Phys 570

Lecture #9

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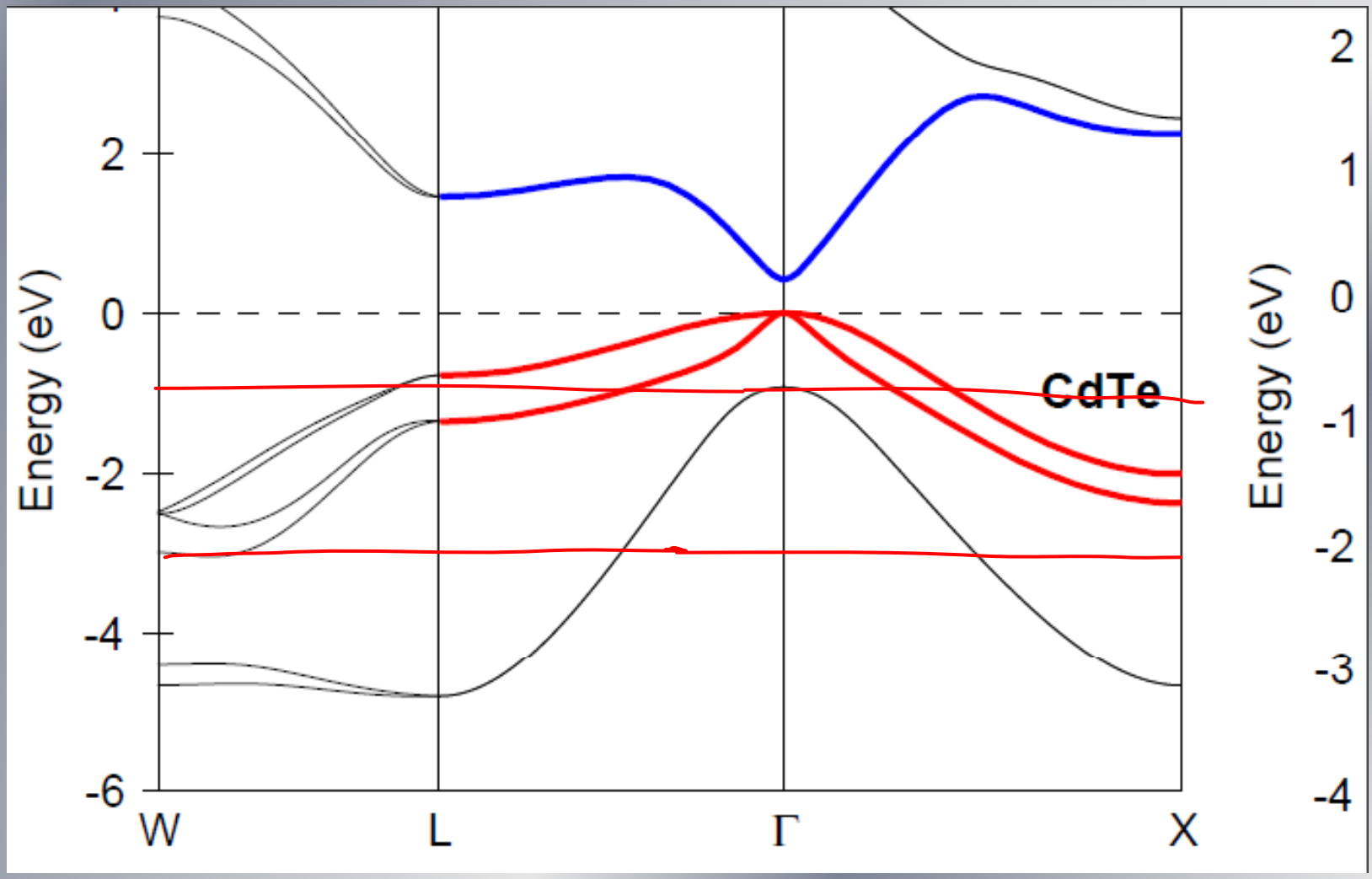
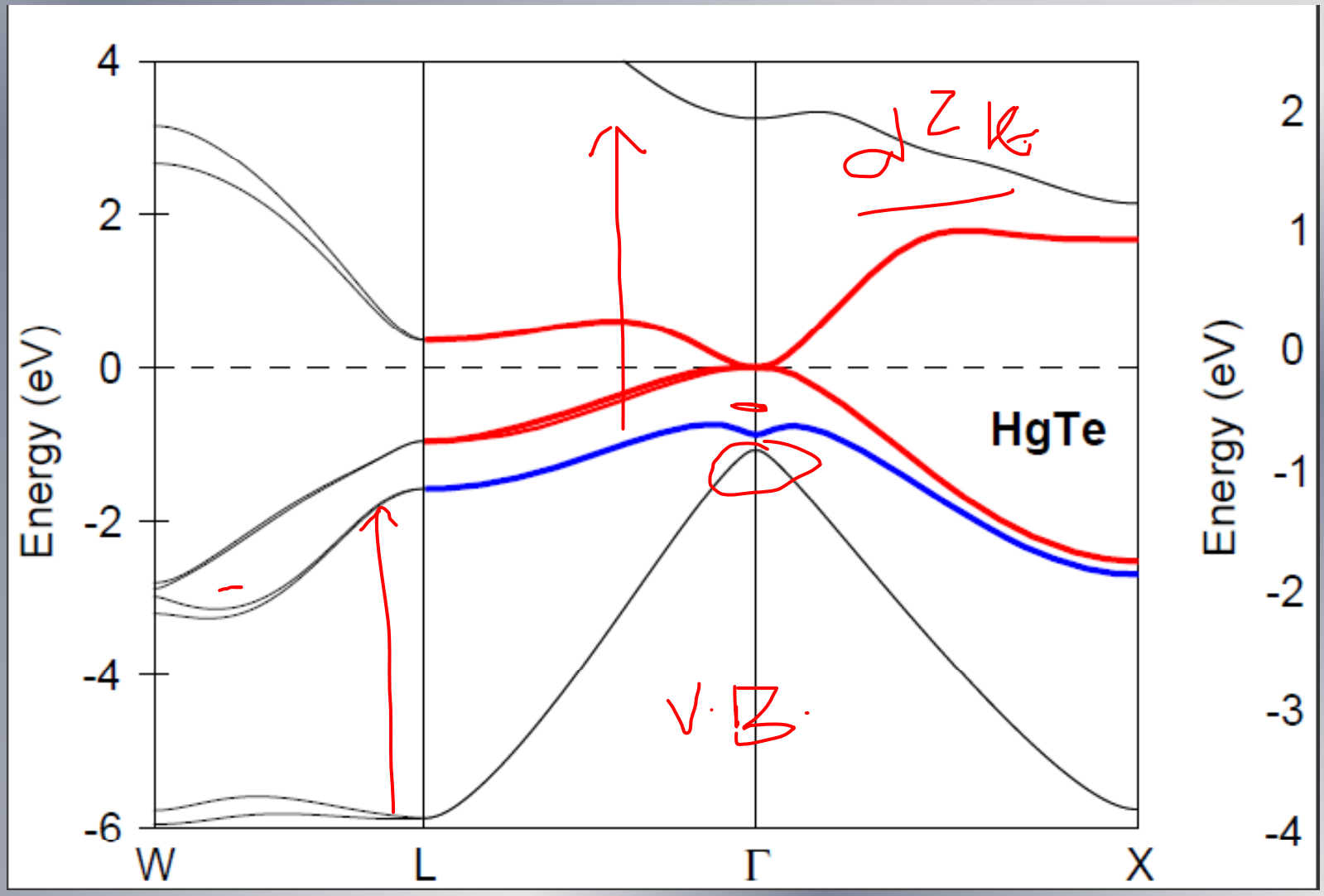
Chapter 8: SEMICONDUCTOR CRYSTALS

Band Structure in CdTe (negative band gap)



Chapter 8: SEMICONDUCTOR CRYSTALS

Band Structure in HgTe (negative band gap)



Chapter 8: SEMICONDUCTOR CRYSTALS

Holes

- The properties of vacant orbitals in an otherwise filled band are important in semiconductor physics and in solid state electronics. Vacant orbitals in a band are commonly called holes, and without holes there would be no transistors.
- A hole acts in applied electric and magnetic fields as if it has a positive charge *+e*. The reason is given in five steps:

1- $K_h = -k_e$ **(17)**

- The total wavevector of the electrons in a filled band is zero: $\Sigma \mathbf{k} = \mathbf{0}$, where the sum is over all states in a Brillouin zone.
- If the band is filled all pairs of orbitals k and ***-k*** are filled, and the total wavevector is zero
- If an electron is missing from an orbital of wavevector $\boldsymbol{k_e}$, the total wavevector of the system is ***-k***, and is attributed to the hole
- The hole is an alternate of a band with one missing electron.

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Electron –Hole Conservation of Total Momentum

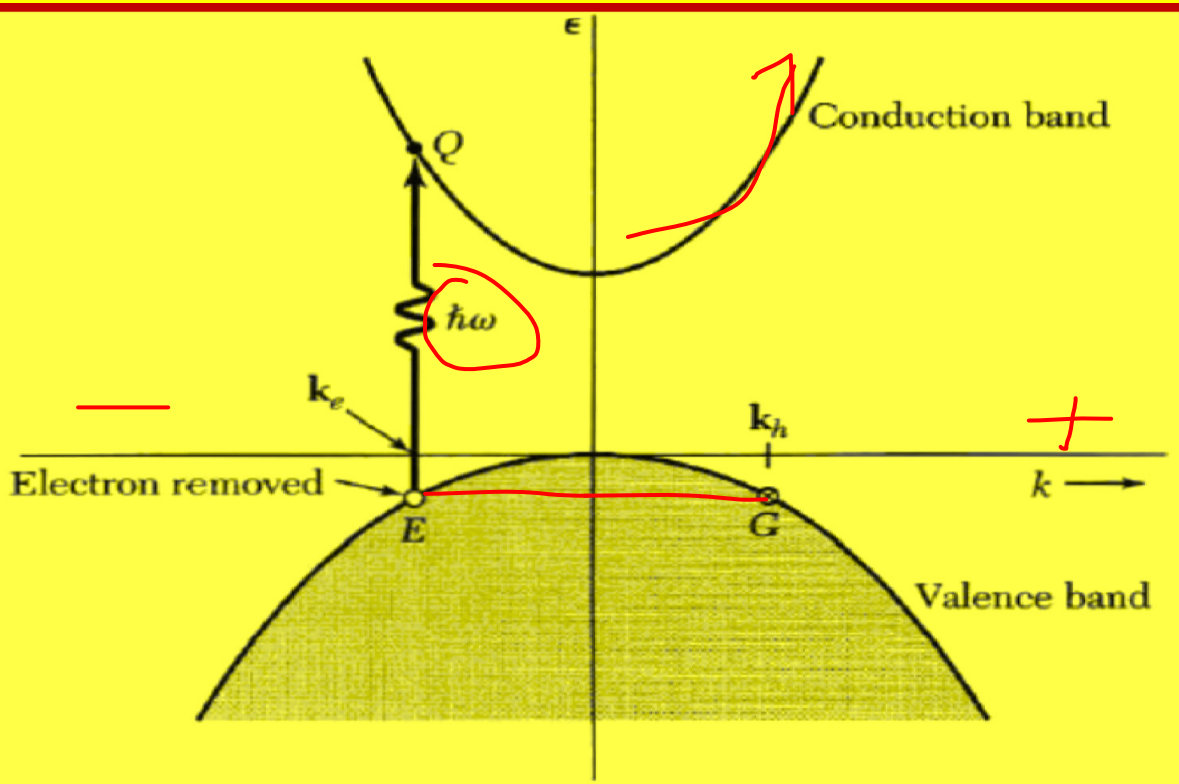

Figure 7 Absorption of a photon of energy $\hbar\omega$ and negligible wavevector takes an electron from E in the filled valence band to Q in the conduction band. If $\mathbf{k}_e$ was the wavevector of the electron at E, it becomes the wavevector of the electron at Q. The total wavevector of the valence band after the absorption is $-\mathbf{k}_e$, and this is the wavevector we must ascribe to the hole if we describe the valence band as occupied by one hole. Thus $\mathbf{k}_h = -\mathbf{k}_e$; the wavevector of the hole is the same as the wavevector of the electron which remains at G. For the entire system the total wavevector after the absorption of the photon is $\mathbf{k}_e + \mathbf{k}_h = 0$, so that the total wavevector is unchanged by the absorption of the photon and the creation of a free electron and free hole.

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Holes

2- $\varepsilon_h(K_h) = -\varepsilon_e(k_e)$ **(18)**

- Here the zero of energy of the valence band is at the top of the band.
- The lower in the band the missing electron lies; the higher the energy of the system.
- The energy of the hole is opposite in sign to the energy of the missing electron, because it takes more work to remove an electron from a low orbital than from a high orbital
- Thus if the band is symmetric: $\varepsilon_e(k_e) = \varepsilon_e(-k_e) = -\varepsilon_h(-k_e) = -\varepsilon_h(k_h)$.

3- $V_h = V_e$ **(19)**

- The velocity of the hole is equal to the velocity of the missing electron

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Electron –Hole Conservation of Total Momentum

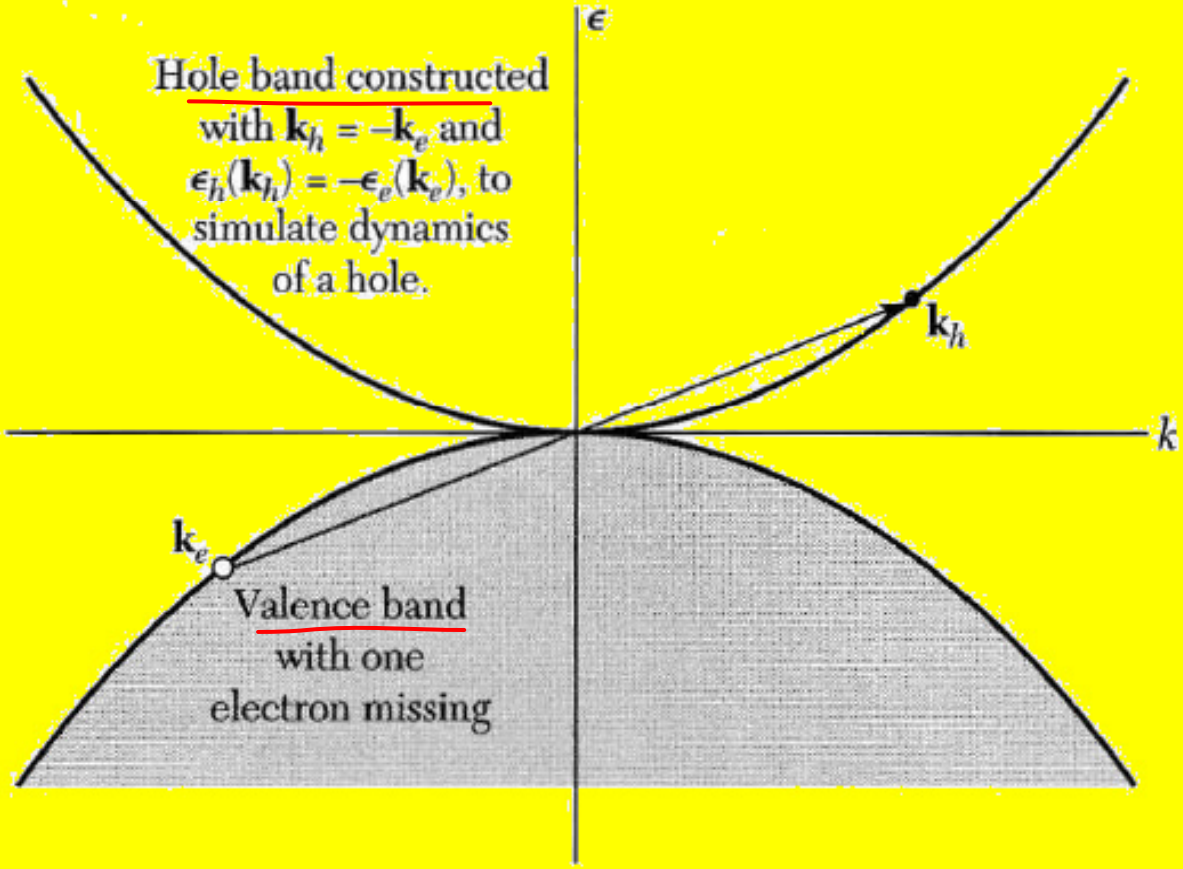

Figure 8 The upper half of the figure shows the hole band that simulates the dynamics of a hole, constructed by inversion of the valence band in the origin. The wavevector and energy of the hole are equal, but opposite in sign, to the wavevector and energy of the empty electron orbital in the valence band. We do not show the disposition of the electron removed from the valence band at $\mathbf{k}_e$.

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Holes

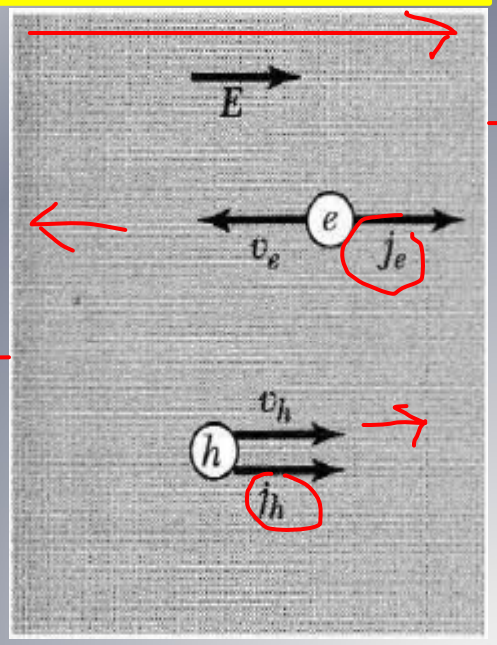
4- $m_h = -m_e$ **(20)**

- We show below that the effective mass is inversely proportional to the curvature $d^2\varepsilon/dk^2$ and for the hole band this has the opposite sign to that for an electron in the valence band. Near the top of the valence band m_e is negative, so that m_h *is positive*

5- $$\hbar \frac{d\mathbf{k}_h}{dt} = e(\mathbf{E} + \frac{1}{c}\mathbf{v}_h \times \mathbf{B}) \qquad (21)$$

- The equation of motion for a hole is that of a particle of positive charge ***e***.
- *Current:*

  $\mathbf{j} = (-e)\mathbf{v}(G) = (-e)[-\mathbf{v}(E)] = e\mathbf{v}(E)$ (23)
- The hole and electron drift velocities are in opposite directions



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Holes and Electrons (Comparison)

- In the next table: We quickly compare between Holes & Electrons. Momentum, Energy, Velocity , mass and Eq. of motion

Hole	Electron	Quantity
$K_h = -k_e$	k_e	Momentum
$\varepsilon_h(k_h) = -\varepsilon_e(k_e)$	$\varepsilon_e(k_e)$	Energy
$V_h = V_e$	V_e	Velocity
$m_h = -m_e$	m_e	Mass
$\hbar \frac{d\mathbf{k}_h}{dt} = e(\mathbf{E} + \frac{1}{c}\mathbf{v}_h \times \mathbf{B})$	$\hbar \frac{d\mathbf{k}_e}{dt} = -e(\mathbf{E} + \frac{1}{c}\mathbf{v}_e \times \mathbf{B})$	Equation of Motion

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*Effective Mass m**

- When we look at the energy-wavevector relation $\varepsilon=(\hbar^2/2m)k^2$ for free electrons, we see that the coefficient of k^2 determines the curvature of ε versus k. Turned about, we can say that 1/m, the reciprocal mass, determines the curvature.
- For electrons in a band there can be regions of unusually high curvature near the band gap at the zone boundary.
- In semiconductors the band width is of the order of 20 eV, while the band gap is of the order of 0.2 to 2 eV.
- Thus, the reciprocal mass is enhanced by a factor 10 to 100, and the effective mass is reduced to 0.1-0.01 of the free electron mass.
- These values apply near the band gap; as we go away from the gap the curvatures and the masses are likely to approach those of free electrons.

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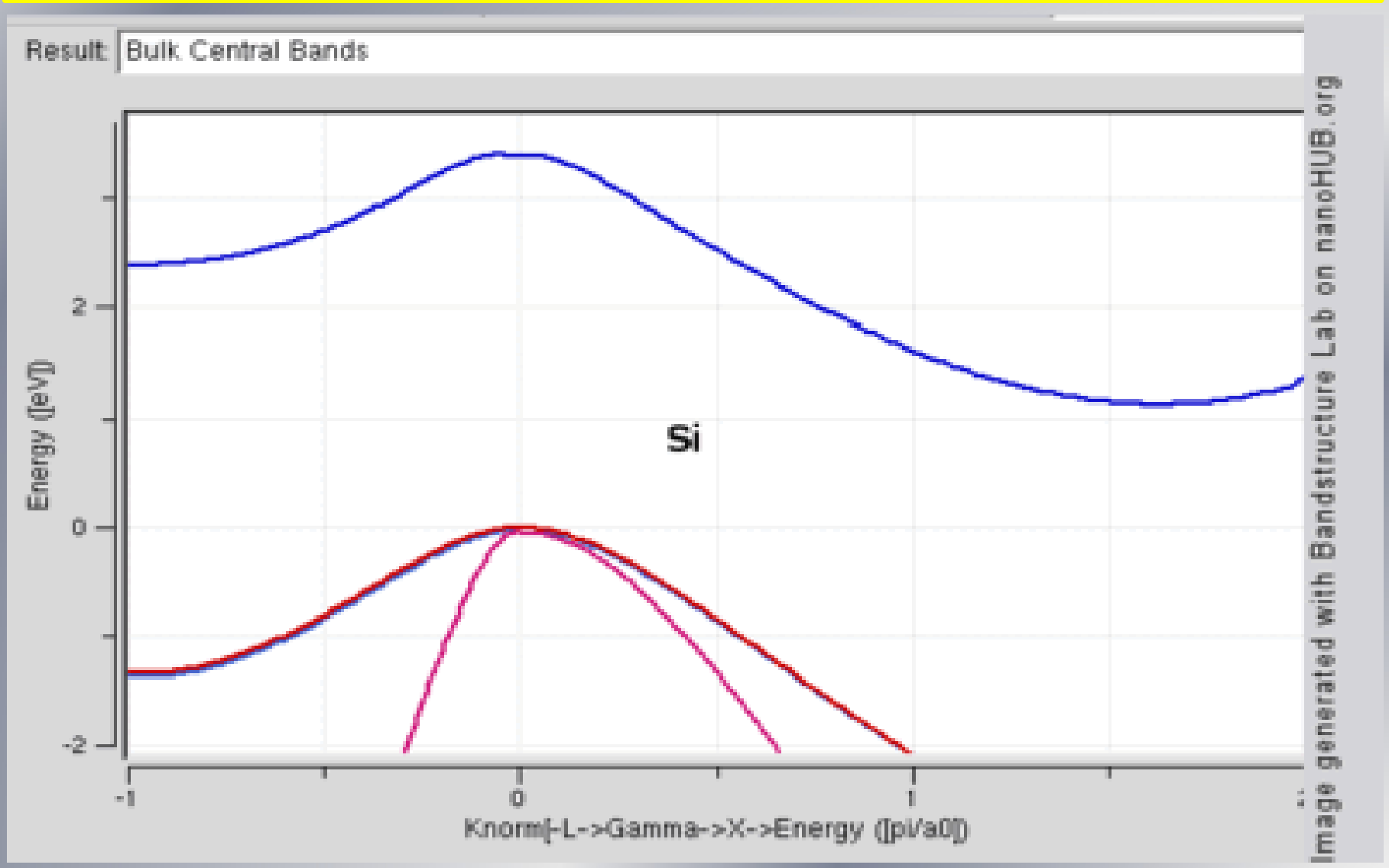
Electron –Hole Conservation of Total Momentum



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*Effective Mass m**

- Quotation from Arabic lectures:
- وللتوضيح أكثر، فإن حركة الإلكترون داخل المادة تخضع لمؤثرات كثيرة بسبب وجود الأنوية بالقرب منه، مما يجعل حركته غير خاضعة لقوانين الحركة المعروفة (قوانين نيوتن). ومن هنا برزت فكرة الكتلة الفعالة كنوع من التعويض حتى نتمكن من الاستمرار في استخدام قوانين الحركة.
- ربما نوضح الموضوع بشكل أفضل كما يلي: تصور شخصا مرتبه 1000 ريال في الشهر، ولكن بما أن الأسعار تتغير، مرات ترتفع و مرات تنخفض، إذن مرتبه (الفعال) قد يصبح 2000 أو 500 ريال. بمعنى قدرته الشرائية تعتمد على المؤثرات الخارجية وليس على مجرد الرقم الذي ينزل في البنك. إذن إذا كانت قيمة هذا الإنسان تعتمد فعليا على قيمة مرتبه الحقيقية، فقيمته تتذبذب بناءا على مؤشرات الأسعار. لو فرض أن الشركة التي تدفع له المرتب، تزيد من قيمته وتخفض بناءا على مؤشرات الأسعار، أذن يصبح مرتبه دائما هو 1000 ريال من حيث القيمة لا من حيث الرقم. فهذا العمل من الشركة مقابل تغير الأسعار مثل استخدام مفهوم الكتلة الفعالة مقابل تأثير الأنوية الأخرى على الإلكترون (تأثير موقعه من الشريحة).

Effective Mass Equation

First differentiate group velocity with time:

Wave function of a free elecron is expressed as: $e^{ik.x}$:

$$v_g = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{d\varepsilon}{dk}$$

Change of energy of electron by the work don by E is:

$$d\varepsilon = \frac{d\varepsilon}{dk}dk = -eEdx = -eEvdt = \frac{-eE}{\hbar}\frac{d\varepsilon}{dk}dt$$

$$\because \frac{dp}{dt} = \frac{d\hbar k}{dt} = \hbar\frac{dk}{dt} = m\frac{dv}{dt}$$

$$\therefore \frac{\hbar}{m}\frac{dk}{dt} = \frac{1}{\hbar}\frac{d}{dt}\frac{d\varepsilon}{dk} = \frac{1}{\hbar}\frac{d^2\varepsilon}{dk^2}\frac{dk}{dt}$$

$$\Rightarrow \frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2\varepsilon}{dk^2} \qquad (28)$$

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Effective Masses in Semiconductors

- In many semiconductors it has been possible to determine by cyclotron resonance the effective masses of carriers in the conduction and valence bands near the band edges.
- The determination of the energy surface is equivalent to a determination of the effective mass.
- Cyclotron resonance in a semiconductor is carried out so that the current carriers are accelerated in helical orbits about the axis of a static magnetic field.
- The angular rotation frequency ω_e *is:*

$$\omega_c = \frac{eB}{m^*} \qquad (30)$$

where m* is the appropriate cyclotron effective mass

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Effective Masses in Semiconductors

- Resonant absorption of energy from an rf electric field perpendicular to the static magnetic field occurs when the rf frequency is equal to the cyclotron frequency.
- Holes and electrons rotate in opposite directions.

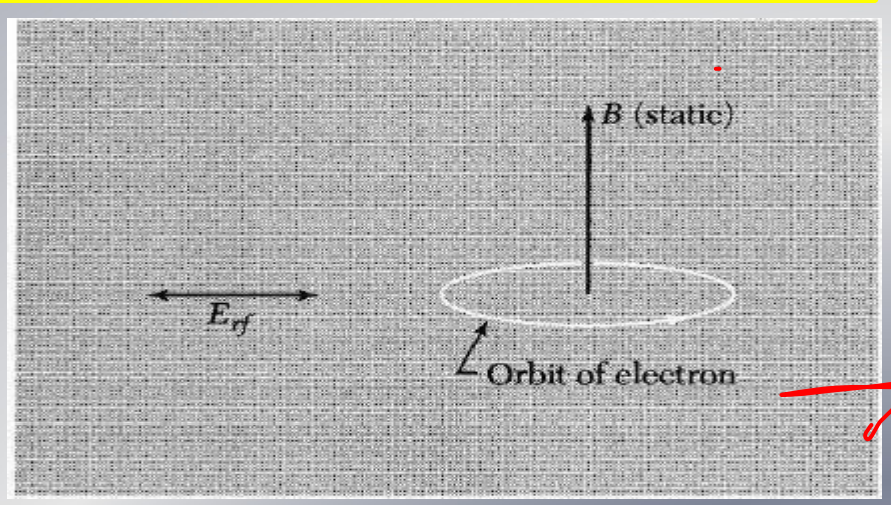

Table 2 Effective masses of electrons and holes in direct-gap semiconductors

Crystal	Electron m_e/m	Heavy hole m_{hh}/m	Light hole m_{lh}/m	Split-off hole m_{soh}/m	Spin-orbit Δ, eV
InSb	0.015	0.39	0.021	(0.11)	0.82
InAs	0.026	0.41	0.025	0.08	0.43
InP	0.073	0.4	(0.078)	(0.15)	0.11
GaSb	0.047	0.3	0.06	(0.14)	0.80
GaAs	0.066	0.5	0.082	0.17	0.34
Cu_2O	0.99	—	0.58	0.69	0.13

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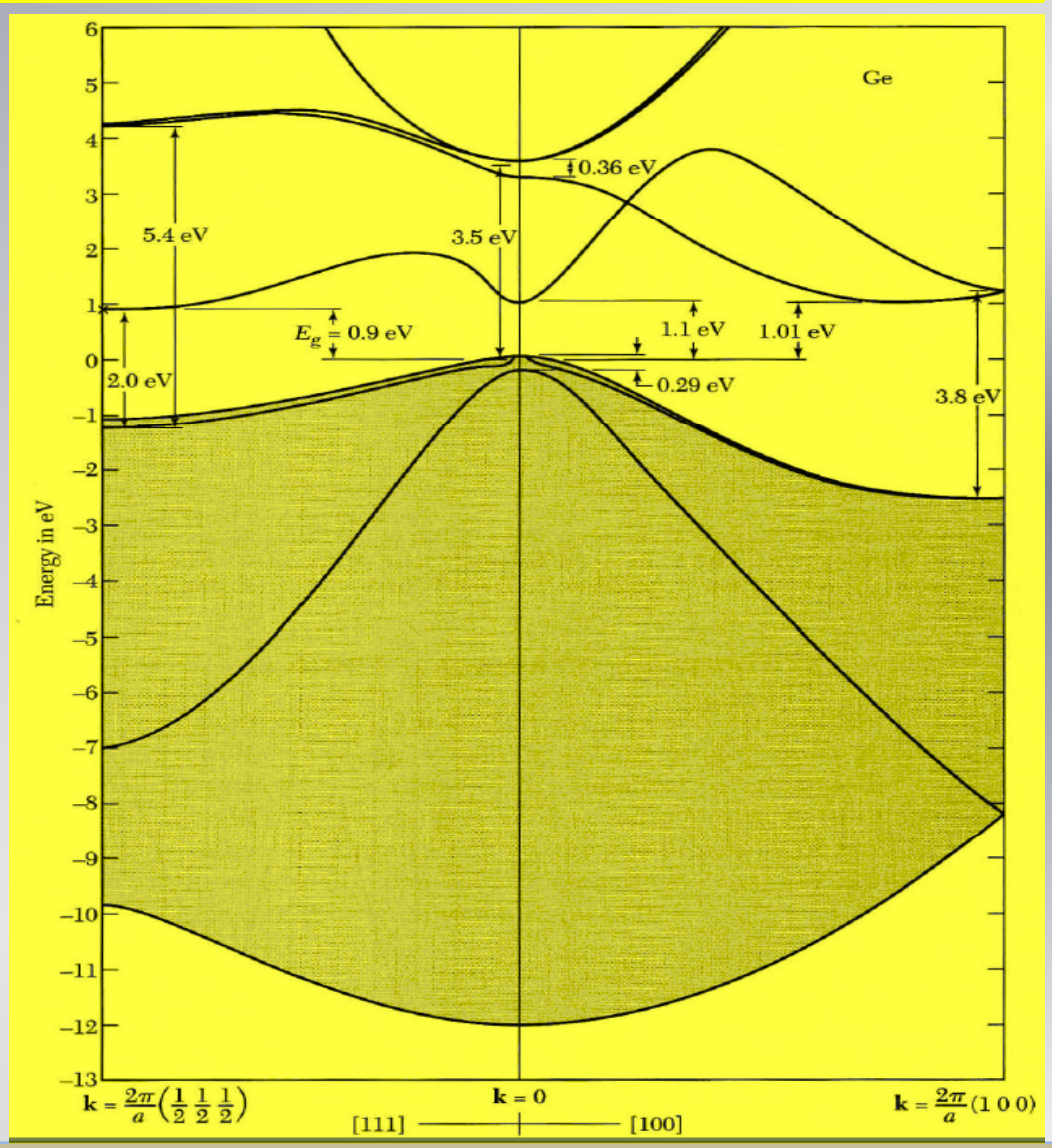
Electron –Hole Conservation of Total Momentum

Figure 14 Calculated band structure of germanium. The general features are in good agreement with experiment. The four valence bands are shown in gray. The fine structure of the valence band edge is caused by spin-orbit splitting. The energy gap is indirect; the conduction band edge is at the point (2π/a)(½½½).



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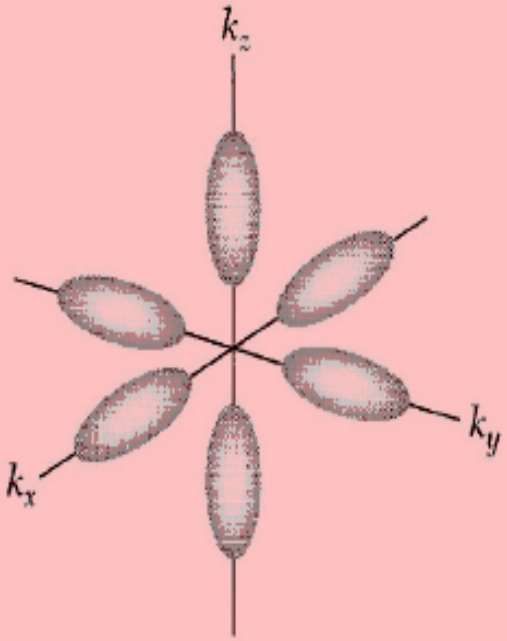
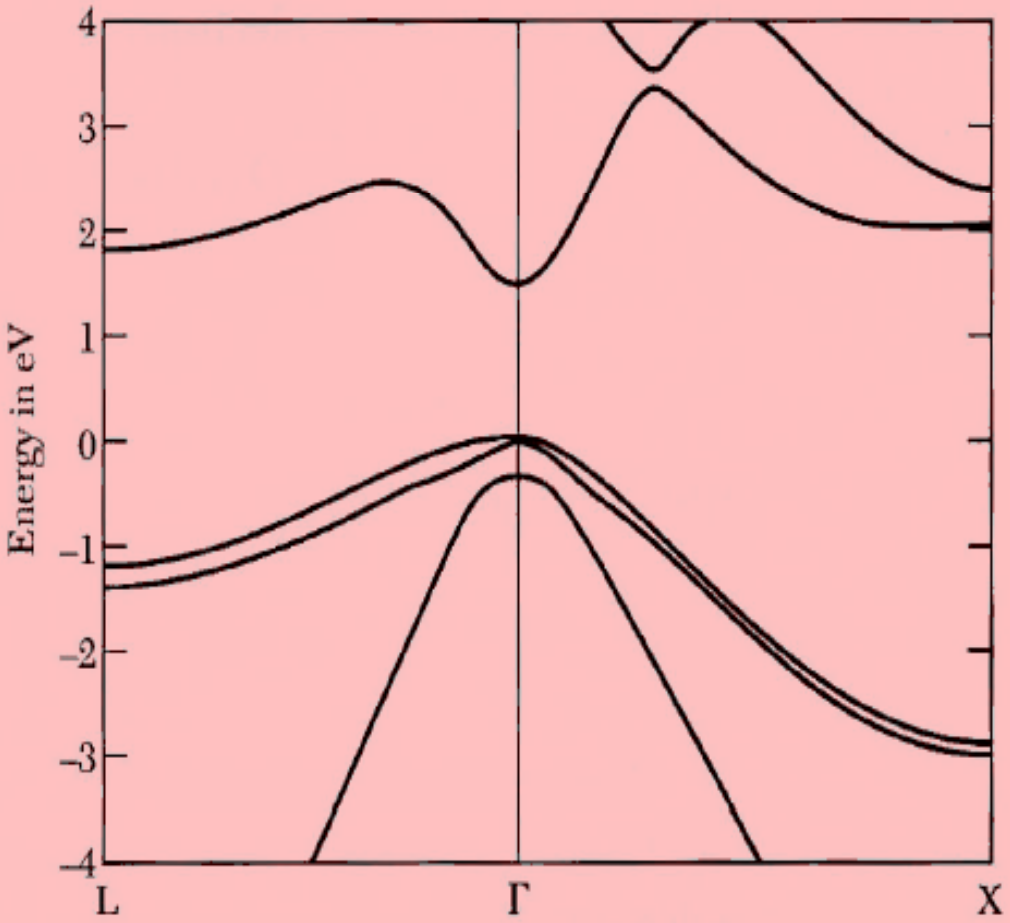


(a)

Figure 17a Constant energy ellipsoids for electrons in silicon, drawn for $m_l/m_t = 5$.



(b)

Figure 17b Band structure of GaAs, after S. G. Louie.

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INTRINSIC CARRIER CONCENTRATION

- We want the concentration of intrinsic carriers as a function of temperature, in terms of the band gap.
- we assume that $\varepsilon-\mu \gg k_B T$, *so that* the Fermi-Dirac distribution function reduces to:

$$f_e \approx e^{\left[\frac{\mu-\varepsilon}{k_B T}\right]} \tag{35}$$

- This is the probability that a conduction electron orbital is occupied, in an approximation valid when *fe << 1.*
- The energy of an electron in the conduction band is:

$$\varepsilon_k = E_c + \frac{\hbar^2 k^2}{2m_e^*} \tag{36}$$

- where E_c is the energy at the conduction band edge.

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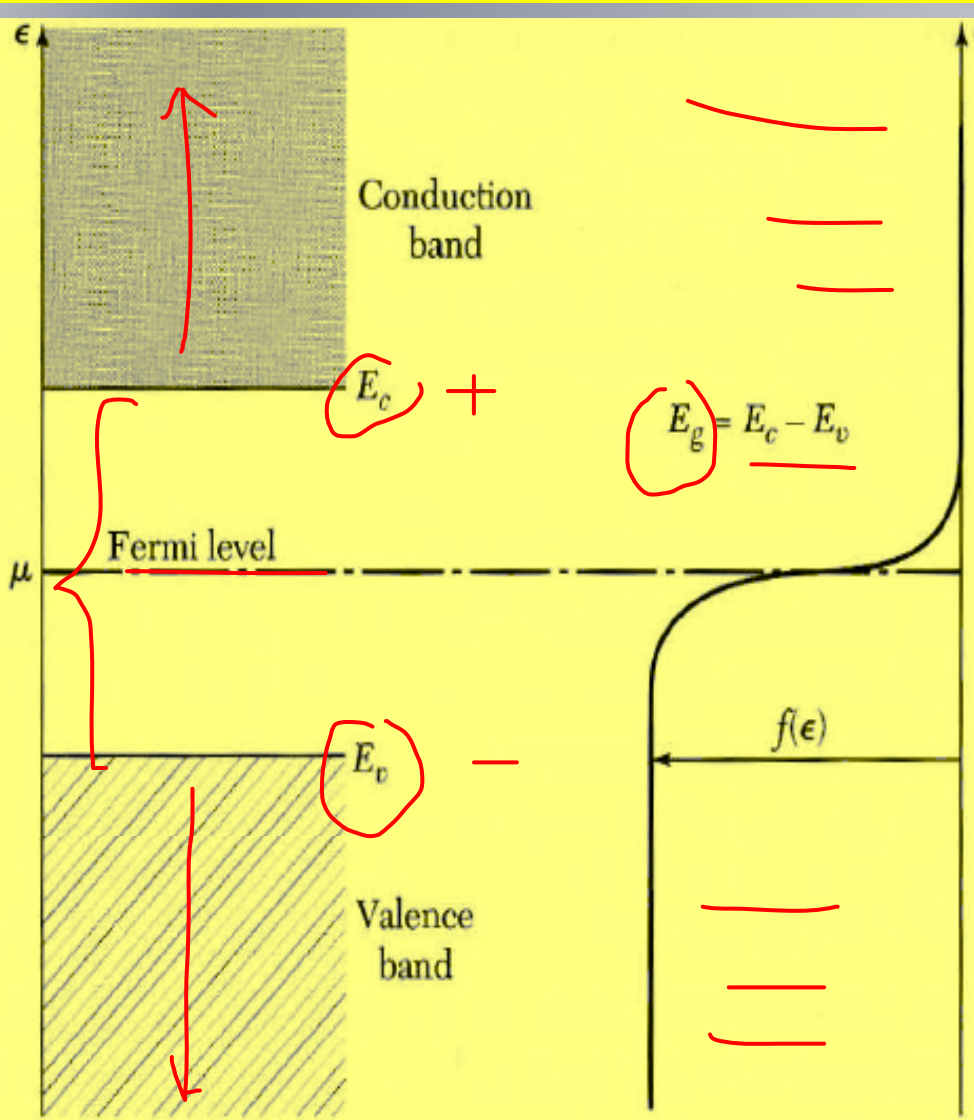

Figure 18 Energy scale for statistical calculations. The Fermi distribution function is shown on the same scale, for a temperature $k_B T \ll E_g$. The Fermi level μ is taken to lie well within the band gap, as for an intrinsic semiconductor. If $\epsilon = \mu$, then $f = \frac{1}{2}$.

- Thus from (6.20) the density of states at ε is:

$$D_e(\varepsilon) = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)(\varepsilon - E_c)^{1/2} \qquad (37)$$

The concentration of electrons in the conduction band is :

$$n = \int_{E_c}^{\infty} D_e(\varepsilon) f_e(\varepsilon) d\varepsilon$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right) e^{\mu/k_B T} \int_{E_c}^{\infty} (\varepsilon - E_c)^{1/2} e^{-\varepsilon/k_B T} d\varepsilon \qquad (38)$$

which integrates to give :

$$n = 2\left(\frac{m_e k_B T}{2\pi\hbar^2}\right)^{3/2} e^{(\mu - E_c)/k_B T} \qquad (39)$$

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INTRINSIC CARRIER CONCENTRATION

- For the holes: $\mu - \varepsilon >> K_B T$

$$f_h = 1 - \frac{1}{\exp\left(\varepsilon - \mu / k_B T\right) + 1} = \frac{1}{\exp\left(\mu - \varepsilon / k_B T\right) + 1} \qquad (40)$$

$$\approx \exp\left[\varepsilon - \mu / k_B T\right]$$

we have:

$$D_h(\varepsilon) = \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}\left(E_v - \varepsilon\right)^{1/2} \qquad (41)$$

$$\therefore p = 2\left(\frac{m^*_h k_B T}{2\pi\hbar^2}\right)^{3/2} e^{(E_c - \mu)/k_B T} \qquad (42)$$

From (39) and (42) we obtain the equilibrium relation:

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 \left(m^*_e m^*_h\right) e^{-E_g/k_B T} \qquad (43)$$