

## Section 8.1: Effective Mass, Density of States and the Fermi Distribution

The density of states has a primary role in determining the gain (or absorption) for semiconductor lasers, light emitting diodes and detectors. This distribution of extended states versus energy determines the range of optical wavelengths involved in the transitions. The bulk materials, without nanostructure, produce a density of states with an energy profile of the form  $E^{(n-2)/2}$  for  $n$  dimensions. Nanostructure embedded within a bulk crystal produces sub-bands and a density of states that differs from that of the bulk. The present section discusses the basics of the density of states for the bulk material and shows how it depends on the effective mass.

### Topic 8.1.1: Effective Mass

The introductory material in Chapter 1 reviewed the formation of bands in bulk semiconductor material. A kinetic energy of a free electron can be plotted as a quadratic dispersion curve in terms of energy  $E$  versus momentum  $p$  or equivalently, angular frequency  $\omega$  versus wave vector  $k$  (or any combination). An electron in a crystal interacts with a periodic potential. This interaction alters the topology of the dispersion curve from a single solid curve into one consisting of disjoint sections that form bands. For example, Figure 8.1.1 shows the structure of the dispersion curves in the extended zone (solid curved lines) and the reduced zone (dotted curved lines) schemes for a 1-D lattice.

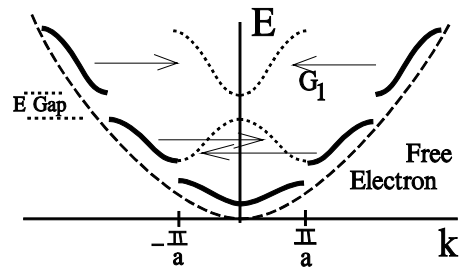


Figure 8.1.1: Comparing the dispersion curves for the free electron and the nearly-free electron. The symbol “ $a$ ” represents the inter-atomic spacing so that  $2\pi/a$  gives the width of the first Brillouin zone.

An electron moving through a crystal experiences the periodic crystal potential due to the atomic charge distribution. The Schrodinger equation incorporates the crystal potential and the mass of the electron. The energy eigenfunctions consist of the Bloch wave functions as discussed in the next section. The crystal potential can be eliminated so long as the Schrodinger’s equation uses the effective mass and the envelope part of the Bloch wave function. The effective mass describes the curvature of the band in which the electron (or hole) moves. If the band diagram has the form  $E = p^2/2m_e$  where  $p = \hbar k$ , then the effective mass  $m_e$  must have the form

$$m_e^{-1} = \frac{\partial^2 E}{\partial p^2} \quad \text{or} \quad m_e^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k^2} \quad (8.1.1)$$

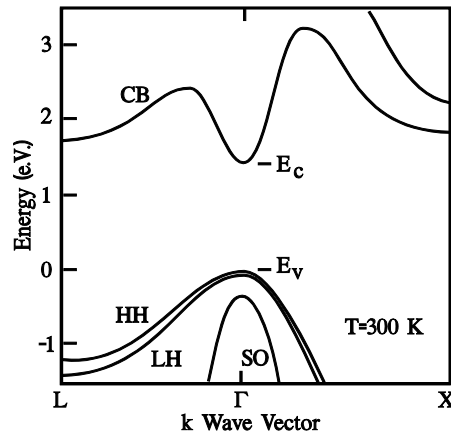


Figure 8.1.2: GaAs Band diagram for two different crystal directions. The bands are conduction band CB, heavy hole HH, light hole LH and split-off SO bands.

This equation shows that the curvature of the band determines the effective mass. As discussed in the companion volume on Solid State and Quantum Theory, the effective mass in 8.1.100 relates the force applied to an electron (not due to the periodic crystal potential) to its group velocity according to  $dv/dt = F/m_e$ .

The effective mass cannot be a scalar since the dispersion curves for two different directions do not necessarily have the same shape as shown in Figure 8.1.2 for bulk GaAs. The band shape depends on the direction of electron motion (i.e.,  $E$  versus  $k$ ). The parabolic band  $E$  versus  $k$  for the 1-D case can be generalized to

$$E = E_c + A(k_x - k_{ox})^2 + B(k_y - k_{oy})^2 + C(k_z - k_{oz})^2 \quad (8.1.2)$$

where the wave vector has the form  $\vec{k} = k_x \tilde{x} + k_y \tilde{y} + k_z \tilde{z}$ . The coordinates  $(k_{ox}, k_{oy}, k_{oz})$  describe the band minimum (or maximum for the valence band) and the coefficients  $A, B, C$  describe the shape of the band along the corresponding direction. If the constants  $A, B, C$  differ then the parabola curvatures differ with direction and therefore the effective mass must also differ with direction.

$$(m_x)^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_x^2} = \frac{2A}{\hbar^2} \quad (m_y)^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_y^2} = \frac{2B}{\hbar^2} \quad (m_z)^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_z^2} = \frac{2C}{\hbar^2} \quad (8.1.3)$$

The acceleration of an electron in the crystal due to non-crystalline forces (i.e., due to forces other than the periodic force caused by the periodic charge distribution).

$$a_x = (m_x)^{-1} F_x = \frac{2AF_x}{\hbar^2} \quad a_y = (m_y)^{-1} F_y = \frac{2BF_y}{\hbar^2} \quad a_z = (m_z)^{-1} F_z = \frac{2CF_z}{\hbar^2} \quad (8.1.4)$$

An average effective mass often appears in formulas such as for the density of states. The average usually appears as a geometric average such as  $\langle m \rangle = (m_x m_y m_z)^{1/3}$  (refer to the companion volume)

Equations 8.1.104 indicate that the effective mass should be represented by a dyad (see Chapter 2)

$$\vec{a} = \vec{m}^{-1} \cdot \vec{F} \quad (8.1.5)$$

Although Equation 8.1.2 is useful for illustration, it does not describe the general band shapes depicted in Figure 8.1.2. At minimum, the coefficients must depend on the components of the wave vector. The companion volume shows the effective mass can be written as

$$\vec{m}^{-1} = \frac{1}{\hbar^2} \nabla_k \nabla_k E \quad (8.1.6)$$

*Example 8.1.1:* Find the effective mass  $m_{ij}$  for the isotropic band

$$E = A\hbar^2 k^2 = A\hbar^2 (k_x^2 + k_y^2 + k_z^2)$$

*Solution:* Using 7.8.12, namely  $(m^{-1})_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}$  produces  $(m^{-1})_{ij} = 2A \delta_{ij}$ .

Therefore the effective mass  $m = \frac{1}{2A}$  must be isotropic.

Topic 8.1.2: Introduction to Boundary Conditions

The previous topic treats the semiconductor bands as continuous. The energy  $E_{\vec{k}}$  versus  $k$  dispersion curve represents the eigenvalues for the time-independent Schrodinger equation for the crystal. Boundary conditions over a finite region of space produce a discrete set of wave vectors  $\{\vec{k}\}$  and hence a discrete set of energy eigenvalues  $\{E_{\vec{k}}\}$ . The energy bands consist of the collection of closely spaced points  $\{(\vec{k}, E_{\vec{k}})\}$  that represent the Bloch eigenfunctions. The envelope part of the block wave function consists of plane waves with wavelength  $\lambda = 2\pi/|\vec{k}|$  and angular frequency  $\omega_k = E_k / \hbar$ .

The Bloch wave functions, as eigenfunctions of the Schrodinger wave, must be normalized over some region of space. In general, either an electron can be confined to a finite region of space as for an atom or it can remain unconfined as for the case of a plane wave. In either case, the wave function must be normalized over a finite volume of space by requiring it to satisfy boundary conditions over a finite region of space. These boundary conditions place conditions on the particle wavelength and hence also on the wave vector. Finite regions of space produce discrete allowed wave vectors and therefore discrete energy values. Two types of boundary conditions, specifically fixed-endpoint and periodic, are typically applied to the electron.

The fixed-endpoint boundary conditions require the particle wave function to have a fixed value at the boundary of the finite region of space. Often the wave function must be zero at both the boundary and outside the finite region since the particle should not be found anywhere except inside the finite region. These fixed-endpoint boundary conditions produce sine and cosine standing waves for the energy eigenfunctions (i.e., the energy basis set). The wave vectors  $\vec{k}$  have only positive components since negative values do not change the form of the basis function. Electrons confined to nanostructure can use this type of boundary condition.

Travelling waves usually require periodic boundary conditions whereby the wave function must repeat every macroscopic distance  $L$ . The plane wave functions comprising the basis set must be normalized over this same distance  $L$  although the wave extends across larger distances. In this case, the wave vectors  $\vec{k}$  have both positive and negative components in order to account for motion along the positive and negative directions. However, the finite size of  $L$  leads to discrete allowed wavelengths, wave vectors, and therefore also energy. Very large regions  $L$  produce very closely spaced wavelengths, wave vectors and energy and therefore approximate a continuum. It is customary to use the length  $L$  of a real crystals as the repetition length for the boundary conditions. In such a case, the size of the crystal sets a minimum spacing for allowed  $k$ .

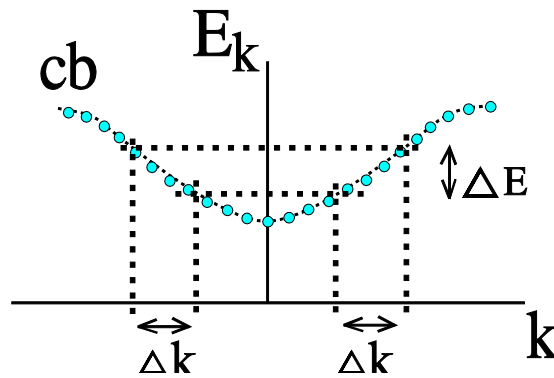


Figure 8.1.3: The density of energy states must be related to the density of k-states.

Once we know the allowed energies for a finite system, we can count the number of allowed states. Figure 8.1.3 shows the discrete states for the conduction band. We can count the number of states  $\Delta N$  in the energy range  $\Delta E$  to find the density of states  $g(E) \sim \Delta N / \Delta E$ . The figure shows how the number of states along the energy axis must be related to the number along the  $k$ -axis. In fact, the total number of states in the range  $\Delta E$  comes from the two regions marked  $\Delta k$ . For 2-D systems, the  $\Delta k$  region corresponds to an annular region between two circles.

*Topic 8.1.3: The Fixed Endpoint Boundary Conditions*

The fixed-endpoint boundary conditions require a wave to be zero at the edges of the bounding region. The fundamental modes fitting the region appear as sine and cosine waves as shown in Figure 8.1.4. The wavelengths cannot be larger than

$$\lambda_1 = 2L$$

In fact, the wave must exactly fit into the distance  $L$  according to the relation

$$\lambda = \frac{2L}{1}, \frac{2L}{2}, \frac{2L}{3}, \dots, \frac{2L}{n}, \dots$$

Therefore, the allowed wave vectors must be

$$k_n = \frac{2\pi}{(2L/n)} = \frac{n\pi}{L} \quad n = 1, 2, 3, \dots \quad (8.1.7)$$

The finite region of space  $0 < x < L$  produces sinusoidal functions

$$B_s = \left\{ \sqrt{\frac{2}{L}} \text{Sin}(k_n x) \right\} \quad (8.1.8)$$

Three-dimensional problems require three-dimensional wave vectors. For a cube, with sides of length  $L$ , the allowed wave vectors can be written as

$$\vec{k} = \frac{n_x \pi}{L} \hat{x} + \frac{n_y \pi}{L} \hat{y} + \frac{n_z \pi}{L} \hat{z} \quad (8.1.9)$$

where  $n_x, n_y, n_z = 0, +1, +2, \dots$  for plane waves. As we will see, traveling waves most naturally use the *periodic* boundary conditions since then the waves don't need to be zero at the boundaries.

*Topic 8.1.4: The Periodic Boundary Condition*

Periodic boundary conditions describe macroscopically sized real crystals. The electron wavefunction must repeat itself every distance  $L$ , which usually matches the physical size of the crystal. For free space or physically large media, the length  $L$  can be increased without bound. We have primary interest in finite physical crystals. In this case, the waves can be imagined to have infinite

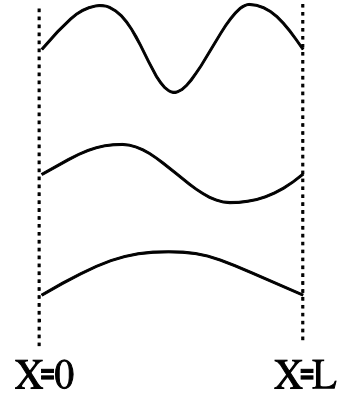


Figure 8.1.4: The endpoint boundary conditions.

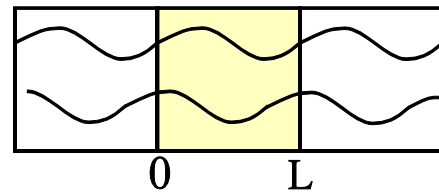


Figure 8.1.5: Repeating the physical crystal every distance  $L$ .

extent by imagining copies of the physical crystal placed next to each other as shown in Figure 8.1.5.

Two allowed modes with the longest wavelengths appear in Figure 8.1.6. The allowed wavelengths must be given by

$$\lambda_n = \frac{L}{n} \quad n = 0, \pm 1, \dots$$

and the allowed 1-D wave vectors must be

$$k_n = \frac{2\pi}{\lambda_n} = \frac{2\pi n}{L} \quad (8.1.10a)$$

The value of  $n$  can assume any non-zero integer value in the range  $(-\infty, \infty)$  for the extended-zone band diagram.

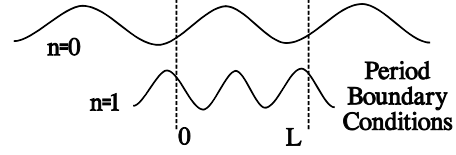


Figure 8.1.6: The first two allowed modes that satisfy the periodic boundary conditions.

The reduced-zone band diagrams use only the first Brillouin zone (FBZ). If we assume an even number of atoms  $N$  spaced apart by lattice constant “ $a$ ” in the 1-D crystal then we can write  $L=Na$  and

$$k_n = \frac{2\pi}{\lambda_n} = \frac{2\pi n}{a N} \quad (8.1.10b)$$

The longest wavelength corresponds to  $L=Na$  so that the closest spacing of  $k$ -values must be  $\Delta k = \frac{2\pi}{L} = \frac{2\pi}{Na}$ . The wavelengths  $\lambda_{\min} = 2a$  correspond to  $k$ -vectors  $k_{\text{FBZ}} = \pi/a$  at the edge of the first Brillouin zone (FBZ). This smallest wavelength sets the maximum integer  $n$  in Equation 8.1.10b.

$$k_n = \frac{2\pi}{\lambda_n} = \frac{2\pi n}{a N} \quad n = \pm 1, \pm 2, \dots, \pm N/2 \quad (8.1.10c)$$

We see that each band (in the reduced band scheme) must have  $N$  states. For crystals with an atomic basis,  $N$  represents the number of unit cells.

Three-dimensional crystals use similar periodic boundary conditions

$$\vec{k} = \frac{2\pi n_x}{L_x} \hat{x} + \frac{2\pi n_y}{L_y} \hat{y} + \frac{2\pi n_z}{L_z} \hat{z} \quad n_x, n_y, n_z = 0, \pm 1, \dots \quad (8.1.11a)$$

where,  $L_x, L_y, L_z$  represent the lengths of the three sides of the normalization volume. The lengths refer to the size of the normalization volume and not necessarily to the crystal. For convenience, we can assume that all of the sides have the same length  $L = L_x = L_y = L_z$ . Consequently, the wave function must be normalized to the volume of a cube. For  $N$  atoms along each edge of the cube ( $N^3$  total atoms), the length  $L$  must be  $L=Na$  and the allowed  $k$ -vectors become

$$\vec{k} = \frac{2\pi n_x}{aN} \hat{x} + \frac{2\pi n_y}{aN} \hat{y} + \frac{2\pi n_z}{aN} \hat{z} \quad n_x, n_y, n_z = 0, \pm 1, \dots \quad (8.1.11b)$$

The size of the crystal sets the smallest spacing of the components of the wave vectors

$$\Delta k_x = \Delta k_y = \Delta k_z = \frac{2\pi}{L} = \frac{2\pi}{aN}$$

The upper limit corresponds to a wave vector  $k^{\text{FBZ}}$  at the edge of the FBZ for which the wave does not propagate. Strong reflections occur for the smallest wavelength  $\lambda = 2a$  so that

$$k_x^{\text{FBZ}} = k_y^{\text{FBZ}} = k_z^{\text{FBZ}} = \frac{\pi}{a}$$

Therefore the allowed wave vectors must be

$$\vec{k} = \frac{2\pi n_x}{L} \hat{x} + \frac{2\pi n_y}{L} \hat{y} + \frac{2\pi n_z}{L} \hat{z} = \frac{2\pi}{a} \frac{n_x}{N} \hat{x} + \frac{2\pi}{a} \frac{n_y}{N} \hat{y} + \frac{2\pi}{a} \frac{n_z}{N} \hat{z} \quad (8.1.11c)$$

$$n_x, n_y, n_z = 0, \pm 1, \dots, \pm N/2$$

Again we see each k-axis has N states corresponding to the number of atoms along the axis. The number of states for the entire 3-D band must be  $N^3$  corresponding to the total number of atoms within the solid. The total number of atoms will be very large for any physically sized crystal (on the order of Avagadro's number). Notice that the k-vectors can have positive or negative values depending on the direction of wave propagation unlike for the fix-endpoint boundary conditions.

The plane waves corresponding to these macroscopic boundary conditions have the form

$$B_{1D} = \left\{ \frac{e^{ik_n x}}{\sqrt{L}} \right\} \quad \text{or} \quad B_{3D} = \left\{ \frac{e^{i\vec{k} \cdot \vec{r}}}{\sqrt{V}} \right\} \quad (8.1.12)$$

where  $V = L^3$  for the 3-D case. These wave functions correspond to the envelope part of the Bloch wave function. The next topics show how the macroscopic boundary conditions determine the density of states.

### Topic 8.1.5: The Density of k-States

The "density of k-states" measures the number of possible modes in a given region of k-space. Consider a *two-dimensional bulk crystal*. Figure 8.1.7 shows a 2-D region of k-space with a point for each k-vector

$$\vec{k} = \frac{2\pi m}{L} \hat{x} + \frac{2\pi n}{L} \hat{y} \quad m, n = 0, \pm 1, \dots$$

from periodic boundary conditions. Consider the horizontal direction for a moment. The distance between adjacent points can be calculated as

$$\frac{2\pi(m+1)}{L} - \frac{2\pi m}{L} = \frac{2\pi}{L}$$

Therefore, each elemental area of k-space

$$\frac{2\pi}{L} \cdot \frac{2\pi}{L} = \left( \frac{2\pi}{L} \right)^2$$

corresponds to precisely one mode. The number of modes per unit area of  $\vec{k}$ -space must then be given by

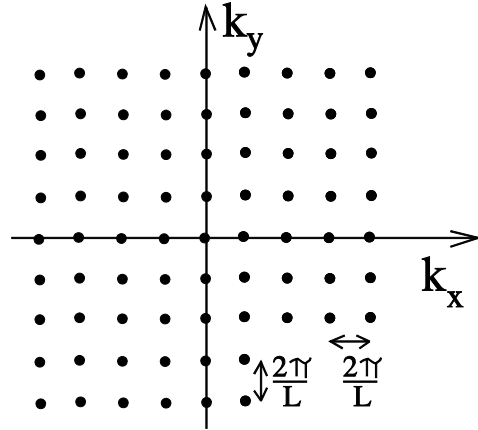


Figure 8.1.7: The allowed values of  $\vec{k}$  as determined by periodic boundary conditions.

$$g_{\vec{k}}^{(2D)} = \frac{1}{(2\pi/L)^2} = \frac{L^2}{4\pi^2} = \frac{A_{\text{xal}}}{4\pi^2} \quad (8.1.13)$$

where  $A_{\text{xal}}$  represents the area of the crystal. Note the use of the “vector  $\vec{k}$ ” as opposed to the “scalar  $k$ ” as a subscript on  $g$ .

In general,  $n$  dimensions produces a  $k$ -spaced density of states (DOS) of

$$g_{\vec{k}}^{(n-D)} = \frac{1}{(2\pi/L)^n} = \left(\frac{L}{2\pi}\right)^n \quad (8.1.14)$$

where bulk crystals can be 3-D, 2-D, or a line of atoms for 1-D.

### *Topic 8.1.6: The Electron Density of Energy States for a 2-D Crystal*

Semiconductor devices (as well as all optical ones) require the density of states. For electronic devices, recall the combination of the Fermi-Dirac distribution  $F(E)$  with the density of energy states  $g(E)$  leads to the number of electrons per crystal volume in a given energy range according to

$$n = \int dE g(E) F(E)$$

This topic finds the density of energy states using a graphical technique. The interested reader should consult the companion volume on the solid state and introduction to quantum theory for more detail.

We need to clearly distinguish the bulk cases from those encountered with reduced dimensional systems such as quantum wells, wires, and dots. These latter systems still have 3-D arrangements of atoms. However, the 3-D pattern of atoms (heterostructure) produces potentials that tend to confine electrons to wells. In this topic, we discuss 2-D and 3-D arrays of atoms without regard to confining the electron to smaller wells. For simplicity, we apply the procedure to portions of the band having a parabolic shape. The density of states for the entire band requires the full dispersion curve  $E=E(k)$  and not just the portion at the top or bottom of the band.

For simplicity of drawing figures, consider the 2-D case for the electronic density of energy states. We want to calculate the number  $N$  of energy states per unit energy, specifically  $g(E) = dN/dE$ , whereas the previous topic calculates the density of  $k$ -states with units of  $k$ -states per unit  $k$ -region. The calculation requires the energy versus wave vector  $k$  in terms of the effective mass  $m_e$

$$E = \frac{\hbar^2 k^2}{2m_e} \quad k^2 = k_x^2 + k_y^2 \quad (8.1.15)$$

where for convenience, we start the energy scale at the bottom of the conduction band so that  $E_c = 0$ . For constant effective mass  $m_e$ , Equation 8.1.15 represents the conduction band only near the minimum. The number  $N$  can be related to  $E$  through Equation 8.1.15 provided we can find the number of states up to the value  $k = |\vec{k}|$ .

To calculate the number of states up to the value  $k$  for the 2-D case, first plot the allowed  $k$ -states and then use  $k$  as the radius of a circle in  $k$ -space (see Figure 8.1.8). The number of states up to radius  $k$  can be calculated as

$$N(k) = \frac{\# \text{ States}}{k\text{-area}} \quad k\text{-area} \quad (8.1.16a)$$

or

$$N(k) = g_k^{2D} \pi k^2 = \left( \frac{L}{2\pi} \right)^2 \pi k^2 = \frac{A_{\text{xal}}}{(2\pi)^2} \pi k^2 \quad (8.1.16b)$$

where  $A_{\text{xal}}$  represents the area of the 2-D crystal. The total number of states per unit energy then becomes

$$g^{2D}(E) = \frac{dN(k)}{dE} = \frac{dk}{dE} \frac{dN}{dk} = \frac{1}{dE/dk} \frac{dN}{dk} \quad (8.1.16c)$$

Dividing out the area  $A_{\text{xal}}$  and substituting Equations 8.1.16b and 8.1.15 provides

$$g_E^{(2D)} = \frac{1}{2\pi} \frac{m_e}{\hbar^2} \quad (\text{no spin}) \quad (8.1.17a)$$

Usually a factor of “2” should be included for the degenerate electron spin

$$g_E^{(2D)} = \frac{1}{\pi} \frac{m_e}{\hbar^2} \quad (\text{spin}) \quad (8.1.17b)$$

Notice that the density of energy states for the 2-D bulk case remains constant above the bottom of the band. In the case of a band increasing upward from a vertex at  $E_c$ , the formula must include the step function  $\theta$ .

$$g_E^{(2D)} = \frac{1}{\pi} \frac{m_e}{\hbar^2} \theta(E - E_c) \quad (\text{spin}) \quad (8.1.17c)$$

The density of state must be zero for energy  $E$  smaller than  $E_c$  and constant for energy larger than  $E_c$ .

In general, an  $n$ -dimensional bulk crystal has the density of energy states (*including spin*) given by

$$g_E^{(3D)} = \frac{\sqrt{2}}{\pi^2 \hbar^3} m_e^{3/2} \sqrt{E - E_c} \theta(E - E_c) \quad (8.1.18a)$$

$$g_E^{(2D)} = \frac{1}{\pi} \frac{m_e}{\hbar^2} \theta(E - E_c) \quad (8.1.18b)$$

$$g_E^{(1D)} = \frac{\pi}{\hbar} \frac{\sqrt{8m_e}}{\sqrt{E - E_c}} \theta(E - E_c) \quad (8.1.18c)$$

where the step function  $\theta$  has a value of one for  $E \geq E_c$  and zero otherwise, and the equations have units of #/xal-vol/energy, #/xal-area/energy, #/xal-length/energy, respectively.

As an example, the 3-D density of energy states can be plotted next to the band diagram as illustrated in Figure 8.1.9. Both the conduction band and heavy-hole valence band produce a density of states that increase as  $\sqrt{E}$ . The effective mass controls the shape of the density of states as illustrated in Figure 8.1.10. The two bands have different curvatures. The boundary conditions

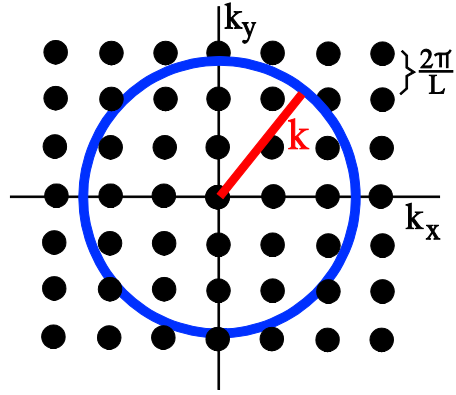


Figure 8.1.8: Number of modes  $N$  in circle of radius  $k$ .

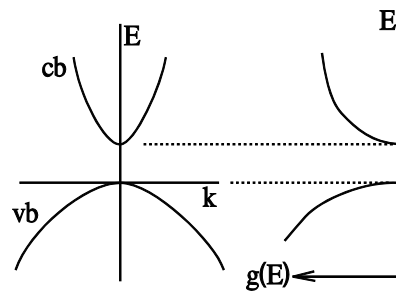


Figure 8.1.9: The conduction and valence band both have a density of states function.

produce equally spaced states along the horizontal k-axis. Let  $\Delta E$  represent a small fixed energy interval. The curvature of the bands produces two different numbers of states within the energy interval. The band with the larger curvature and therefore smaller effective mass has fewer states within the energy interval. The flatter band with the larger effective mass has more states within the interval.

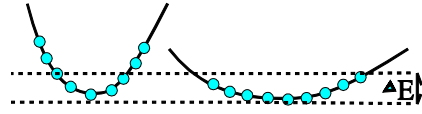


Figure 8.1.10: Bands with different curvatures have different numbers of states in a fixed energy interval.

*Topic 8.1.7: Overlapping Bands*

Gallium Arsenide has overlapping heavy hole (HH) and light hole (LH) valence bands as shown in Figure 8.1.11. We will find overlapping sub-bands for the reduced dimensional structures such as quantum wells. Each band must have states corresponding to the allowed discrete wave vectors k. Therefore the number of states within the energy range  $\Delta E$  must include states from both the HH and LH bands.

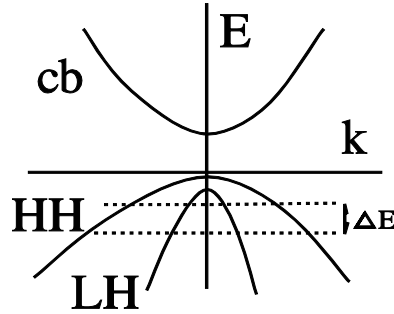


Figure 8.1.11: Light and heavy hole valence bands.

We now discuss the method for calculating the density of states for overlapping bands. The calculation for the quantum well sub-bands will be very similar. For simplicity, let  $-E \rightarrow E$  in Figure 8.1.11 and consider two the overlapping bands now with positive curvature as shown in Figure 8.1.12. We demonstrate that the density of states must be given by

$$g_E^{(3D)}(E) = \frac{m_1^{3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - E_1} \Theta(E - E_1) + \frac{m_2^{3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - E_2} \Theta(E - E_2) \quad (8.1.19)$$

The figure shows that the density of states must be zero below  $E_1$ . As  $E$  increases, we eventually encounter band #1 starting at energy  $E_1$  where the states start. The density of states (3-D crystal) must therefore increase as  $\sqrt{E - E_1}$  according to Equation 8.1.18. At energy  $E_2$ , the number of states in band 2 must be included. The density of states in band 2 increases as  $\sqrt{E - E_2}$  again according to Equation 8.1.18. To find the total number of states for energy larger than  $E_2$ , we must add the states from bands 1 and 2. Therefore, we find Equation 8.1.19.

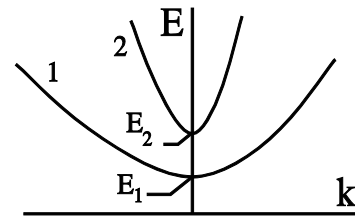


Figure 8.1.12: Two over-lapping 3-D bands (inverted for convenience).

*Topic 8.1.8: Density of States from Fixed-Endpoint Boundary Conditions*

The topics in the present section find the density of states using the periodic boundary conditions. The length  $L$  in Figure 8.1.6 appears to be rather arbitrary. For the fixed-endpoint boundary conditions, the length  $L$  matches the physical length of the crystal. We make the same requirement for the length  $L$  in the periodic boundary conditions as illustrated in Figure 8.1.5. However, the fixed-endpoint conditions might seem to give the more accurate density of states since electrons must surely be confined

to the crystal and cannot therefore be standing wave that repeat every length  $L$ . Let's examine how the choice of the type of boundary conditions affects the density of states. We will find that both types give precisely the same density of energy state function.

The following table compares the wavelength, wave vectors and minimum wave vector spacing using periodic and fixed-endpoint boundary conditions for a 2-D crystal (for example).

<u>Periodic BCs</u>		<u>Fixed-Endpoint BCs</u>	
$\lambda_x = L/m$	$\lambda_y = L/n$	$\lambda_x = 2L/m$	$\lambda_y = 2L/n$
$k_x = 2\pi m/L$	$k_y = 2\pi n/L$	$k_x = \pi m/L$	$k_y = \pi n/L$
$\Delta k_x = 2\pi/L$	$\Delta k_y = 2\pi/L$	$\Delta k_x = \pi m/L$	$\Delta k_y = \pi n/L$
Travelling waves		Standing waves	
m,n can be positive and negative		m,n must be non-negative	

The periodic boundary conditions produce twice the spacing between allowed  $k$  values as does the fixed-endpoint ones. Figure 8.1.13 shows the periodic boundary conditions (PBC) produce density of  $k$ -states 4 times smaller than that from the fixed-endpoint boundary conditions (FEBC)

$$g_{k(\text{pbc})}^{(2D)} = \frac{g_{k(\text{febc})}^{(2D)}}{4} \quad (8.1.20a)$$

Next, we see that constant energy circle covers 4 times the area for the PBCs as it does for the FEBCs.

$$A_{\text{pbc}} = 4A_{\text{febc}} \quad (8.1.20b)$$

The density of energy states can then be calculated from the product of Equations 8.1.20. We find the same result for either set of boundary conditions.

$$g(E) = g_{k(\text{pbc})}^{(2D)} A_{(\text{pbc})} = \frac{g_{k(\text{febc})}^{(2D)}}{4} 4A_{(\text{febc})} = g_{k(\text{febc})}^{(2D)} A_{(\text{febc})} \quad (8.1.20c)$$

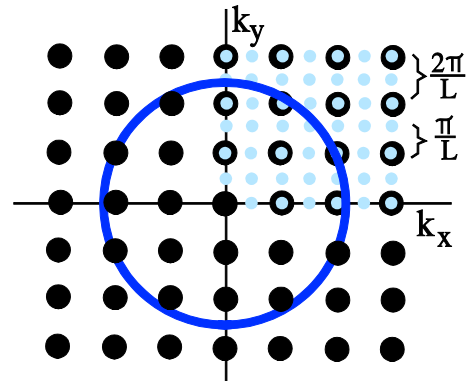


Figure 8.1.13: Large dots represent allowed  $k$  for periodic BC while the small dots represent the fixed-endpoint BCs.

Topic 8.1.9: Changing Summations to integrals

The density-of-states can be used to convert summations to integrals. Suppose we start with a summation of coefficients  $C_{\vec{k}}$  of the form

$$S = \sum_{\vec{k}} C_{\vec{k}}$$

The index  $\vec{k}$  on the summation means to sum over allowed values of  $k_x, k_y, k_z$ ; i.e., think of the two dimensional plot in the previous topics and imagine that  $C_{\vec{k}}$  has a different value at each point on the plot. For one dimension, a plot of “ $C_k$  vs.  $k$ ” might appear as in Figure 8.1.14. Suppose the allowed values of “ $k$ ” are close to one another. Let  $\Delta k_i$  be a small interval along the  $k$ -axis but assume that it contains 4 of the “ $k$ ” points. Let  $k_i$  be the center of each of these intervals. The figure shows that

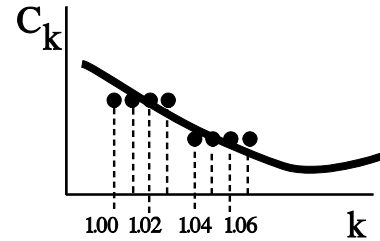


Figure 8.1.14: Example of closely spaced modes.

$$S = (C_{1.00} + C_{1.01} + C_{1.02} + C_{1.03}) + (C_{1.04} + C_{1.05} + C_{1.06} + C_{1.07}) + \dots$$

The sum can be recast into

$$S = 4C_{1.00} + 4C_{1.04} + \dots = \sum [g(k)\Delta k] C_k \equiv \sum C(k)g(k)\Delta k \cong \int dk C(k)g(k)$$

where, for the figure,  $\Delta k = 0.04$  and  $g(k) = 4/0.04 = 100$  (states per  $k$ -length).

Alternatively, suppose a slowly varying function  $f(x)$  is defined at the points in the set  $\{x_1, x_2, \dots\}$  where the points  $x_i$  are equally spaced and separated by the common distance  $\Delta x$ . The summation can be rewritten as

$$\sum_i f(x_i) = \sum_i \frac{1}{\Delta x_i} f(x_i) \Delta x_i$$

We recognize the quantity  $1/\Delta x$  as the density of states; that is,  $g = 1/\Delta x$ . Recognizing the second summation as an integral for sufficiently small  $\Delta x$ , the summation can be written as

$$\sum_i f(x_i) \cong \int dx g(x) f(x) \tag{8.1.21}$$

The last expression generalizes to a 3-D case most commonly applied to the wave vectors discussed in the preceding topics.

$$\sum_{\vec{k}} f(\vec{k}) \rightarrow \int d^3k g(\vec{k}) f(\vec{k}) = \frac{V}{(2\pi)^3} \int d^3k f(\vec{k}) \tag{8.1.22}$$

where  $V$  represents the normalization volume coming from periodic boundary conditions. We essentially use this last integral when we find the total number of discrete states within a sphere or circle.

*Topic 8.1.10: A Brief Review of the Fermi-Dirac Distribution*

At thermal equilibrium the number of electrons occupying a conduction band state or a valence band state can be written as

$$F_e = \frac{1}{1 + e^{\frac{E-E_f}{kT}}} \quad (8.1.23a)$$

where  $E_f$  represents the Fermi level. The average number of electrons per state can range between 0 and 1. Equation 8.1.23 can be interpreted as a probability. At  $E = E_f$ , the probability has the value of 0.5. The probability of a hole occupying a state necessarily has the form

$$F_h(E) = 1 - F_e = \frac{1}{1 + e^{\frac{E-E_f}{kT}}} \quad (8.1.23b)$$

If the states in either case have energy at least several  $kT$  away from the Fermi level then these two equations reduce to the Boltzman distribution for electrons in the conduction band and holes in the valence band, respectively.

$$F_e = e^{-\frac{E-E_f}{kT}} \quad F_h = e^{+\frac{E-E_f}{kT}} \quad (8.1.23c)$$

These do not apply to electrons in the valence band or holes in the conduction bands since otherwise the Fermi functions would be larger than 1 for sufficiently large energy.

The number of electrons over a range of energy must be given as follows

$$n = \sum_{\text{energy}} \#e = \sum_{\text{energy}} \frac{\#e}{\text{State}} \frac{\#States}{\text{Energy}} \rightarrow \int dE F_e(E) g(E) \quad (8.1.24)$$

As discussed in solid state and device physics books, the doping level determines the placement of  $E_f$ . The law of mass action  $np = n_i^2$  holds regardless of the doping lever where  $n_i$  refers to the number of electrons at thermal equilibrium without doping ( $n_i = p_i$ ).

*Topic 8.1.11: The Quasi Fermi Levels*

Thermal equilibrium requires the number of electrons and holes to satisfy the Fermi-Dirac distribution. There exists only one Fermi level  $E_f$  as shown on the left side of Figure 8.1.15. Non-thermal generation of carriers (such as photogeneration or injection) produces more carriers than should be present for temperature  $T$  as dictated by the Fermi-Dirac distribution. Therefore, the distribution does not obey the Fermi-Dirac distribution and the position of the Fermi level  $E_f$  cannot simultaneously describe the number of free electrons and holes. Instead, the

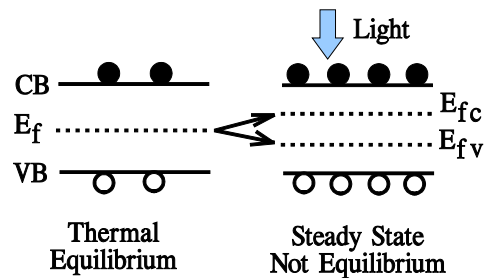


Figure 8.1.15: Non-thermal generation of carriers splits a single Fermi level  $E_f$  into two quasi Fermi levels  $E_{fc}$  and  $E_{fv}$ . Both cases are maintained at the same temperature  $T$ .

Fermi level splits into two quasi Fermi levels  $E_{fc}$  and  $E_{fv}$  for the conduction and valence electrons, respectively.

The probability of an electron occupying a state in the conduction and valence bands, respectively, becomes

$$F_c(E) = \frac{1}{1 + \text{Exp}\left(\frac{E - E_{fc}}{kT}\right)} \quad (8.1.25a)$$

$$F_v(E) = \frac{1}{1 + \text{Exp}\left(\frac{E - E_{fv}}{kT}\right)} \quad (8.1.25b)$$

The probability of a valence or conduction band state being empty must be  $1 - F_v$  and  $1 - F_c$ , respectively.

The quasi Fermi functions provide the number of electrons in the conduction and valence bands. The number of conduction electrons, for example, can be written as

$$n = \int_{E_g}^{\infty} dE g_c(E) F_c(E) \quad (8.1.26)$$

The quasi Fermi *level* fixes the number of electrons as will now be demonstrated. This is important for lasers since the separation of the quasi fermi levels must generally be larger than the band gap. In the parabolic band approximation for a 3-D bulk crystal, the number of electrons must be

$$n = \int_{E_g}^{\infty} dE C m_e^{3/2} \frac{\sqrt{E - E_g}}{1 + e^{\frac{E - E_{fc}}{kT}}} \quad (8.1.27)$$

where C denotes constants associated with the 3-D bulk density of states  $C = \sqrt{2}/(\pi^2 \hbar^3)$ .

Setting

$$\xi = \frac{E - E_g}{kT} \quad d = \frac{E_{fc} - E_g}{kT} \quad (8.1.28)$$

where “d” signifies the difference in energy between the quasi-Fermi level  $E_{fc}$  and the

band gap energy  $E_g$ . Equation 8.1.27 for the total number of electrons in the conduction band can be rearranged into either of two equivalent forms

$$n = C(kT)^{3/2} m_e^{3/2} F(d) \quad (8.1.29a)$$

$$n = C(kT)^{3/2} (m_e d)^{3/2} F_d(d) \quad (8.1.29b)$$

where the functions F and  $F_d$  are

$$F(d) = \int_0^{\infty} d\xi \frac{\sqrt{\xi}}{1 + e^{\xi - d}} \quad F_d = \int_0^{\infty} d\xi \frac{\sqrt{\xi/d^3}}{1 + e^{\xi - d}} \quad (8.1.29c)$$

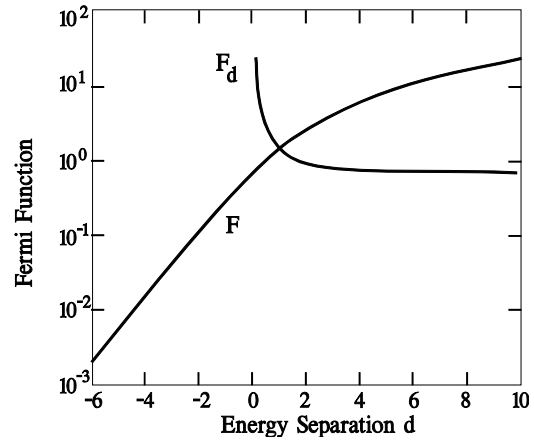


Figure 8.1.16: A plot of the Fermi F and  $F_d$ .

These equations differ only by the placement of the energy separation  $d$ . Equation 8.1.29b incorporates the energy separation  $d$  with the effective mass whereas Equation 8.1.29a includes it in the function  $F_d$ . Figure 8.1.16 plots both functions. In particular, notice  $F_d$  approaches 0.7 for large energy separation  $d > 2$  or equivalently  $E_{fc} > E_g + 2kT$ . Therefore, the number of electrons can be characterized by  $m_e d$  in Equation 8.1.29b when the quasi-Fermi level is more than several  $kT$  beyond the band edge. The number of electrons becomes approximately

$$n \cong 0.7 C (kT)^{3/2} (m_e d)^{3/2} \cong \frac{(kT)^{3/2}}{\pi^2 \hbar^3} (m_e d)^{3/2} \quad (8.1.30)$$

where  $m_e$  represents the effective mass of the electron and  $d = (E_{fc} - E_g)/kT$ .