VE320 Intro to Semiconductor Devices

Chapter 1 & 2 & 3

Ziyi Wang

UM-SJTU Joint Institute

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   - Density of States Function
   - Statistical Mechanics

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Lattice Types

- Simple cubic: $\#\text{atom} = \frac{1}{8} \times 8 = 1$, $r(\text{atom}) = \frac{a}{2}$
- Body-centered cubic: $\#\text{atom} = \frac{1}{8} \times 8 + 1 = 2$, $r(\text{atom}) = \frac{\sqrt{3}a}{4}$
- Face-centered cubic: $\#\text{atom} = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$, $r(\text{atom}) = \frac{\sqrt{2}a}{4}$
- Volume Density $= \frac{\#\text{atoms per unit cell}}{\text{volume of unit cell}}$
- Surface Density $= \frac{\#\text{atoms per lattice plane}}{\text{area of lattice plane}}$

Miller Index

- Steps:
  - Find the intersection (∞ if parallel to the axis)
  - Write the reciprocal
  - Times the lowest common denominator
- All parallel planes are equivalent.
- [*hkl*]: Crystal direction
  (*hkl*): Crystal plane direction
  [*hkl*] direction is perpendicular to the (*hkl*) plane in the simple cubic lattice.

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Basic: Wave-particle Duality

- For matters: $p = mv$, $E = \frac{1}{2}mv^2$
- For photons: $p = \frac{h\nu}{c}$, $E = h\nu$, $\nu = \frac{\lambda}{c}$
- For both: $k = \frac{2\pi}{\lambda}$, $p = \frac{h}{\lambda}$, $\hbar = \frac{h}{2\pi}$

Basic Concepts

- Wave function: $\Psi(x)$
- Probability density function: $|\Psi(x)|^2 = \Psi(x) \times \Psi^*(x)$.
  Note: In quantum mechanics, we cannot determine the exact coordinates of a particle, only the probability that it is at a certain coordinate position.
- Schrodinger Equation:

$$\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2m}{\hbar}(E - V(x))\Psi(x) = 0$$

  where m: mass of the particle, V(x): potential function, E: total energy of the particle.
- Boundary condition:
  - $\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1$
  - $\Psi(x)$ must be finite and continuous
  - $\partial\Psi(x)/\partial x$ must be finite and continuous

Solution of 2nd Order DE

- $\frac{\partial^2 y}{\partial x^2} = k^2 y$

$$y = Ae^{kx} + Be^{-kx}$$

- $\frac{\partial^2 y}{\partial x^2} = -k^2 y$

$$\begin{aligned} y &= Ae^{ikx} + Be^{-ikx} \\ &= C\sin(kx) + D\cos(kx) \end{aligned}$$

Electrons in Free Space

- Suppose $V(x) = 0$

$$\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi(x) = 0$$

- General solution:

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}$$

  where the wave number $k = \sqrt{\frac{2mE}{\hbar}}$.

- Particles in free space behave as traveling waves, and we have $k = \sqrt{\frac{2mE}{\hbar}} = \frac{p}{\hbar}$, $\lambda = \frac{h}{p} = \frac{2\pi}{k}$.

Electrons in Infinite Quantum Well

- $\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi(x) = 0, \begin{cases} V(x) = +\infty, & x \leq 0 \text{ or } x \geq a \\ V(x) = 0, & 0 < x < a \end{cases}$
- General solution:

$$\Psi(x) = A_1 \cos kx + A_2 \sin kx$$

- Boundary condition:

$$\Psi(x = 0) = \Psi(x = a) = 0$$

$$\int_0^a \Psi(x)\Psi^*(x) = 1$$

- Conclusion:

$$A_1 = 0, A_2 = \sqrt{\frac{2}{a}}, k_n = \frac{n\pi}{a}, n = 1, 2, 3, \cdots$$

$$\Psi(x) = \sqrt{\frac{2}{a}} \sin k_n x, \quad E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

Electrons in Finite Quantum Well

- $\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi(x) = 0, \begin{cases} V(x) = V_0, & x \leq 0 \text{ or } x \geq a \\ V(x) = 0, & 0 < x < a \end{cases}$
- General solution:

$$\Psi(x) = \begin{cases} Ae^{-ik_1 x} + Be^{ik_1 x}, & k_1 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}, x \leq 0 \text{ or } x \geq a \\ Ce^{-ik_2 x} + De^{ik_2 x}, & k_2 = \sqrt{\frac{2mE}{\hbar^2}}, 0 < x < a \end{cases}$$

- Boundary condition:

$$\Psi(x)|_{x=0,a} \text{ continuous}$$

$$\Psi'(x)|_{x=0,a} \text{ continuous}$$

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x) = 1$$

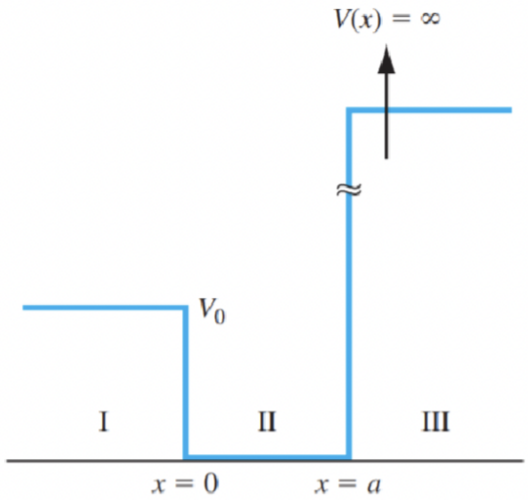
- Conclusion: Depending on the relationship between E and V_0, $\Psi(x)$ is different.

Exercise

Homework 1 Exercise 1.7

Exercise 1.7

Consider the one-dimensional potential function shown in Figure 1. Assume the total energy of an electron is $E < V_0$. (a) Write the wave solutions that apply in each region. (b) Write the set of equations that result from applying the boundary conditions. (c) Show explicitly why, or why not, the energy levels of the electron are quantized.



Exercise

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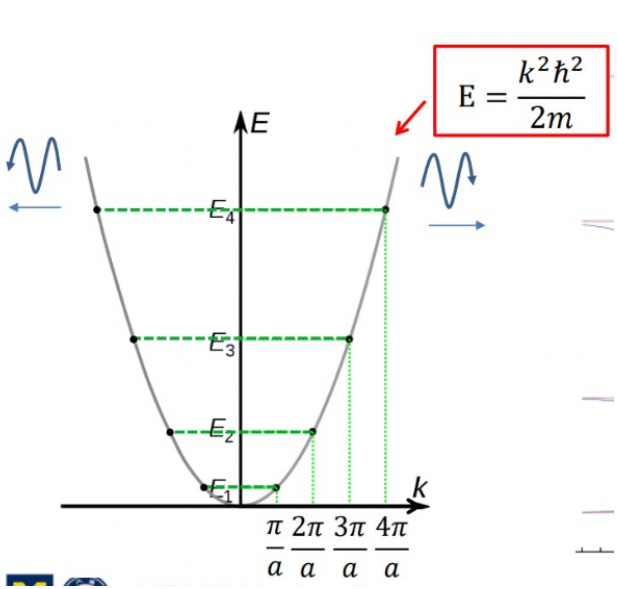
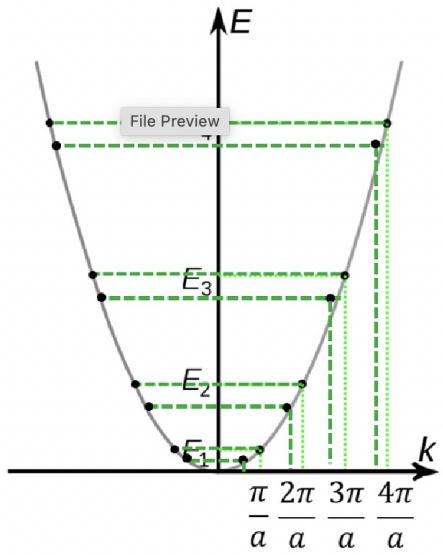
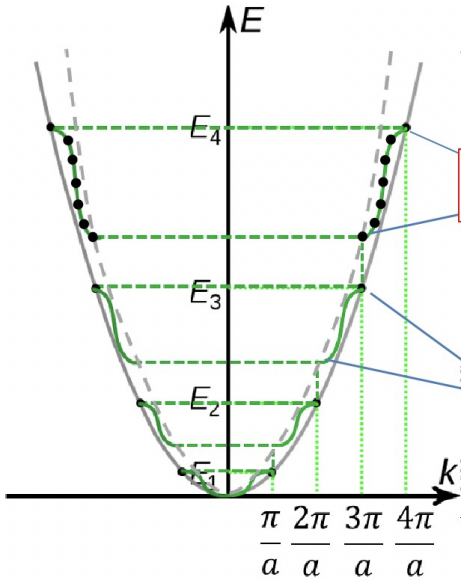
Energy Bands



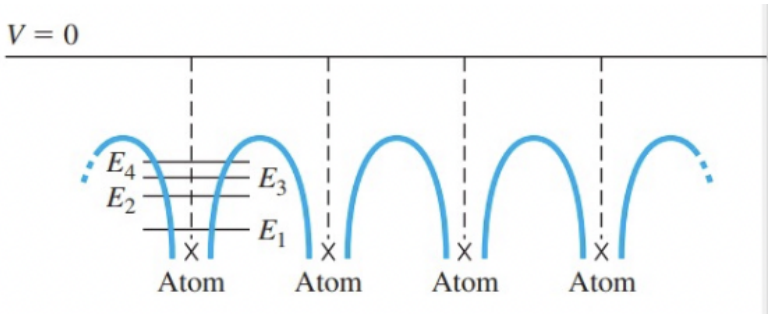
(a) Isolated atom



(b) 2 atoms



(c) N atoms



(d) Potential function of 1-D crystal

Figure: Energy bands

1-D Kronig-Penny Model

- Idealized model of one dimensional single crystal

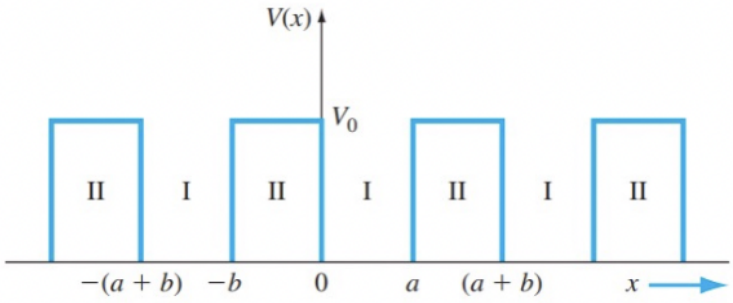


Figure: Potential function of 1-D crystal in KP model

- Bloch theorem: $\Psi(x) = u(x)e^{jkx}$
- Conclusion:

$$P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

where $P' = \frac{mV_0 ba}{\hbar^2}$. This equation gives the condition that the Schrodinger wave equation has a solution.

Energy Bands in K Space

- Consider the E-k relation of particles in the lattice.
- Let $f(\alpha a) = P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$

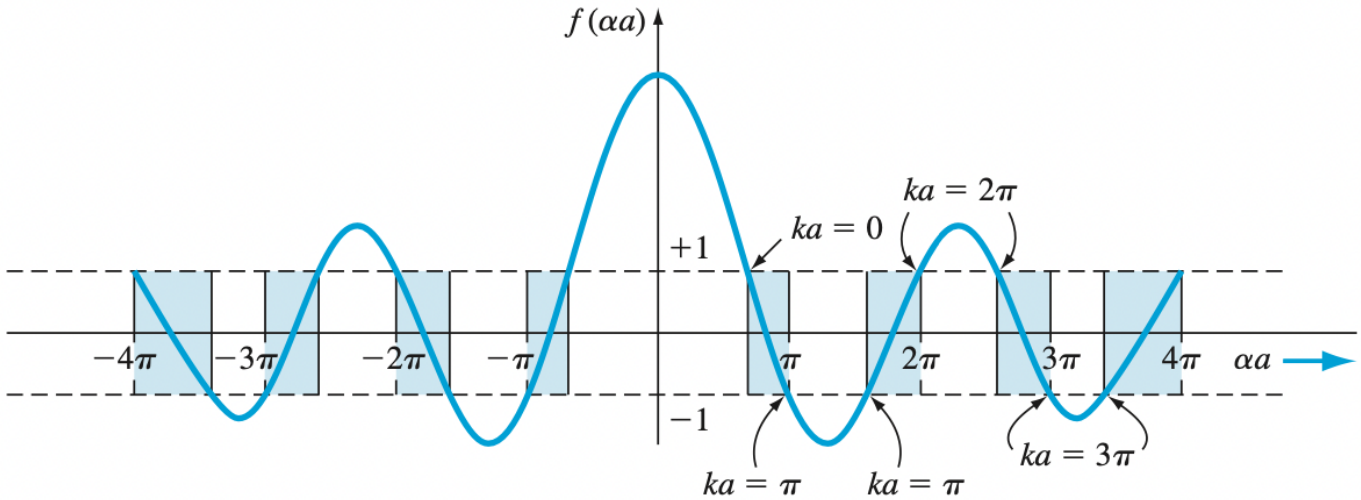


Figure: The entire $f(\alpha a)$ function

where the shared areas show the allowed values of αa corresponding to real values of k.

The E versus k diagram

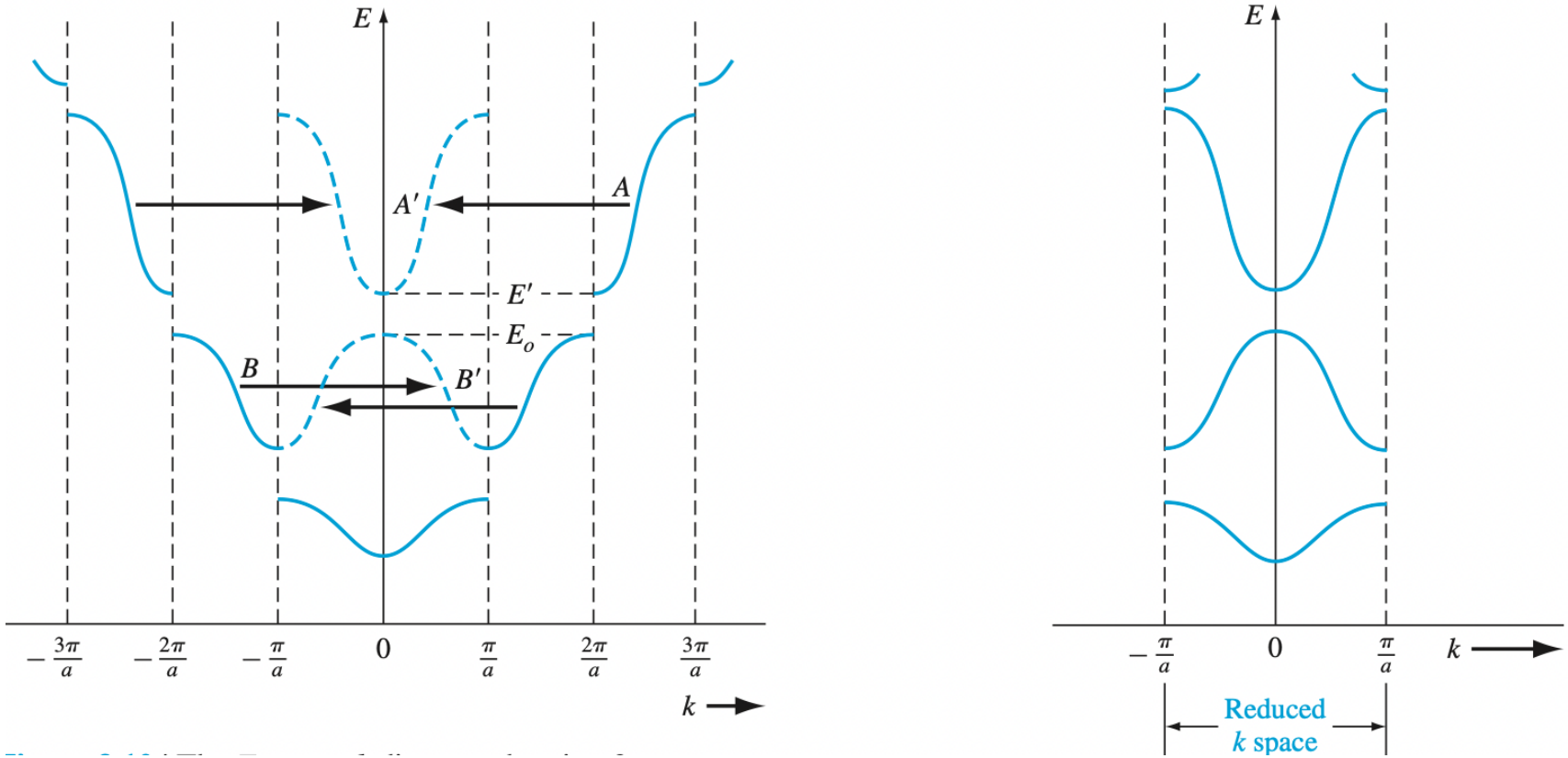


Figure: E vs. k diagram

Energy bands

- Metal:
- Insulator:
- Semiconductor:

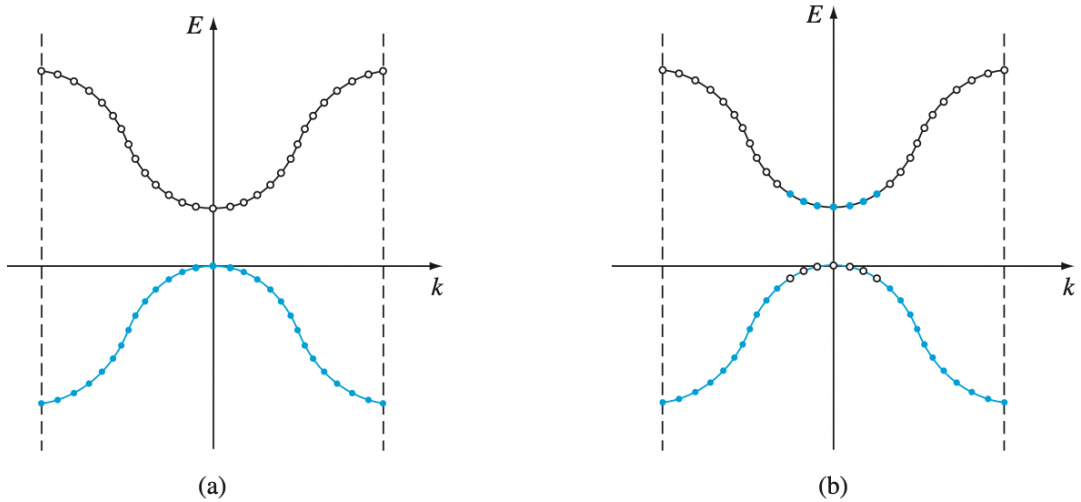


Figure: E-k diagram of semiconductor. (a)T=0K; (b)T>0K

- Drift current density: $J = qNv_d = q\sum_{i=1}^{N} v_i$.

Effective Mass

- Background: for the electrons in the lattice,

$$F_{\text{total}} = F_{\text{ext}} + F_{\text{int}} = ma$$

where m is the static mass of the electron. Consider only the external force,

$$F_{\text{ext}} = m^* a$$

where m^* is the effective mass of the electron.

- For electron in free space, we have $E = \frac{\hbar^2 k^2}{2m}$, i.e.,

$$\frac{1}{\hbar}\frac{dE}{dk} = v$$

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m}$$

Effective Mass

- For electrons at the bottom of the conduction band, $E - E_c = C_1(k)^2$, i.e.,

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}$$

- For electrons at the top of the valance band, $E - E_v = -C_2(k)^2$, i.e.,

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$$

  which is equivalent to holes with positive mass and positive charge.

- $$E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}(k - k_1)^2$$

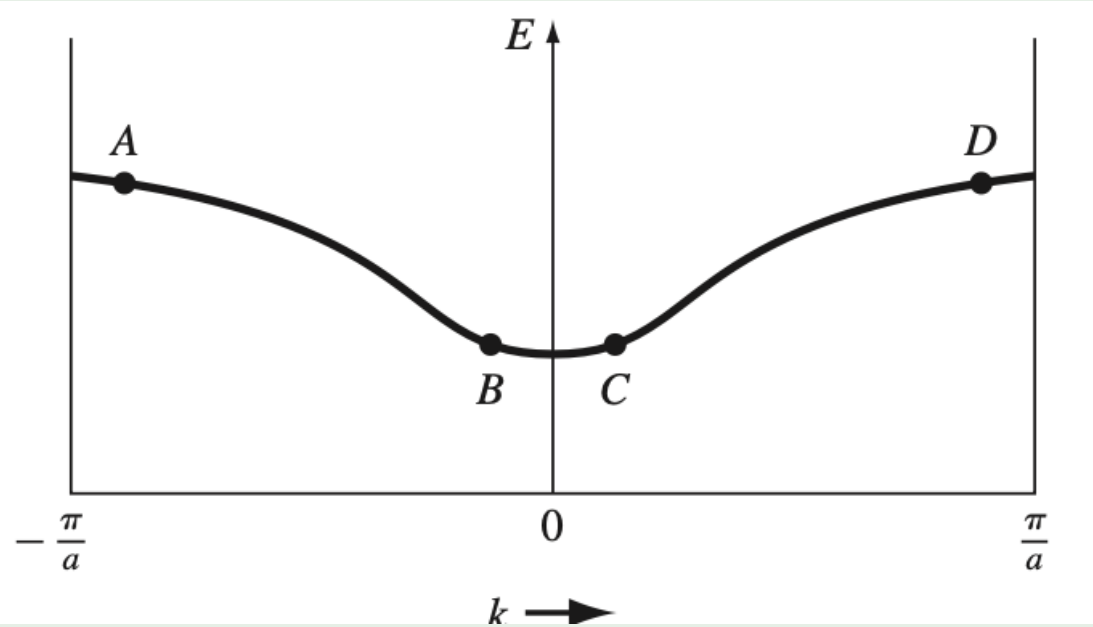
  $$E = E(k) = E_v - \frac{\hbar^2}{2m_p^*}(k - k_2)^2$$

  where m_n^* and m_p^* are effective mass of electrons and holes.

Exercise

Effective mass

The E versus k diagram for a particular allowed energy band is shown in Figure below. Determine (a) the sign of the effective mass and (b) the direction of velocity for a particle at each of the four positions shown.



Exercise

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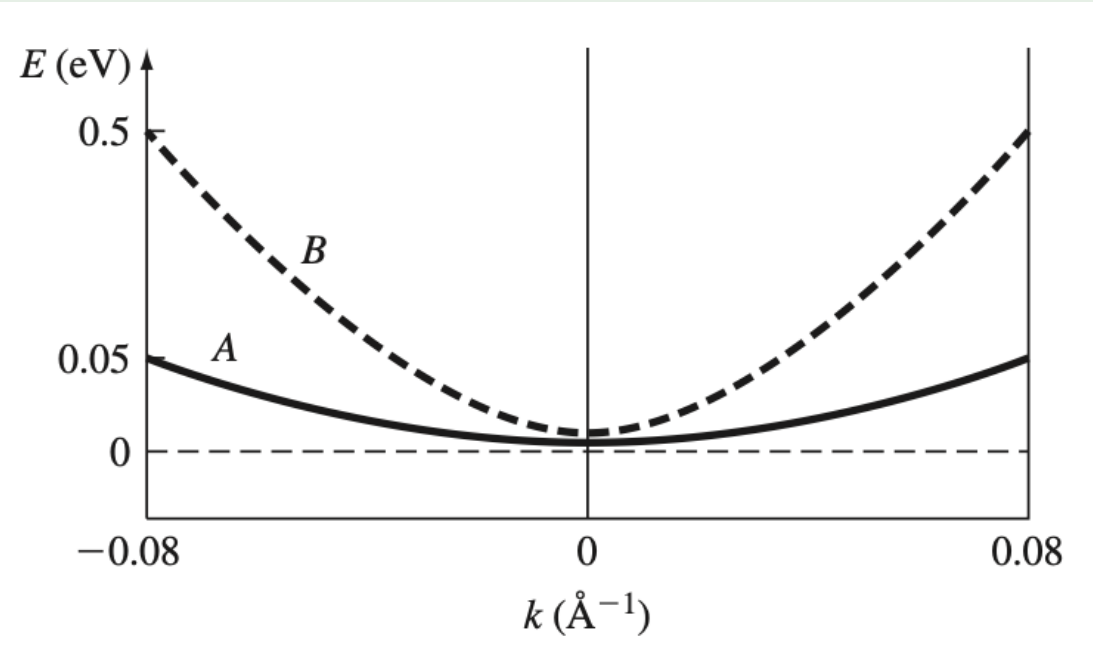
Effective mass

Figure below shows the parabolic E versus k relationship in the conduction band for an electron in two particular semiconductor materials. Determine the effective mass (in units of the free electron mass) of the two electrons.



Exercise

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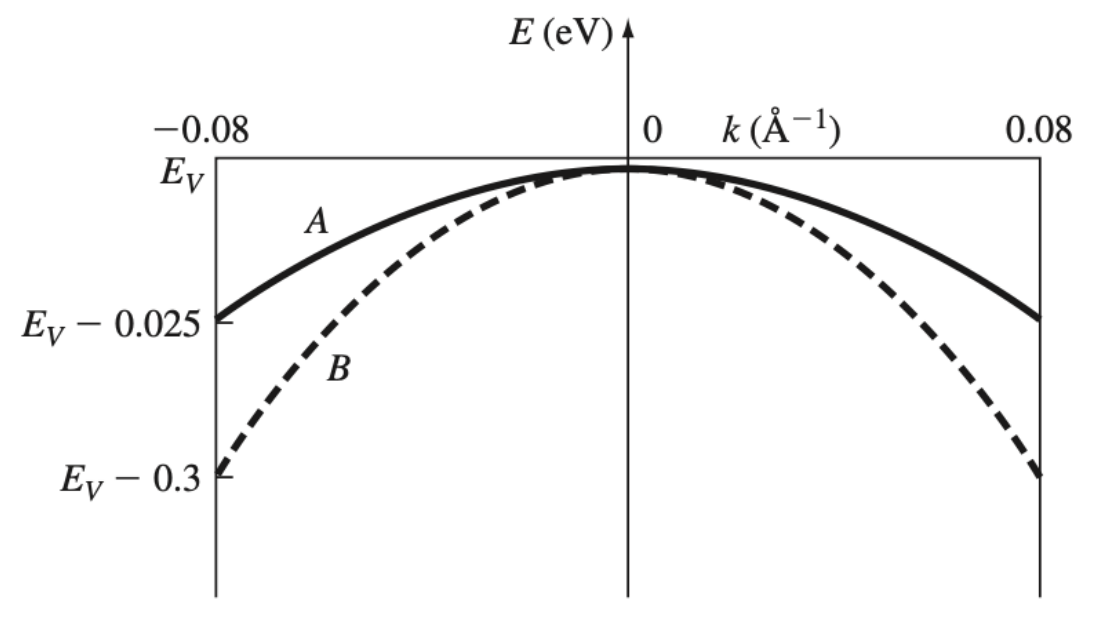
Effective mass

Figure below shows the parabolic E versus k relationship in the valence band for a hole in two particular semiconductor materials. Determine the effective mass (in units of the free electron mass) of the two holes.



Exercise

Exercise

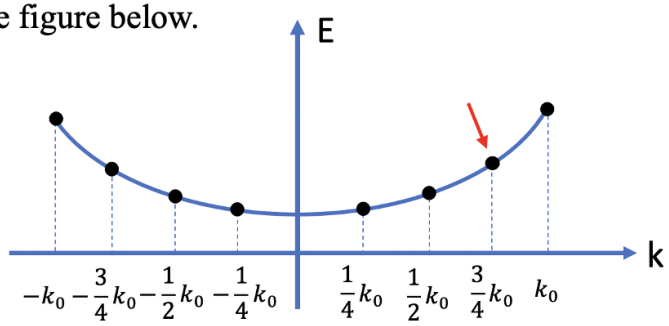
Problem Example 1

1. In a quantum system, the wavenumber k and energy E is quantized as shown in Figure 1. Please answer the following questions:

a) Write the static wavefunction of the dot ($k = \frac{3}{4}k_0$) that the red arrow is pointing to. Find the wavelength of this wavefunction.

b) If all the states are filled with electrons, how many electrons can be filled in the figure below? The electron spin is not considered.

c) If the effective mass of this quantum system is m_n^*, can this system allow an electron to have a quantized energy of $\frac{\hbar^2 k_0^2}{9m_n^*}$? If yes, mark the state of this electron in the figure below. How about a quantized energy of $\frac{\hbar^2 k_0^2}{8m_n^*}$? If yes, mark the state of this electron in the figure below.



Exercise

Density of States Function Derivation

Density of States Function

- For electrons in the lattice, $E = \frac{\hbar^2 k^2}{2m}$,

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E}$$

- For electrons at the bottom of the conduction band, $E - E_c = \frac{\hbar^2 k^2}{2m_n^*}$,

$$g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3}\sqrt{E - E_c}, \quad E \geq E_c$$

- For holes at the top of the valance band, $E_v - E = \frac{\hbar^2 k^2}{2m_p^*}$,

$$g_v(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3}\sqrt{E_v - E}, \quad E \leq E_v$$

- There is no energy states in the forbidden band, $g(E) = 0$, when $E_v < E < E_c$.

Fermi-Dirac Probability Function

- Fermi level E_F: hypothetical levels with a 50% probability of electron occupancy in thermodynamic equilibrium.
- $f_F(E)$ represents the possibility that a quantum state of energy E is occupied by an electron

$$f_F(E) = \frac{1}{1 + \exp(\frac{E - E_F}{kT})}$$

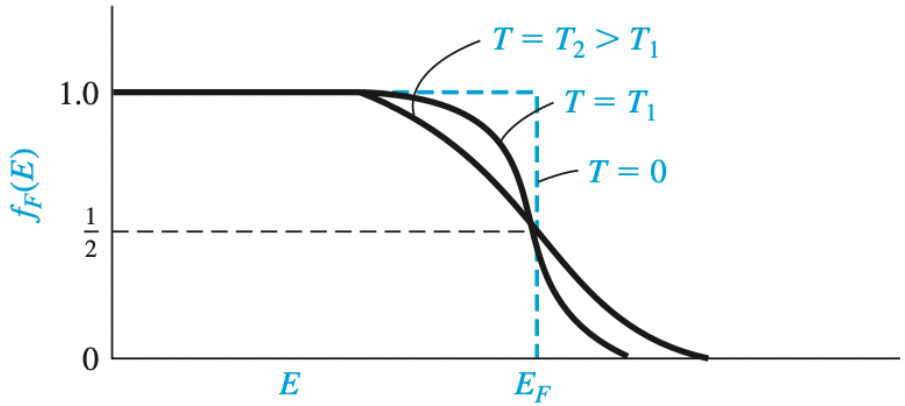


Figure: The Fermi probability function versus energy for different temperatures.

Exercise

Different distributions

Assume that the Fermi energy level for a particular material is 6.25 eV and that the electrons in this material follow the Fermi–Dirac distribution function. Calculate the temperature at which there is a 1 percent probability that a state 0.30 eV below the Fermi energy level will not contain an electron.

Boltzmann Distribution

- When $\exp(\frac{E-E_F}{kT} \gg 1)$ $(E - E_F > 3kT)$,

$$f_F(E) \approx \exp(-\frac{E - E_F}{kT})$$

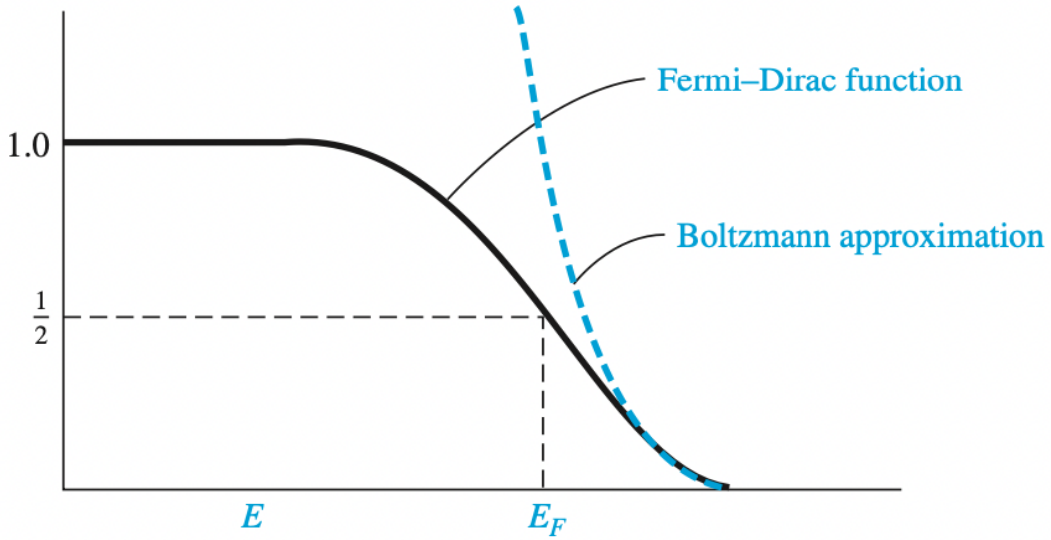


Figure: The Fermi–Dirac probability function and the Maxwell–Boltzmann approximation.

Exercise

Different distributions

Calculate the energy, in terms of kT and E_F, at which the difference between the Boltzmann approximation and the Fermi–Dirac function is 5 percent of the Fermi function.