f - q \cdot \Phi_m$$

Emitted electrons

ε

300K

$q\Phi_m$

ε_f

0K

0   N(ε)

vacuum level
(electron escapes from metal)

Light photon
Energy:
$\varepsilon = h.f$
h= "Planck's Constant"
=6.63x10^-34 J.sec

Example 2.4