

Part 2. The Quantum Particle in a Box

Part 2. The Quantum Particle in a Box

The goal of this class is to calculate the behavior of electronic materials and devices. In Part 1, we have developed techniques for calculating the energy levels of electron states. In this part, we will learn the principles of electron statistics and fill the states with electrons. Then in the following sections, we will apply a voltage to set the electrons in motion, and examine non-equilibrium properties like current flow, and the operation of electronic switches.

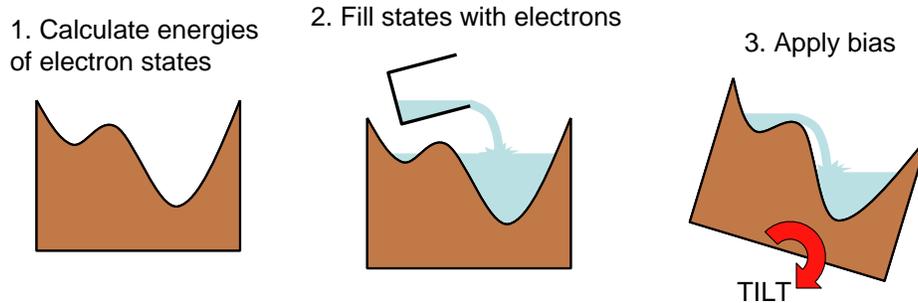


Fig. 2.1. The next two parts in diagram form.

How many electrons? Fermi-Dirac Statistics

In the previous section, we determined the allowed energy levels of a particle in a quantum well. Each energy level and its associated wavefunction is known as a ‘state’. The **Pauli exclusion principle** forbids multiple identical electrons from occupying the same state simultaneously. Thus, one might expect that each state in the conductor can possess only a single electron. But electrons also possess *spin*, a purely quantum mechanical characteristic. For any given orientation, the spin of an electron may be measured to be $+1/2$ or $-1/2$. We refer to these electrons as spin up or spin down.

Spin up electrons are different to spin down electrons. Thus the exclusion principle allows *two* electrons per state: one spin up and one spin down.

Next, if we were to add electrons to an otherwise ‘empty’ material, and then left the electrons alone, they would ultimately occupy their *equilibrium* distribution.

As you might imagine, at equilibrium, the lowest energy states are filled first, and then the next lowest, and so on. At $T = 0\text{K}$, state filling proceeds this way until there are no electrons left. Thus, at $T = 0\text{K}$, the distribution of electrons is given by

$$f(E, \mu) = u(\mu - E), \quad (2.1)$$

where u is the unit step function. Equation (2.1) shows that all states are filled below a characteristic energy, μ , known as the **chemical potential**. When used to describe electrons, the chemical potential is also often known as the Fermi Energy, $E_F = \mu$. Here, we will follow a convention that uses μ to symbolize the chemical potential of a contact, and E_F to describe the chemical potential of a conductor.

Introduction to Nanoelectronics

Equilibrium requires that the electrons have the same temperature as the material that holds them. At higher temperatures, additional thermal energy can excite some of the electrons above the chemical potential, blurring the distribution at the Fermi Energy; see Fig. 2.2.

For arbitrary temperature, the electrons are described by the Fermi Dirac distribution:

$$f(E, \mu) = \frac{1}{1 + \exp\left[\frac{E - \mu}{kT}\right]} \quad (2.2)$$

Note that Eq. (2.2) reduces to Eq. (2.1) at the $T = 0\text{K}$ limit. At the Fermi Energy, $E = E_F = \mu$, the states are half full.

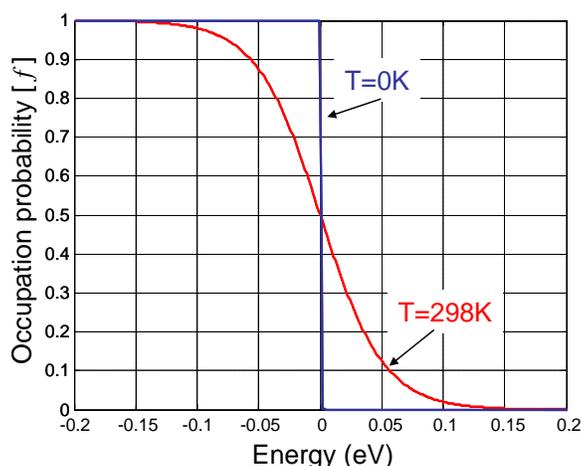


Fig. 2.2. The occupation probability for electrons at two different temperatures. The chemical potential in this example is $\mu = 0$.

It is convenient to relate the Fermi Energy to the number of electrons. But to do so, we need to know the energy distribution of the allowed states. This is usually summarized by a function known as the density of states (DOS), which we represent by $g(E)$. There will be much more about the DOS later in this section. It is defined as the number of states in a conductor per unit energy. It is used to calculate the number of electrons in a material.

$$n = \int_{-\infty}^{+\infty} g(E) f(E, \mu) dE \quad (2.3)$$

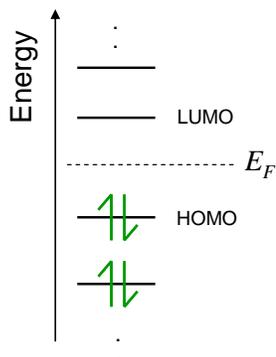


Fig. 2.3. At left, we show a possible energy structure for a molecule at $T = 0\text{K}$. You can think of a molecule as a little dot that confines electrons in every direction. Thus, like the 1 dimensional quantum well studied previously, the energy levels, or states, in a molecule are discrete. For a molecule each state is often described as a molecular orbital. Below the Fermi energy, each molecular orbital, contains two electrons, one spin up and one spin down. We represent these electrons with upward and downward pointing arrows. The highest occupied molecular orbital is frequently abbreviated as the HOMO. The lowest unoccupied molecular orbital is the LUMO.

Part 2. The Quantum Particle in a Box

Current

The electron distribution within a material determines its conductivity. As an example, let's consider some moving electrons in a Gaussian wavepacket. The wavepacket in turn can be described by the weighted superposition of plane waves. Now, we know from the previous section that, if the wavepacket is not centered on $k = 0$ in k -space, then it will move and current will flow.

There is another way to look at this. Note that there are plane wave components with both $+k_z$ and $-k_z$ wavenumbers. Thus, *even when the electron is stationary, components of the wavepacket are traveling in both directions*. But if each component moving in the $+k_z$ direction is balanced by a component moving in the $-k_z$ direction, there is no net current.

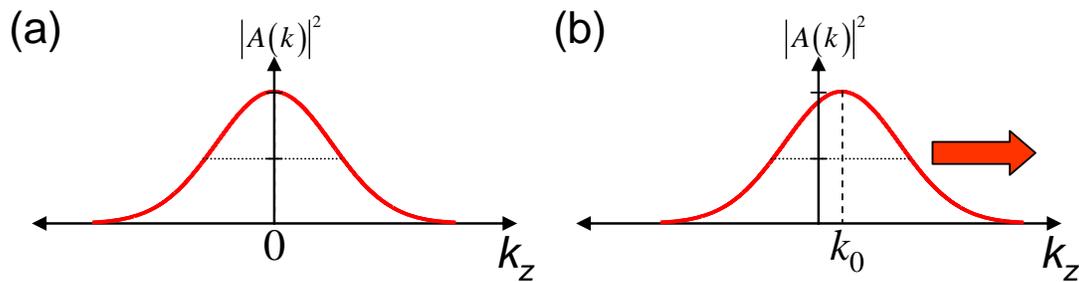


Fig. 2.4. (a) A wavepacket with no net velocity. Note that each plane wave component with a $+k_z$ wavenumber is compensated by a plane wave component with a $-k_z$ wavenumber. (b) A wavepacket with a net velocity in the positive z direction is asymmetric about $k_z = 0$.

We'll show in this section that we can apply a similar analysis to electrons within a conductor. For example, electrons in a wire occupy states with different wavenumbers, known as k -states. Each of these states can be modeled by a plane wave and there are states that propagate in both directions.

Recall that for a plane wave

$$E = \frac{\hbar^2 k_z^2}{2m} \quad (2.4)$$

This relation between energy and wavenumber is known as a dispersion relation. For plane waves it is a parabolic curve. Below the curve there are no electron states. Thus, the electrons reside within a certain *band* of energies.[†]

[†] Strictly a band needs an upper as well as a lower limit to the allowed energy, whereas the simple plane wave model yields only a lower limit. Later we'll also find upper limits in more accurate models of materials. Note also that 0-d materials such as molecules or quantum dots do not have bands because the electrons are confined in all directions and cannot be modeled by a plane wave in any direction.

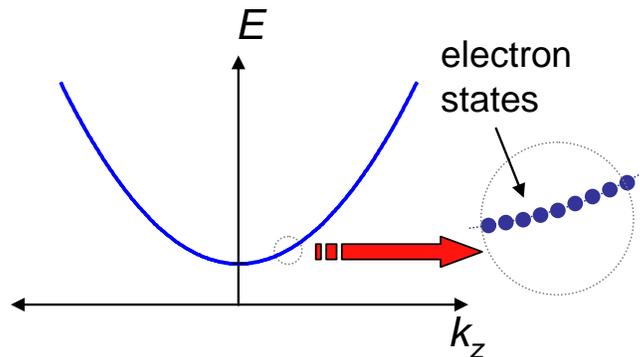


Fig. 2.5. Electrons in a wire occupy states with different energies and wavenumbers.

Under equilibrium conditions, the wire is filled with electrons up to the Fermi energy, E_F . The electrons fill both $+k_z$ and $-k_z$ states, and propagate *equally* in both directions. No current flows. We say that these electrons are compensated.

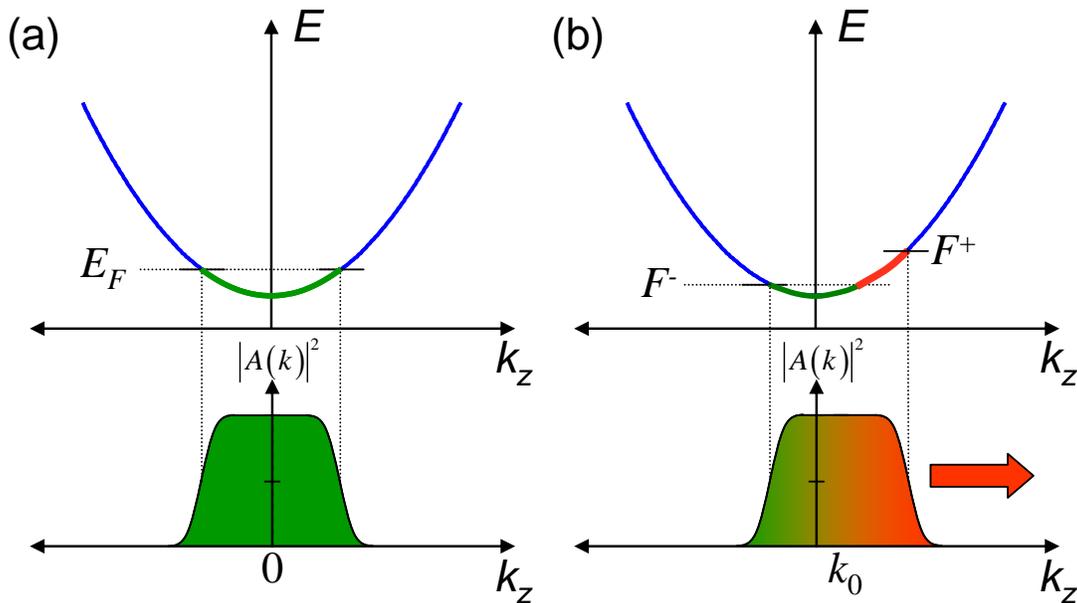
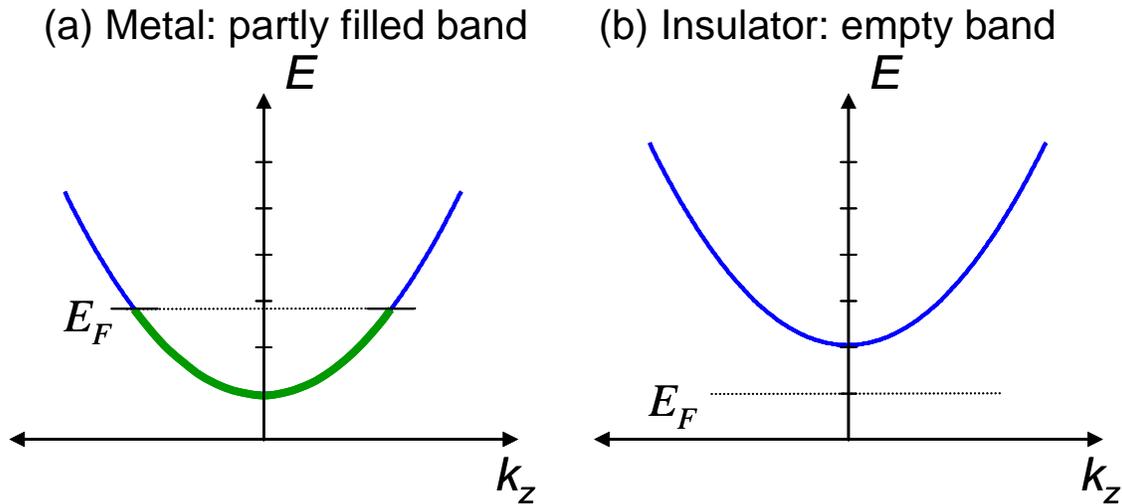


Fig. 2.6. (a) Under equilibrium conditions, electrons fill up the lowest energy k -states first. Since equal numbers of $+k_z$ and $-k_z$ states are filled there is no net current. (b) When $+k_z$ and $-k_z$ states are filled to different levels, there is a net current.

For a net current to flow there must be difference in the number of electrons moving in each direction. Thus, electrons traveling in one direction cannot be in equilibrium with electrons traveling in the other. We define two *quasi* Fermi levels: F^+ is the energy level when the states with $k_z > 0$ are half full, F^- is the corresponding energy level for states with $k_z < 0$. We can see that current flow is associated with a difference in the quasi

Part 2. The Quantum Particle in a Box

Fermi levels, *and* the presence of electron states between the quasi Fermi levels. If there are no electrons between F^+ and F^- , then the material is an insulator and cannot conduct



charge.

Fig. 2.7. Examples of a metal **(a)**, and an insulator **(b)**.

To summarize: current is carried by *uncompensated* electrons.

Metals and Insulators

Metals are good conductors; a small difference between F^+ and F^- yields a large difference between the number of electrons in $+k_z$ and $-k_z$ states. This is possible if the bands are partially filled at equilibrium.

If there are no electrons between F^+ and F^- , then the material is an insulator and cannot conduct charge. This occurs if the bands are completely empty or completely full at equilibrium. We have not yet encountered a band that can be completely filled. These will come later in the class.

Thus, to calculate the current in a material, we must determine the number of electrons in states that lie between the quasi Fermi levels. It is often convenient to approximate Eq. (2.2) when calculating the number of electrons in a material. There are two limiting cases:

(i) degenerate limit: $E_F - E_C \gg kT$.

As shown in Fig. 2.8 (a), here the bottom of the band, E_C , is much less than the Fermi energy, E_F , and the distribution function is modeled by a unit step:

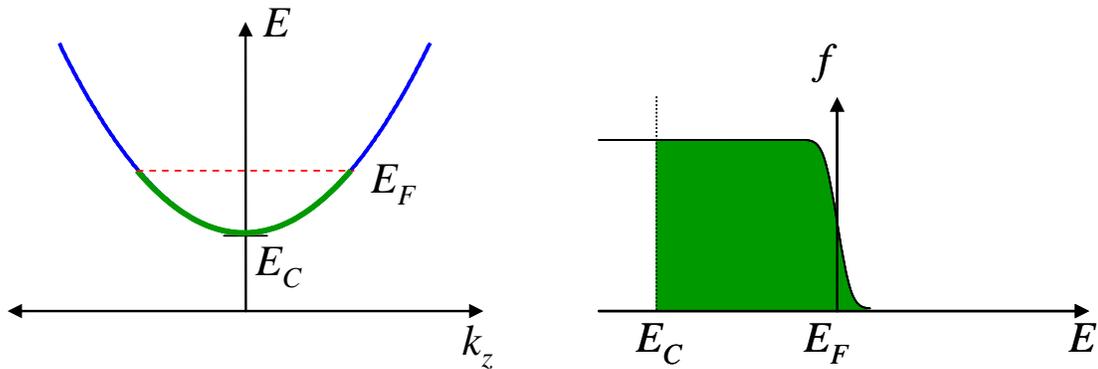
$$f(E) = u(E_F - E) \quad (2.5)$$

(ii) **non-degenerate limit:** $E_C - E_F \gg kT$.

As shown in Fig. 2.8 (b), here $E_C \geq E_F$ and the distribution function reduces to the Boltzmann distribution:

$$f(E) = \exp[-(E - E_F)/kT] \quad (2.6)$$

(a) **Degenerate limit:** $f = u(E_F - E)$



(b) **Non-degenerate limit:** $f = \exp[-(E - E_F)/kT]$

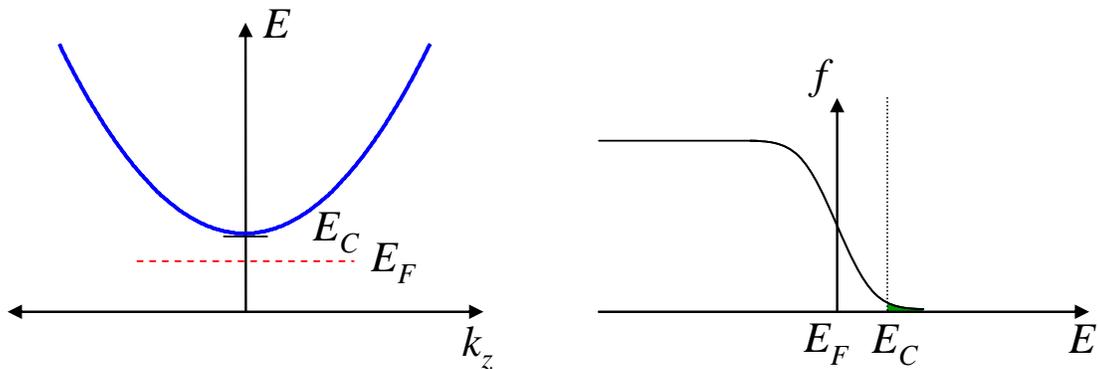


Fig. 2.8. Two limiting cases when calculating the number of electrons in a material. **(a)** If E_F is within a band, then thermal blurring of the electron distribution is not significant, and we can simply integrate up to E_F . This is the so-called degenerate case. **(b)** On the other hand, if the filled states are due solely to thermal excitation above E_F , the filling fraction falls off exponentially. This is the non-degenerate limit.

Part 2. The Quantum Particle in a Box

The Density of States

To determine whether a material is a metal or an insulator, and to calculate the magnitude of the current under applied bias, we need the density of states (DOS), which as you recall is a measure of the number of states in a conductor per unit energy. In this part, we will calculate the DOS for a variety of different conductors.

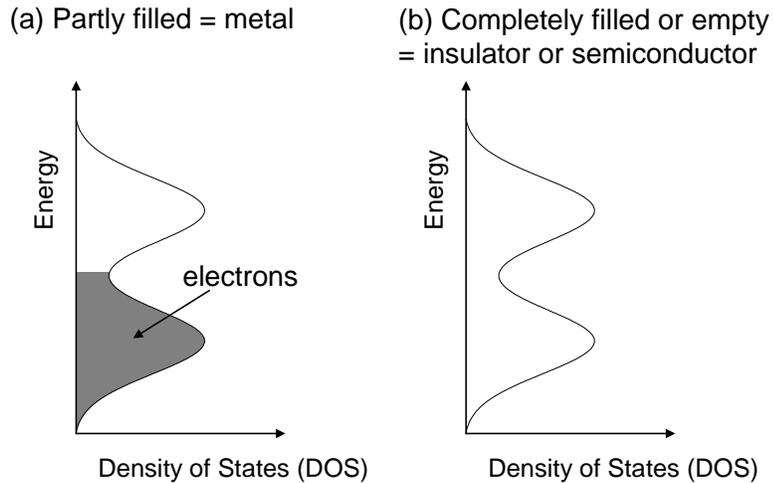


Fig. 2.9. Partly filled states give metallic behavior, while completely filled or empty states correspond to insulators or semiconductors.

To calculate the density of states we will employ two assumptions: (i) we will model the conductor as a homogeneous box, and (ii) we will assume periodic boundary conditions.

The particle in a box

Modeling our electronic material as a box allows us to ignore atoms and assume that the material is perfectly homogeneous. We will consider boxes in different dimensions: either three dimensions (typical bulk materials), 2-d (quantum wells), 1-d (quantum wires), or 0-dimensions (this is a quantum dot). The label 'quantum' here refers to the confinement of electrons. When we say that an electron is 'confined' in a low dimensional material we mean that critical dimensions of the material are on the order of the wavelength of an electron. We've seen that when particles are confined, their energy levels become discrete.

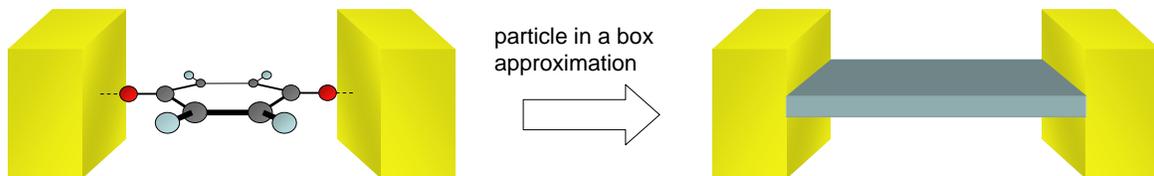


Fig. 2.10. The 'particle in a box' takes a complex structure like a molecule and approximates it by a homogeneous box. All details, such as atoms, are ignored.

Introduction to Nanoelectronics

In quantum dots, electrons are confined in all three dimensions, in quantum wires, electrons are confined in only two dimensions and so on. So when we say that a given structure is 2-d, we mean that the electron is *unconfined* in 2 dimensions. In the unconfined directions, we will assume that the electron is described by a plane wave.

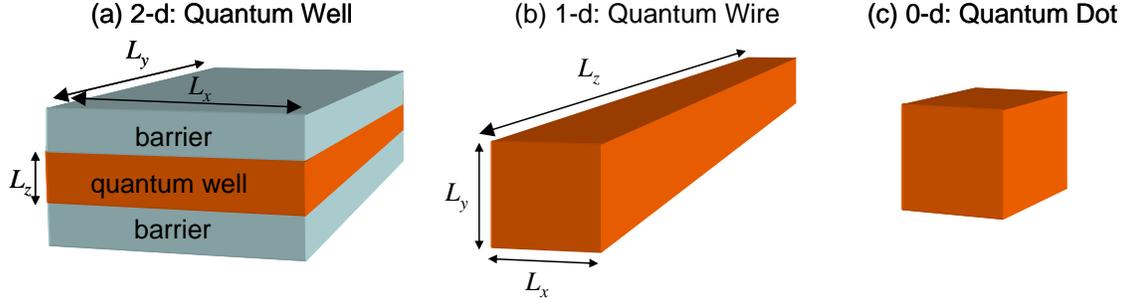


Fig. 2.11. (a) In quantum wells, electrons are confined only in one dimension. Quantum wells are usually implemented by burying the confining material within a barrier material. (b) Quantum wires confine electrons in two dimensions. The electron is not confined along the wire. (c) In a quantum dot, an electron is confined in three dimensions.

The Schrödinger Equation in Higher Dimensions

Analyzing quantum wells and bulk materials requires that we solve the Schrödinger Equation in 2-d and 3-d. The equation in 1-d

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x) \quad (2.7)$$

is extended to higher dimensions as follows:

(i) The Kinetic Energy operator

In 1-d

$$\hat{T} = \frac{\hat{p}_x^2}{2m} \quad (2.8)$$

Now, the magnitude of the momentum in 3-d can be written

$$|\mathbf{p}|^2 = p_x^2 + p_y^2 + p_z^2 \quad (2.9)$$

Where p_x , p_y and p_z are the components of momentum on the x , y and z axes, respectively. It follows that in 3-d

$$\hat{T} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m} = -\frac{\hbar^2}{2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) \quad (2.10)$$

(ii) Separable Potential – Quantum Well

A quantum well is shown in Fig. 2.11 (a). We will assume that the potential can be separated into x , y , and z dependent terms

$$V(x, y, z) = V_x(x) + V_y(y) + V_z(z) \quad (2.11)$$

For example, a quantum well potential is given by

Part 2. The Quantum Particle in a Box

$$\begin{aligned} V_x(x) &= 0 \\ V_y(y) &= 0 \\ V_z(z) &= V_0 u(z-L) + V_0 u(-z) \end{aligned} \quad (2.12)$$

where in the infinite square well approximation $V_0 \rightarrow \infty$, and u is the unit step function.

For potentials of this form the Schrödinger Equation can be separated:

$$\begin{aligned} \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_x(x) \right] \psi(x, y, z) + \left[-\frac{\hbar^2}{2m} \frac{d^2}{dy^2} + V_y(y) \right] \psi(x, y, z) \\ + \left[-\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + V_z(z) \right] \psi(x, y, z) = (E_x + E_y + E_z) \psi(x, y, z) \end{aligned} \quad (2.13)$$

The wavefunction can also be separated

$$\psi(x, y, z) = \psi_x(x) \psi_y(y) \psi_z(z) \quad (2.14)$$

From Eqs. (1.118) and (1.119), the solutions to the infinite quantum well potential are

$$\psi(x, y, z) = \psi_x(x) \psi_y(y) \psi_z(z) = \sqrt{\frac{2}{L}} \sin\left(n \frac{\pi z}{L}\right) \cdot \exp[ik_x x] \cdot \exp[ik_y y] \quad (2.15)$$

with

$$E = E_x + E_y + E_z = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} + \frac{n^2 \hbar^2 \pi^2}{2mL^2} \quad (2.16)$$

This dispersion relation is shown in Fig. 2.12 for the lowest three modes of the quantum well.

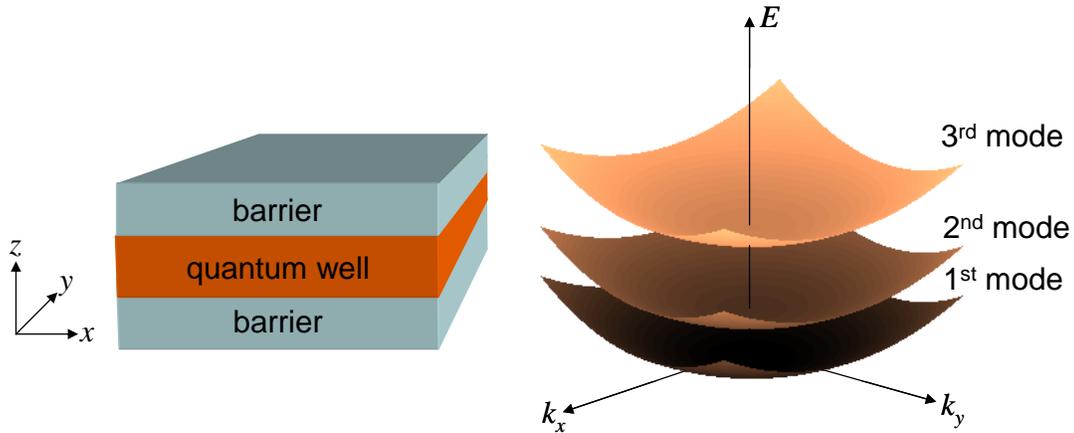


Fig. 2.12. A quantum well confines electrons in 1 dimension.

(ii) Separable Potential – Quantum Wire

A quantum wire with rectangular cross-section is shown in Fig. 2.11(b). Again, we will assume that the potential is infinite at the boundaries of the wire:

$$V(x, y, z) = V_0 u(-x) + V_0 u(x - L_x) + V_0 u(-y) + V_0 u(y - L_y), \quad (2.17)$$

where $V_0 \rightarrow \infty$. The associated wavefunction is confined in the x - y plane and composed of plane waves in the z direction, thus we chose the trial wavefunction

$$\psi(x, y, z) = \psi(x, y) e^{ik_z z} \quad (2.18)$$

Inserting Eq. (2.18) into the Schrödinger equation gives (for $0 \leq x \leq L_x$ and $0 \leq y \leq L_y$):

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x, y) - \frac{\hbar^2}{2m} \frac{d^2}{dy^2} \psi(x, y) + \frac{\hbar^2 k_z^2}{2m} \psi(x, y) = E \psi(x, y) \quad (2.19)$$

Since the potential goes to infinity at the edges of the wire, $\psi(x=0) = \psi(x=L_x) = \psi(y=0) = \psi(y=L_y) = 0$. Thus, the solution is

$$\psi(x, y) = \psi_0 \sin(k_x x) \sin(k_y y), \quad (2.20)$$

where

$$k_x = \frac{n_x \pi}{L_x}, \quad n_x = 1, 2, \dots, \quad k_y = \frac{n_y \pi}{L_y}, \quad n_y = 1, 2, \dots \quad (2.21)$$

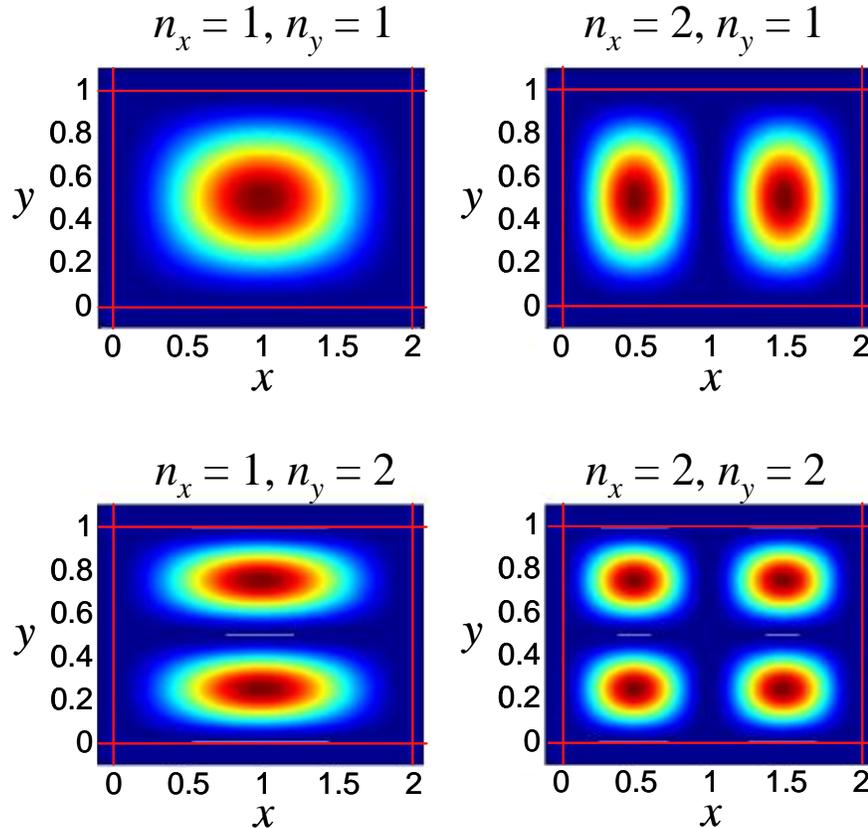


Fig. 2.13. The first four modes of the quantum wire. Since in this example, $L_x > L_y$ the $n_x = 2, n_y = 1$ mode has lower energy than the $n_x = 1, n_y = 2$ mode.

Part 2. The Quantum Particle in a Box

Thus, the constraint in the x - and y -directions defines the discrete energy levels

$$E_{n_x, n_y} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right), \quad n_x, n_y = 1, 2, \dots \quad (2.22)$$

The total energy is

$$E_{n_x, n_y} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right) + \frac{\hbar^2 k_z^2}{2m}, \quad n_x, n_y = 1, 2, \dots \quad (2.23)$$

This dispersion relation is plotted in Fig. 2.14 for the lowest three modes.

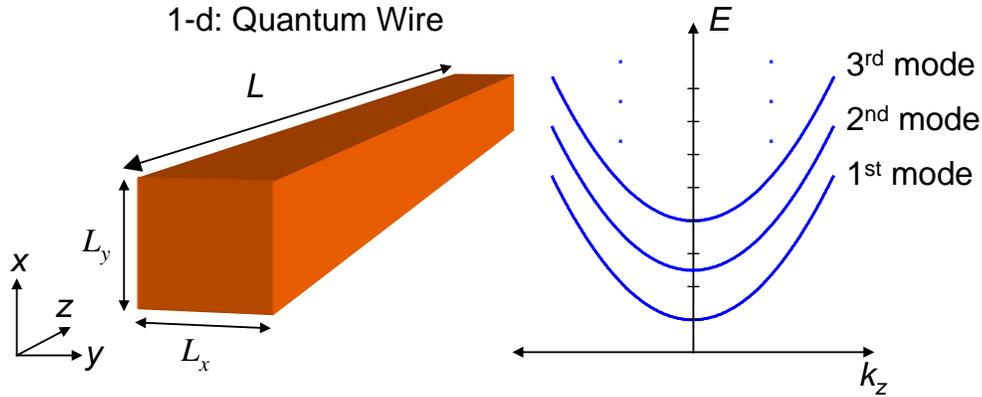


Fig. 2.14. A quantum wire confines electrons in 2 dimensions.

The 0-d DOS: single molecules and quantum dots confined in 3-d

The 0-d DOS is a special case because the particle is confined in all directions.

Like a particle in a well with discrete energy levels, we might assume that the density of states in a 0-d might be a series of delta functions at the allowed energy levels. This is indeed true for an *isolated* 0-d particle.

The lifetime of a charge in an orbital of an isolated particle is infinite. From the uncertainty principle, infinite lifetimes are associated with perfectly discrete energy states in the isolated molecule, i.e. if $\Delta t \rightarrow \infty$, $\Delta E \rightarrow 0$.

But when, for example, a molecule is brought in contact with a metal electrode, the electron may eventually escape into the metal. Now, the electron's lifetime on the molecule is finite, and hence the molecule's energy levels should also exhibit a finite width. Thus, molecular energy levels are broadened in a coupled metal-molecule system – the greater the coupling, the greater the broadening of the molecular energy levels.

Let's assume that there are two electrons in the molecular orbital. Let's assume that the lifetime of these electrons on the molecule is τ . Furthermore, let's assume that the decay of the electron probability on the molecule is exponential. Then the time dependence of the electron probability in the molecular orbital is:

$$|\psi(t)|^2 = \frac{2}{\tau} \exp\left[-\frac{t}{\tau}\right] u(t) \quad (2.24)$$

One choice for the corresponding wavefunction is

$$\psi(t) = \sqrt{\frac{2}{\tau}} \exp\left[-i\frac{E_0 t}{\hbar} - \frac{t}{2\tau}\right] u(t) \quad (2.25)$$

We have included a complex term in the exponent to account for the phase rotation of the electron. The characteristic angular frequency of the phase rotation is E_0/\hbar , where E_0 is the energy of the molecular orbital in the isolated molecule.

Next we use a Fourier transform to convert from the time to the energy domain. The Fourier transform of $\psi(t)$ gives

$$A(\omega) = \frac{\sqrt{2/\tau}}{1/2\tau + i(E_0/\hbar - \omega)} \quad (2.26)$$

Now from the definition of normalization in angular frequency we require that

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} |A(\omega)|^2 d\omega = \int_{-\infty}^{\infty} g(E) dE \quad (2.27)$$

where $g(E)$ is the density of states. Thus,

$$g(E) = \frac{1}{2\pi} |A(\omega)|^2 \frac{d\omega}{dE} = \frac{2}{\pi} \frac{\hbar/2\tau}{(E - E_0)^2 + (\hbar/2\tau)^2} \quad (2.28)$$

This function is known as a Lorentzian – it is characteristic of an exponential decay in the time domain; see Fig. 2.15. The width of the Lorentzian at half its peak value (full width at half maximum, or FWHM) is \hbar/τ . The coupling between the molecule and the contact can be described either by the lifetime of the electron on the molecule τ , or a coupling energy, Γ , equal to the FWHM of the Lorentzian density of states and given by

$$\Gamma = \hbar/\tau \quad (2.29)$$

Thus, as expected, a stronger interaction between a molecule and a contact is correlated with a shorter electron lifetime on the molecule and a broader molecular density of states. In well coupled systems Γ may approach 1 eV, corresponding to an electron lifetime of $\tau \sim 4$ fs.

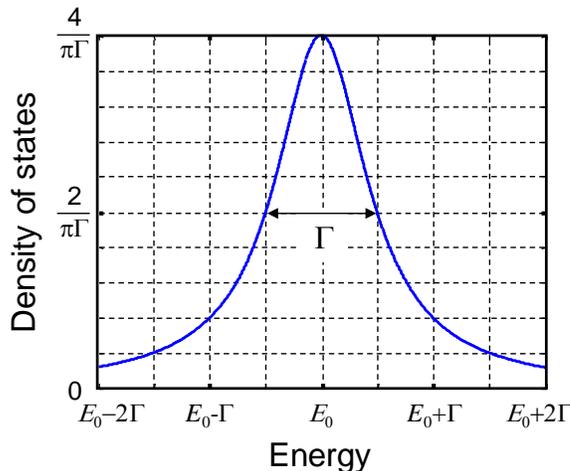


Fig. 2.15. The density of states in a molecule is broadened when the molecule is brought in contact with a metal. The effect is significant if the molecule is small, and the lifetime of electrons on the molecule changes dramatically in the presence of the metal.

Part 2. The Quantum Particle in a Box

Periodic boundary conditions

Usually, our material does not exist in isolation, but rather it may be connected to contacts, for example. So we have a problem: When determining its energy structure, how do we treat the boundaries between our material and the rest of the physical world?

First of all, if the material is big enough (for example, if a quantum wire is long enough), the boundaries will not significantly affect the electron states in the majority of the material. If this is true, we can choose any *boundary conditions* that are convenient. Indeed, we shall continue for the moment assuming that we can choose convenient boundary conditions. But note that in nanoscale devices, boundary conditions can be problematic; see the previous discussion on 0-d materials coupled to contacts.

When boundaries do not dominate the properties of the material, the usual choice is *periodic boundary conditions*. As shown in Fig. 2.16, to apply periodic boundary conditions, we take the wavefunction of the material, and make infinite copies in the unconfined directions. This gives us the ability to analyze electrons traveling in those directions in the material. After all, if just a single, isolated copy of the material was studied, the material could not support traveling electrons, only standing waves.

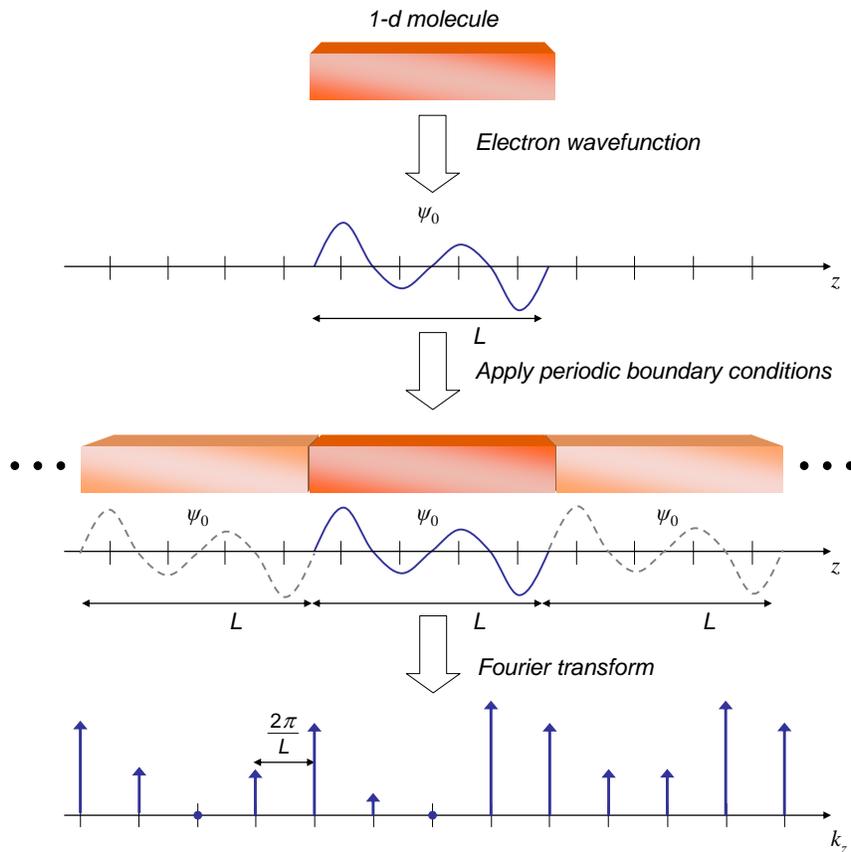


Fig. 2.16. Given periodic boundary conditions, only certain k values are allowed in the 'unconfined' direction of a quantum wire.

Introduction to Nanoelectronics

But forcing periodicity in real space affects the Fourier transform of the wavefunction. In k -space, the periodic wavefunction is discrete. For example, on the long axis of a quantum wire of length L , the allowed k -values are spaced by

$$\Delta k = \frac{2\pi}{L} \quad (2.30)$$

Each allowed k -value corresponds to a plane wave, and each allowed k -value corresponds to a discrete electron wavefunction with a characteristic energy. As we shall see, knowing the separation of k -states in k -space allows us to easily *count* the number of electron states in the material.

The other way to think about the limitation to certain discrete k values in a periodic material is to recall that any periodic structure supports modes. Consequently, there are only certain allowed wavevectors for delocalized electrons in a periodic molecule. We characterize these modes by their wavevector, k given by $k = 2\pi n / Na_0 = 2\pi n / L$, where L is the length of the molecule. The allowed k states are therefore:

$$k = 0, \pm \frac{2\pi}{L}, \pm \frac{4\pi}{L}, \pm \frac{6\pi}{L}, \dots \quad (2.31)$$

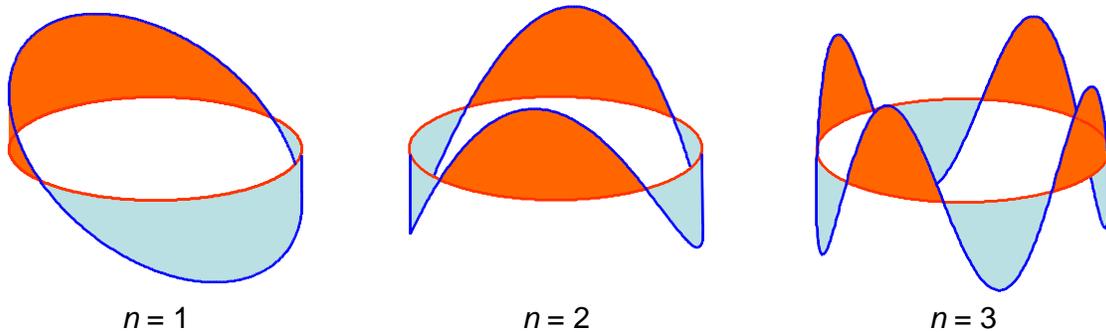


Fig. 2.17. Several modes on a ring. Because the ring is periodic, only the wavevectors, $k = 2\pi n / L$ give stable states, where L is the perimeter of the ring and n is an integer.

Thus, in a conductor where we have applied periodic boundary conditions, the spacing of the allowed k states is determined by the length of conductor.

The 1-d DOS: quantum wires confined in 2-d

The density of states, $g(E)$ is defined as the number of allowed states within energy range dE , i.e. the total number of states within the energy range $-\infty < E < E_F$ is

$$n_s(E_F) = \int_{-\infty}^{E_F} g(E) dE \quad (2.32)$$

To determine $g(E)$ we will count k states and then use the relation between E and k (known as the dispersion relation) to change variables from k to E .

We showed above that the energy of electrons in a quantum wire is

Part 2. The Quantum Particle in a Box

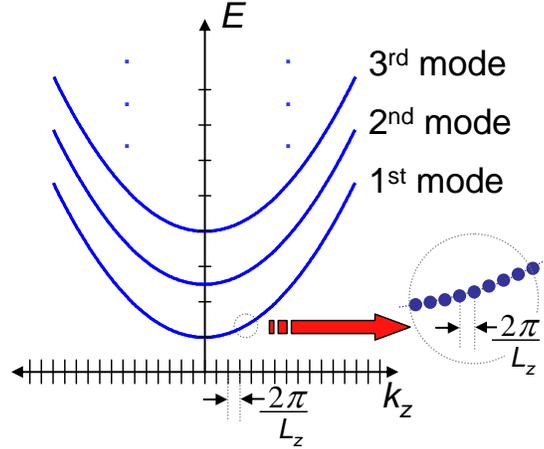


Fig. 2.18. The dispersion relation of a quantum wire after application of periodic boundary conditions.

$$E_{n_x, n_y} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} \right) + \frac{\hbar^2 k_z^2}{2m}, \quad n_x, n_y = 1, 2, \dots \quad (2.33)$$

Thus, counting the x - y modes is straight forward, since in the confined potential they are discrete. But to count the modes in the z -direction we impose *periodic boundary conditions*.

This should be OK if the wire is sufficiently long since the boundaries of the wire are then less significant. Periodic boundary conditions cause k_z to be quantized, and each allowed value of k -space occupies a length $2\pi/L_z$.

For convenience, we will integrate with respect to the magnitude of k_z . Since we are integrating $|k_z|$ from 0 to ∞ , not $-\infty < k_z < \infty$, there is an extra factor of two to account for modes with negative k_z , and an additional factor of two to account for the two possible electron spins per k state.

$$n_s(|k_z|) = 2 \times 2 \times \int_0^{|k_z|} \frac{1}{2\pi/L_z} dk. \quad (2.34)$$

Next we need to change variables in Eq. (2.34), i.e. we need $g(E)$ where

$$n_s(E_F) = \int_{-\infty}^{E_F} g(E) dE \quad (2.35)$$

Now $|k_z|$ is related to the energy by

$$E - E_{n_x, n_y} = \frac{\hbar^2 |k_z|^2}{2m}, \quad E \geq E_{n_x, n_y} \quad (2.36)$$

Using the dispersion relation of Eq. (2.36) in Eq. (2.34) gives,

$$g(E) dE = \frac{2L}{\pi} \sqrt{\frac{m}{2\hbar^2}} \sum_{n_x, n_y} \frac{u(E - E_{n_x, n_y})}{\sqrt{E - E_{n_x, n_y}}} dE, \quad (2.37)$$

where u is the unit step function. The DOS is plotted in Fig. 2.19. Note that the flat region in the dispersion relation as $k \rightarrow 0$ yields infinite peaks in the DOS at the bottom of each band. The peaks have finite area, however, since the wire contains a finite number of states.

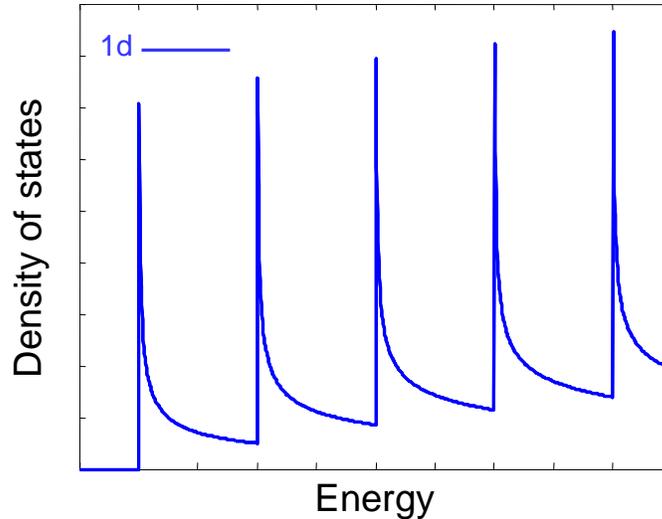


Fig. 2.19. The density of states for a quantum wire (1d).

Periodic Boundary Conditions in 2-d

Applying periodic boundary conditions to 2d materials follows the same principles as in 1d.

Let's assume that the long axes of the quantum well are aligned with the x and y axes, and that the dimensions of the quantum well are $L_x \times L_y$. When we apply periodic boundary conditions, the infinite system is periodic on both the x -axis (period L_x) and the y -axis (period L_y).

First, let's consider periodicity on the x -axis; see Fig. 2.20.

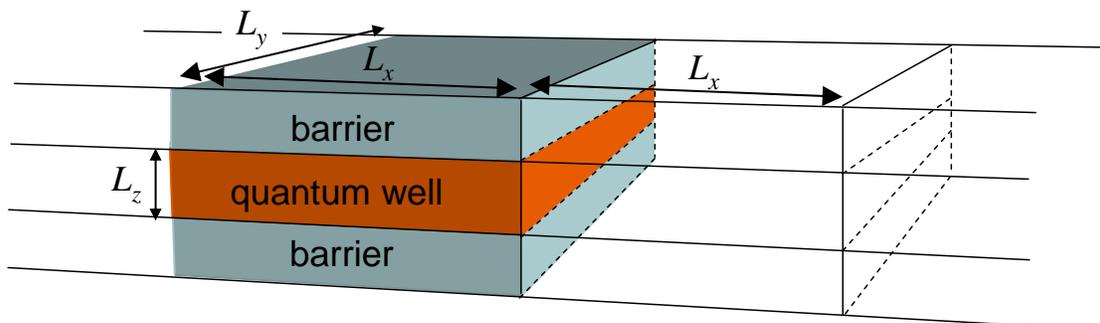


Fig. 2.20. The quantum well, assuming periodic boundary conditions on the x -axis.

Part 2. The Quantum Particle in a Box

On the x -axis the wavefunction is a plane wave.

$$\psi_x(x) = \exp[ik_x x] \quad (2.38)$$

Under periodic boundary conditions, only discrete k_x values are allowed

$$k_x = n_x \frac{2\pi}{L_x} \quad (2.39)$$

where n_x is an integer.

Similarly, for periodicity on the y -axis:

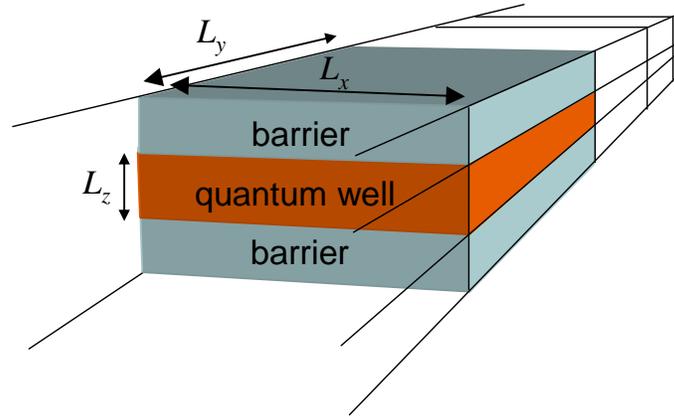


Fig. 2.21. The quantum well, assuming periodic boundary conditions on the y -axis.

the wavefunction on the y -axis

$$\psi_y(y) = \exp[ik_y y] \quad (2.40)$$

is restricted to discrete k_y values:

$$k_y = n_y \frac{2\pi}{L_y} \quad (2.41)$$

where n_y is an integer.

Thus, in k -space the allowed k -states are spaced regularly, with:

$$\Delta k_x = \frac{2\pi}{L_x}, \quad \Delta k_y = \frac{2\pi}{L_y} \quad (2.42)$$

Overall, the area occupied in k -space per k -state is:

$$\Delta k^2 = \Delta k_x \Delta k_y = \frac{2\pi}{L_x} \frac{2\pi}{L_y} = \frac{4\pi^2}{A} \quad (2.43)$$

where A is the area of the quantum well.

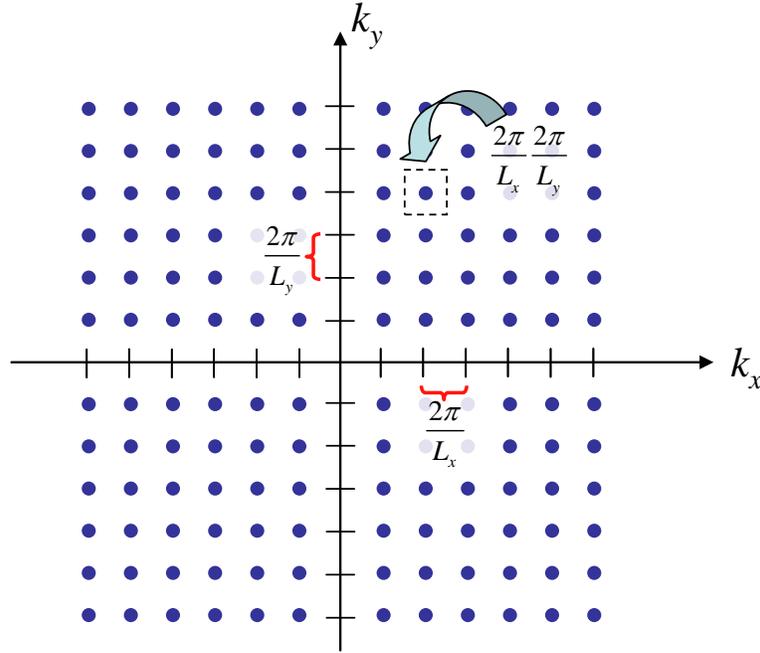


Fig. 2.22. In k -space only certain discrete values are allowed. Each state occupies an area of $4\pi^2/L_x L_y$.

The 2-d DOS: quantum wells confined in 1-d

We showed above that the energy of electrons in a quantum well is

$$E = \frac{\hbar^2 \pi^2}{2mL_z^2} n^2 + \frac{\hbar^2 (k_x^2 + k_y^2)}{2m}, \quad n = 1, 2, \dots \quad (2.44)$$

For the DOS calculation, the specifics of the confining potential are irrelevant; we note only that the electron is unconfined in two dimensions. If the quantum well has area $L_x \times L_y$, then each allowed value of k -space occupies an area of $2\pi/L_x \times 2\pi/L_y$.

It is convenient to convert to cylindrical coordinates (k, ϕ, z) where k is the magnitude of the k -vector in the x - y plane. The number of states within a ring of thickness dk is then

$$n_s(k) dk = 2 \times \frac{1}{4\pi^2/A} \times 2\pi k dk \quad (2.45)$$

where $A = L_x \times L_y$, and again we have multiplied by two to account for the electron spin.

Now k is related to the energy by

$$E - E_n = \frac{\hbar^2 k^2}{2m}, \quad E \geq E_n \quad (2.46)$$

Thus, from Eq. (2.46),

Part 2. The Quantum Particle in a Box

$$g(E)dE = \frac{Am}{\pi\hbar^2} \sum_n u(E - E_n) dE, \quad (2.47)$$

where u is the unit step function. The DOS is plotted in Fig. 2.24.

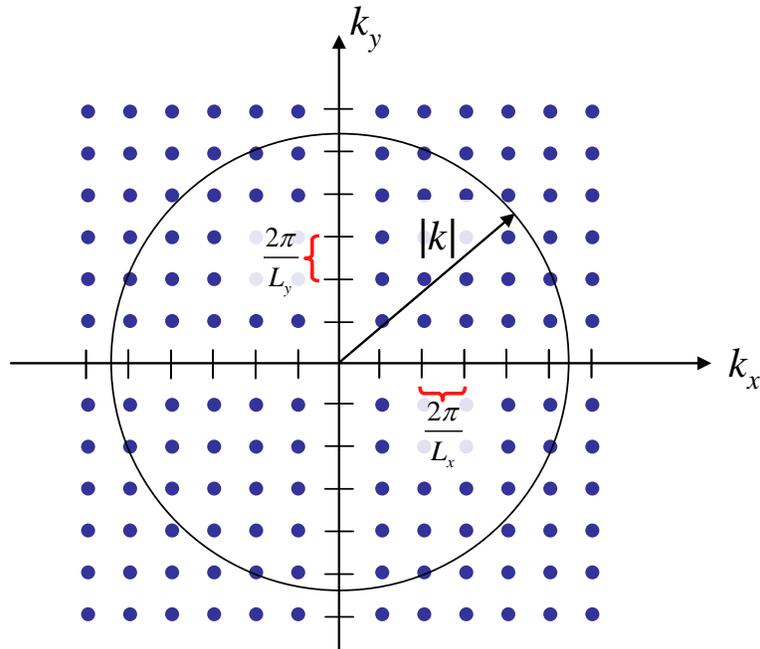


Fig. 2.23. We calculate the number of k -states within a circle of radius $|k|$.

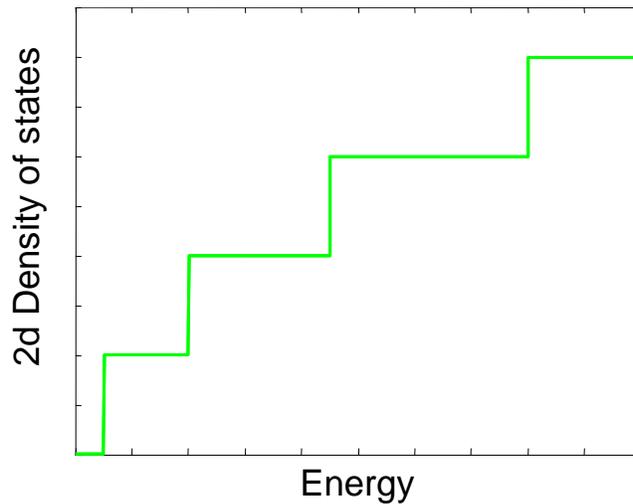


Fig. 2.24. The density of states for a quantum well (2d).

Periodic boundary conditions in 3-d

In three dimensions, again only discrete values of k are allowed. This time the *volume* of k -space per allowed state is

$$\Delta k^3 = \Delta k_x \Delta k_y \Delta k_z = \frac{2\pi}{L_x} \frac{2\pi}{L_y} \frac{2\pi}{L_z} = \frac{8\pi^3}{V} \quad (2.48)$$

where V is the volume of the material.

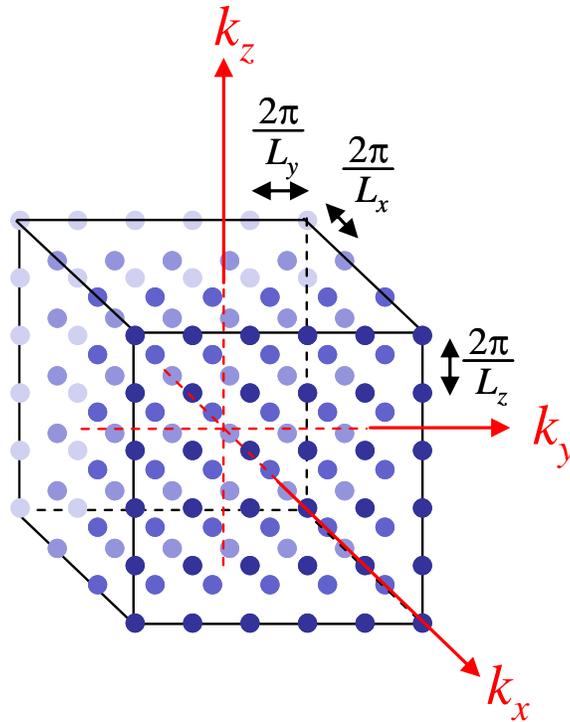


Fig. 2.25. In k -space only certain discrete values are allowed. Each state occupies a volume of $8\pi^3/L_x L_y L_z$.

In summary, the k -space occupied per state is

1-d	$\Delta k = \frac{2\pi}{L}$
2-d	$\Delta k^2 = \frac{4\pi^2}{A}$
3-d	$\Delta k^3 = \frac{8\pi^3}{V}$

Table 2.1. The k -space occupied per state in 1, 2 and 3 dimensions.

Part 2. The Quantum Particle in a Box

The 3-d DOS: bulk materials with no confinement

In 3-d, there is no electron confinement. The only constraint on k_x , k_y , or k_z are the periodic boundary conditions. We have just shown that if the system has volume $L_x \times L_y \times L_z$ then each allowed value of k -space occupies a volume of $2\pi/L_x \times 2\pi/L_y \times 2\pi/L_z = 8\pi^3/V$.

To determine the number of allowed states, we will integrate over all k -space. It is convenient to do this in spherical coordinates. If k is the magnitude of the \mathbf{k} vector, the number of modes within a spherical shell of thickness dk is then

$$n_s(k) dk = 2 \times \frac{1}{8\pi^3/V} \times 4\pi k^2 dk. \quad (2.49)$$

where $V = L_x \times L_y \times L_z$, $V = L_x \times L_y \times L_z$, and the factor of two accounts for electron spin.

The unconfined wavefunctions within our 3-d box are plane waves in all directions, i.e. the wavefunction could be described by

$$\psi(x, y, z) = \psi_0 e^{ik_x x} e^{ik_y y} e^{ik_z z} \quad (2.50)$$

Substituting into the Schrödinger Equation gives

$$-\frac{\hbar^2}{2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) \psi = E\psi \quad (2.51)$$

Which gives

$$\frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2) = E \quad (2.52)$$

Rearranging:

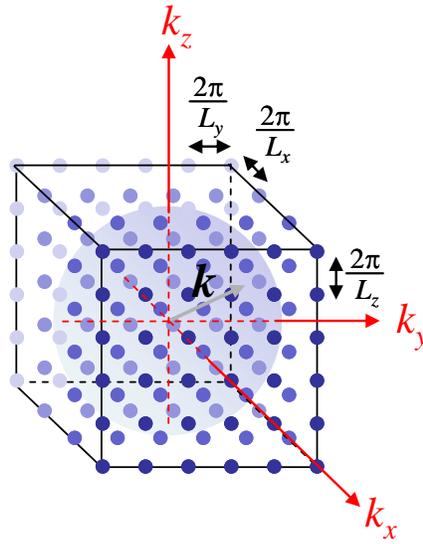


Fig. 2.26. Construction used for calculating the DOS for a 3d system.

$$E = \frac{\hbar^2 k^2}{2m} \quad (2.53)$$

Using Eq. (2.53) to relate E to k gives:

$$g(E)dE = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{E} dE \quad (2.54)$$

where $g(E)$ is the density of states per unit energy.

A comparison of the density of states in 1-d, 2-d and 3-d materials is shown in Fig. 2.27.

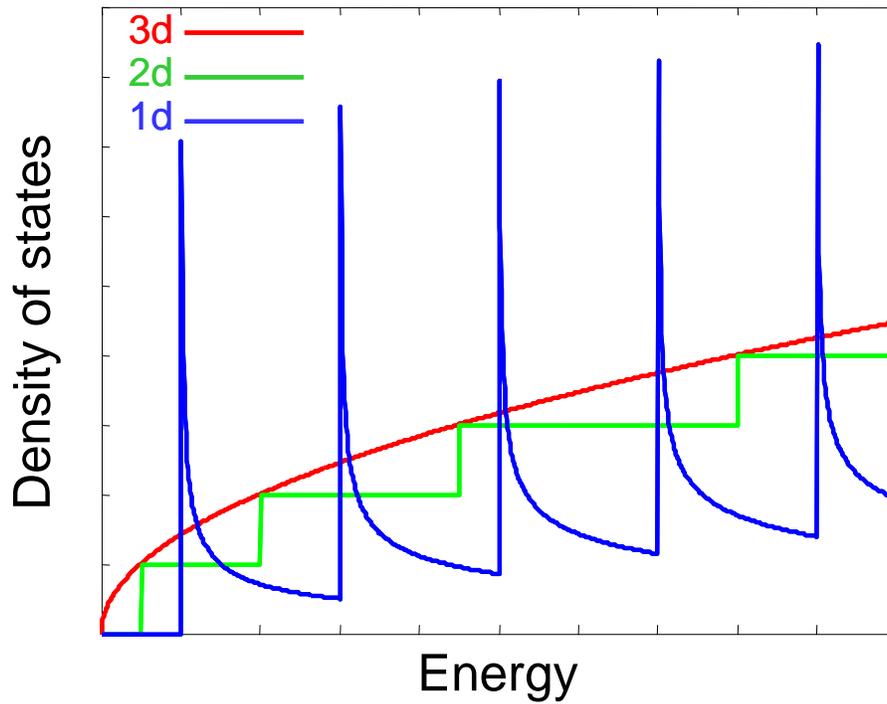


Fig. 2.27. Normalized densities of states for bulk materials (3d), quantum wells (2d), and molecular wires (1d).

Part 2. The Quantum Particle in a Box

Problems

1. i) Using MATLAB, generate Fig. 2.13.

ii) If $L_y = L_x \cdot \sqrt{\frac{3}{5}}$ which mode has a lower energy $\{n_x = 3, n_y = 1\}$ or $\{n_x = 2, n_y = 2\}$

2. The transistor illustrated below has an oxide ($\epsilon = 4\epsilon_0$) thickness $d = 1.2\text{nm}$ and channel depth $L_z = 2.5\text{nm}$. Considering the channel as a quantum well, how many modes are filled when a voltage $V=1\text{V}$ is applied to the gate?



Fig. 2.28. A simple model of a modern transistor.

Hint: calculate the charge in the channel using the expression for a parallel plate capacitor.

3. A particular conductor of length L has the dispersion relation:

$$\begin{aligned} E_1(k) &= 5 + 2V \cos(ka) \\ E_2(k) &= 10 - 2V \cos(ka) \end{aligned}, \quad |k| < \frac{\pi}{a}$$

where V and a are positive constants.

- i) Sketch the dispersion relation.
- ii) Calculate the density of states in terms of E , V , and a .

4. In general, the degenerate approximation for the electron distribution function $f(E, E_F)$ works when the density of states is large and slowly varying above and below the Fermi level. The non degenerate approximation works best when the density of states at the Fermi level is much smaller than the density of states at higher energies.

Here, we consider these approximations in a Gaussian density of states. The Gaussian varies fairly slowly near its center, but it decreases extremely rapidly in its tails. The electron population in a Gaussian density of states is given by

$$n = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(E/\sigma)^2} f(E, E_F) dE,$$

Introduction to Nanoelectronics

where $f(E, E_F)$ is the Fermi function. For a particular range of the Fermi level, E_F , the electron population may be approximated as:

$$n \approx \int_{-\infty}^{E_F} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}(E/\sigma)^2} dE$$

This is the degenerate limit.

As the Fermi level decreases, the electron population is better calculated in the non-degenerate limit. Derive the minimum Fermi level E_F for the degenerate limit to hold as a function of temperature T and standard deviation σ .

Hint: estimate the minimum Fermi level by examining the energetic distribution of electrons in the non-degenerate limit.

MIT OpenCourseWare
<http://ocw.mit.edu>

6.701 / 6.719 Introduction to Nanoelectronics
Spring 2010

For information about citing these materials or our Terms of Use, visit: <http://ocw.mit.edu/terms>.