

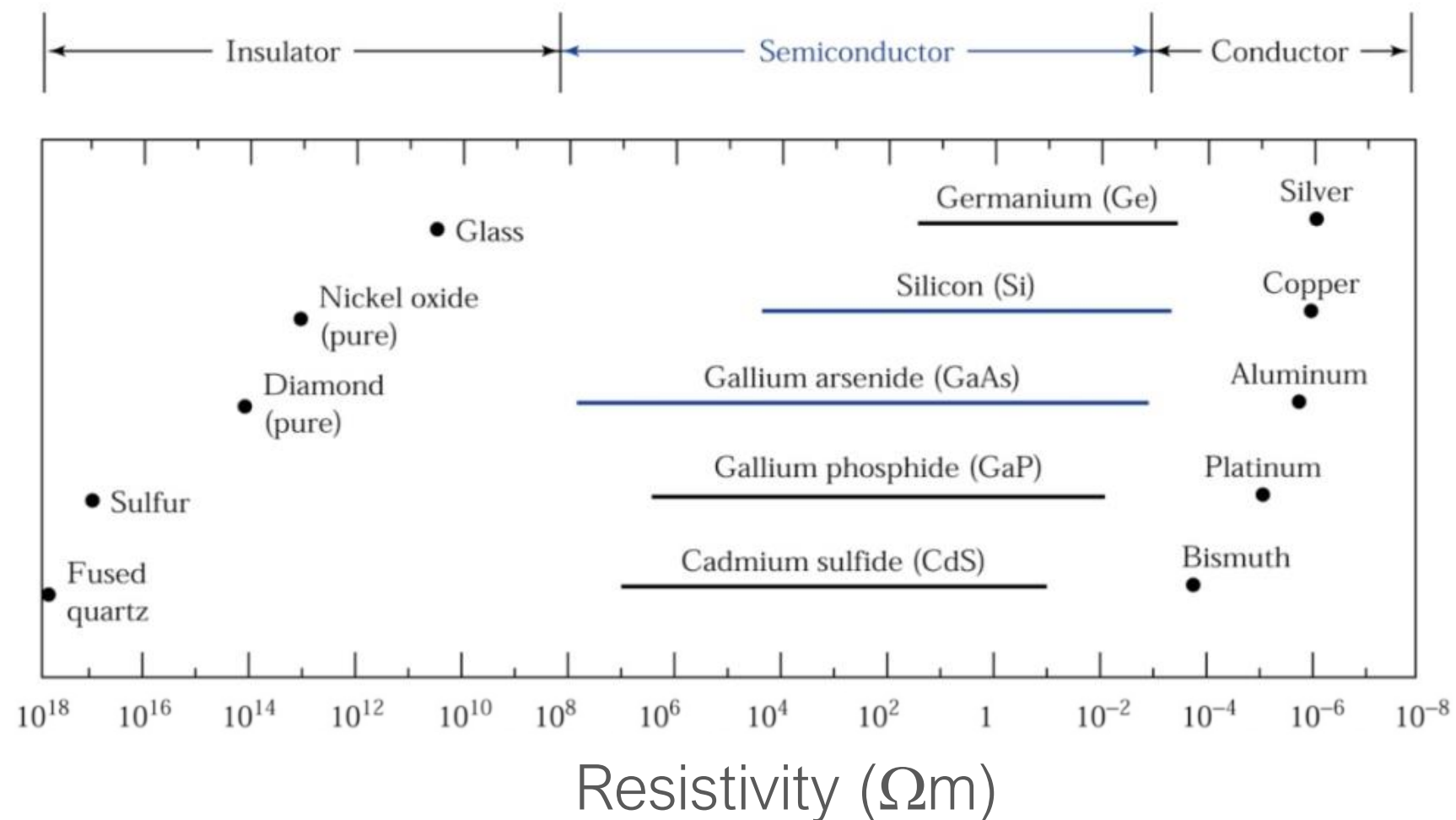
# Aims & objectives (second part)

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- Describe the influence of the periodic lattice potential on the electron  $E$ - $k$  dispersion: appearance of 'energy bands' and energy 'band gaps'
- Describe how Bragg reflection of electron waves leads to standing wave states for  $k$ -vectors at the zone boundaries
- Be able to construct the Reduced Zone Scheme  $E$ - $k$  dispersion from the Extended Zone Scheme
- Explain how scenarios involving partial- or complete- filling of energy bands can account for metallic, semiconducting, and insulating, electrical behaviour
- Explain using the energy band picture why no current flow is expected when an electric field is applied to an insulator
- Appreciate how thermally induced electron-hole pair production is accommodated in the energy band picture for semiconductors
- Explain why the Fermi Level should be placed in the middle of the band gap for semiconductors
- Be able to derive the carrier density formula  $n(T)$  for intrinsic semiconductors and appreciate role of band gap size for distinguishing between insulators/semiconductors
- Rationalise the existence of electron holes by considering the current contribution of a nearly-full valence band
- Understand the role of photons in induced pair-production and Direct/Indirect semiconductors
- Derivation and meaning of the effective mass  $m^*$
- Inspection of bandstructures to identify effective masses of carriers in the conduction and valence bands

# Semiconductors

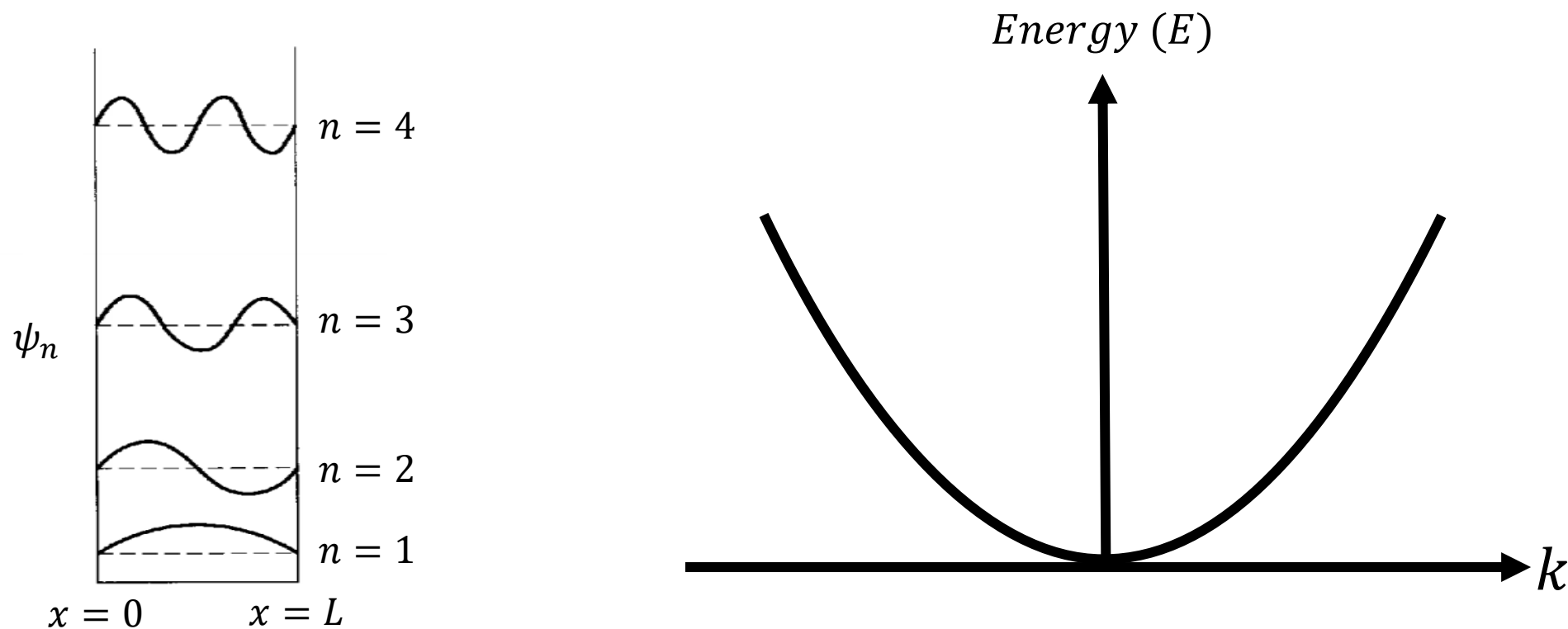
- Another look at the figure below shows semiconductors can be “tuned” to exhibit the broadest range of conductivity – GaAs alone can be processed such that  $\rho$  spans  $10^{11}(\Omega\text{m})$



- We can crudely expect high conductivity in metals where there are free electrons available and virtually no conductivity in insulators where all the outer electrons are involved in covalent bonding.
- We need to refine this picture to explain the vast ranges and how materials with the same bonding types have very different values.

# Energy band theory - Free-electron gas revisited

- Free electron gas: allowed electron states have energy that can be expressed as a quasi-continuous quadratic function of  $k$ -vector



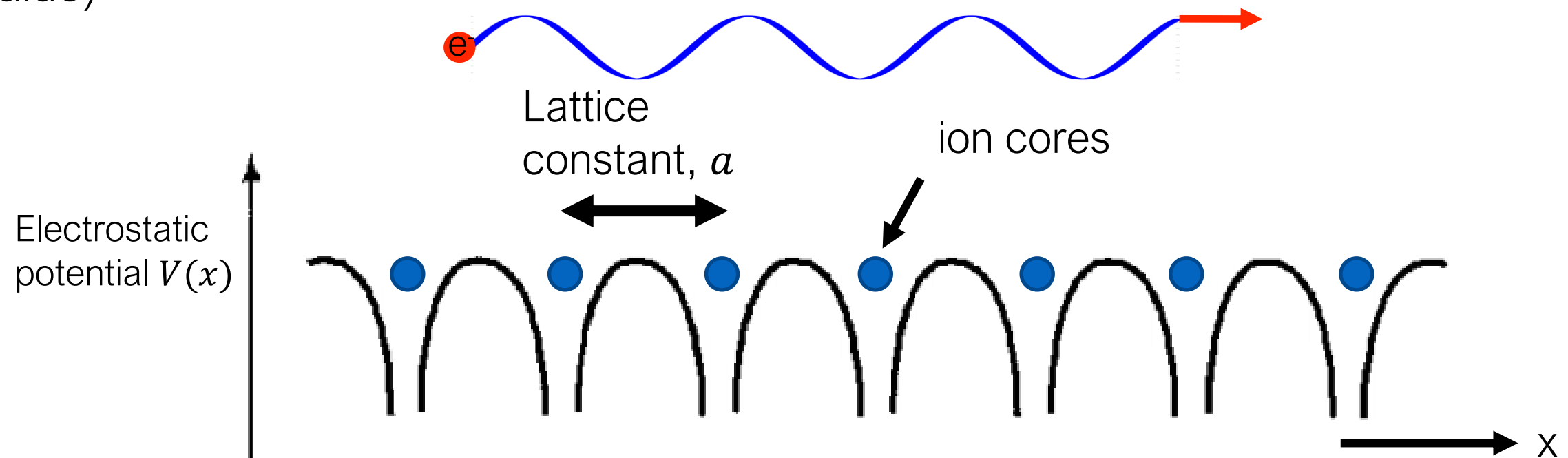
$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi(r) \quad V(r) = 0 \text{ within the well}$$

- When periodic boundary conditions are considered, electron wavefunctions are described by freely propagating plane waves:

$$\psi_k(r) = Ae^{i\underline{k}.\underline{r}}$$

# Energy band theory – electrons in a periodic potential

- A more sophisticated approach to dealing with the ionic potential is to include a periodic potential energy function in the TISE (rather than an assumed constant value)



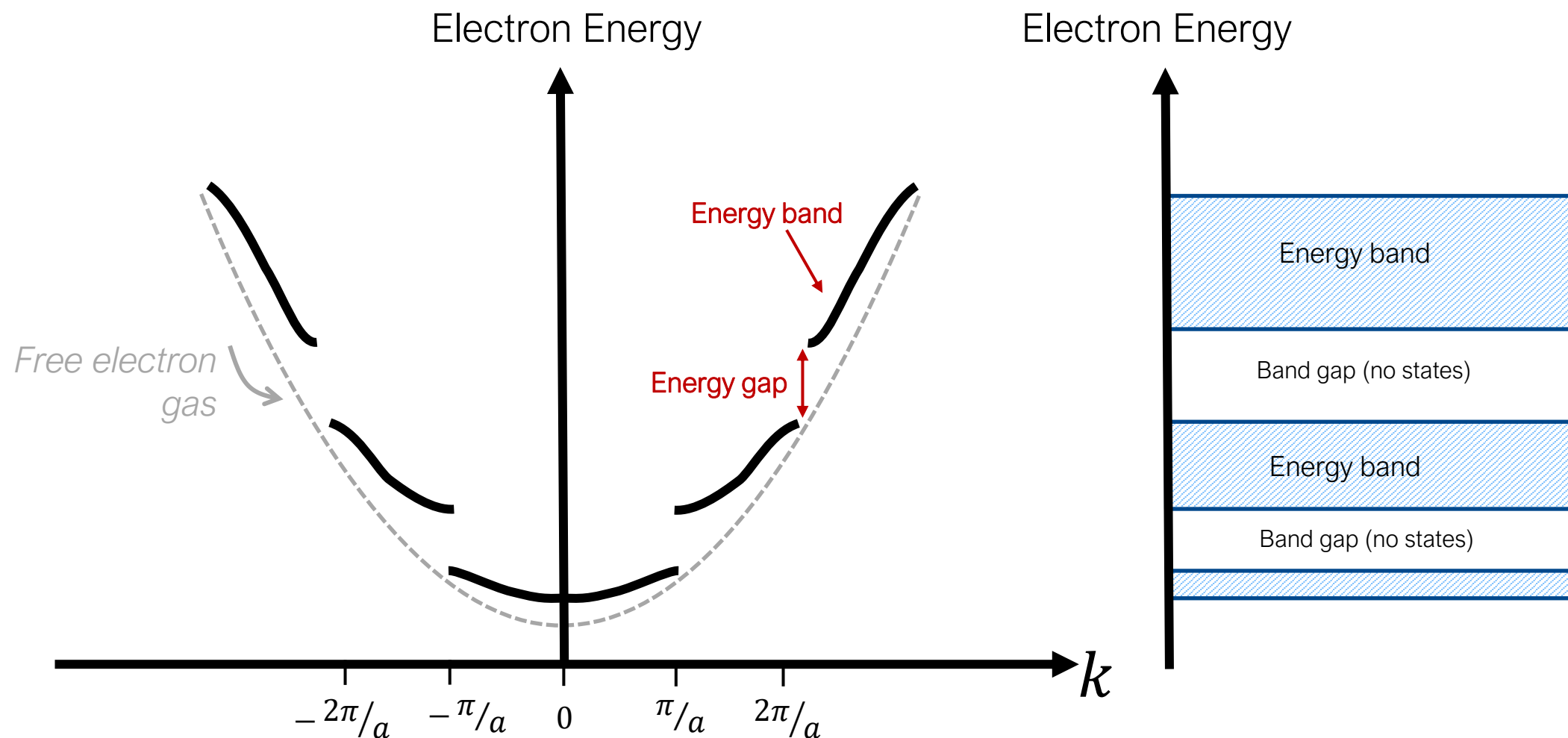
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x) = E\psi$$

where  $V(x) = V(x + ma)$   
( $m$  is any integer no. of lattice periods)

- Stationary solutions to TISE exist and involve modulating plane wave solutions by a function  $u(x)$  that has periodicity of the lattice, i.e.  $u(x) = u(x + ma)$  such that:  $\psi_k = Ae^{ikx} \cdot u_k(x)$
- Result: the effect of a (perfectly) periodic lattice can be completely accounted for with no expectation of scattering by static ions – the electron waves can travel freely without attenuation over time

# Energy band theory – electrons in a periodic potential

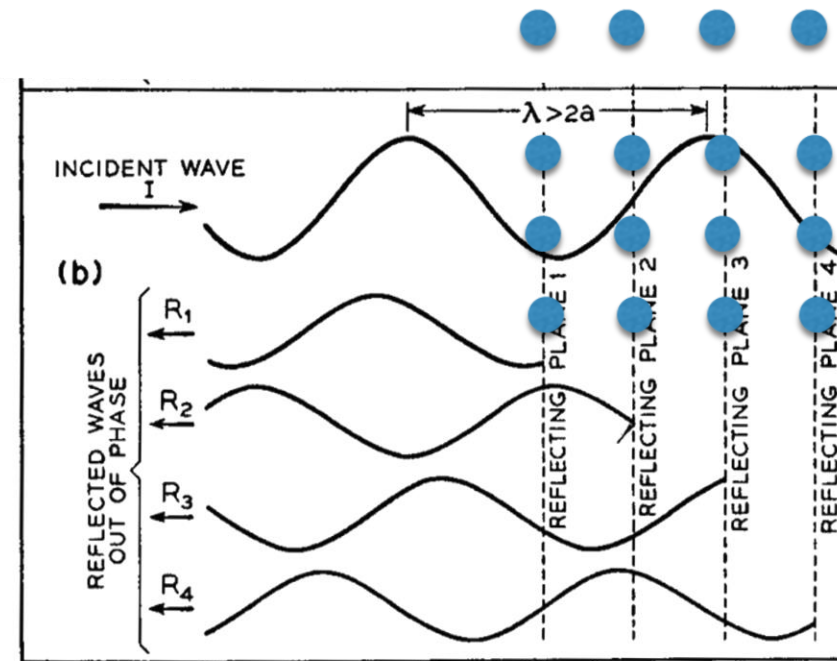
- How is the  $E$ - $k$  dispersion affected by the effect of the periodic potential?



- The free-electron  $E$ - $k$  function becomes **distorted** and **discontinuities** in energy appear where there are no states i.e. “**energy band gaps**”
- The band-gaps appear at  $k = \pm n\pi/a$ . At these  $k$ -points, forward propagating electron waves combine with those partially-reflected by the lattice ions and form standing wave states (critical condition when  $\lambda = 2a$ )

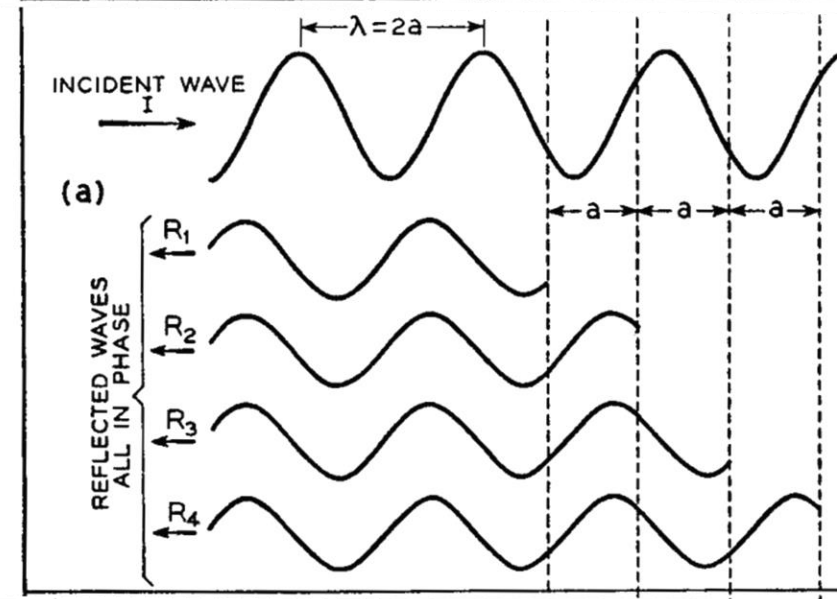
## Real-space schematic of wave behaviour:

Far from Bragg k-condition being satisfied: reflected waves destructively interfere and resulting travelling electron wave propagates relatively undisturbed



far from  $k = \pm \frac{\pi}{a}$

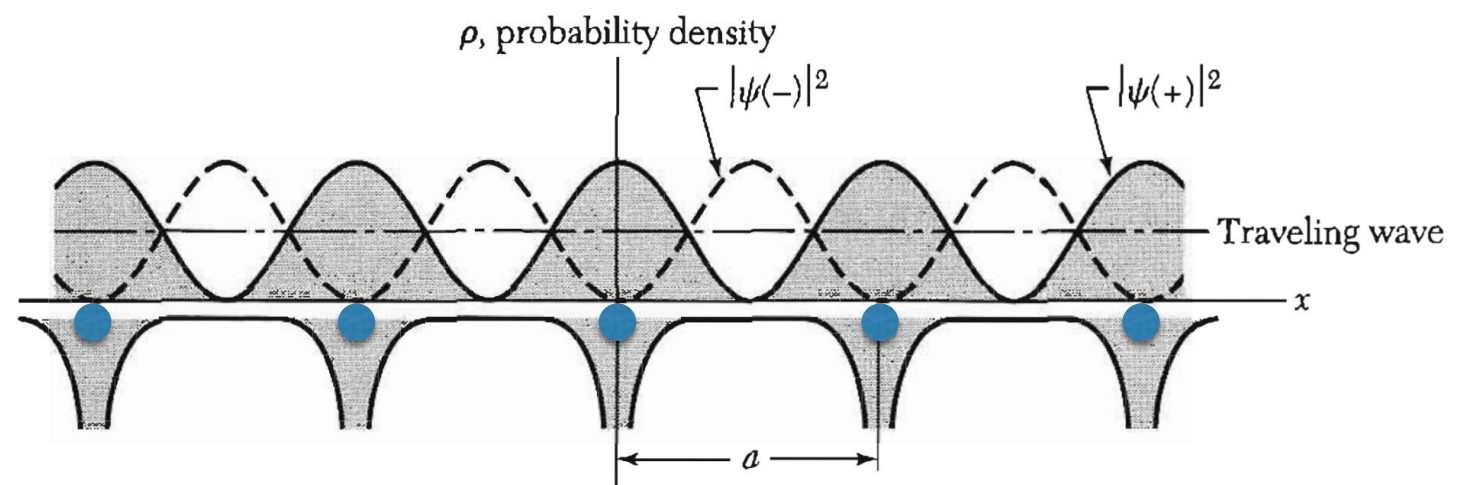
Bragg condition satisfied for travelling electron waves normally incident on a periodic lattice of ions when  $\lambda = 2a$ ; interference with partially reflected waves results in formation of a standing wave overall



when  $k = \pm \frac{\pi}{a}$

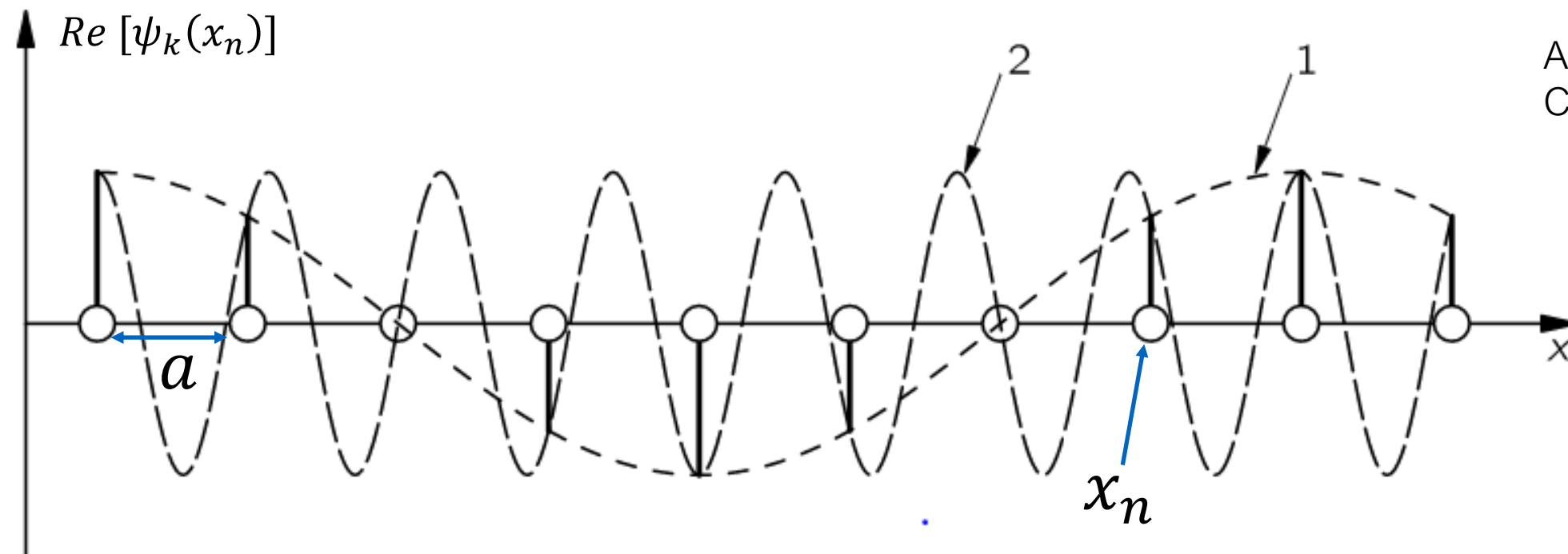
FIG. 5-8—Phase Relations between Reflected Waves, Showing Critical Condition for  $\lambda = 2a$ .

Standing wave states develop with charge density concentrated either close to the ion cores or between them. Different electrostatic energy in each case gives rise to the two distinct energy states seen at  $k = \pi/a$  ( $\lambda = 2a$ )





# Electron propagation through a discrete periodic lattice



After Feynman Lectures,  
Ch13

Fig. 13-4. Two values of  $k$  which represent the same physical situation; curve 1 is for  $k = -\pi/4a$  curve 2 is for  $k = 7\pi/4a$

Electron  $k$ -states with values differing by integer multiples of  $\frac{2\pi}{a}$  give the same amplitude at equivalent atomic sites  $x_n$  and can therefore represent the same state

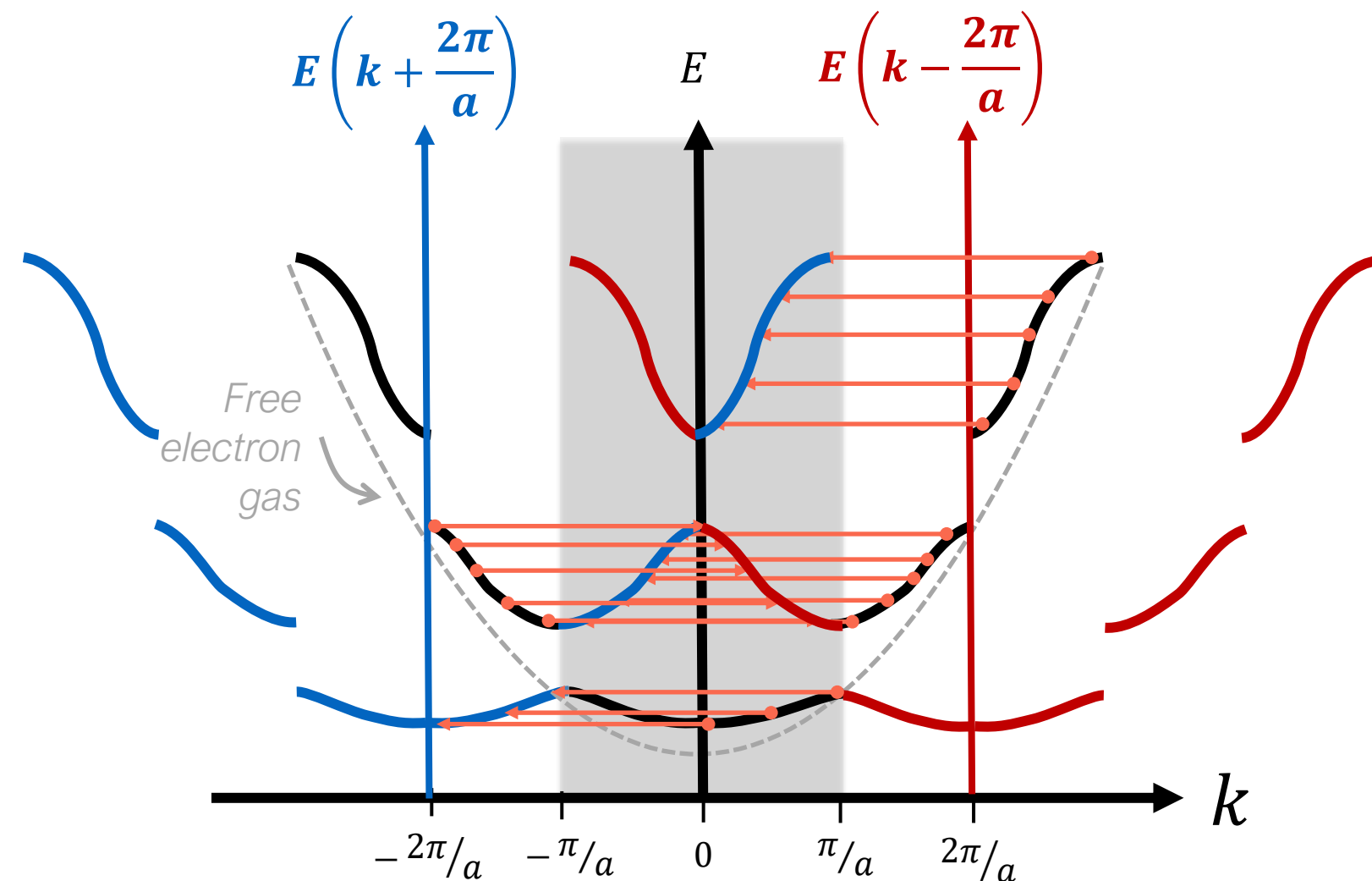
$$\psi_k(x_n) = Ae^{ikx_n} \quad \text{Consider } k' = k + \frac{2\pi}{a} \quad x_n = na$$

$$\psi_{k'}(x_n) = Ae^{ik'x_n} = Ae^{ikx_n} \cdot e^{i\frac{2\pi x_n}{a}} = Ae^{ikx_n} = \psi_k(x_n)$$

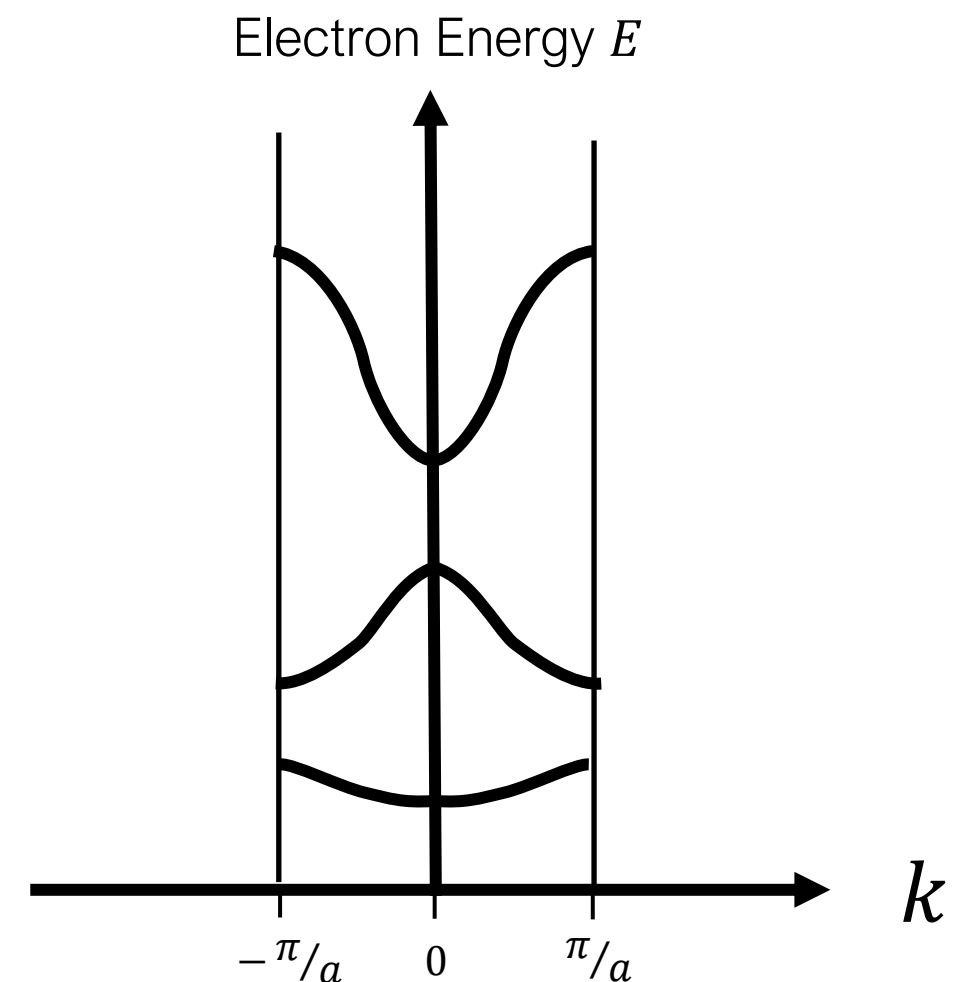
# Zone representation schemes

- The periodicity of the lattice imposes a condition that electron wave states are equivalent insofar as  $E\left(k \pm \frac{2\pi n}{a}\right) = E(k)$  for a given band

Extended zone scheme



Reduced zone scheme (1<sup>st</sup> BZ)



- All physically distinct electron states are captured in a region of  $k$ -space from  $-\pi/a$  to  $+\pi/a$  (the 1<sup>st</sup> Brillouin Zone). The  $E$ - $k$  dispersion plot becomes multi-valued in energy for a given  $k$  value in the reduced scheme.

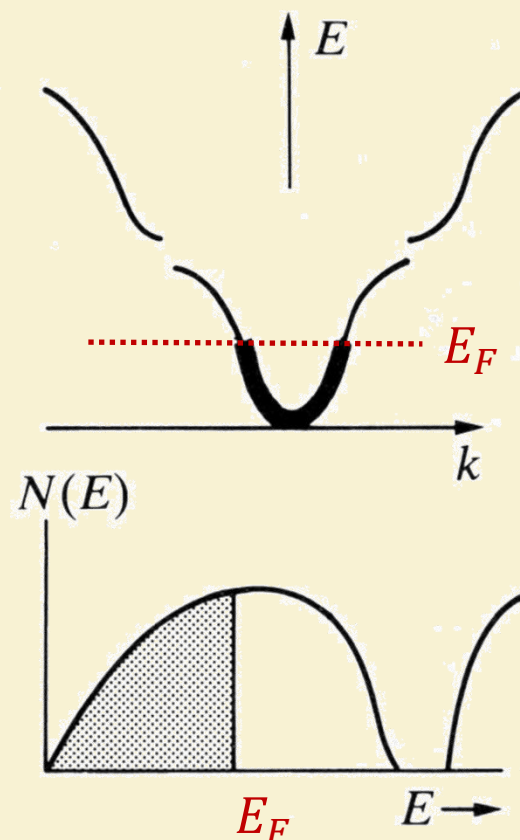


# Metals, semiconductors and insulators

- The idea of energy bands and band-gaps has dramatic implications for the behaviour of conduction in solids when the band occupancy is also considered

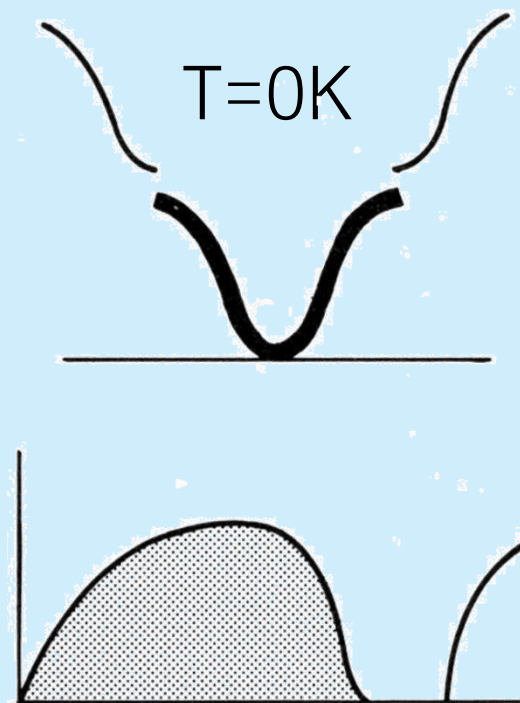
## Metal

Alkali metals (e.g. Na, Li, K) have one outer electron. The band is partially filled at all temperatures and conduction can occur under applied fields

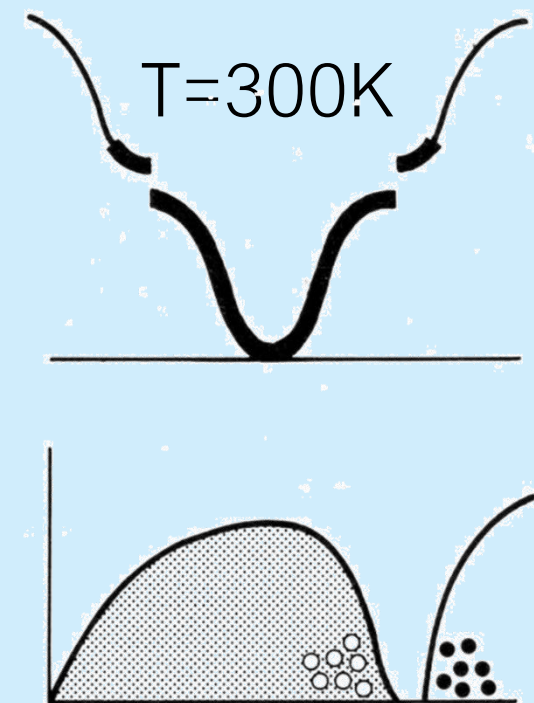


## Insulator / semiconductor

For systems where any populated energy bands are all full, no net change in electrons among  $k$ -states can occur so the material is an **insulator**

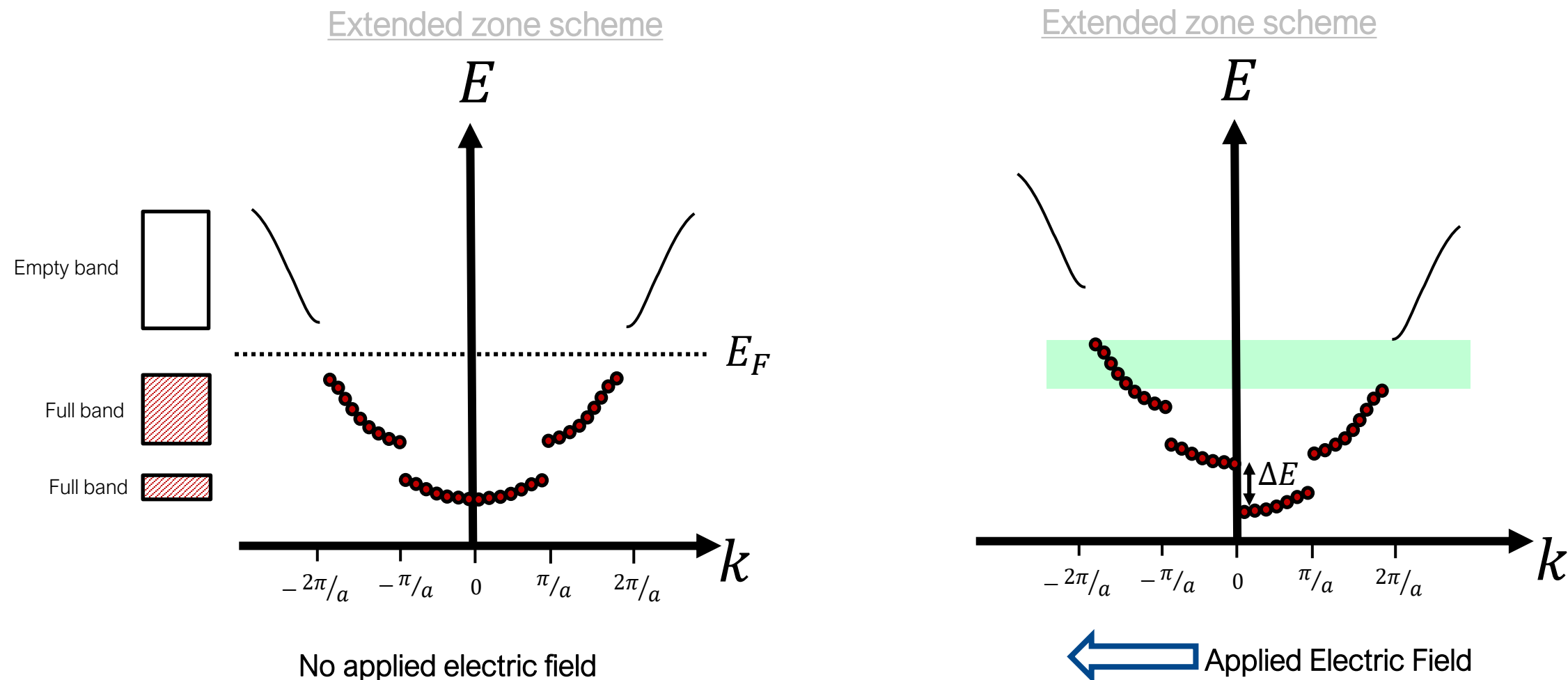


If the band gap is small enough ( $\Delta E \sim 1\text{ eV}$ ), thermal energy can excite electrons into next band. Electrons in the higher bands can respond to applied fields and conduct – the material is a **semiconductor**.



# What happens to the energy bands in an insulator at $T = 0K$ under an applied field?

- The key difference from the metallic case is that we now have only completely full or completely empty bands (none are partially filled)



- Key point: full or empty bands **do not** contribute to conduction. Only partially filled bands contribute to current flow. Each partially filled band gives an independent contribution to the total current.

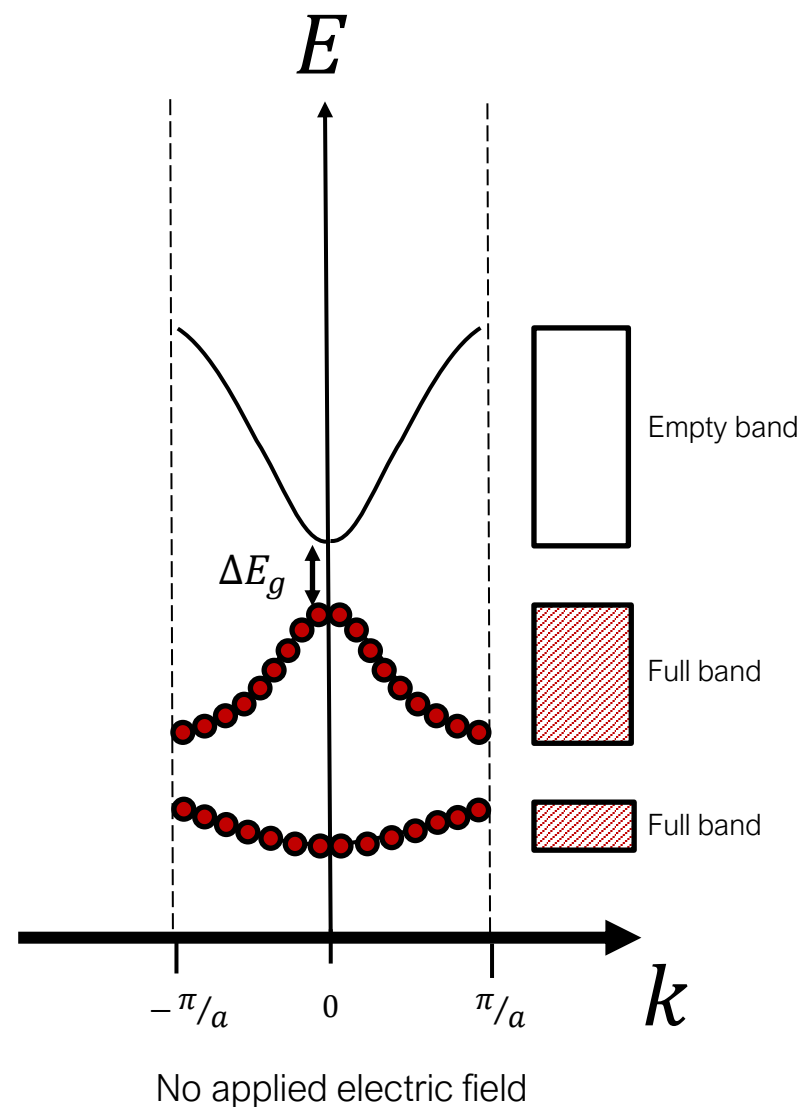
# Thermal electron/hole pair generation in semiconductors

- If temperature is high enough, and the band-gap narrow enough, electrons from the lower energy band can be thermally promoted into the higher energy band that was empty at  $T = 0K$

- These electrons can change energy state under applied field and contribute to current
- However, since both the upper and lower energy bands are partially filled, independent contributions to conduction are anticipated from both bands
- The vacant orbitals left behind in the nearly-full energy band will respond to applied fields as if they were carrying positive charge and are known as 'holes'

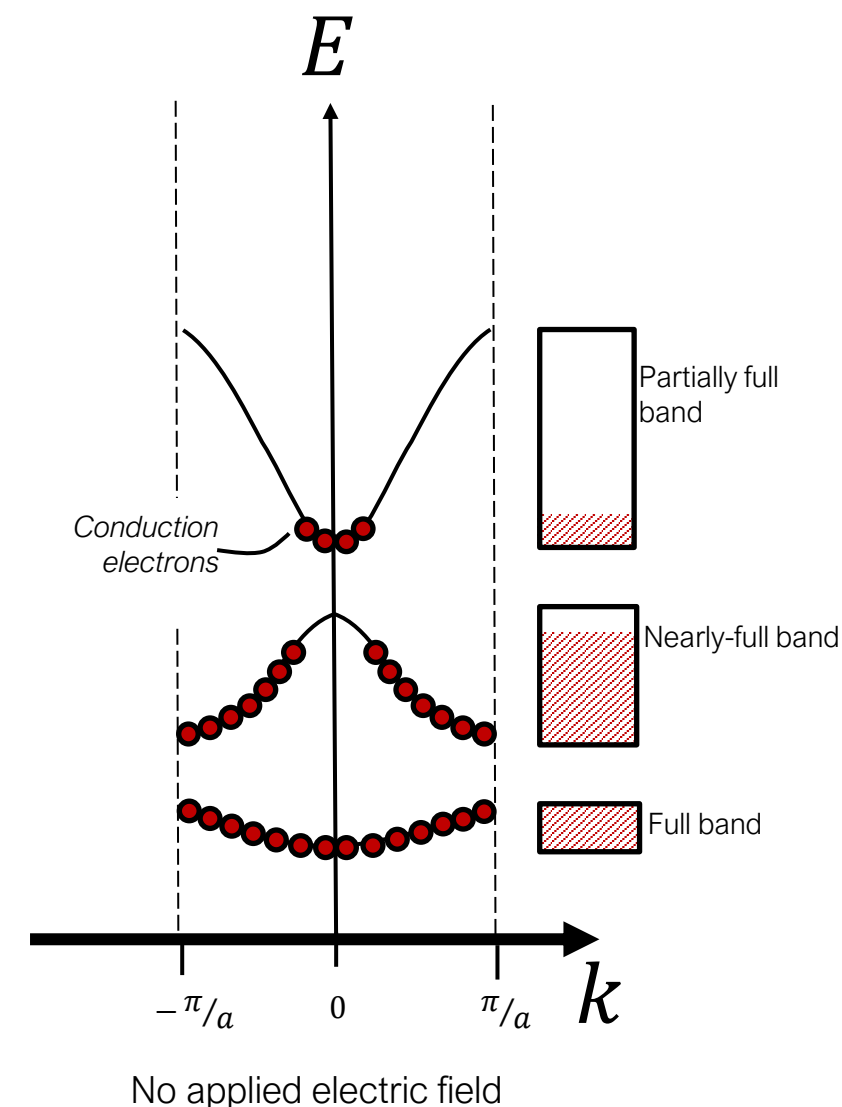
## Reduced zone scheme

(a)  $T = 0K$



Only full or empty bands, insulating behavior is expected when field applied

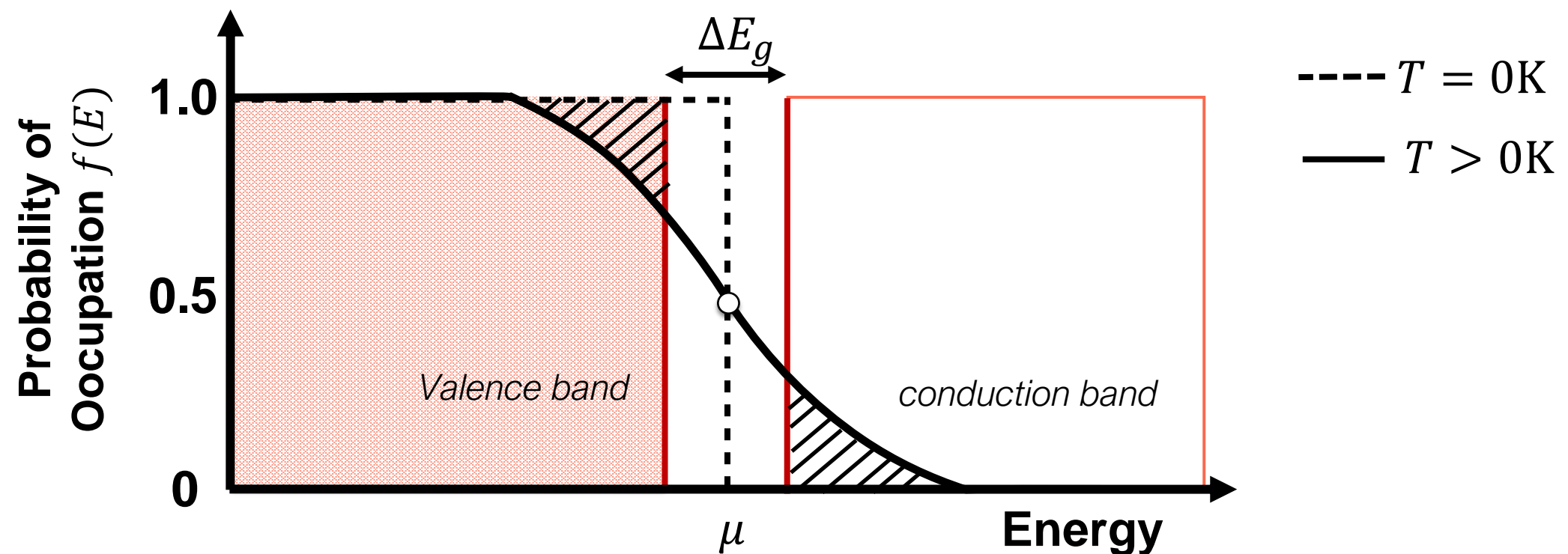
(b)  $T > 0K$



Electrons thermally promoted into higher band with large number of adjacent free energy states; current can flow under applied field

# Where is the Fermi level in a semiconductor?

- Since at  $T = 0\text{ K}$  the probability of state occupancy goes from 1 to 0 at the top of the valence band (where the highest energy filled state is), it is tempting to put  $E_F$  here (as seen for a metal at  $T = 0\text{ K}$ ) but this is incorrect for an intrinsic semiconductor
- Plot schematic flat energy bands on their side (energy along x-axis) and overlay the FD distribution at some temperature  $T > 0\text{ K}$  to help understand where the Fermi level should be:

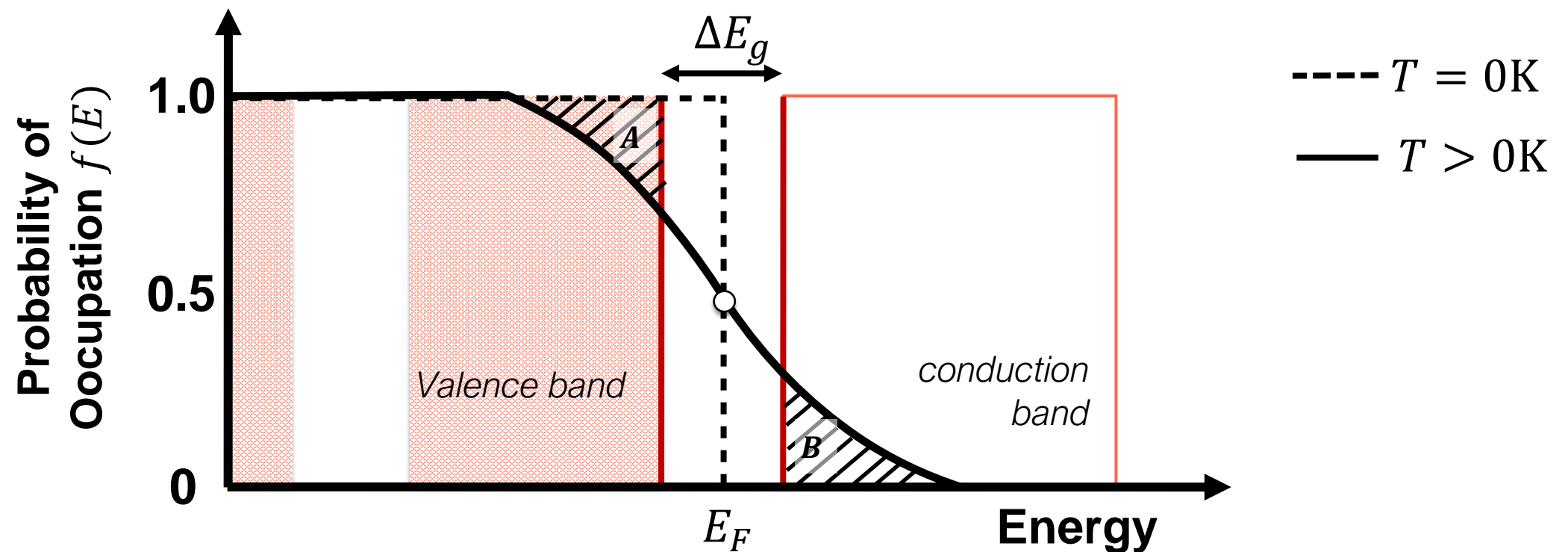


- At  $T > 0\text{ K}$  for an intrinsic semiconductor, the number of electrons missing from the valence band (due to thermal excitation) must be found in the conduction band i.e. the total number of electrons in the semiconductor is conserved
- This will only be true if the Fermi level  $\mu$  is located at the mid-point of the bandgap (due to the symmetry of FD function about  $\mu$ ). Otherwise, the implied number of electrons in the conduction band will be different than the number of electrons missing from the valence band as shown on next slide

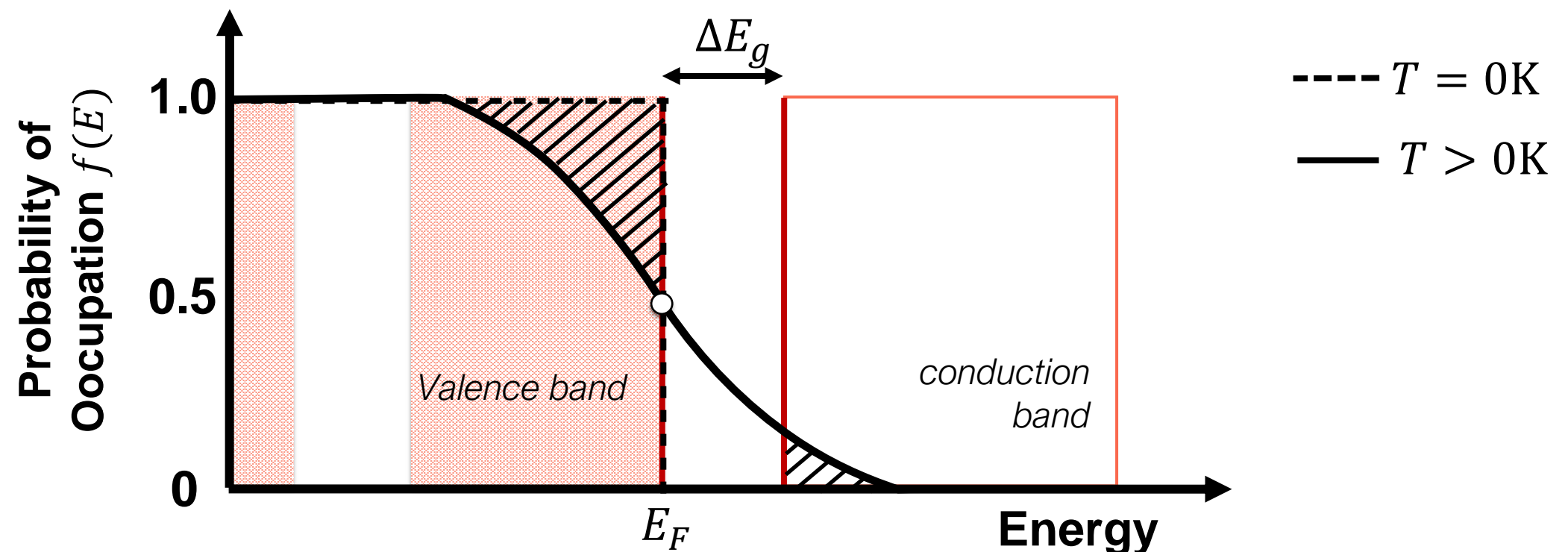
# Where is the Fermi Energy ( $T = 0K$ ) in a semiconductor?

- At  $T > 0K$  for an intrinsic semiconductor, the number of electrons missing from the valence band must be found in the conduction band i.e. the total number of electrons is conserved

If  $E_F$  is at midpoint of band gap:



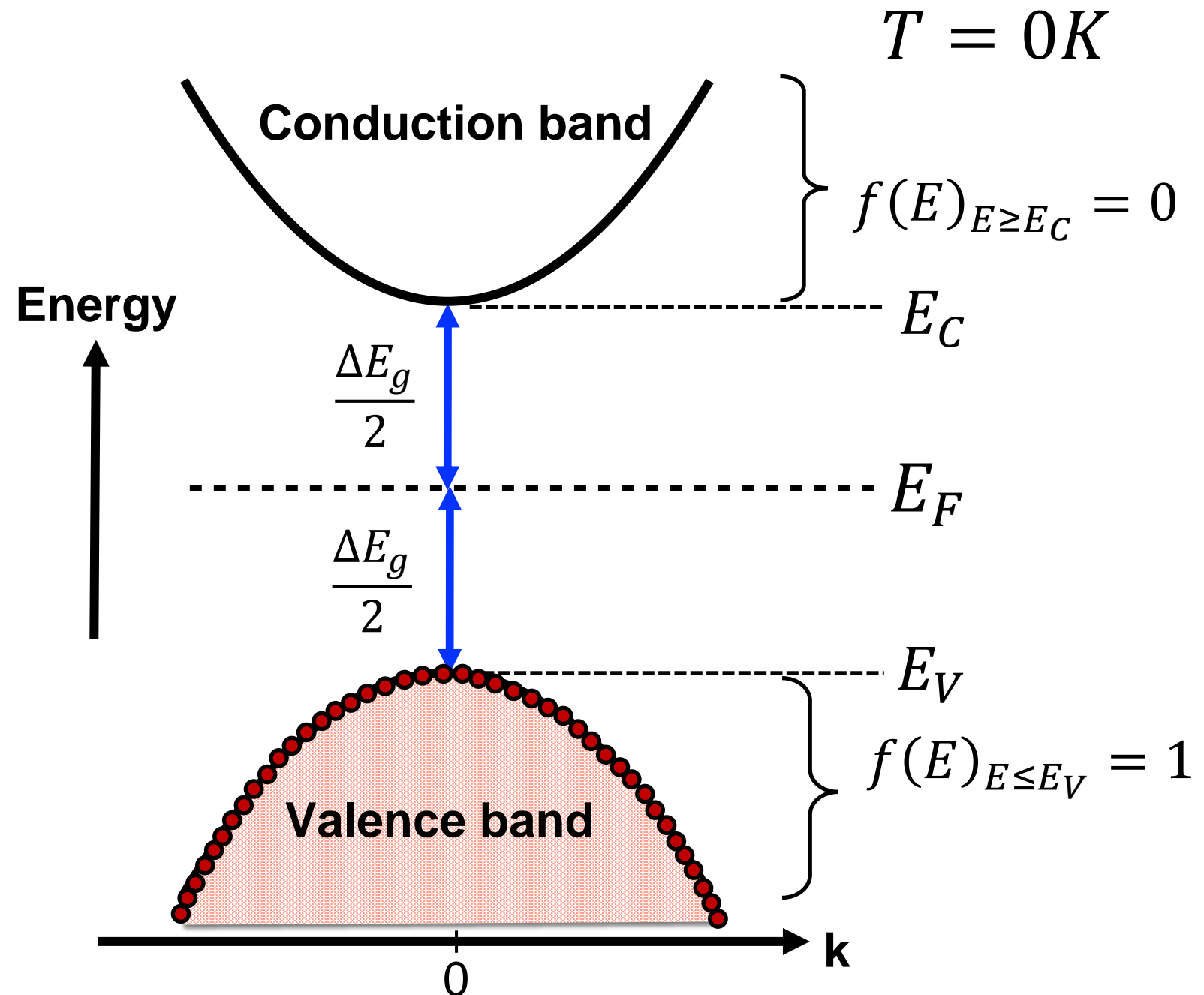
If  $E_F$  is not at midpoint of band gap:



# Where is the Fermi Energy ( $T = 0K$ ) in an intrinsic semiconductor?

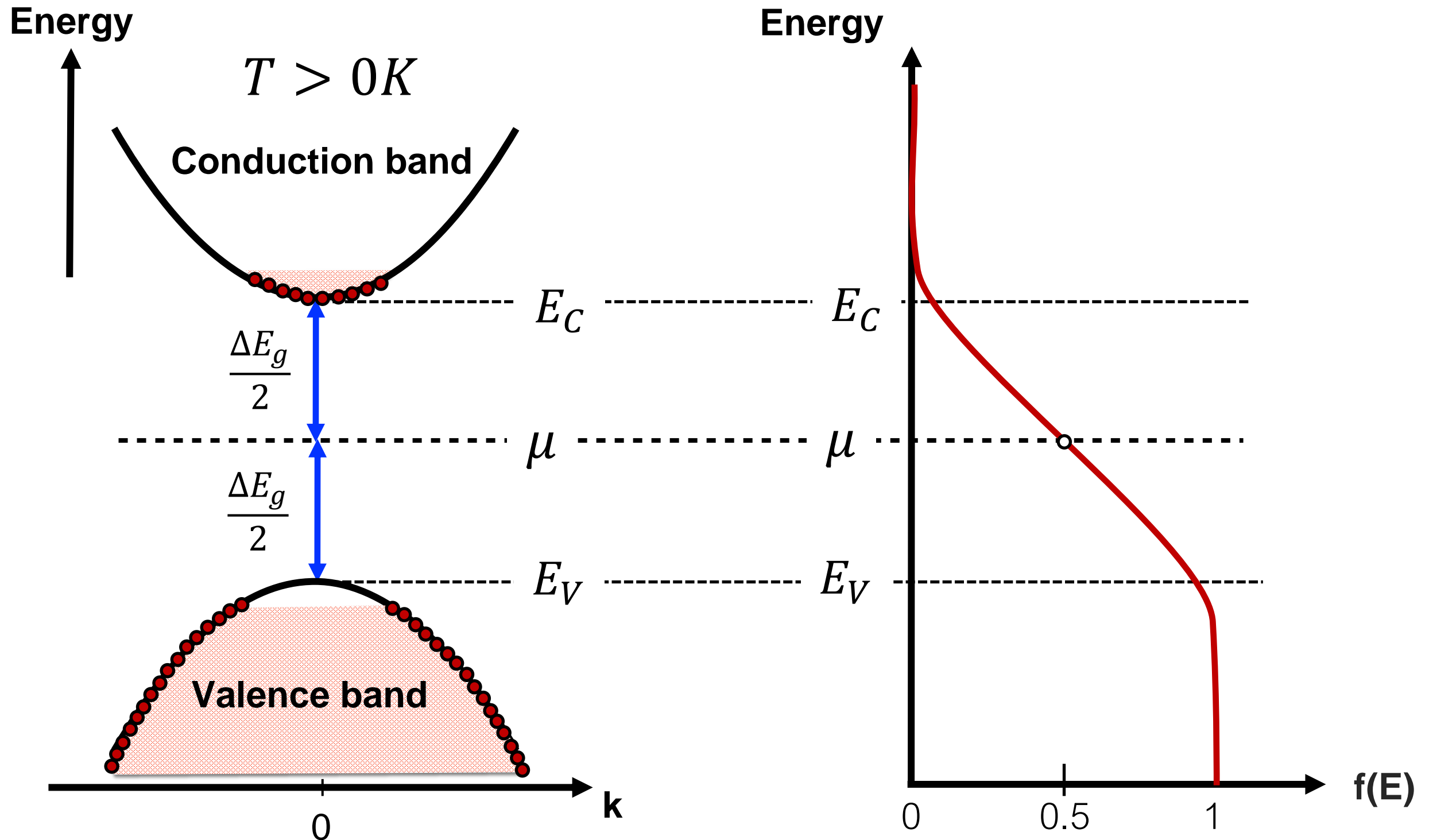
'Fermi Energy' is defined as the energy where  $f(E) = 1/2$  at  $T = 0 K$

[Fermi Level  $\mu(T)$  is defined as the energy where  $f(E) = 1/2$  at  $T > 0 K$ ]



- At  $T = 0 K$ , all energy states in the lower band are populated with probability of unity, i.e.  $f(E) = 1$  for  $E \leq E_V$ .
- For a pure semiconductor  $E_F$  is located in the centre of the energy band gap at  $E_F = E_V + \frac{\Delta E_g}{2}$  (or equivalently  $E_F = E_C - \frac{\Delta E_g}{2}$ )

# Fermi Level ( $T > 0K$ ) in an intrinsic semiconductor



- The Fermi Level positioned mid-gap ensures the number of thermally generated electrons in the conduction band equals the number of holes in the valence band. This picture will change when we later consider the effect of doping.



# Derivation of electron carrier density $n(T)$ in the conduction band at $T > 0$ K

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- We will use our earlier expression for counting up the number of electrons in a defined interval of energy, in this case all energies above the bottom of the conduction band  $E_C$ . For convenience, the upper bound of the integral is set to infinity instead of  $E_{max}$  since negligible error is introduced

$$n_c = \int_{E_C}^{\infty} D(E)f(E)dE$$

- For the Fermi-Dirac function, if we assume the band gap  $\Delta E_g \gg k_B T$  then for energies close to the bottom of the conduction band  $(E - \mu) \gg k_B T$  also, and:

$$f(E) = \frac{1}{1 + e^{\left(\frac{E-\mu}{k_B T}\right)}} \approx \frac{1}{e^{\left(\frac{E-\mu}{k_B T}\right)}} \quad \text{i.e. use classical Boltzmann statistics}$$

- We can use our derived expression for the density of states of an electron band in the free-electron fermi gas. Here the conduction band has minimum value  $E_C$ , rather than zero, so  $E \rightarrow (E - E_C)$  to set the new zero at  $E_C$  for the density of states

$$D(E) = \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E - E_C)^{\frac{1}{2}} \quad D(E) \text{ here is number of states per unit energy per unit volume}$$

- We can now evaluate the integral for the expected total number of electrons per unit volume in the conduction band ( $n_c$ ) at a given temperature  $T$ :

$$n_c = \int_{E_C}^{\infty} D(E) f(E) dE$$

$$n_c = \int_{E_C}^{\infty} \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} (E - E_C)^{\frac{1}{2}} \cdot e^{-\left( \frac{E - \mu}{k_B T} \right)} dE$$

- Take terms not dependent on  $E$  outside integral:

$$n_c = \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} e^{\left( \frac{\mu}{k_B T} \right)} \int_{E_C}^{\infty} (E - E_C)^{\frac{1}{2}} \cdot e^{-\left( \frac{E}{k_B T} \right)} dE$$

- To calculate the integral, move towards changing the variable of integration from  $E$  to  $(E - E_C)/k_B T$ :

$$n_c = \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} e^{\left( \frac{\mu}{k_B T} \right)} e^{\left( \frac{-E_C}{k_B T} \right)} (k_B T) \int_{E_C}^{\infty} \left( \frac{E - E_C}{k_B T} \right)^{\frac{1}{2}} \cdot e^{-\left( \frac{E - E_C}{k_B T} \right)} dE$$

- Now replace  $dE$  with  $d((E - E_C)/k_B T)$

$$n_c = \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} e^{\left( \frac{\mu - E_C}{k_B T} \right)} (k_B T)^{\frac{3}{2}} \underbrace{\int_0^\infty \left( \frac{E - E_C}{k_B T} \right)^{\frac{1}{2}} \cdot e^{-\left( \frac{E - E_C}{k_B T} \right)} d \left( \frac{E - E_C}{k_B T} \right)}_{\int_0^\infty x^{\frac{1}{2}} \cdot e^{-x} dx = \frac{\sqrt{\pi}}{2}}$$

$$n_c = \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{\frac{3}{2}} e^{\left( \frac{\mu - E_C}{k_B T} \right)} (k_B T)^{\frac{3}{2}} \frac{\sqrt{\pi}}{2}$$

$$n_c = 2 \left( \frac{m k_B T}{2\pi \hbar^2} \right)^{\frac{3}{2}} e^{\left( \frac{\mu - E_C}{k_B T} \right)}$$

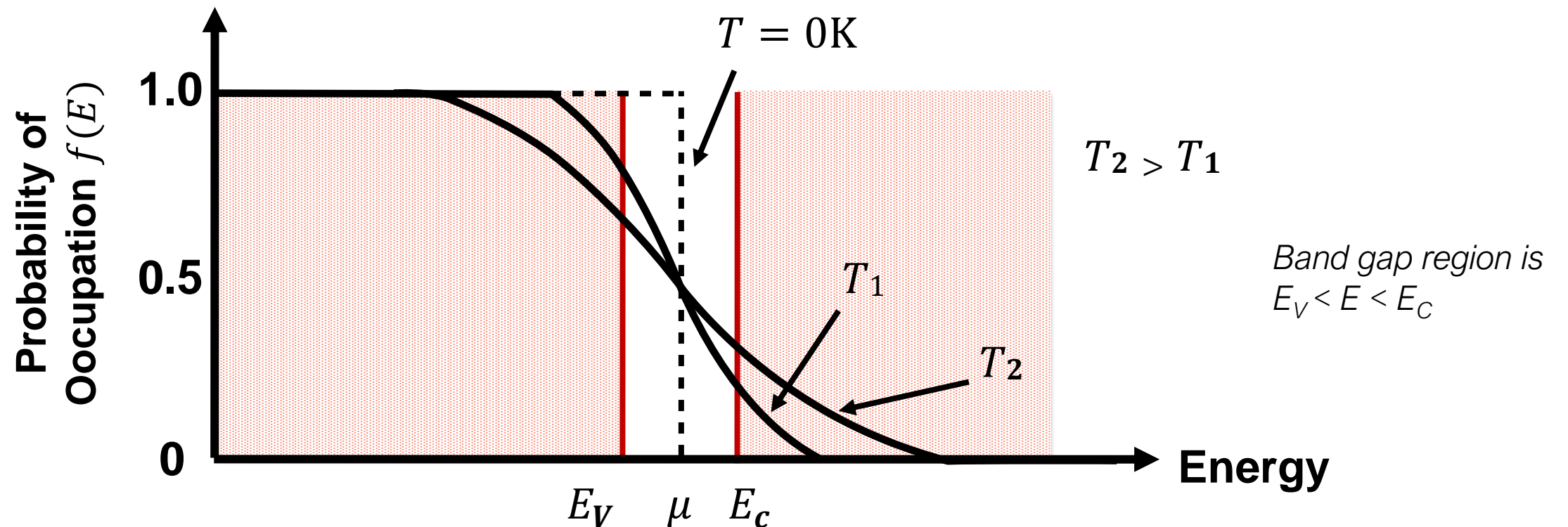
- The conduction band carrier density, usually just denoted as  $n$ , is exponentially dependent on temperature
- The prefactor term does not depend as strongly on temperature and is approximated as a constant:

$$n(T) = C e^{-\left( \frac{E_C - \mu}{k_B T} \right)} \quad \text{where } C = 2 \left( \frac{m k_B T}{2\pi \hbar^2} \right)^{\frac{3}{2}}$$

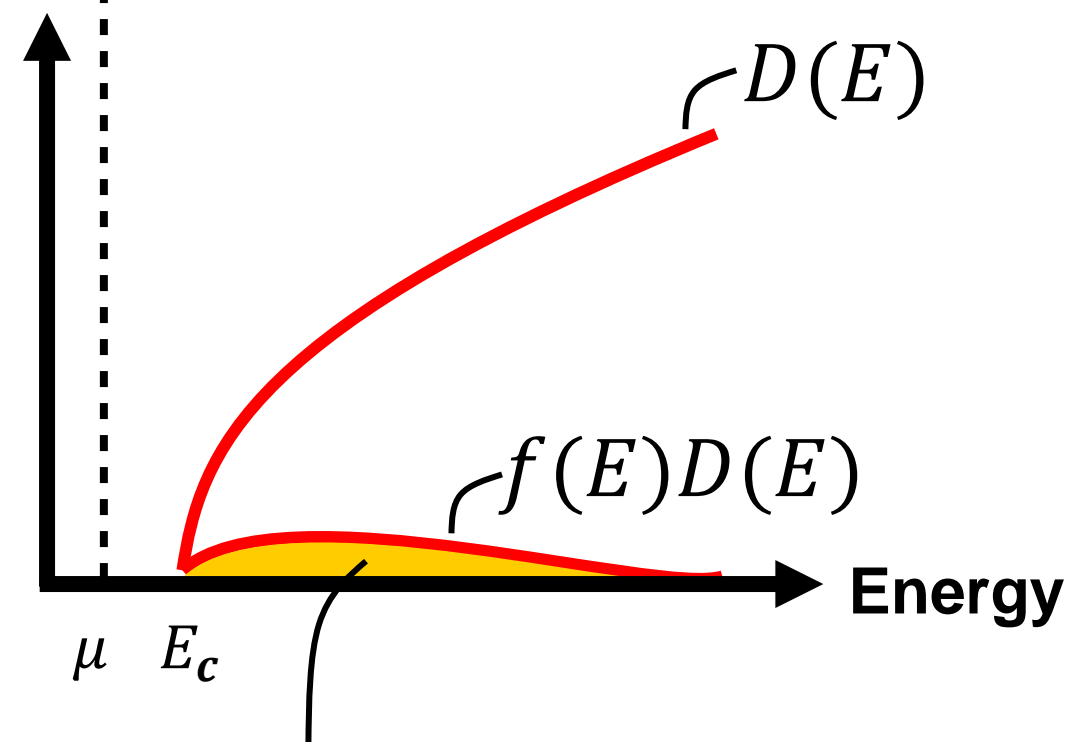
- Assuming the Fermi level to be mid band-gap for an intrinsic semiconductor  $(E_C - \mu) = \Delta E_g / 2$ :

$$n(T) = C e^{-\left( \frac{\Delta E_g}{2 k_B T} \right)}$$

# Temperature dependence of electron distribution



As the temperature increases the probability of occupation at the conduction band edge increases. However, only the 'tail' of the FD function is relevant for  $E > E_C$  so we can approximate it using the Boltzmann distribution



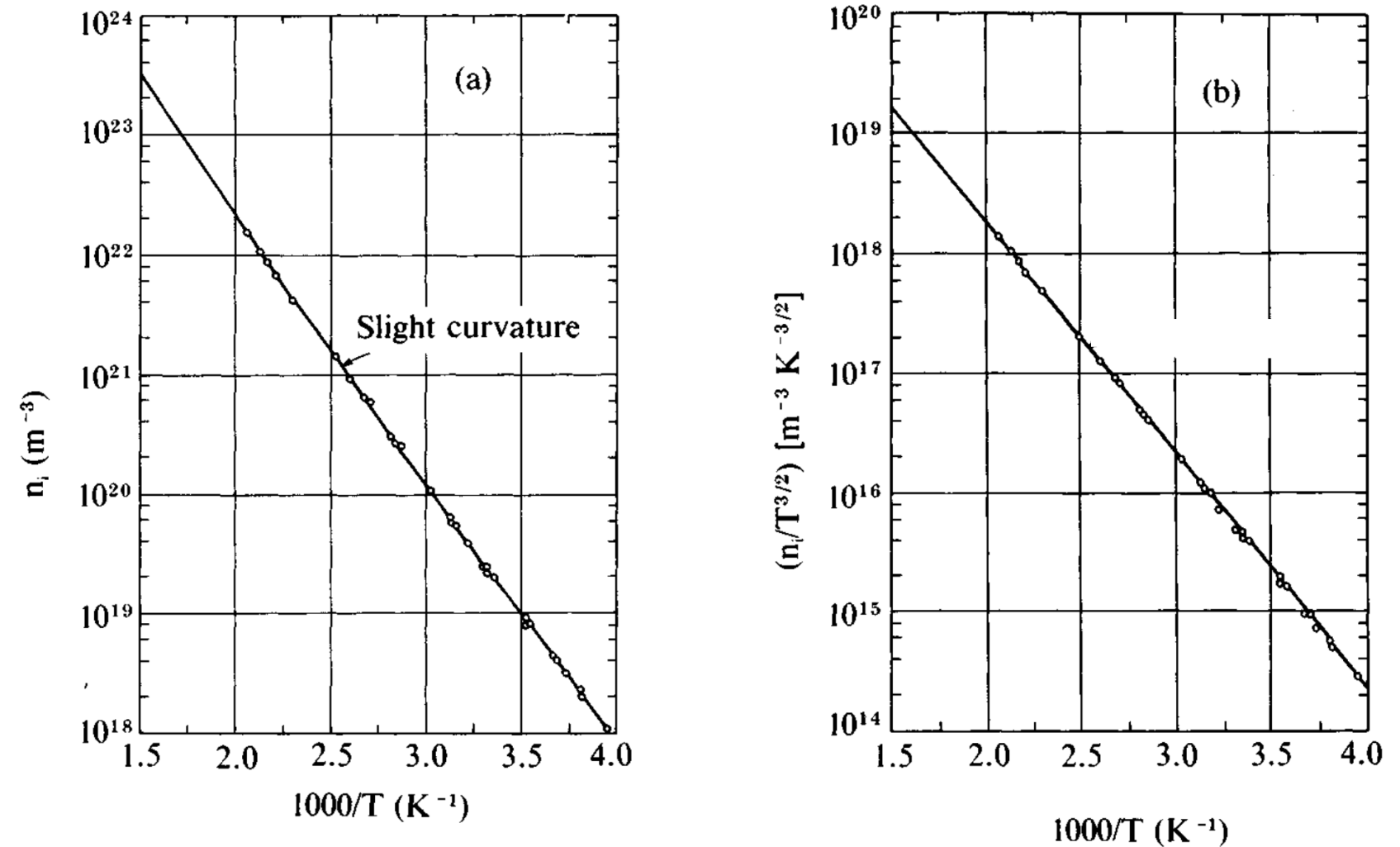
The orange shaded area is  $n(T)$ , the electron density in the conduction band

After J S Blakemore  
 “Solid state physics”  
 pp305

$$n(T) = \int_{E_C}^{\infty} D(E)f(E)dE$$

$$n(T) \approx C e^{-\left(\frac{\Delta E_g}{2k_B T}\right)}$$

$$\text{where } C \propto T^{\frac{3}{2}}$$



**Figure 4-7** (a), Semilogarithmic presentation of intrinsic concentration as a function of reciprocal temperature for germanium. The experimental points are the data of Morin and Maita, Phys. Rev. **96**, 28 (1954). Note the slight curvature caused by the  $T^{3/2}$  temperature dependence of  $(N_c N_v)^{1/2}$ . (b), The same data replotted with  $(n_i/T^{3/2})$  as ordinate. This can be interpreted in terms of Equation 4-20. The points shown are based on experimental measurements of the Hall effect.

- Intrinsic semiconducting behaviour can generally be verified by resistance vs temperature measurements and the carrier density vs temperature can be determined by Hall Effect measurements as a function of temperature

- We are now in a position to obtain an estimate for the number of electrons per unit volume in the conduction band at a given temperature:

$$n(T) = C e^{-\left(\frac{E_c - \mu}{k_B T}\right)}$$

From earlier band diagram see that:  $E_c - \mu \approx \frac{\Delta E_g}{2}$

$$\therefore n(T) = C e^{\left(\frac{-\Delta E_g}{2k_B T}\right)}$$

- For many semiconductors and insulators,  $C \sim 10^{25} \text{ m}^{-3}$
- For Si we have  $\Delta E_g = 1.11 \text{ eV}$ , at  $T = 300 \text{ K}$  with  $C = 3 \times 10^{25} \text{ m}^{-3}$

$$n(T) \approx (3 \times 10^{25}) e^{-\left(\frac{(1.11)(1.6 \times 10^{-19})}{2(1.38 \times 10^{-23})(300)}\right)} = (3 \times 10^{25})(4.8 \times 10^{-10}) \text{ m}^{-3}$$

$$n(T) \approx 1.45 \times 10^{16} \text{ m}^{-3}$$

- If we do the same for diamond with  $\Delta E_g = 5.5 \text{ eV}$ :

$$n(T) \approx 2 \times 10^{-21} \text{ m}^{-3}$$

- A factor of 5 change in the bandgap leads to 37 orders of magnitude difference in the electron population in the conduction band! These vastly different results depending on  $\Delta E_g$  accounts for the difference between semiconductors and insulators. Remember for metals  $n$  is in the range of  $10^{28} \text{ m}^{-3}$

# The energy gap between valence and conduction bands is characteristic of insulators and semiconductors

**Values of the energy gap for sample insulators and semiconductors:**

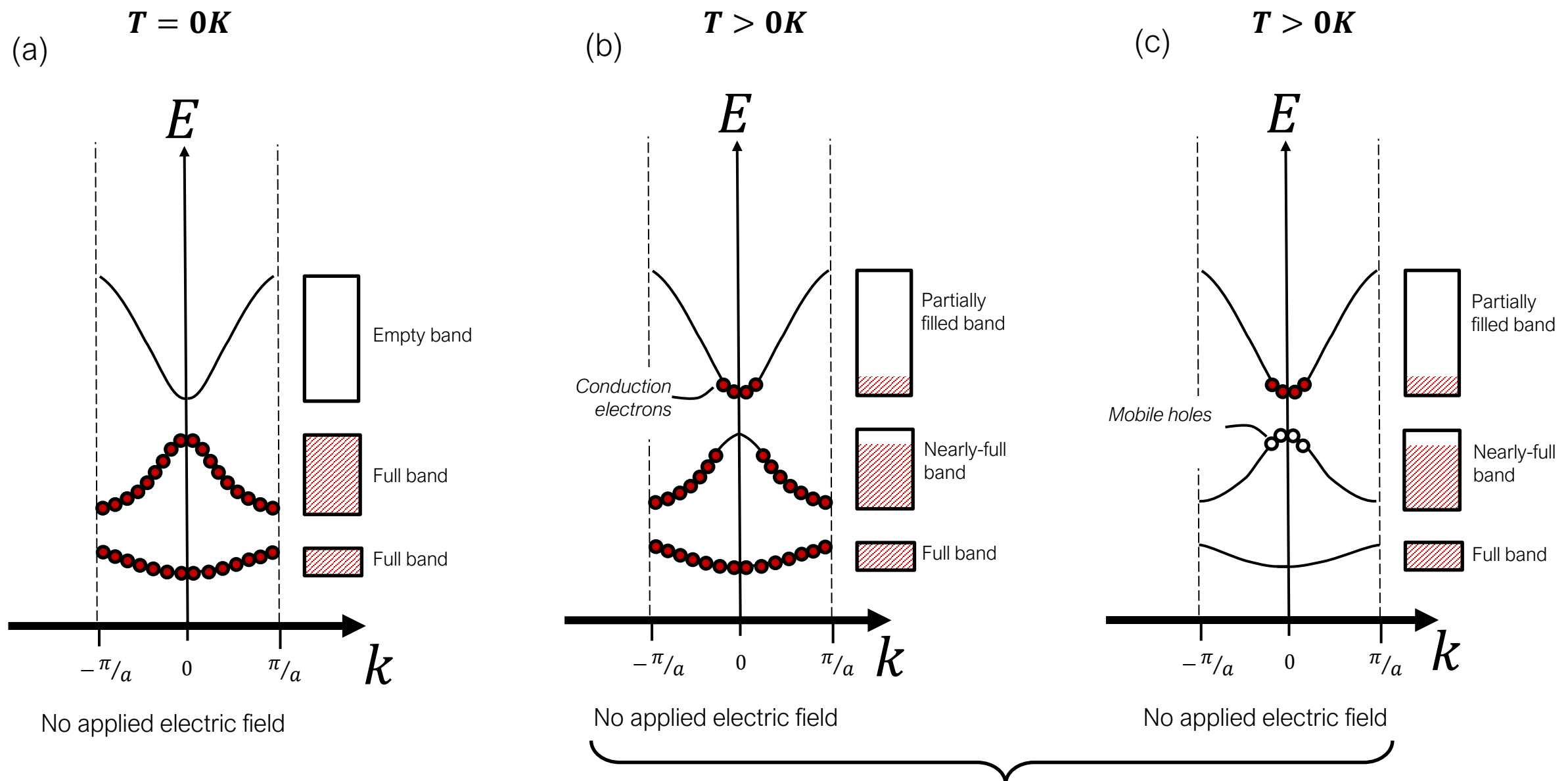
	$E_g$ (eV)
Diamond	5.5
Silicon Carbide	2.3
Galium Arsenide	1.43
Silicon	1.11
Germanium	0.67
Indium antimonide	0.18

- The distinction between insulators and semiconductors is based on the energy width of the band-gap, band gap values of ~several eV leads to insulating behaviour (e.g. SiC, diamond)
- Band-gaps of order ~ 1eV give semiconducting behaviour at room temperature



# Electron/hole pair generation in semiconductors (again)

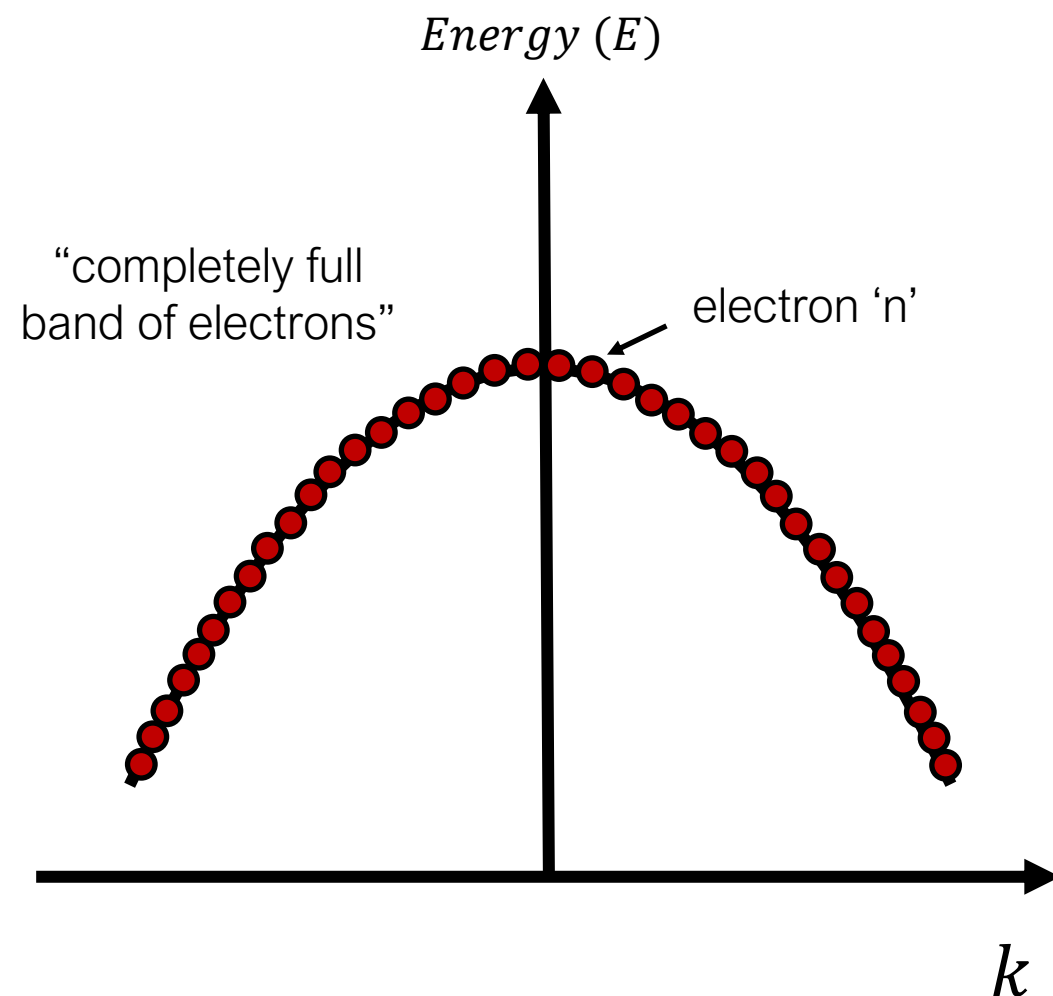
- The classical theory of conduction was unable to explain 'anomalous' Hall voltage measurements that suggested current flow was due to positive charge movement in some materials.
- The energy band picture for semiconductors can account for this through the existence and movement of positively charged electron-holes - vacancies in a nearly-full band.



(b) and (c) show equivalent ways of describing the effect of a nearly-full band of electrons

# Rationalising the behaviour of electron-holes

- The hole concept is an abstraction that gives a convenient way of describing the behaviour of electrons in a nearly-full band
- Examine the case of a full-band at  $T = 0K$  which then becomes a nearly-full band at elevated temperature due to thermal carrier generation:



- For every occupied +ve k-state moving with some velocity  $v_m$  there is also an occupied -ve k-state with  $k_m$  that has the same speed but in the opposite direction  $-v_m$  i.e. no current flows overall:

$$J_{tot} = \frac{-e}{V} \sum_m v_m = 0 \quad V = \text{volume of crystal}$$

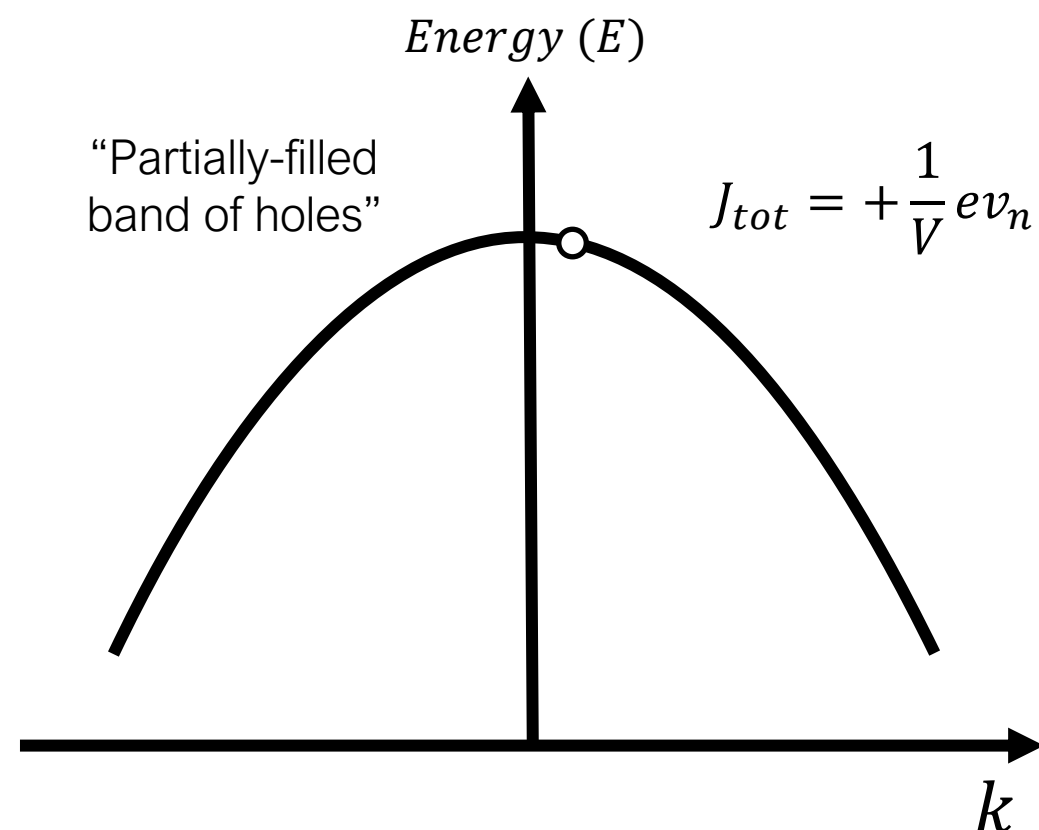
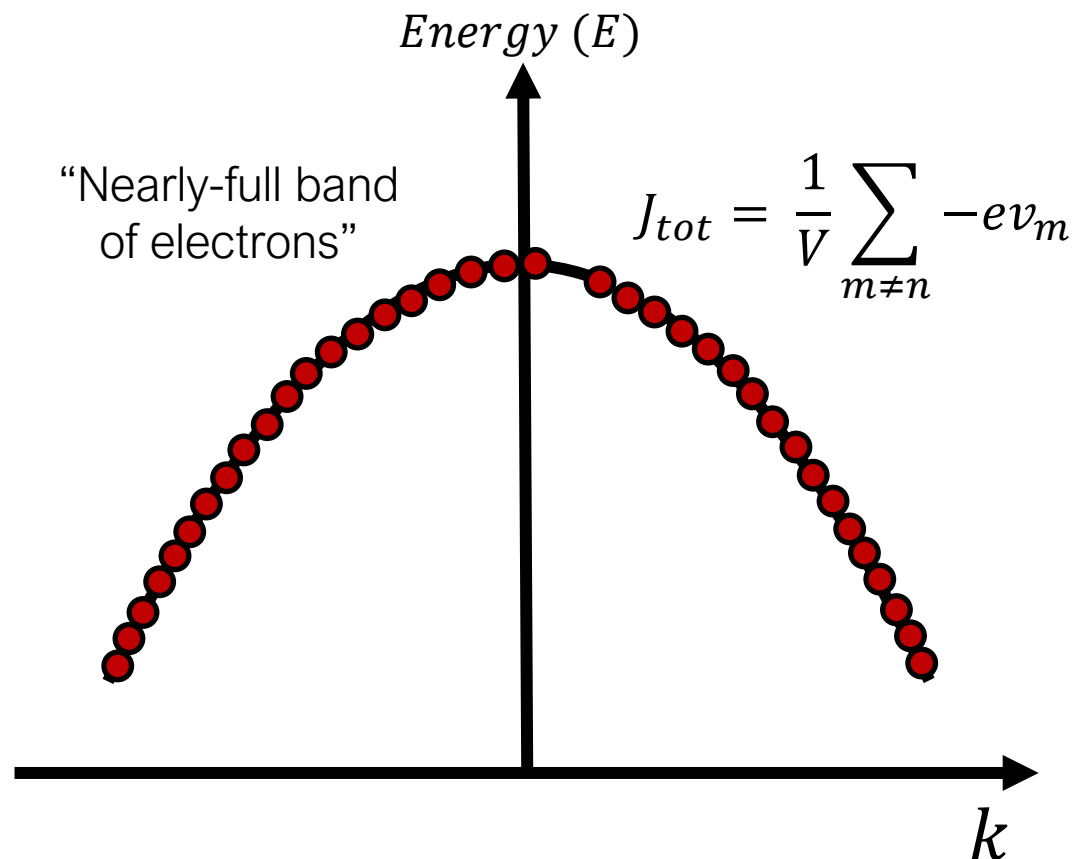
- Arbitrarily single out an occupied single state 'n' and take it outside the summation

$$J_{tot} = -\frac{e}{V} v_n - \frac{e}{V} \sum_{m \neq n} v_m = 0$$

hence

$$+\frac{e}{V} v_n = \frac{-e}{V} \sum_{m \neq n} v_m$$

# Rationalising the behaviour of electron-holes



- Now, consider the case where the single electron in some state ‘n’ is removed from the band. Now the total current due to the band is non-zero:

$$J_{tot} = \frac{-e}{V} \sum_{m \neq n} v_m \neq 0$$

But since  $\frac{-e}{V} \sum_{m \neq n} v_m = + \frac{e}{V} v_n$

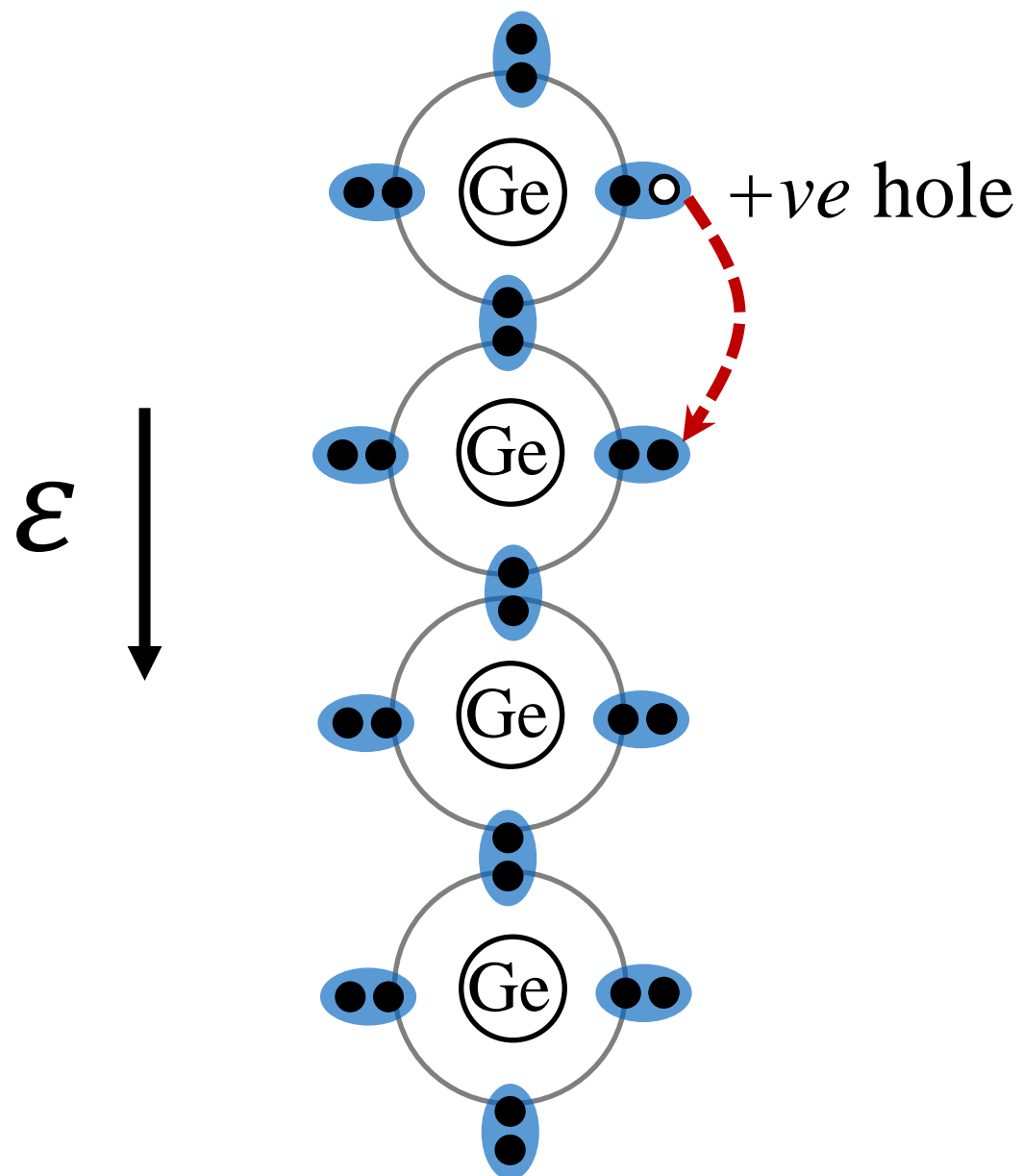
$$J_{tot} = + \frac{e}{V} v_n$$

- i.e. we see that the behavior of the nearly-full electron band is equivalent to an otherwise empty band with a single positively charged electron (a ‘hole’)
- The current due to a ‘hole’ corresponds to a charge +e moving with the velocity associated with the missing quantum state:

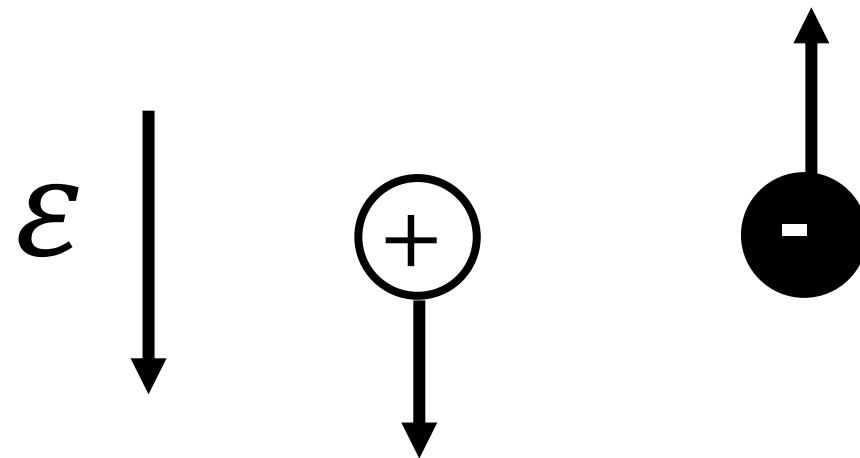
$$J_{hole} = + \frac{1}{V} e v_n$$

# Electric-field motion of electron-holes

- The vacancy moves under applied E-fields in the same way as a positively charged particle is expected to, and is therefore considered as a **positively charged** quasiparticle called an electron “**hole**” with charge  $+e$
- Electron and hole movement under fields contribute *independently* to current



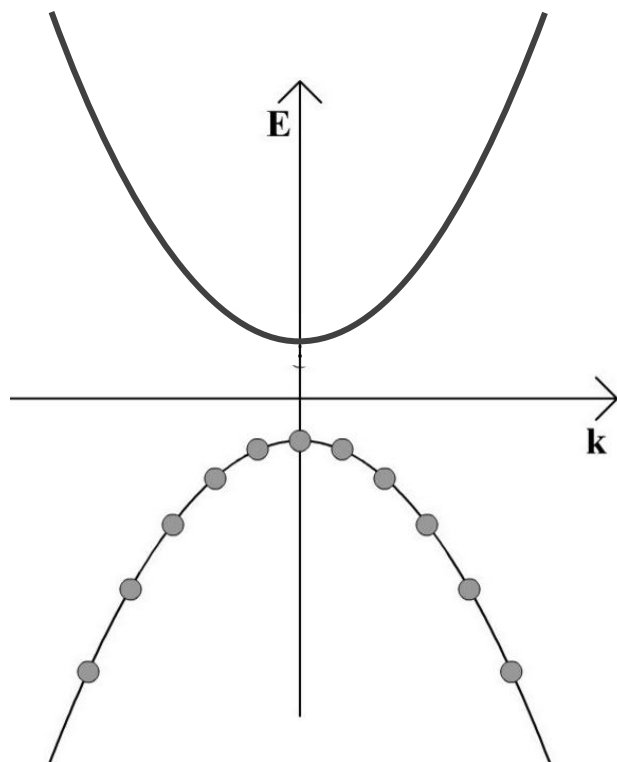
Direction of motion under  $\mathcal{E}$ -field



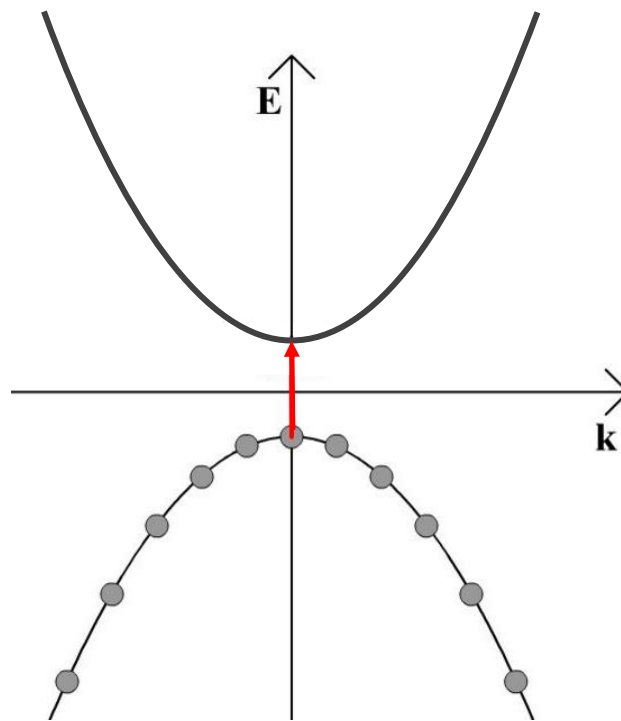
# Energy-wavevector plots for semiconductors

- We know from metals that the energy levels of electrons can be described by a parabolic  $E(k)$  relationship
- The lower energy valence band is typically well approximated as an inverted parabola near the top of the band (close to  $k = 0$ )

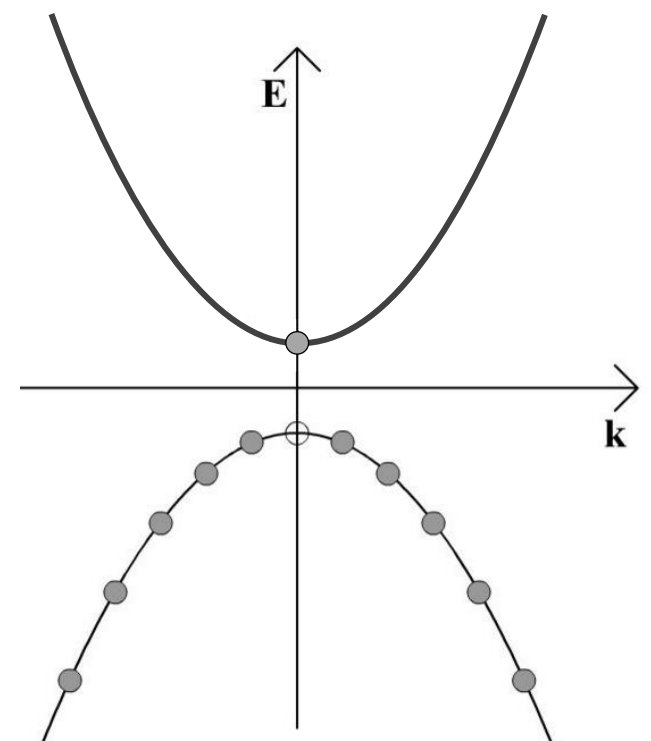
Empty conduction band:



Electron thermally excited across the energy gap:



An electron-hole pair is produced:

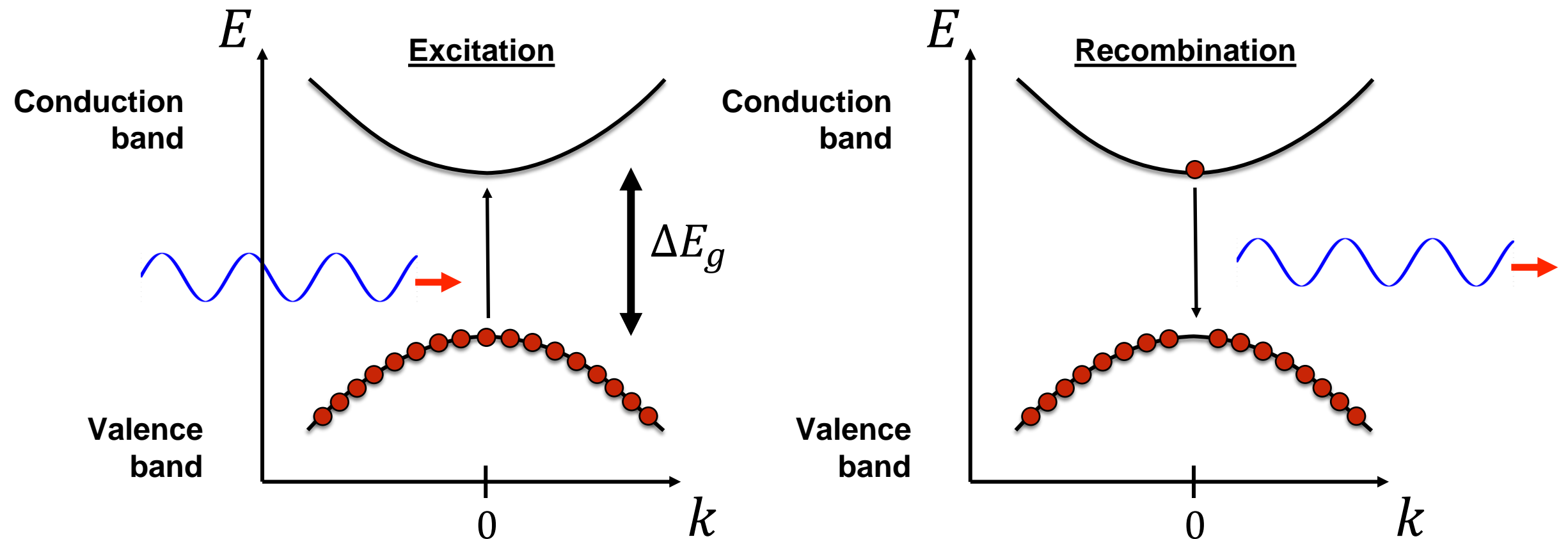


$$n_i = p_i$$

in an “intrinsic” (elementally-pure) semiconductor (subscript  $i$  refers to intrinsic)

# Photon induced electron/hole pair generation

- Up to now we have considered thermal agitations at temperature  $T$  as responsible for populating the conduction band
- The energy required to promote an electron into the conduction band can also be provided by absorption of photons with frequency beyond a threshold value



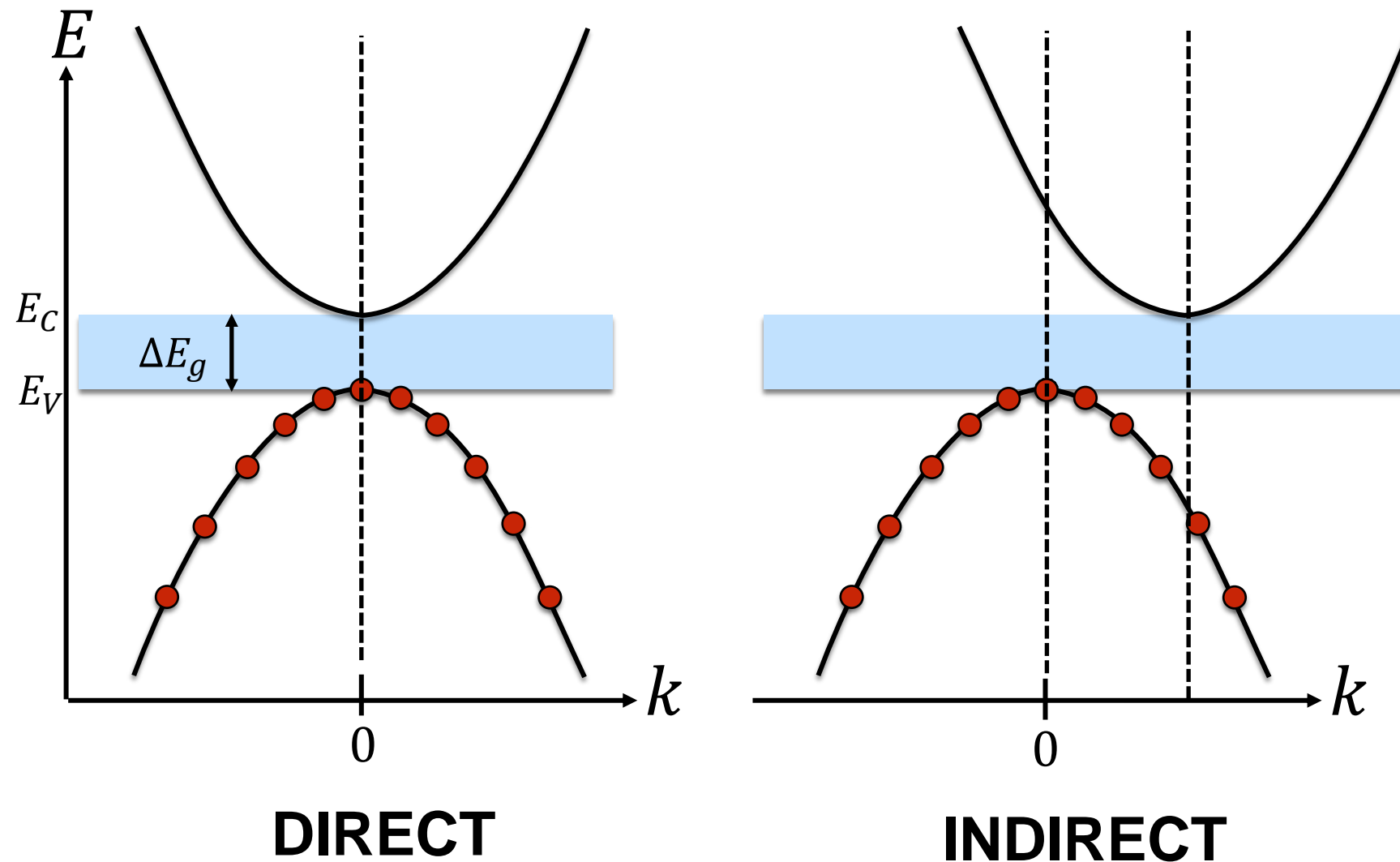
- Minimum threshold frequency to promote electrons over the gap is

Photon energy:  $E = hf$

Minimum frequency  
for creation of  
electron/hole pair:  $f_{min} = \frac{\Delta E_g}{h}$

# Direct & Indirect semiconductors

- Absorption of a photon of the correct energy is not the whole picture. We also need to consider conservation of  $k$ -vector (momentum) between the initial/final electron energy states.

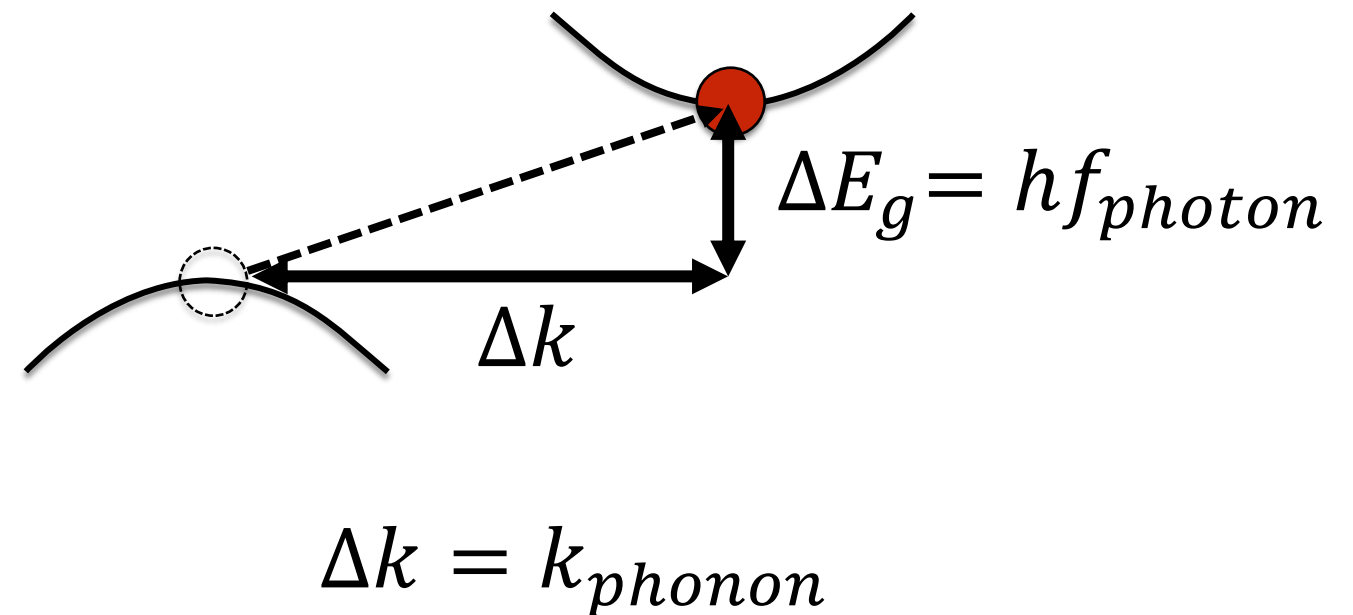
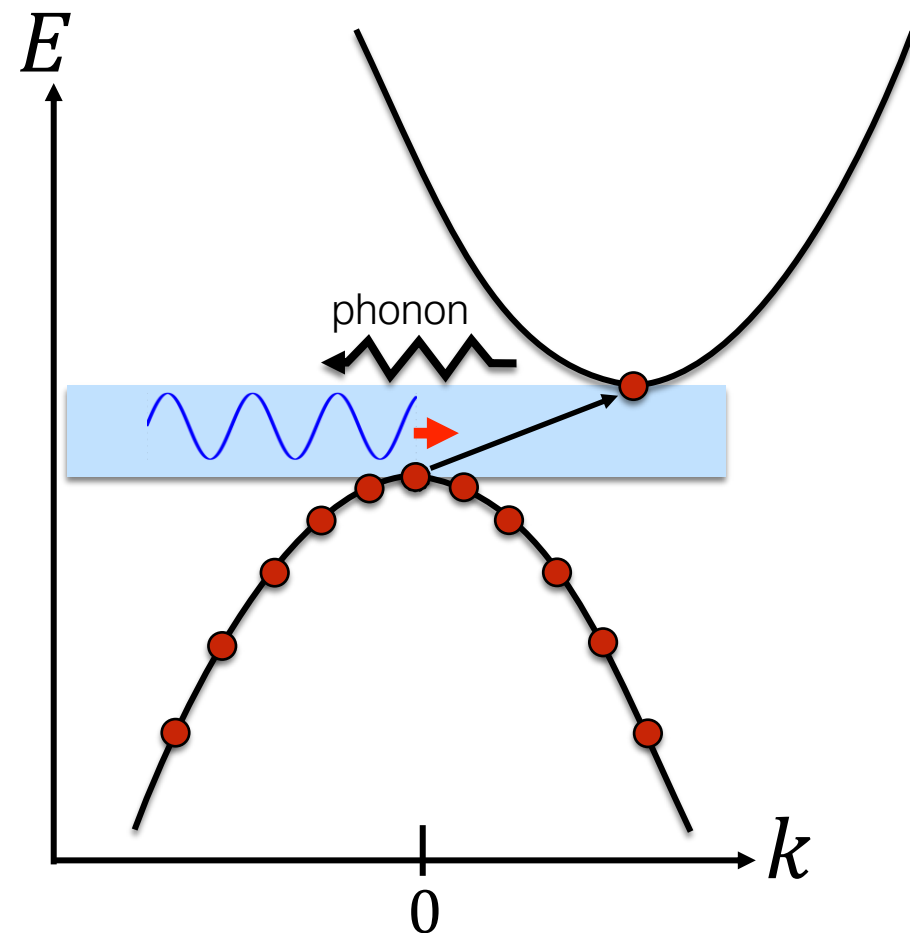


“**Direct**” semiconductor: the top of the valence band and bottom of conduction band ( $\Delta E_g$ ) occur at the same  $k$ -states for both bands. During a recombination event, change in the electron  $k$ -state  $\Delta k = 0$  (i.e. no change in momentum) and a photon can be emitted directly



# Direct & Indirect semiconductors

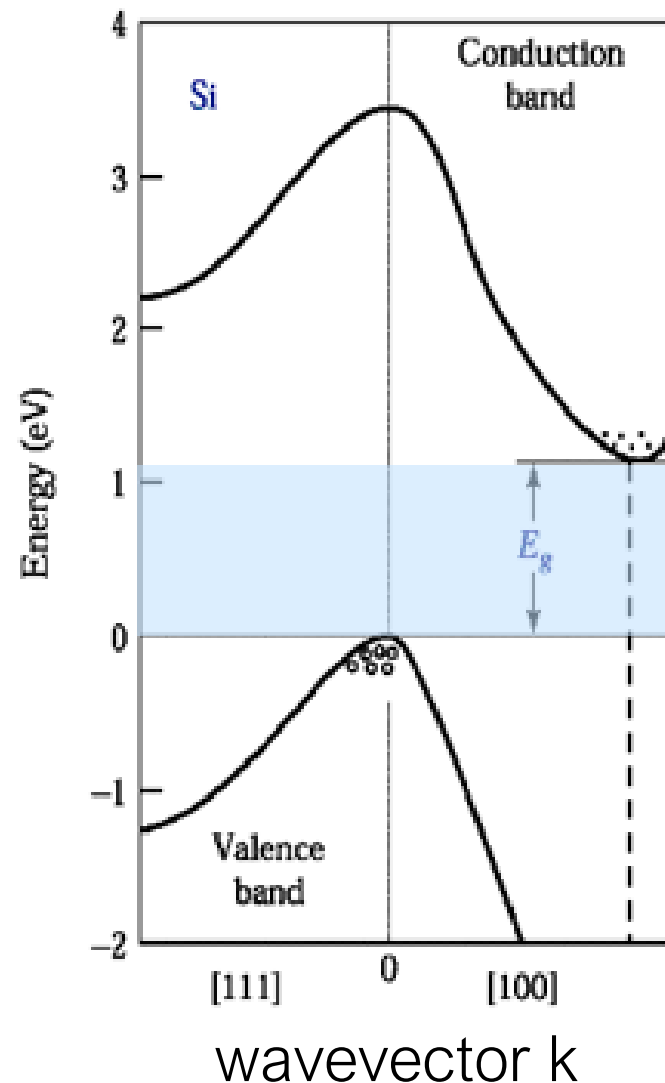
## INDIRECT



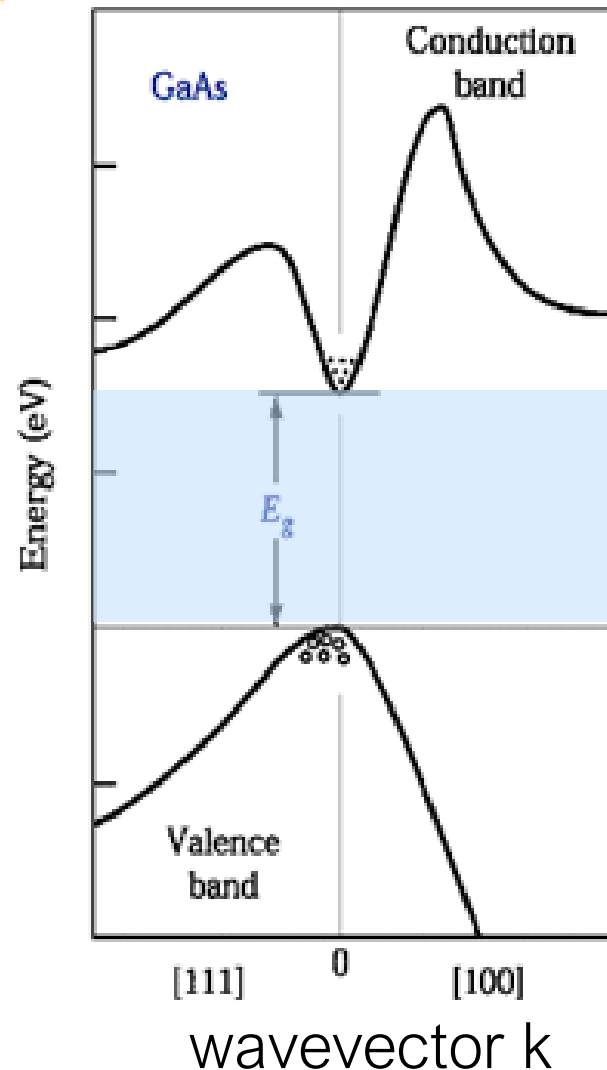
“Indirect” semiconductor: Minimum energy of conduction band and maximum of valence band occur at different  $k$ -states (momentum states). Conservation of momentum requires **phonon** emission/absorption to take up the difference between initial/final electron momentum states.

# Real Direct & Indirect semiconductor band structures

Silicon band structure



Gallium Arsenide band structure



- Silicon has an indirect bandgap whereas Gallium Arsenide has a direct bandgap
- Rate of electron-hole recombination (and photon emission) is less for Si due to necessity of absorption/emission of a phonon with the appropriate momentum, hence Si is not efficient for optical devices such as light emitting diodes
- Direct bandgap semiconductors are used for optical devices

## Additional important points for reading bandstructure diagrams:

- Note that the zero of the energy scale has been set to the highest occupied energy level at  $T = 0K$ . This indicates a full valence band and tells us right away we are dealing with a semiconductor or insulator and not a metal
- The size of the bandgap indicates that the material is likely to be a semiconductor at room temperature
- The  $k$ -axis is labelled in terms of crystallographic directions, indicating different  $E-k$  profiles along different crystal axes (anisotropy). The  $k = 0$  point is often called the “ $\Gamma$  –point”

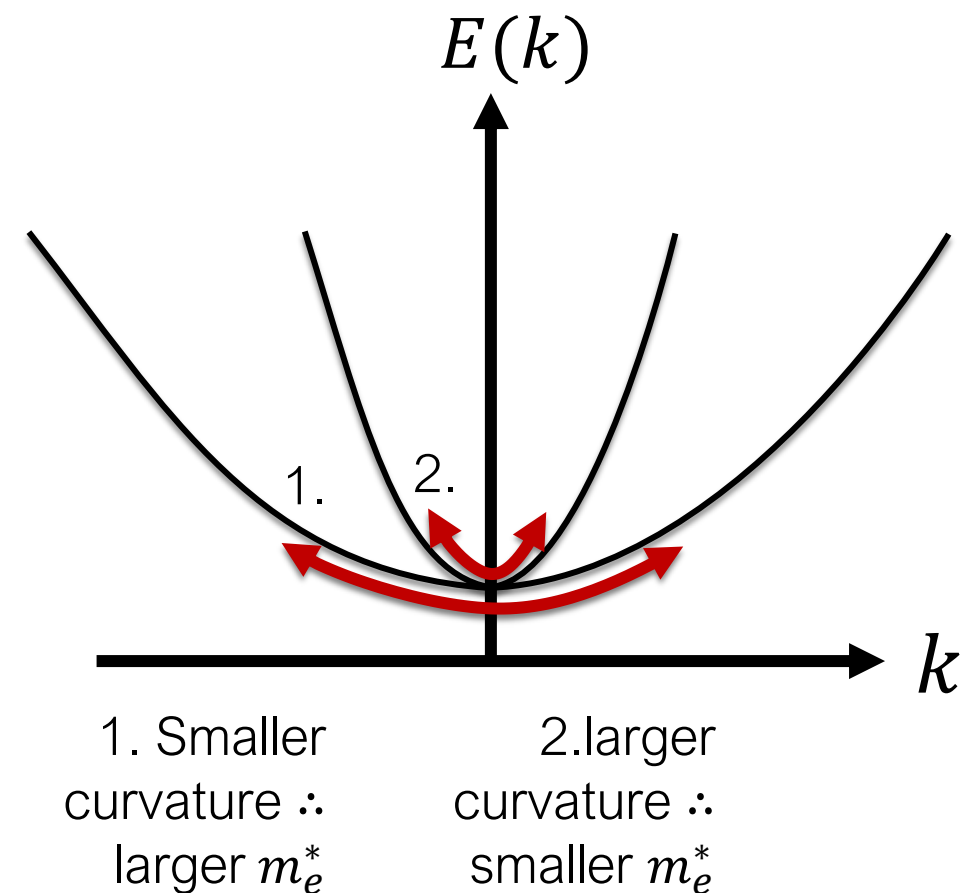
# The effective mass $m^*$

- What will be the influence of the periodic potential on electrons when we are considering the effect of electric fields (compared to free electron gas picture)?
- We can account for this by considering an electron travelling through the crystal to respond to applied fields as if it has an “**effective mass**”  $m_e^*$ . This allows us to continue to treat the electron as a freely propagating particle but with a renormalised mass which accounts for the lattice interactions
- Examining the  $E(k)$  relationship for a parabolic band for example:

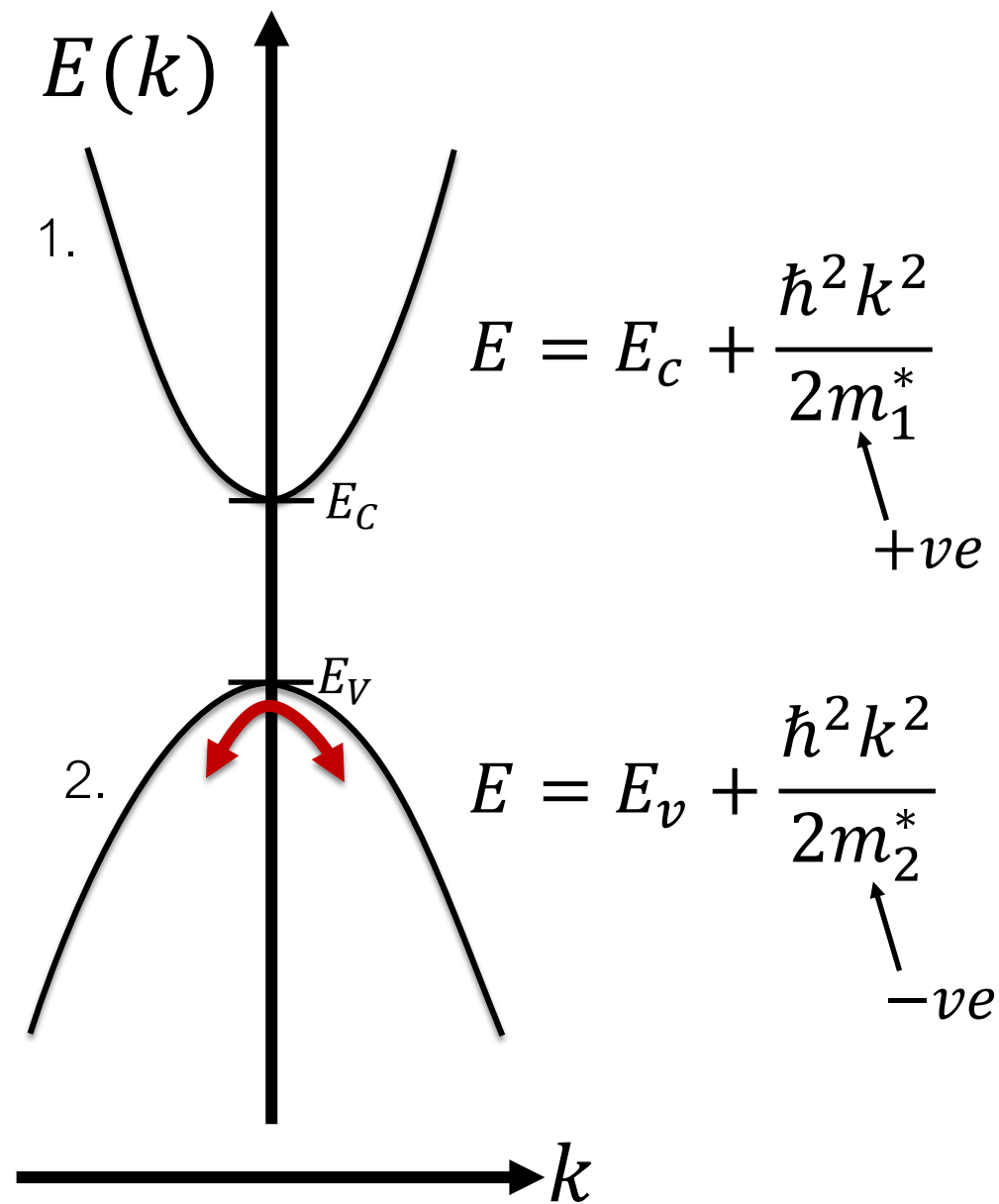
$$E(k) = \frac{\hbar^2 k^2}{2m_e^*}$$

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m_e^*} \quad \text{and} \quad \frac{d^2 E}{dk^2} = \frac{\hbar^2}{m_e^*}$$

$$\therefore m_e^* = \hbar^2 \left[ \frac{d^2 E}{dk^2} \right]^{-1}$$



- The effective mass for a given k-state is proportional to the **local inverse curvature** of the band



\*Shockley reasons that the hole must have a positive mass to be consistent with a current being developed in the same direction as the field (as is observed experimentally)

- Looking at the curvature of a nearly-full electron band near  $k = 0$  we see that the effective mass  $m_e^*$  is a negative number

$$m_2^* = \hbar^2 \left[ \frac{d^2 E}{dk^2} \right]^{-1} = -ve$$

- In other words, the electrons in the nearly-full band respond to applied E-fields as if they have a negative mass!
- Resolution: electrons still have the same bare mass  $m_0$  but  $m_e^*$  also takes into account the interaction forces with the lattice (so that we don't have to consider them separately)
- In the negative mass region, electrons are accelerated in the E-field direction (usually accelerated counter to E-field direction)
- The nearly-full band carrier contribution can be described by holes which have both **positive charge** and **positive effective mass**

# The effective mass

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- We can also denote effective mass for holes as  $m_h^*$
- Revisit our analysis for the conductivity to take electron and hole conduction into account. Note that we now anticipate different drift velocity for electrons and holes:

$$\text{electrons } v_e = - \left[ \frac{e\tau_e}{m_e^*} \right] \varepsilon \qquad \text{holes } v_h = \left[ \frac{e\tau_h}{m_h^*} \right] \varepsilon$$

- We use the general definition of the drift velocity to define the ‘mobility’, a measure of how easily the charge carriers move through the lattice

$$v = \mu \varepsilon \qquad \text{where mobility } \mu = \frac{e\tau}{m^*}$$

- Value of  $\mu$  depends on the material considered, charge type (electron or hole) and temperature

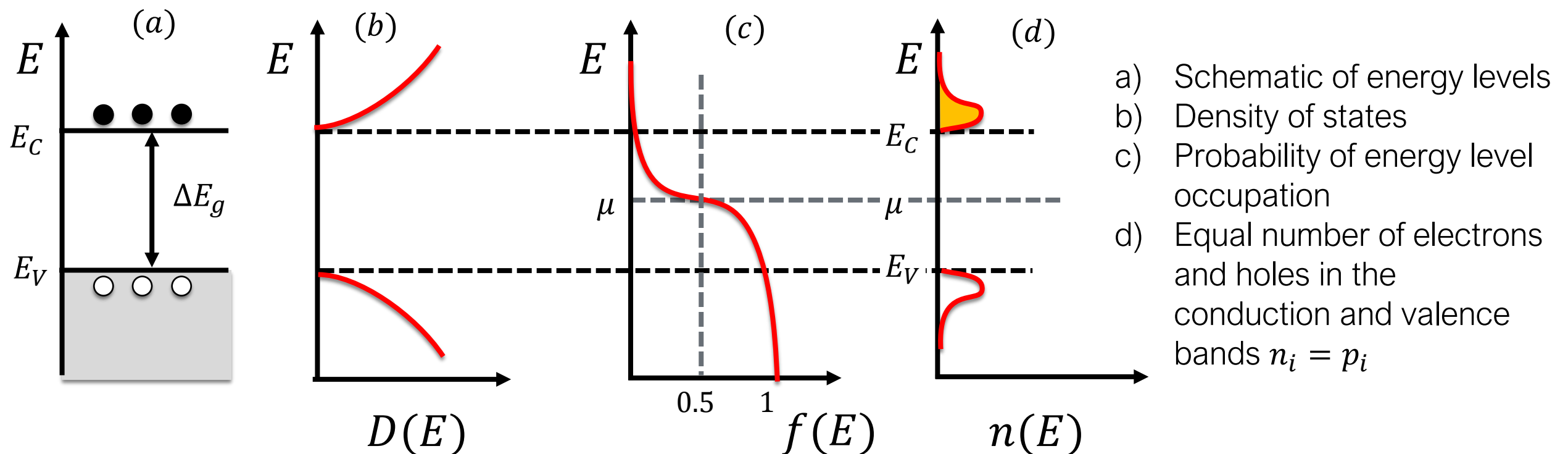
$$\text{electron mobility } \mu_e = \frac{e\tau_e}{m_e^*} \qquad \text{hole mobility } \mu_h = \frac{e\tau_h}{m_h^*}$$

- The conductivity can then be written:

$$\sigma = \frac{ne^2\tau}{m_e} = ne\mu \quad \text{becomes } \sigma = e(n_i\mu_e + p_i\mu_h)$$

# Intrinsic semiconductors (summary)

- So far, we have only considered generation of electron/hole pairs by thermal excitation or by photon absorption as the only means to create mobile carrier pairs in a pure semiconductor (“intrinsic”)
- The number of electrons equals the number of holes at all temperatures in an intrinsic semiconductor i.e.  $n_i = p_i$
- Incorporation of impurity species onto lattice sites in the semiconductor enables the magnitude of conductivity and the majority carrier charge type (p- or n-type) to be controlled
- Important plots as a function of energy (y-axis) for an *intrinsic* semiconductor:



Note, probability of electron energy level occupancy:  $f(E) \approx e^{-\left(\frac{E-\mu}{k_B T}\right)}$

$\therefore$  probability of hole occupancy in valence band:  $1 - f(E) \approx 1 - e^{-\left(\frac{E-\mu}{k_B T}\right)}$