within non-relativistic quantum mechanics. The conditions under which special relativity is important might seem far removed from ordinary semiconductors, but electrons move at a significant fraction of the speed of light when they pass close to a nucleus. This leads to an effect called spin–orbit coupling, which has a profound effect on the top of the valence band and therefore on the behaviour of holes. This will be described in Section 2.6.3.

Returning to the problem at hand, we can define a density of states in k-space such that $N_{1\mathrm{D}}(k)\,\delta k$ is the number of allowed states in the range k to $k + \delta k$. It is given by

$$N_{1\mathrm{D}}(k)\delta k = 2\frac{L}{2\pi}\delta k. \tag{1.86}$$

The factor of 2 accounts for the spin, $L/2\pi$ is the density of points, and the range δk cancels to leave $N_{1\mathrm{D}}(k) = L/\pi$. This is proportional to the volume (length) of the system, which makes sense: we would expect to double the number of states if we doubled the size of the system. Usually one takes this factor out to leave a density of states per unit length, which is $n_{1\mathrm{D}}(k) = N_{1\mathrm{D}}(k)/L = 1/\pi$.

The next task is to turn this into a density of states in energy. Figure 1.7 shows how the allowed values of k, which are evenly spaced, map to allowed values in energy through the dispersion relation $E = \varepsilon(k)$. These energies lie in a continuous band for $E \geq 0$ in a large system. The figure shows a parabola but the theory works for a more general dispersion relation. The resulting values of energy get further apart as k rises, so the density of states falls with increasing energy. A range δk in wave number corresponds to a range in energy of $\delta E = (dE/dk)\delta k$. The number of states in this range can be written in terms of $n_{1\mathrm{D}}(k)$ or in terms of the density of states in energy per unit volume $n_{1\mathrm{D}}(E)$. The two expressions must give the same number of states, so

$$n_{1\mathrm{D}}(E)\delta E = n_{1\mathrm{D}}(E)\frac{dE}{dk}\delta k = 2n_{1\mathrm{D}}(k)\delta k. \tag{1.87}$$

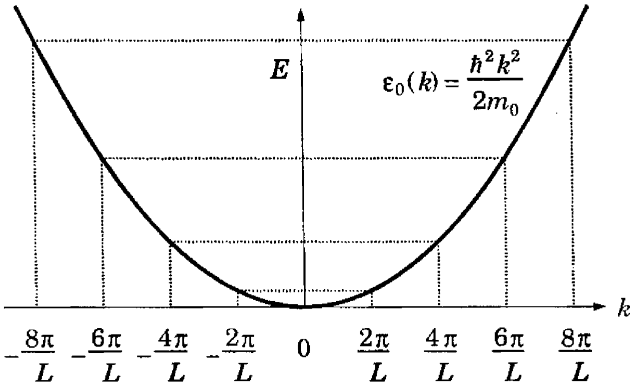

FIGURE 1.7. Dispersion relation $\varepsilon_0(k)$ for free electrons, showing how the allowed values of k map onto ε.

The factor of 2 in front of $n_{1D}(k)$ arises because of the two directions of motion: there is one range δk for $k > 0$ and another for $k < 0$. Note that the same symbol n_{1D} is used to represent the density of states in k and E; this is bad mathematics but typical usage in physics, where one rapidly tends to run out of variants of n and E to denote commonly used quantities. It shouldn't lead to confusion provided that the argument k or E is always included. Thus $n_{1D}(E) = (2/\pi)/(d\varepsilon/dk)$. This can be simplified using the group velocity $v = d\omega/dk = (1/\hbar)(d\varepsilon/dk)$, giving

$$n_{1D}(E) = \frac{2}{\pi\hbar v(E)}. \tag{1.88}$$

We shall see in Section 5.7.1 that the current depends on the product of the velocity and the density of states. Equation (1.88) shows that this is a constant in one dimension, which in turn leads to a quantized conductance.

Substituting the velocity for the special case of free electrons gives

$$n_{1D}(E) = \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}. \tag{1.89}$$

The density of states diverges as $E^{-1/2}$ as $E \to 0$, a characteristic feature of one dimension.

1.7.2 THREE DIMENSIONS

In three dimensions, put the electrons into a box of volume $\Omega = L_x \times L_y \times L_z$. The wave functions are travelling waves in each direction with periodic boundary conditions, just as in the one-dimensional case, and their product gives

$$\phi_{lnm}(\mathbf{R}) = \frac{1}{\sqrt{L_x L_y L_z}} \exp[i(k_x x + k_y y + k_z z)] = \frac{1}{\sqrt{\Omega}} \exp(i\mathbf{K}\cdot\mathbf{R}). \tag{1.90}$$

Remember our convention that upper-case letters are used for three-dimensional positions and wave vectors. The product of three waves has been written as a three-dimensional plane wave using the scalar product. Similarly, the allowed values of K in each of the three directions can be combined into three-dimensional wave vectors

$$\mathbf{K} = \left(\frac{2\pi l}{L_x}, \frac{2\pi m}{L_y}, \frac{2\pi n}{L_z}\right), \qquad l, m, n = 0, \pm 1, \pm 2, \ldots. \tag{1.91}$$

These can be plotted as points in a three-dimensional $\mathbf{K}$-space with (k_x, k_y, k_z) as axes, where they form an evenly spaced rectangular mesh. Each unit cell encloses volume $(2\pi/L_x)(2\pi/L_y)(2\pi/L_z) = (2\pi)^3/\Omega$. Thus the density of allowed states is $N_{3D}(\mathbf{K}) = 2\Omega/(2\pi)^3$, where the 2 accounts for spin. Dividing by the volume gives the density of states in $\mathbf{K}$-space per unit volume of the system in real space, $n_{3D}(\mathbf{K}) = 2/(2\pi)^3$. This is again a constant, and generalizes in an obvious way to d dimensions as $n_d(\mathbf{K}) = 2/(2\pi)^d$.

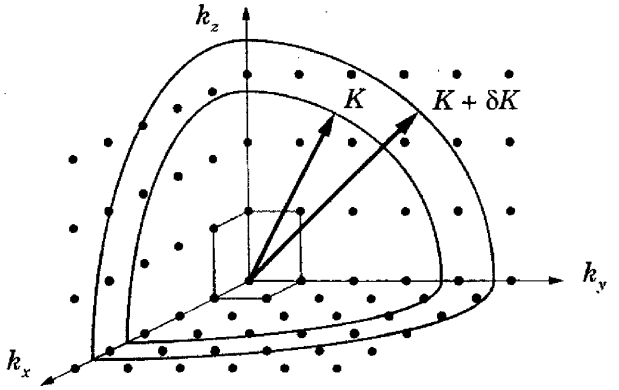

FIGURE 1.8. Construction in **K**-space to calculate the density of states for free electrons in three dimensions. The shells have radii K and $K + \delta K$, corresponding to energies ε and $\varepsilon + \delta\varepsilon$.

Now we need to derive the density of states as a function of energy. Consider free electrons only, because the calculation is more complicated for a general function $\varepsilon(\mathbf{K})$. Figure 1.8 shows two spheres about the origin in **K**-space, one with radius K and the other with radius $K + \delta K$. The volume of the shell between these two spheres is $4\pi K^2 \delta K$. The number of states in the shell is found from the product of this volume and the density of states $n_{3D}(\mathbf{K})$, giving $(K^2/\pi^2)\delta K$. The separation δK corresponds to a difference in energy of

$$\delta E = \frac{dE}{dK}\delta K = \frac{\hbar^2 K}{m}\delta K. \tag{1.92}$$

The number of states in the shell is given in terms of the density of states in energy by $n(E)\delta E$. Equating the two expressions yields $n_{3D}(E)\delta E = n_{3D}(E)(\hbar^2 K/m)\delta K = (K^2/\pi^2)\delta K$, whence

$$n_{3D}(E) = \frac{mK}{\pi^2\hbar^2} = \frac{m}{\pi^2\hbar^3}\sqrt{2mE}. \tag{1.93}$$

The square root is characteristic of three dimensions. Its singularity at the bottom of the band is much weaker than the one-dimensional result of $E^{-1/2}$. In general the density of states shows a stronger feature at the bottom of the band in fewer dimensions. Optical properties such as absorption are strongly influenced by the density of states, and low-dimensional systems are preferred for optoelectronic devices because their density of states is larger at the bottom of the band. The density of states for free electrons in one, two, and three dimensions is plotted in Figure 1.9. In all cases a low mass is associated with a low density of states.

The density of states for a three-dimensional crystal is more complicated because the surfaces of constant energy in **K**-space are not spheres. Further singularities of $n(E)$ appear inside bands, and provide fruitful material for optical spectroscopy. A simpler case arises if the energy depends on only the magnitude of **K** but not

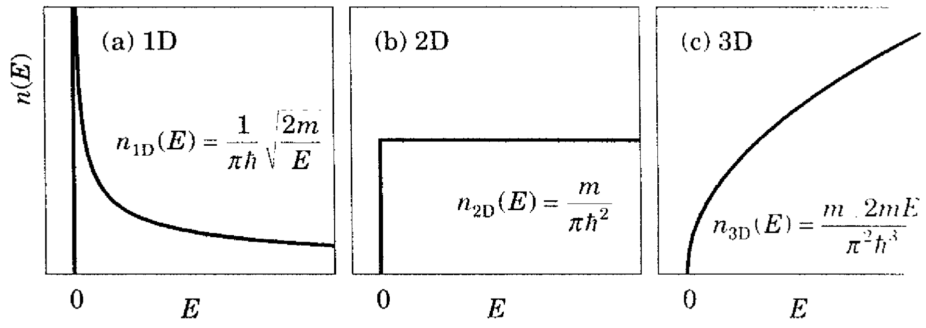

FIGURE 1.9. Densities of states for free electrons in one, two, and three dimensions.

its direction. In this case the surfaces of constant energy remain spherical and t derivation of $n(E)$ proceeds as before except for the form of $\varepsilon(K)$. For examp the conduction band of GaAs is often modelled by the expression

$$\varepsilon(K)[1+\alpha\varepsilon(K)] = \frac{\hbar^2 K^2}{2m_0 m_e}. \qquad (1.$$

This takes account of the fact that the band is not parabolic for high energies, w $\alpha \approx 0.6\,\text{eV}^{-1}$.

1.7.3 A GENERAL DEFINITION OF THE DENSITY OF STATES

A general definition of the density of states is often useful. Let the states of a syst have energies ε_n. Then the density of states in energy can be written as

$$N(E) = \sum_n \delta(E - \varepsilon_n), \qquad (1.$$

where $\delta(E)$ is the Dirac δ-function. This is the total density of states, not that unit volume. We shall now justify this definition and see how it is related to previous calculations.

First, it is clear that equation (1.95) makes sense only if we integrate over because of the δ-functions. Consider

$$\int_{E_1}^{E_2} N(E)\,dE = \int_{E_1}^{E_2} \sum_n \delta(E-\varepsilon_n)\,dE = \sum_n \int_{E_1}^{E_2} \delta(E-\varepsilon_n)\,dE. \qquad (1.$$

This is illustrated in Figure 1.10. If the energy of a state n lies within the range integration from E_1 to E_2, the integral over $\delta(E-\varepsilon_n)$ gives unity by definition the energy ε_n lies outside the range of integration, on the other hand, there is contribution because the weight of the δ-function is concentrated entirely at $E =$ Thus the integral gives 1 for all states in the range $E_1 \le \varepsilon_n \le E_2$ and zero for th

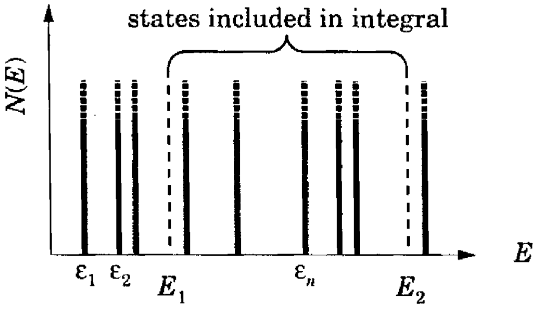

FIGURE 1.10. The 'δ-function' definition of the density of states integrating to count the states between E_1 and E_2.

outside. Performing the sum next, we see that it adds up to the total number of states between E_1 and E_2. This is exactly what we would expect from an integral over $N(E)$, and shows that equation (1.95) is a valid definition of the density of states.

To confirm that it works, consider free electrons in one dimension again. In this case we can label the states by their wave number k and the definition (1.95) becomes

$$N(E) = 2 \sum_{k=-\infty}^{\infty} \delta[E - \varepsilon_0(k)]. \tag{1.97}$$

The factor of 2 is for spin. Next, turn the sum into an integral, assuming a large system. We have already seen how to do this: the density of states in k-space is $L/2\pi$, so the sum becomes

$$N(E) = \frac{L}{\pi} \int_{-\infty}^{\infty} \delta[E - \varepsilon_0(k)]\,dk. \tag{1.98}$$

There is still a function inside the δ-function, which is a nuisance, so change the variable of integration from k to $z = \varepsilon_0(k) = \hbar^2 k^2/2m$. This requires

$$dk = \frac{dk}{dz}dz = \frac{1}{\hbar}\sqrt{\frac{m}{2z}}\,dz, \tag{1.99}$$

and the integral becomes

$$N(E) = \frac{2L}{\pi\hbar} \int_0^{\infty} \sqrt{\frac{m}{2z}}\,\delta(E - z)\,dz. \tag{1.100}$$

The 2 in the prefactor comes from the two signs of k for each value of the energy z. Now the integral is trivial, as the only contribution is at $z = E$ when $E > 0$, and we finally get

$$N(E) = \frac{2L}{\pi\hbar}\sqrt{\frac{m}{2E}} = \frac{L}{\pi\hbar}\sqrt{\frac{2m}{E}} \tag{1.101}$$

as before.