

Section 7.16: Introduction to Density of States

Many physical phenomena depend on the number of states within an energy range (energy density of states). When a semiconductor absorbs light for example, electrons can be promoted from occupied valence states to empty conduction states. The energy of the photons must match the energy difference between the occupied and the empty states. Without the empty states, the transitions cannot occur. More occupied valence states and more unoccupied conduction states mean the possibility of greater transition rates and therefore higher levels of absorption. The same reasoning applies to thermal transitions.

The discussion distinguishes between localized and extended states only in their role in semiconductor processes. The localized states provide a convenient starting picture for developing the energy density of states. All bands in a semiconductor consist of extended states. This section discusses density of states for electrons in bulk and heterostructure with special focus on reduced dimensional structures such as quantum wells, quantum wires and quantum dots. Sections 7.5 and 7.6 discuss the origin and meaning of subbands. For bulk semiconductors, we indicate how satellite valleys in the bands affect the density of states. The discussion includes the reduced density of states necessary for light emitters and absorbers.

Topic 7.16.1: Introduction to Localized and Extended States

The “localized states” refer to traps and recombination centers. Electrons (or holes) moving in a semiconductor collide with the traps and become immobilized. The localized electron or hole has a wavefunction with finite size. For example, Figure 7.16.1 shows an electron caught in a trap; the electron has a Gaussian shaped wavefunction. The trap can be thought of as finitely deep square well potential. The localized states occur in the bulk or at the surface of a semiconductor. The surface states trap either electrons or holes or act as surface recombination centers.

The position of the state within the band gap determines whether it behaves as a trap or as a recombination center. Shallowly trapped electrons require little energy to become free. A semiconductor at room temperature supplies sufficient numbers of phonons to release the electron. States near the center tend to be recombination centers since few phonons have enough energy to release the electron. Eventually a free hole encounters the trapped electron and recombines with it. Therefore the depth of the trap controls the rate of release and determines its function for recombination and optical processes.

The localized surface and bulk states affect the efficiency of electronic and optoelectronic components. As just mentioned, the localized states can function as recombination centers that lower the efficiency of the device. For example, consider a light emitting diode operating under forward bias. The recombination centers provide recombination current that does not contribute to the optical emission. Therefore the

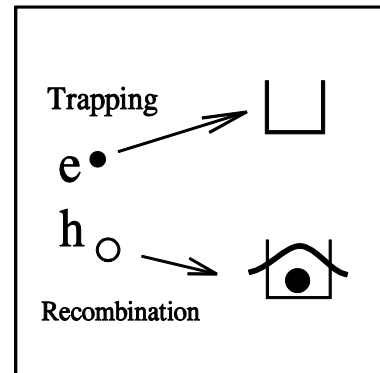


Figure 7.16.1: Trapping states with localized wavefunctions.

efficiency of the bias current for producing light must be reduced as compared with the case for a high quality semiconductor without recombination or trapping centers.

The extended states refer to plane waves with infinite extent and to electrons (or holes) with unrestricted motion within the semiconductor. In particular, they describe electrons and holes within the valence or conduction band. The Bloch wave function has the plane wave as the envelope function. A finite system can support only certain plane waves which gives rise to the quantized energy and discrete states. The boundary conditions produce the allowed wave vectors.

Topic 7.16.2: Definition of the Density of States

In this topic, we discuss the counting procedure for the energy density of states. We start with the localized states for simplicity.

The energy density of states (EDOS) function measures the number of energy states in each unit interval of energy and in each unit volume of the crystal

$$g(E) = \frac{\text{\#states}}{\text{Energy} * \text{XalVol}} \quad (7.16.1)$$

We need to explore the reasons for dividing by the energy and the crystal volume.

First we discuss the reason for the “per unit energy”. Suppose we have a system with the energy levels shown at the left of Figure 7.16.1. Assume for now the number of states occurs in a unit volume of material (say 1 cm³). Maybe the system consists of a few quantum wells with slightly different widths distributed throughout the material. The figure shows the energy levels from all of the wells in the unit volume. The figure shows 4 energy states in the energy interval between 3 and 4 eV. The density of states at E=3.5 must be

$$g(3.5) = \frac{\text{\#states}}{\text{Energy} \times \text{Vol}} = \frac{4}{1\text{eV} \times 1\text{cm}^3} = 4$$

Similarly, between four and five electron volts, we find two states and the density of states function has the value $g(4.5) = 2$ and so on. Essentially, we just add up the number of states at each energy. The graph shows the number of states vs. energy; for illustration, the graph has been flipped over on its side. Generally we use finer energy scales and the material has larger numbers of states (10^{17}) so that the graph generally appears much smoother than the one in Figure 7.16.1 since the energy levels essentially form a continuum. The “per unit energy” characterizes the type of state and the type of material.

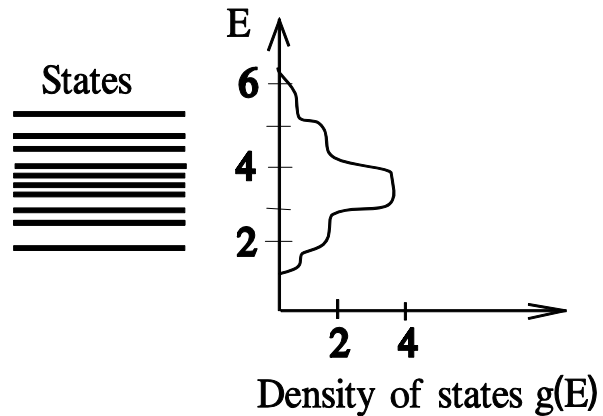


Figure 7.16: The density of states for the discrete levels shown on the left-hand side. The plot assumes the system has unit volume (1 cm³) and the levels have energy measured in eV.

The definition of density of states uses “per unit crystal volume” in order to remove geometrical considerations from the measure of the type of state. Obviously, if each unit volume has N_v traps given by

$$N_v = \int_0^\infty dE g(E) = \int d(\text{energy}) \frac{\# \text{states}}{\text{Energy} * \text{vol}} = \frac{\# \text{states}}{\text{vol}} \quad (7.16.2)$$

then the volume V must have $N = N_v V$ traps. Changing the volume changes the total number. To obtain a measure of the “type of state”, we need to remove the trivial dependence on crystal volume.

What are the states? The states can be those in an atom. The states can also be traps that an electron momentarily occupies until being released back into the conduction band. The states might be recombination centers that electrons enter where they recombine with holes. Traps and recombination centers can be produced by defects in the crystal. Surface states occur on the surface of semiconductors as an inevitable consequence of the interrupted crystal structure. The density of defects can be low within the interior of the semiconductor and high near the surface; as a result, the density of states can depend on position.

Let’s consider several of examples. First, suppose a crystal has two discrete states (i.e. single states) in each unit volume of crystal. Figure 9.10.2 shows the two states on the left side of the graph. The density-of-state function consists of two Dirac delta functions of the form

$$g(E) = \delta(E - E_1) + \delta(E - E_2)$$

Integrating over energy gives the number of states in each unit volume

$$N_v = \int_0^\infty dE g(E) = \int_0^\infty dE [\delta(E - E_1) + \delta(E - E_2)] = 2$$

If the crystal has the size $1 \times 4 \text{ cm}^3$ then the total number of states in the entire crystal must given by

$$N = \int_0^4 dV N_v = 8$$

as illustrated in Figure 9.10.3. Although this example shows a uniform distribution of states within the volume V , the number of states per unit volume N_v can depend on the position within the crystal. For example, the growth conditions of the crystal can vary or perhaps the surface becomes damaged after growth.

As a second example, consider localized states near the conduction band of a semiconductor as might occur for amorphous silicon. Figure 7.16.4 shows a sequence of graphs. The first graph shows the distribution of states versus the position “ x ” within the semiconductor. Notice that the states come closer together (in energy) near the conduction band edge. As a note, amorphous materials have mobility edges rather than band edges. The second graph shows the density of states function versus energy. A sharp Gaussian spike represents the number of states at each energy. At 7 electron volts, the material has six states (traps) per unit length in the

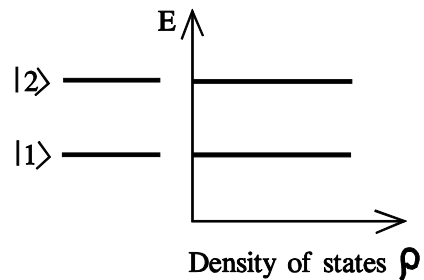


Figure 7.16.2: The density of states for two discrete states shown on the left side.

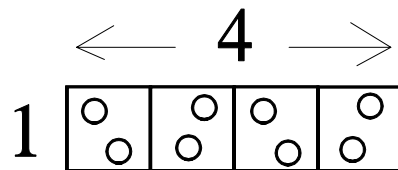


Figure 7.16.3: Each unit volume has two states and the full volume has 8.

semiconductor as shown in the first graph. The second graph shows a spike at seven electron volts. Actual amorphous silicon has very large numbers of traps near the upper mobility edge and they form a continuum as represented in the third graph. This example shows how the density of states depends on position and how closely spaced discrete levels form a continuum.

As a final example for localized states, let's consider the role of localized states for nanoscale devices. Suppose a small cube of length L represents a small electronic device. Suppose electrons and holes are created in the bulk and on the surface either by electrical or optical pumping. Suppose the device should function when carriers recombine in the bulk of the material (for example, the device might be a small LED). However, some of the carriers will recombine at surface states, which does not contribute to the device operation. We can reasonably assume the bulk and surface recombination rates depend on the total number of states at the surface and in the bulk. The surface recombination rates must be

$$R_{\text{bulk}} = C_v N_v V = C_v N_v L^3 \quad R_{\text{surf}} = C_A N_A A = C_A N_A L^2 \quad (7.16.3)$$

where C_v, C_A are constants, N_v, N_A represent the total number of states per volume and area. We therefore see the ration of surface to bulk recombination rates must be

$$\frac{R_{\text{surf}}}{R_{\text{bulk}}} = \frac{C_A N_A L^2}{C_v N_v L^3} \sim \frac{1}{L} \quad (7.16.4)$$

We therefore see that surface recombination can dominate the bulk recombination at sufficiently small sizes. For a device intended to operate using traditional bulk processes, the surface states pose significant problems and can completely destroy the device efficiency. For recombination involving phonons, the surface becomes the prime heating agent.

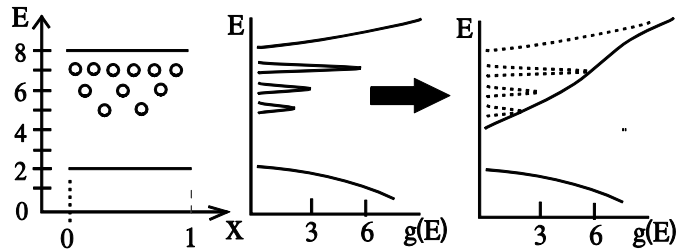


Figure 7.16.4: Transition from discrete localized states to the continuum.

Topic 7.16.3: Relation between Density of Extended States and Boundary Conditions

So far we have discussed the density of states for the localized states. We can add up the number of extended states using similar techniques. However, the extended states correspond to plane waves characterized by a wave vector \vec{k} and angular frequency ω_k . For electron and hole wave functions, the band diagrams inter-relate the wave vector and angular frequency. Therefore allowed values of energy $E = \hbar\omega$ must be related to allowed values of k .

The electron can be either confined to a finite region of space or not confined at all. Confining an electron to a finite region of space places conditions on the allowed electron wavelength and hence also on the allowed wave vectors. Finite regions of space produce discrete allowed wave vectors and therefore discrete energy values. Boundary conditions mathematically model the effect of the finite regions. Either fixed-endpoint conditions or periodic boundary conditions can be applied to the wavefunction for the confined electron. The fixed-endpoint boundary conditions produce sine and cosine standing waves for the energy eigenfunctions. The wave vectors \vec{k} have only positive components as given by the Fourier summations in Chapter 2. The periodic boundary conditions over a finite distance L usually applies to planewaves even though the wave must be restricted to length L . In this case, the wave vectors \vec{k} have both positive and negative components. We apply these periodic conditions to macroscopic size L as opposed to the quantum well or wire. For those electrons not confined to finite regions, we apply the periodic boundary conditions over the length L . Here the length L appears artificial in order to provide normalization for an infinitely sized wave. Nevertheless, the finite size of L leads to discrete allowed wavelengths, wave vectors, and therefore also energy. For infinitely sized regions, we can let the repetition length L increase unbounded. The allowed wavelengths, wave vectors and energy become infinitesimally close together and essentially form a continuum. The transition from the Fourier series to the Fourier transform appears very similar to this procedure for letting L increase without bound. In real crystals with finite sizes, the length of the crystal must be identical with the repetition size. In such a case, the size of the crystal sets a minimum spacing for allowed k . We find that each atom contributes one state to each band. The number of states in each band must be the same as the number of atoms N .

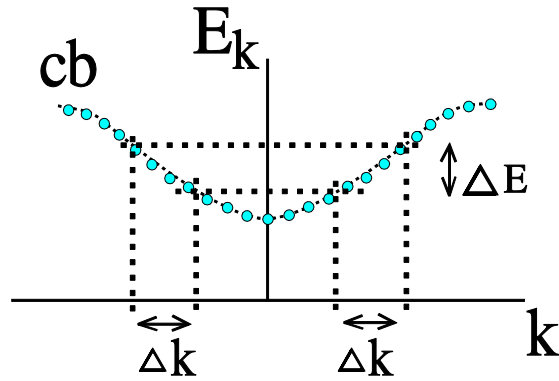


Figure 7.16.5: The density of energy states must be related to the density of k -states.

Once we know the allowed energies for a finite system, we can count the number of allowed states. Figure 7.16.5 shows the discrete states for the conduction band. We can count the number of states in the energy range ΔE to find $g(E)$. However, the figure makes it clear that 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 ΔE comes from

the two regions marked Δk . For 2-D systems the Δk region corresponds to an annular region between two circles as depicted in Figure 3.7.3 for phonons.

Topic 7.16.4: 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 7.16.6. The wavelengths can be no 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

$$k_n = \frac{2\pi}{(2L/n)} = \frac{n\pi}{L} \quad n = 1, 2, 3, \dots \quad (7.16.5)$$

The integer “ n ” must be positive when using the Fourier series expansion in Sine and Cosine basis set given by

$$B = \left\{ \frac{1}{\sqrt{2L}}, \frac{1}{\sqrt{L}} \cos(k_n x), \frac{1}{\sqrt{L}} \sin(k_n x) \right\} \quad (7.16.6)$$

On the other hand, the integers n must be positive and negative $n = 0, \pm 1, \pm 2, \dots$ for the equivalent basis set

$$B' = \left\{ \frac{e^{ik_n x}}{\sqrt{2L}} \right\} \quad (7.16.7)$$

Although the range of “ n ” is larger for the exponential basis set, the two sets contain the same number of basis functions.

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

$$\vec{k} = \frac{n_x \pi}{L} \hat{x} + \frac{n_y \pi}{L} \hat{y} + \frac{n_z \pi}{L} \hat{z} \quad (7.16.8)$$

where $n_x, n_y, n_z = 0, \pm 1, \dots$ 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.

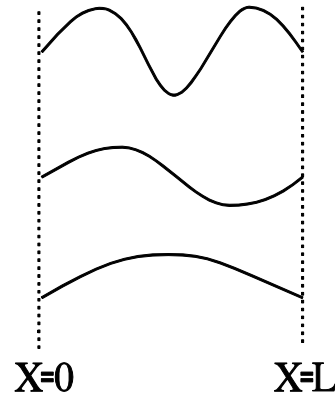


Figure 7.16.6: The endpoint boundary conditions.

Topic 7.16.5: 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 infinitely sized media, such as free space, the length L can be increased without bound. We are primarily interested in finite physical crystals. In this case, the waves can be imagined to have infinite extent by imagining copies of the physical crystal next to each other as shown in Figure 7.16.7.

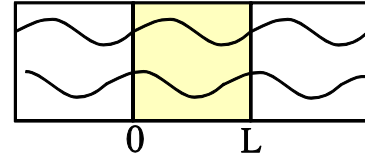


Figure 7.16.7: Repeating the physical crystal every distance L .

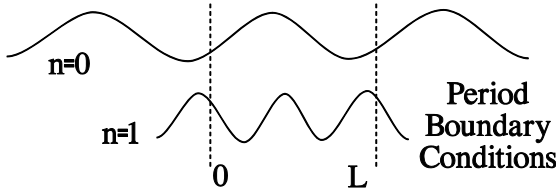


Figure 7.16.8: The first two allowed modes that satisfy the periodic boundary conditions.

Two allowed modes with the longest wavelengths appear in Figure 7.16.8. 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

$$k_n = \frac{2\pi}{\lambda_n} = \frac{2\pi n}{L} \quad (7.16.9a)$$

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

$$k_n = \frac{2\pi}{\lambda_n} = \frac{2\pi}{a} \frac{n}{N} \quad (7.16.9b)$$

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 smallest wavelength of interest must be $\lambda_{\max} = 2a$ corresponding to the edge of the first Brillouin zone at $k_{\text{FBZ}} = \pi/a$. Therefore the allowed wave vectors can be written as

$$k_n = \frac{2\pi}{\lambda_n} = \frac{2\pi}{a} \frac{n}{N} \quad n = \pm 1, \pm 2, \dots, \pm N/2 \quad (7.16.9c)$$

We see that each band must have N states. For crystals with an atomic basis, N represents the number of unit cells.

The periodic boundary conditions apply similarly to three-dimensional cubic systems to give an allowed set of wave vectors

$$\vec{k} = \frac{2\pi n_x}{L} \hat{x} + \frac{2\pi n_y}{L} \hat{y} + \frac{2\pi n_z}{L} \hat{z} \quad n_x, n_y, n_z = 0, \pm 1, \dots \quad (7.16.10a)$$

where the same length “ L ” appears in all three terms. This requires the wavefunction to be normalized to the volume of a cube. In principle, all three terms in Equation 7.16.10 could have different denominators but it doesn’t change the calculation of the density of states. Let’s assume N atoms along each edge of the cube (N^3 total atoms) then length L must be $L=Na$ and the allowed k -vectors have the form

$$\vec{k} = \frac{2\pi n_x}{aN} \hat{x} + \frac{2\pi n_y}{aN} \hat{y} + \frac{2\pi n_z}{aN} \hat{z} \quad n_x, n_y, n_z = 0, \pm 1, \dots \quad (7.16.10b)$$

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

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

However, we place an upper limit on the wave vectors not required by the periodic boundary conditions. The upper limit occurs at the edge of the FBZ where the wave can no longer propagate. The smallest wavelength of $\lambda = 2a$ produces components of the wave vector

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

Therefore the allowed wave vectors must be

$$\vec{k} = \frac{2\pi n_x}{a N} \hat{x} + \frac{2\pi n_y}{a N} \hat{y} + \frac{2\pi n_z}{a N} \hat{z} \quad n_x, n_y, n_z = 0, \pm 1, \dots, \pm N/2 \quad (7.16.10c)$$

Again we see each 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).

Topic 7.16.4: The Density of k-States

The “density of k-states” measures the number of possible modes in a given region of k-space. Figure 7.16.3 shows a *two-dimensional region* of k-space for the vectors

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

that assumes periodic boundary conditions. Consider just 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

$$g_{\vec{k}}^{(2D)} = \frac{1}{(2\pi/L)^2} = \frac{L^2}{4\pi^2} = \frac{A_{\text{xal}}}{4\pi^2} \quad (7.16.11)$$

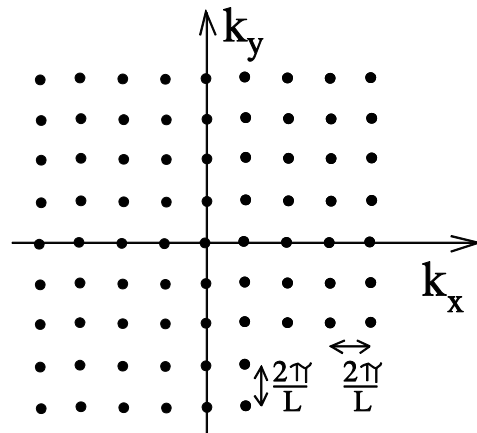


Figure 7.16.3: The allowed values of \vec{k} as determined by periodic boundary conditions.

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

The same type of calculation provides the density of states for a *three-dimensional* crystal. In this case, we find one mode in each elemental volume of k -space

$$g_{\vec{k}}^{(3D)} = \frac{1}{(2\pi/L)^3} = \frac{L^3}{8\pi^3} = \frac{V_{\text{xal}}}{8\pi^3} \quad (7.16.12)$$

where V_{xal} is the total volume of the crystal (in direct space). Many times the “density of k -states” has units of “#modes per unit crystal volume per unit k -space volume” thereby requiring us to divide the last equation by V_{xal} . The density of k -states becomes

$$g_{\vec{k}}^{(3D)} = \frac{1}{8\pi^3} \quad (7.16.13)$$

We can likewise surmise the density of states for the 1-D crystal

$$g_{\vec{k}}^{(1D)} = \frac{1}{(2\pi/L)} = \frac{L}{2\pi} \quad (7.16.14)$$

The previous equations show that the density of states for n -dimensions can be written as

$$g_{\vec{k}}^{(n-D)} = \frac{1}{(2\pi/L)^n} = \left(\frac{L}{2\pi}\right)^n \quad (7.16.15)$$

Topic 7.16.5: The Electron Density of Energy States for a 2-D Crystal

In this topic and the next topic, we discuss the density of energy states for 2-D and 3-D arrays of atoms. We need to clearly distinguish these cases from those encountered with reduce 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, let’s first consider the 2-D case for the electronic density of energy states. We need the energy versus wave vector \mathbf{k} . Keep in mind that the \mathbf{k} -vector refers to the envelope of the Bloch wavefunction and therefore we must use the effective mass. We can write the energy dispersion relation for the electron near the bottom of the conduction band as

$$E = \frac{\hbar^2 \mathbf{k}^2}{2m_e} \quad (7.16.16)$$

where we have shifted the energy scale for convenience to set the bottom of the conduction band at $E_c = 0$. This last equation does not represent the full band $E = E(\vec{k})$ but only a portion of it. The previous topic calculated the number of k -states per unit wave-number without restriction to the shape of the dispersion curve.

Now we determine the number of energy states in each unit interval of energy E . We have seen that the number of energy states must be related to the number of allowed k -states as discussed in Topic 7.16.3.

Equation 7.16.16 relates the magnitude of the wave vector to the energy of the wave. We want to know how many states fall within each unit interval of energy. We therefore need to know how many states fall within each unit length represented by $k = |\vec{k}|$. Therefore, first find the number of states per unit k -length. Figure 7.16.4 shows the total number of states within the k -space area of a circle of radius “ κ ” is given by

$$N_T = \text{total number} = \sum_{k-\text{area}} \frac{\text{number}}{k-\text{area}} \Delta(k-\text{area}) \quad (7.16.1)$$

which can be rewritten as

$$N_T = \int g_k^{(2D)} (dk |k| d\phi) \quad (7.16.18)$$

Substituting for the density of k -states and using a dummy variable κ provides

$$N_T = \int_0^{\kappa} \kappa d\kappa \int_0^{2\pi} d\phi g_k^{(2D)} = \int_0^{\kappa} \kappa d\kappa \int_0^{2\pi} d\phi \frac{A_{\text{xal}}}{4\pi^2} = \int_0^{\kappa} \kappa d\kappa \frac{A_{\text{xal}}}{4\pi^2} 2\pi \quad (7.16.19)$$

Integrating over k provides

$$N_T = \frac{A_{\text{xal}}}{4\pi^2} \pi \kappa^2 = g_k^{(2D)} A_{k-\text{sp}} \quad (7.16.20)$$

where $A_{k-\text{sp}} = \pi \kappa^2$ gives the area of the circle. We could have written Equation 7.16.20 right from the start since $g_k^{(2D)}$ is independent of k . The density of states per unit “*magnitude* k ” can be found if desired from the last equation by differentiating

$$g_k^{(2D)} = \frac{\partial N_T}{\partial k} = \frac{A_{\text{xal}} k}{2\pi}$$

Notice that this last equation differs from Equation 7.16.11 because this one gives the number of states per unit k -length whereas 7.16.11 gives the number of states per unit k -area.

We can find the density of energy states by solving for the magnitude of the wave vector in the dispersion relation $E = \hbar^2 k^2 / (2m_e)$ and then substituting into Equation 7.16.20.

$$N_T = g_k^{(2D)} A_{k-\text{sp}} = \frac{A_{\text{xal}}}{4\pi^2} \pi k^2 = \frac{A_{\text{xal}}}{2\pi} \frac{m_e}{\hbar^2} E$$

Therefore, the number of states per unit energy must be given by

$$g_E^{(2D)} = \frac{\partial N_T}{\partial E} = \frac{A_{\text{xal}}}{2\pi} \frac{m_e}{\hbar^2} \quad (7.16.21a)$$

where A_{xal} represents the area of the 2-D crystal. Usually, the physical size of the crystal is removed from the crystal to write

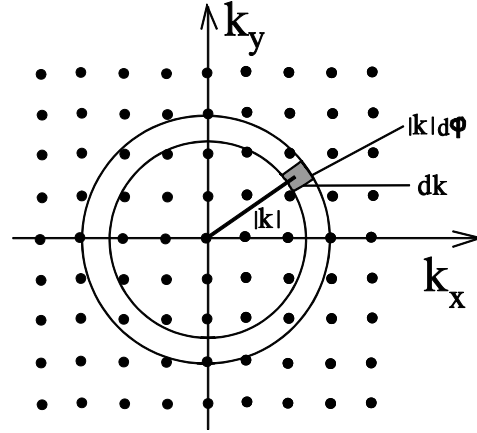


Figure 7.16.4: The number of modes in length dk (over the angular range of 2π) depends on the radius k .

$$g_E^{(2D)} = \frac{1}{2\pi} \frac{m_e}{\hbar^2} \quad (7.16.21b)$$

Notice that the 2-D density of energy states does not depend on the energy.

Topic 7.16.6: The Electron Density of Energy States for a 3-D Crystal

The *three-dimensional* case proceeds in a similar fashion to the 2-D case. We know that the density of states in k-space is

$$g_k^{(3D)} = \frac{V_{\text{xal}}}{8\pi^3}$$

The total number of states to a radius of κ is given by

$$N_T = \int_0^\kappa dk \int_0^{2\pi} k d\phi \int_0^\pi d\theta k \text{Sin } \theta g_k^{(3D)}$$

where the integral is given in spherical coordinates with a differential volume element of $(dk)(k d\phi)(d\theta k \text{Sin } \theta)$

The two angular integrals can be evaluated since the density of states does not depend on the angles. Using a dummy variable κ , we find

$$N_T = 4\pi \int_0^\kappa dk \kappa^2 g_k^{(3D)} = 4\pi \int_0^\kappa dk \kappa^2 \frac{V_{\text{xal}}}{(2\pi)^3} = \frac{V_{\text{xal}}}{(2\pi)^3} 4\pi \int_0^\kappa dk \kappa^2 \quad (7.16.22)$$

This last equation gives the total number of states in a k-space sphere of radius k

$$N_T = g_k^{(3D)} V_{\text{k-sph}} = \frac{V_{\text{xal}}}{(2\pi)^3} \frac{4\pi}{3} k^3 \quad (7.16.23)$$

The density of states in “*magnitude* k-space” can be written if desired by differentiating either Equation 7.16.22 or 7.16.23 to find

$$g_k^{(3D)} = \frac{\partial N_T}{\partial k} = \frac{V_{\text{xal}} k^2}{2\pi^2} \quad (7.16.24)$$

The density of states for E-space comes from differentiating Equation 7.16.23 and using the dispersion relation $E = \hbar^2 k^2 / (2m_e)$

$$g_E^{(3D)} = \frac{dN_T}{dE} = \frac{dk}{dE} \frac{dN_T}{dk} = \left(\frac{dE}{dk} \right)^{-1} \frac{d}{dk} \left(\frac{V_{\text{xal}}}{(2\pi)^3} \frac{4\pi}{3} k^3 \right) = \frac{m_e}{\hbar^2 k} \frac{4\pi V_{\text{xal}} k^2}{(2\pi)^3} = \frac{m_e V_{\text{xal}}}{2\pi^2 \hbar^2} k \quad (7.16.25)$$

The density of energy states must be written in terms of energy. The dispersion relation then provides

$$g_E^{(3D)} = \frac{m_e V_{\text{xal}}}{2\pi^2 \hbar^2} \sqrt{\frac{2m_e E}{\hbar^2}} = \frac{m_e^{3/2} V_{\text{xal}}}{\sqrt{2} \pi^2 \hbar^3} \sqrt{E} \quad (7.16.26a)$$

Usually we divide out the crystal volume as appropriate for the definition of density of energy states to get

$$g_E^{(3D)} = \frac{m_e^{3/2}}{\sqrt{2} \pi^2 \hbar^3} \sqrt{E} \quad (7.16.26b)$$

As an important note, the electron can have either spin up or spin down. Often time, the spin degeneracy can be included in the density of states by multiplying by 2.

The 3-D density of energy states can be plotted next to the band diagram as illustrated in Figure 7.16.5. Both the conduction band and heavy hole valence band produces a density of states. The two bands have different density of states although they both increase as \sqrt{E} . Notice the conduction band has been shifted back to its proper location and the density of states for the conduction band actually increases as $\sqrt{E - E_c}$ where E_c represents the bottom of the conduction band. The effective mass controls the shape of the density of states.

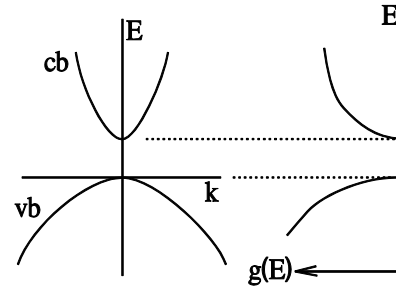


Figure 7.16.5: The conduction and valence band both have a density of states function.

We can see the reason that the effective mass enters into the formula (7.16.26) for the density of states from Figure 7.16.6. The two depicted bands have different curvatures. The boundary conditions produce equally spaced states along the horizontal k-axis. Let ΔE 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.

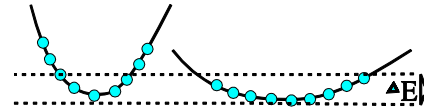


Figure 7.16.6: Different curvatures place different numbers of states in a fixed energy interval.

Topic 7.16.7: General Relation Between the g_k and g_E Mode Density

The previous topic shows how to find the k-space and E-space density of states. More generally, we can trace through the development of the previous two topic to find a general formula relating the density of states for the *magnitude* of \vec{k} (c.f., Equation 7.16.24) and the density of energy states. We just need to realize that we integrating over $|\vec{k}|$ up to some value κ must give the same number of states as integrating the energy E up to some value Ω . For example in 2-D, the radius of the circle in Figure 7.16.4 can be written in terms of either $k = |\vec{k}|$ or $E = \hbar^2 k^2 / (2m_e)$. Therefore, the dispersion relation relates the limits of the integral to give the same number of states within the circle $\Omega = \hbar^2 \kappa^2 / (2m_e)$. The total number of states can be written in two ways

$$\int_0^{\kappa} dk g_k = N_T = \int_0^{\Omega} dE g_E \quad (7.16.27)$$

Similar considerations can be applied to a variety of density of states including those for phonons and EM waves traveling in free space. Therefore, we expect

$$g_k dk = g_E dE \quad (7.16.28)$$

since κ, Ω are assumed to describe the same “region of mode space” as discussed below.

To see that relation 7.16.28 holds, consider the electron dispersion relation near the bottom of the conduction band $E = \frac{\hbar^2 k^2}{2m_e}$. Equation 7.16.27 becomes

$$\int_0^E dE' g_E(E') = N_T = \int_0^k dk' g_k(k')$$

Differentiate both sides with respect to E.

$$\frac{d}{dE} \int_0^E dE' g_E(E') = N_T = \frac{d}{dE} \int_0^k dk' g_k(k')$$

$$g_E(E) = \frac{dk}{dE} \frac{d}{dk} \int_0^k dk' g_k(k') = \frac{dk}{dE} g_k(k)$$

Therefore,

$$g_E(E) dE = g_k(k) dk$$

Topic 7.16.9: Tensor Effective Mass and Density of States

So far we have assumed symmetric bands in k_x, k_y, k_z . Now we repeat the derivation using the tensor effective mass

$$\left(m^{-1}\right)_{ij} = \frac{1}{\hbar^2} \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} E \quad (7.16.29)$$

from Sections 7.12 and 7.13.

We must use ellipsoid-shaped constant energy surfaces for the unsymmetrical band unlike the the spherical constant energy surfaces for the symmetrical bands. We can see this as follows. The energy as a function of the components of the wave vector can be written as

$$E = \frac{\hbar^2}{2} \sum_{ij} \left(m^{-1}\right)_{ij} k_i k_j \quad (7.16.30a)$$

For a diagonal mass matrix

$$\underline{m} = \begin{pmatrix} m_x & 0 & 0 \\ 0 & m_y & 0 \\ 0 & 0 & m_z \end{pmatrix} \quad (7.16.30b)$$

we find the energy relation

$$E = \frac{\hbar^2}{2} \left[\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z} \right] \quad (7.16.31c)$$

We put this last dispersion relation in the standard form for an ellipse

$$1 = \frac{k_x^2}{\left(\sqrt{\frac{2m_x E}{\hbar^2}}\right)^2} + \frac{k_y^2}{\left(\sqrt{\frac{2m_y E}{\hbar^2}}\right)^2} + \frac{k_z^2}{\left(\sqrt{\frac{2m_z E}{\hbar^2}}\right)^2} \quad (7.16.32a)$$

which can be written as

$$1 = \frac{k_x^2}{a^2} + \frac{k_y^2}{b^2} + \frac{k_z^2}{c^2} \quad \text{with} \quad a = \sqrt{\frac{2m_x E}{\hbar^2}} \quad b = \sqrt{\frac{2m_y E}{\hbar^2}} \quad c = \sqrt{\frac{2m_z E}{\hbar^2}} \quad (7.16.32b)$$

We now determine the density of states by finding the number of states within the constant energy surface as illustrated in Figure 7.16.7. As before, the density of states in \bar{k} space is

$$g_{\bar{k}}^{(3D)} = \frac{V_{\text{xal}}}{8\pi^3} \quad (7.16.33)$$

The volume of the ellipsoid can be written as

$$V = \frac{4\pi}{3} abc \quad (7.16.34)$$

The number of states within the constant energy surface must be

$$N(E) = g_{\bar{k}}^{(3D)} V = \frac{V_{\text{xal}}}{8\pi^3} \frac{4\pi}{3} abc = \frac{V_{\text{xal}}}{6\pi^2} \left(\frac{2}{\hbar^2} \right)^{3/2} E^{3/2} \sqrt{m_x m_y m_z} \quad (7.16.35)$$

The density of energy states can be written as

$$g(E) = \frac{dN}{dE} = \frac{V_{\text{xal}} m_e^{3/2}}{\sqrt{2} \pi^2 \hbar^3} \sqrt{E} \quad (7.16.36a)$$

where the effective mass must be

$$m_e = (m_x m_y m_z)^{1/3} \quad (7.16.36b)$$

Taking into account the two possible directions for electron spin and dividing out the crystal volume, we find

$$g(E) = \frac{dN}{dE} = \frac{\sqrt{2} m_e^{3/2}}{\pi^2 \hbar^3} \sqrt{E} \quad (7.16.36c)$$

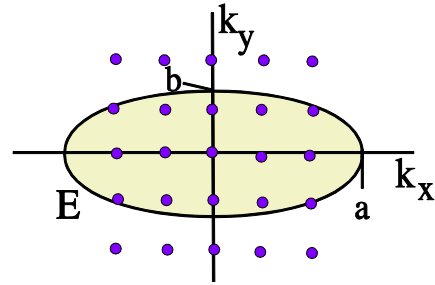


Figure 7.16.7: An ellipse in k -space as a constant energy surface.

Topic 7.16.9: Overlapping Bands

Gallium Arsenide has overlapping heavy hole (HH) and light hole (LH) valence bands as shown in Figure 7.16.10. 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 ΔE must include states from both the HH and LH bands.

We now discuss the method for calculating the density of states for overlapping sub-bands. For simplicity, consider two overlapping bands with positive curvature as shown in Figure 7.16.10. We can easily demonstrate that the density of states must be given by

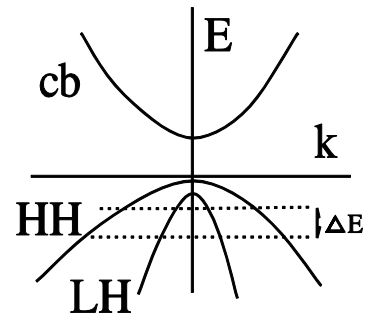


Figure 7.16.10: Light and heavy hole valence bands.

$$g_E^{(3D)}(E) = \frac{m_1^{3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - E_1} \Theta(E - E_1) + \frac{m_2^{3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - E_2} \Theta(E - E_2) \quad (7.16.37)$$

where the step function has the definition

$$\Theta(E - E_1) = \begin{cases} 0 & E < E_1 \\ +1 & E \geq E_1 \end{cases}$$

We can intuitively see that Equation 7.16.37 holds. At $E=0$, there isn't any band structure and therefore there can't be any states. 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 7.16.26. At energy E_2 , the number of

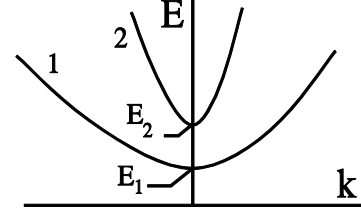


Figure 7.16.11: Two overlapping 3-D bands (inverted for convenience).

states in band 2 must be included. The density of states in band 2 increases as $\sqrt{E - E_2}$ again according to Equation 7.16.27. 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 7.16.37.

The density of states can also be demonstrated using relation 7.16.28 $g_E(E)dE = g_k(k)dk$. Looking at the band #1, the dispersion relation can be written as

$$E = E_1 + \frac{\hbar^2 k^2}{2m_1} \quad E > E_1 \quad (7.16.38a)$$

where, unlike in Topic 7.16.6, the bottom of the band remains shifted from $E=0$ and where m_1 represents the effective mass for band #1. The $|\vec{k}|$ density of states relation in Equation 7.16.24 remains unchanged

$$g_k^{(3D)} = \frac{\partial N_T}{\partial k} = \frac{V_{\text{vol}} k^2}{2\pi^2} \quad (7.16.38b)$$

Therefore, Equation 7.16.28 provides

$$g_E^{(1)}(E) = g_k(k) \left(\frac{dE}{dk} \right)^{-1} = \frac{V_{\text{vol}} k^2}{2\pi^2} \left(\frac{\hbar^2 k}{m_1} \right)^{-1} = \frac{m_1}{\hbar^2 2\pi^2} k \quad (7.16.39)$$

However, solving for k in Equation 7.16.38a, we find

$$k = \sqrt{\frac{2m_1}{\hbar^2} (E - E_1)} \Theta(E - E_1)$$

where the step function ensures k does not become imaginary. Therefore, we find

$$g_E^{(1)}(E) = \frac{m_1^{3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - E_1} \Theta(E - E_1) \quad (7.16.40a)$$

Similar reasoning applied to band 2 provides

$$g_E^{(2)}(E) = \frac{m_2^{3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - E_2} \Theta(E - E_2) \quad (7.16.40b)$$

Therefore, the total density of states can be found just by adding Equations 7.16.40 together

$$g_E(E) = g_E^{(1)}(E) + g_E^{(2)}(E) = \frac{m_1^{3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - E_1} \Theta(E - E_1) + \frac{m_2^{3/2}}{\sqrt{2} \pi^2 \hbar^2} \sqrt{E - E_2} \Theta(E - E_2)$$

as required.

Topic 7.16.11: Density of States from Periodic and Fixed-Endpoint Boundary Conditions

The topics in the present section find the density of states using the periodic boundary conditions. The length L in Figures 7.16.7 and 7.16.8 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 7.16.7. 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 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>
$\lambda_x = L/m \quad \lambda_y = L/n$	$\lambda_x = 2L/m \quad \lambda_y = 2L/n$
$k_x = 2\pi m/L \quad k_y = 2\pi n/L$	$k_x = \pi m/L \quad k_y = \pi n/L$
$\Delta k_x = 2\pi/L \quad \Delta k_y = 2\pi/L$	$\Delta k_x = \pi/L \quad \Delta k_y = \pi/L$
Travelling waves	Standing waves
m,n can be positive and negative	m,n must be non-negative

The spacing between allowed k values is twice the size for the periodic boundary conditions compared with the fixed-endpoint ones. As shown in Figure 7.16.12, the density of k -states from the periodic boundary conditions (PBC) must be 25% that for the fixed-endpoint boundary conditions (FEBC)

$$g_{\vec{k}(\text{pbc})}^{(2D)} = \frac{g_{\vec{k}(\text{febc})}^{(2D)}}{4} \quad (7.16.41a)$$

Next, we see that the portion of the area of the constant energy circle covering the allowed states for the periodic boundary conditions is 4 times that for the fixed-endpoint conditions.

$$A_{\text{pbc}} = 4A_{\text{febc}} \quad (7.16.41b)$$

The density of energy states can then be calculated from the product of Equations 7.16.41. We find the same result for either set of boundary conditions.

$$g(E) = g_{\vec{k}(\text{pbc})}^{(2D)} A_{(\text{pbc})} = \frac{g_{\vec{k}(\text{febc})}^{(2D)}}{4} 4A_{(\text{febc})} = g_{\vec{k}(\text{febc})}^{(2D)} A_{(\text{febc})} \quad (7.16.41c)$$

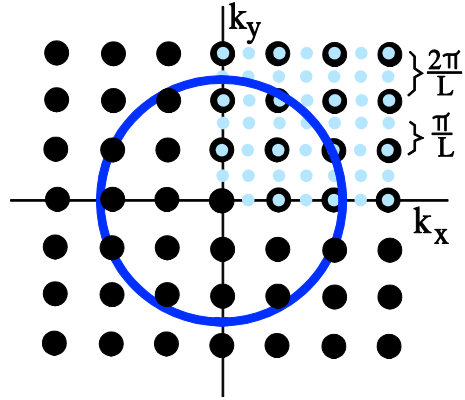


Figure 7.16.12: Full black circles represent allowed \vec{k} for periodic BC while the sky-blue circles represent the fixed-endpoint BCs.

Topic 7.16.12: Changing Summations to integrals

We often use the density-of-states (i.e., density-of-modes) to find the total number of carriers when we know the number per state (Fermi-Dirac Distribution). However the same reasoning applies to other quantities besides the number of carriers. Lets call the amount of some quantity per state as amount/state. We can write

$$\text{total amount} = \sum \frac{\text{amount}}{\text{state}} \cdot \frac{\#\text{states}}{\text{k-space}} \cdot \Delta(\text{k-space})$$

Let $A(\vec{k})$ be the “amount” per state at wave vector \vec{k} and let $g_{\vec{k}}$ be the \vec{k} -space density-of-modes. The “total amount” can be written by

$$\text{total amount} = \int_{\text{k-vol}} A(\vec{k}) g_{\vec{k}} d^3\vec{k}$$

The differential $d^3\vec{k}$ represents a small element of volume in \vec{k} -space such as, for example, the volume element in the previous topic of the form

$$d^3\vec{k} = k^2 \sin \theta dk d\phi d\theta$$

The density-of-states and density-of-modes 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 the figure. Suppose the allowed values of “ k ” are close

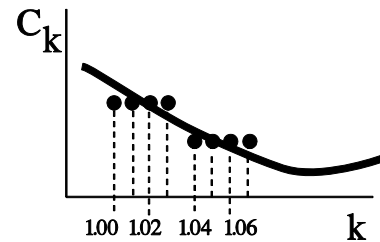


Figure 7.16.13: Example of closely spaced modes.

to one another. Let ΔK_i be a small interval along the k -axis; this interval is small but assume that it contains many of the “ k ” points. Let K_i be the center of each of these

intervals. The figure shows that

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

The sum can be recast into

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

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

Now let prove the above conjecture in general -- it works for any slowly varying function $f(x)$. Suppose f 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 Δx . 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 Δx , the summation can be written as

$$\sum_i f(x_i) \cong \int dx g(x) f(x) \tag{7.16.42}$$

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

$$\sum_{\vec{k}} f(\vec{k}) \rightarrow \int d^3k g(\vec{k}) f(\vec{k}) = \frac{V}{(2\pi)^3} \int d^3k f(\vec{k}) \tag{7.16.43}$$

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 7.16.13: Comment on Probability

The previous topic discusses the use of the density of states for computing summations. This topic points out the difference between the average/probability and the density of states function.

Suppose that repeated measurement of a random variable X produces a discrete set x_1, x_2, x_3, \dots . The average value of that set is given by

$$\langle x \rangle = \frac{1}{N} \sum_{i=1}^N x_i$$

Suppose we plot the value of X vs. the measurement number as shown in Figure 7.16.14. Suppose, for example, that x_1, x_5 have the same value as x_1 , that

x_2, x_3, x_6 have the same value as x_2 , that x_4, x_7 have the same value as x_4 , and $N=7$. The summation can be written as

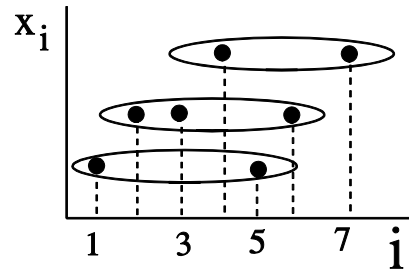


Figure 7.16.14: Regrouping points for calculations involving probability.

$$\langle x \rangle = \frac{1}{N} \sum_{i=1}^N x_i = \frac{1}{N} (2x_1 + 3x_2 + 2x_4)$$

The probability of x_1 occurring is $P(x_1) = 2/7$. Similarly, the probability of x_2, x_4 is given by $P(x_2) = 3/7$ and $P(x_4) = 2/7$. Now the average value can be written as

$$\langle x \rangle = \frac{1}{N} \sum_{i=1}^N x_i = \sum_{x_i} x_i P(x_i)$$

At this point, it should be clear that the indices are unnecessary. The average value can be written as

$$\langle x \rangle = \frac{1}{N} \sum_{i=1}^N x_i = \sum_x x P(x)$$

The point is this: the summation over the N observations can be rearranged into a summation over the observed values. The figure shows that this is a horizontal grouping and does not involve the number of states i per unit i -space. Instead, the average is more related to the number of states per unit x -space. This is more apparent for the integral version.

From calculus

$$\langle f(x) \rangle = \frac{1}{L} \int_0^L dx f(x) = \sum_i f(x_i) \frac{1}{L} \Delta x_i$$

By re-grouping the possible values of $y_i = f(x_i)$ into like values, the summation can be rewritten as before

$$\langle f(x) \rangle = \frac{1}{L} \int_0^L dx f(x) = \int y_i \rho(y_i) dy_i = \int y \rho(y) dy$$

where ρ is the probability density. The advantage of the formula using the probability density is that we do not need to know the functional form of $f(x)$.