

Tight Binding Chain (Interlude and Preview)

11

In the previous two chapters we considered the properties of vibrational waves (phonons) in a one-dimensional system. At this point, we are going to make a bit of an excursion to consider electrons in solids again. The point of this excursion, besides being a preview of much of the physics that will reoccur later on, is to make the point that all waves in periodic environments (in crystals) are similar. In the previous two chapters we considered vibrational waves, whereas in this chapter we will consider electron waves (remember that in quantum mechanics particles are just as well considered to be waves!).

11.1 Tight Binding Model in One Dimension

We described the molecular orbital, tight binding, or LCAO picture for molecules previously in Section 6.2.2. Here we will consider a chain of such molecular orbitals to represent orbitals in a macroscopic (one-dimensional) solid as shown in Fig. 11.1.

In this picture, there is a single orbital on atom n which we call $|n\rangle$. For convenience we will assume that the system has periodic boundary conditions (i.e., there are N sites, and site N is the same as site 0).¹ Further, we assume that all of the orbitals are orthogonal to each other.²

$$\langle n|m\rangle = \delta_{n,m} \quad (11.1)$$

Let us now take a general trial wavefunction of the form

$$|\Psi\rangle = \sum_n \phi_n |n\rangle$$

As we discussed for the tight-binding model (see Eq. 6.4 and Exercise 6.4) the effective Schroedinger equation can be written as²

$$\sum_m H_{nm} \phi_m = E \phi_n \quad (11.2)$$

where H_{nm} is the matrix element of the Hamiltonian

$$H_{nm} = \langle n|H|m\rangle$$

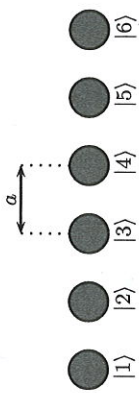


Fig. 11.1 The tight binding chain. There is one orbital on each atom, and electrons are allowed to hop from one atom to the neighboring atom.

¹As in Section 6.2.2 this is not a great approximation, particularly when the atoms get close to each other. Doing it more correctly, however, only adds algebraic complexity and is not all that enlightening. See Exercise 6.5 and 11.3, where we work through the calculation more correctly.

²Another way to get this effective equation is to start with the real Schroedinger equation $H|\psi\rangle = E|\psi\rangle$, insert a complete set $1 = \sum_m |m\rangle\langle m|$ between H and $|\psi\rangle$ and then apply $\langle n|$ from the left on both sides to obtain Eq. 11.2 where $\phi_n = \langle n|\psi\rangle$. If the set $|m\rangle$ were really complete set (which it is not) this would be a good derivation. However, to the extent that these orbitals approximate a complete set, this is an approximate derivation. More precisely one should interpret this as a variational approximation as discussed in Exercise 6.2.

is not the m^{th} , an electron on the m^{th} atom can be transferred (can hop) to the n^{th} atom. Generally this can only happen if n and m are very close to each other. Thus, we write

$$\sum_{j \neq m} \langle n | V_j | m \rangle = \begin{cases} V_0 & n = m \\ -t & n = m \pm 1 \\ 0 & \text{otherwise} \end{cases} \quad (11.3)$$

which defines both V_0 and t . (The V_0 term here does not hop an electron from one site to another, but rather just shifts the energy on a given site.) Note that by translational invariance of the system, we expect that the result should depend only on $n - m$, which this form does. These two types of terms V_0 and t are entirely analogous to the two types of terms $V_{\alpha\alpha}$ and t that we met in Section 6.2.2 when we studied covalent bonding of two atoms.³ The situation here is similar except that now there are many nuclei instead of just two.

With the above matrix elements we obtain

$$H_{n,m} = \epsilon_0 \delta_{n,m} - t (\delta_{n+1,m} + \delta_{n-1,m}) \quad (11.4)$$

where we have now defined⁴

$$\epsilon_0 = \epsilon_{\text{atomic}} + V_0$$

The Hamiltonian is a very heavily studied model, known as the tight binding chain. Here t is known as the hopping term, as it allows the Hamiltonian (which generates time evolution) to move the electron from one site to another, and it has dimensions of energy. It stands to reason that the magnitude of t depends on how close together the orbitals are becoming large when the orbitals are close together and decaying exponentially when they are far apart.

11.2 Solution of the Tight Binding Chain

The solution of the tight binding model in one dimension (the tight binding chain) is very analogous to what we did to study vibrations (and hence the point of presenting the tight binding model at this point!). We propose an ansatz solution⁵

$$\phi_n = \frac{e^{-ikna}}{\sqrt{N}} \quad (11.5)$$

where the denominator is included for normalization where there are N sites in the system. We now plug this ansatz into the Schroedinger equation Eq. 11.2. Note that in this case (as compared to the vibrational case) there is no frequency in the exponent of our ansatz. This is simply because we are trying to solve the time-independent Schroedinger equation. Had we used the time-dependent Schroedinger equation, we would need a factor of $e^{i\omega t}$ as well!

As mentioned previously when we studied the molecular orbital model in Section 6.2.2, this Schroedinger equation is actually a variational approximation. For example, instead of finding the exact ground state, it finds the best possible ground state made up of the orbitals that we have it in the model.

One can make the variational approach increasingly better by expanding the Hilbert space and putting more orbitals into the model. For example, instead of having only one orbital $|n\rangle$ at a given site, one could consider many $|n, \alpha\rangle$ where α runs from 1 to some number p . As p is increased the approach becomes increasingly more accurate and eventually essentially exact. This method of using tight-binding-like orbitals is increasingly well approximate the exact Schroedinger equation is known as LCAO (linear combination of atomic orbitals). However, one complication (which we treat in Exercise 11.3) is that when we add many more orbitals we typically have to give up our nice orthogonality assumption. $\langle n, \alpha | m, \beta \rangle = \delta_{nm} \delta_{\alpha\beta}$ no longer holds. This makes the effective Schroedinger equation a bit more complicated, but not fundamentally different (see comments in Section 6.2.2).

At any rate, in the current chapter we will work with only one orbital per site, and we assume the orthogonality Eq. 11.1.

We write the Hamiltonian as

$$H = K + \sum_j V_j$$

where $K = \mathbf{p}^2 / (2m)$ is the kinetic energy and V_j is the Coulomb interaction of the electron at position \mathbf{r} with the nucleus at site j ,

$$V_j = V(\mathbf{r} - \mathbf{R}_j)$$

where \mathbf{R}_j is the position of the j^{th} nucleus. With these definitions we have

$$H|m\rangle = (K + V_m)|m\rangle + \sum_{j \neq m} V_j|m\rangle$$

Now, we should recognize that $K + V_m$ is the Hamiltonian which would have if there were only a single nucleus (the m^{th} nucleus) and other nuclei in the system. Thus, if we take the tight-binding orbitals $|m\rangle$ to be the atomic orbitals, then we have

$$(K + V_m)|m\rangle = \epsilon_{\text{atomic}}|m\rangle$$

where ϵ_{atomic} is the energy of an electron on nucleus m in the absence of any other nuclei. Thus we can write

$$H_{n,m} = \langle n | H | m \rangle = \epsilon_{\text{atomic}} \delta_{n,m} + \sum_{j \neq m} \langle n | V_j | m \rangle \quad (11.6)$$

We now have to figure out what the final term of this equation is. The meaning of this term is that, via the interaction with some nucleus j

³Just to be confusing, atomic physicists sometimes use J where I have used t here.

⁴Once again ϵ_0 is not a dielectric constant or the permittivity of free space, but rather just the energy of having an electron sit on a site.

⁵Recall that in Section 4.5 we ran into a puzzle that the mean free path of electrons in metals seems unreasonably long. The fact that electrons hopping between orbitals form eigenstates which are plane waves (i.e., are delocalized across the entire system) hints towards the solution to this puzzle. We will return to reconsider this issue in more detail in Section 15.2.

As mentioned previously when we studied the molecular orbital model (Section 6.2.2), this Schrödinger equation is actually a variational approximation. For example, instead of finding the exact ground state, it finds the best possible ground state made up of the orbitals that we have put in the model.

One can make the variational approach increasingly better by expanding the Hilbert space and putting more orbitals into the model. For example, instead of having only one orbital $|n\rangle$ at a given site, one could consider many $|n, \alpha\rangle$ where α runs from 1 to some number p . As p is increased the approach becomes increasingly more accurate and eventually is essentially exact. This method of using tight-binding-like orbitals is increasingly well approximate the exact Schrödinger equation is known as LCAO (linear combination of atomic orbitals). However, one complication (which we treat in Exercise 11.3) is that when we add many more orbitals we typically have to give up our nice orthogonality assumption, i.e., $\langle n, \alpha | m, \beta \rangle = \delta_{nm} \delta_{\alpha\beta}$ no longer holds. This makes the effective Schrödinger equation a bit more complicated, but not fundamentally different (see comments in Section 6.2.2).

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is not the m^{th} , an electron on the m^{th} atom can be transferred to the n^{th} atom. Generally this can only happen very close to each other. Thus, we write

$$\sum_{j \neq m} \langle n | V_j | m \rangle = \begin{cases} V_0 & n = m \\ -t & n = m \pm 1 \\ 0 & \text{otherwise} \end{cases}$$

which defines both V_0 and t . (The V_0 term here does not mean one site to another, but rather just shifts the energy state that by translational invariance of the system, we should expect to find. V_0 and t are entirely analogous to the two types of terms V_0 and t that we met in Section 6.2.2 when we discussed the tight-binding model.) The situation here is similar to that of two atoms.³ With the above matrix elements we obtain

$$H_{n,m} = \epsilon_0 \delta_{n,m} - t (\delta_{n+1,m} + \delta_{n-1,m})$$

where we have now defined⁴

$$\epsilon_0 = \epsilon_{\text{atomic}} + V_0$$

This Hamiltonian is a very heavily studied model, known as the tight-binding model. Here t is known as the hopping term, and ϵ_0 is the energy of an electron on a single atom. The Hamiltonian (which generates time evolution) to move an electron from one site to another, and it has dimensions of energy. The hopping term t is the magnitude of t depends on how close together the atoms are. For large t , the orbitals are close together and the hopping term is large. For small t , the orbitals are far apart.

11.2 Solution of the Tight Binding Model

The solution of the tight binding model in one dimension (the tight-binding chain) is very analogous to what we did to study the free electron gas. The point of presenting the tight binding model at this point is to show that the tight binding model can be used to propose an ansatz solution⁵

$$\phi_n = \frac{e^{-ikna}}{\sqrt{N}}$$

where the denominator is included for normalization of the wave function. We now plug this ansatz into the Schrödinger equation Eq. 11.2. Note that in this case (as compared to the free electron gas) there is no frequency in the exponent of our wave function because we are trying to solve the time-independent Schrödinger equation. Had we used the time-dependent Schrödinger equation we would need a factor of $e^{i\omega t}$ as well!

As with vibrations, it is obvious that $k \rightarrow k + 2\pi/a$ gives the same solution. Further, if we consider the system to have periodic boundary conditions with N sites (length $L = Na$), the allowed values of k are quantized in units of $2\pi/L$. As with Eq. 9.6 there are precisely N possible different solutions of the form of Eq. 11.5.

Plugging the ansatz into the left side of the Schroedinger equation 11.2 and then using Eq. 11.4 gives us

$$\sum_m H_{n,m} \phi_m = \epsilon_0 \frac{e^{-ikna}}{\sqrt{N}} - t \left(\frac{e^{-ik(n+1)a}}{\sqrt{N}} + \frac{e^{-ik(n-1)a}}{\sqrt{N}} \right)$$

which we set equal to the right side of the Schroedinger equation

$$E \phi_n = E \frac{e^{-ikna}}{\sqrt{N}}$$

to obtain the spectrum

$$E = \epsilon_0 - 2t \cos(ka) \quad (11.6)$$

which looks rather similar to the phonon spectrum of the one-dimensional monatomic chain which was (see Eq. 9.2)

$$\omega^2 = 2 \frac{\kappa}{m} - 2 \frac{\kappa}{m} \cos(ka)$$

Note however, that in the electronic case one obtains the energy *whereas* in the phonon case one obtains the *square* of the frequency.⁶

The dispersion curve of the tight binding chain (Eq. 11.6) is shown in Fig. 11.2. Analogous to the phonon case, it is periodic in $k \rightarrow k + 2\pi/a$. Further, analogous to the phonon case, the dispersion always has a group velocity (is flat) for $k = n\pi/a$ for n any integer (i.e., at the Brillouin zone boundary).

Note that unlike free electrons, the electron dispersion here has maximum energy as well as a minimum energy. Electrons only have eigenstates within a certain energy *band*. The word "band" is used to describe the energy range for which eigenstates exist, as well as to describe one connected branch of the dispersion curve. (In this plot there is only a single mode at each k , hence one branch, hence a *band*.)

The energy difference from the bottom of the band to the top is known as the *bandwidth*. Within this bandwidth (between the top and bottom of the band) for any energy there exists at least one k state having that energy. For energies outside the bandwidth there are no k -states with that energy.

The bandwidth (which in this model is $4t$) is determined by the magnitude of the hopping, which depends on the distance between nearest atoms. As a function of the interatomic spacing the bandwidth changes roughly as shown in Fig. 11.3. On the right of this diagram there are N sites each one being an atomic orbital $|\alpha\rangle$. On the left of the diagram there are N states form a band, yet as discussed above in this section, there are

precisely N states (this should not surprise us, being that we have not changed the dimension of the Hilbert state, we have just expressed it in terms of the complete set of eigenstates of the Hamiltonian). Note that the average energy of a state in this band remains always ϵ_0 .

By allowing hopping between orbitals, some of the eigenstates in the band have decreased in energy from the energy ϵ_0 of the atomic eigenstate and some of the eigenstates have increased in energy. This is entirely analogous to what we found in Section 6.2.2 when we found bonding and antibonding orbitals form when we allow hopping between two atoms. In both cases, the hopping splits the energy levels (originally into some higher energy states and some lower energy states.

Aside: Note that if the band is not completely filled, the *total* energy of all of the electrons *decreases* as the atoms are moved together and the band width increases (since the average energy remains zero, but some of the higher energy states are not filled). This decrease in energy is precisely the binding force of a "metallic bond" which we discussed in Section 6.4.⁸ We also mentioned previously that one property of metals is that they are typically soft and malleable. This is a result of the fact that the electrons that hold the atoms together are mobile—in other words, because they are mobile, they can readjust their positions somewhat as the crystal is deformed.

Near the bottom of the band, the dispersion is parabolic. For the dispersion Eq. 11.6, expanding for small k , we obtain

$$E(k) = \text{Constant} + ta^2k^2$$

which tells us that for $t < 0$, the energy minimum is at the Brillouin zone boundary $k = \pi/a$. In this case we would expand for k close to π/a instead of k close to 0. The resulting parabolic behavior is similar to that of free electrons which have a dispersion

$$E_{free}(k) = \frac{\hbar^2 k^2}{2m}$$

we can therefore view the bottom of the band as being almost like free electrons, except that we have to define a new *effective mass* which we call m^* such that

$$\frac{\hbar^2 k^2}{2m^*} = ta^2k^2$$

which gives us

$$m^* = \frac{\hbar^2}{2ta^2}$$

In other words, the *effective mass* m^* is defined such that the dispersion at the bottom of the band is exactly like the dispersion of free particles with mass m^* . (We will discuss effective mass in much more depth in Chapter 17. This is just a quick first look at it.) Note that this mass has nothing to do with the actual mass of the electron, but rather depends on the hopping matrix element t . Further, we should keep in mind that m^* that enters into the dispersion relationship is actually the crystal momentum, not the actual momentum of the electron (recall that crystal

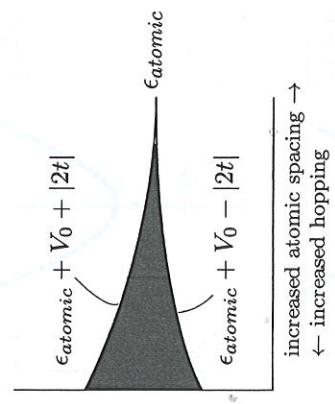


Fig. 11.3 Caricature of the dependence of bandwidth on interatomic spacing. On the far right there is no hopping and the energy of every state in the band is ϵ_0 . As hopping increases (towards the left) the energies of states in the band spread out. At each value of hopping there are eigenstates with energies within the shaded region, but not outside the shaded region.

⁸ Of course, we have not considered the repulsive force between neighboring nuclei, so the nuclei do not get too close together. As in the case of the covalent bond considered in Section 6.2.2, some of the Coulomb repulsion between nuclei will be canceled by V_{cross} (here V_0), the attraction of the electron on a given site to other nuclei.

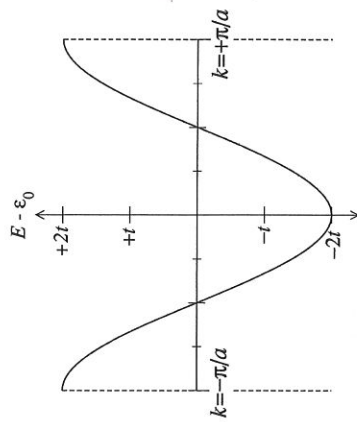


Fig. 11.2 Dispersion of the tight binding chain. Energy is plotted versus wavevector in the first Brillouin zone.

⁶This difference is due to the fact that the time dependent Schrödinger equation has one time derivative, but Newton's equation of motion ($F = ma$) has two.

⁷Since the hopping t depends on an overlap between orbitals on adjacent atoms (see Eq. 11.3 and comments thereafter), in the limit that the atoms are well separated, the bandwidth will decrease exponentially as the atoms are pulled further apart.

As with vibrations, it is obvious that $k \rightarrow k + 2\pi/a$ gives the same solution. Further, if we consider the system to have periodic boundary conditions with N sites (length $L = Na$), the allowed values of k are quantized in units of $2\pi/L$. As with Eq. 9.6 there are precisely N possible different solutions of the form of Eq. 11.5.

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Aside: Note that if the band is not completely filled, the *total* energy of the electrons *decreases* as the atoms are moved together and the band *narrows* (since the average energy remains zero, but some of the higher energy states are not filled). This decrease in energy is precisely the binding force “metallic bond” which we discussed in Section 6.4.⁸ We also mentioned previously one property of metals is that they are typically soft and malleable. This is a result of the fact that the electrons that hold the atoms together are mobile, because they are mobile, they can readjust their positions somewhat as the crystal is deformed.

Near the bottom of the band, the dispersion is parabolic. For dispersion Eq. 11.6, expanding for small k , we obtain

$$E(k) = \text{Constant} + t a^2 k^2$$

that for $t < 0$, the energy minimum is at the Brillouin zone boundary $k = \pi/a$. In this case we would expand for k close to π/a instead of k close to 0.) The resulting parabolic behavior is similar to that of free electrons which have a dispersion

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which gives us

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In other words, the *effective mass* m^* is defined such that the dispersion of the bottom of the band is exactly like the dispersion of free particles of mass m^* . (We will discuss effective mass in much more depth in Chapter 17. This is just a quick first look at it.) Note that this mass is not the same as the actual mass of the electron, but rather depends on the hopping matrix element t . Further, we should keep in mind that the k that enters into the dispersion relationship is actually the crystal momentum, not the actual momentum of the electron (recall that cr

momentum is defined only modulo $2\pi/a$. However, so long as we stay at very small k , then there is no need to worry about the periodicity of ϵ which occurs. Nonetheless, we should keep in mind that if electrons scatter off of other electrons, or off of phonons, it is crystal momentum that is conserved (see the discussion in Section 9.4).

11.3 Introduction to Electrons Filling Bands

We now imagine that our tight binding model is actually made up of atoms and each atom "donates" one electron into the band (i.e., the atom has *valence* one). Since there are N possible k -states in the band and electrons are fermions, you might guess that this would precisely fill the band. However, there are two possible spin states for an electron at each k , so in fact, this then only half-fills the band. This is depicted in the top of Fig. 11.4. The filled states (shaded) in this picture are filled with both up and down spins.

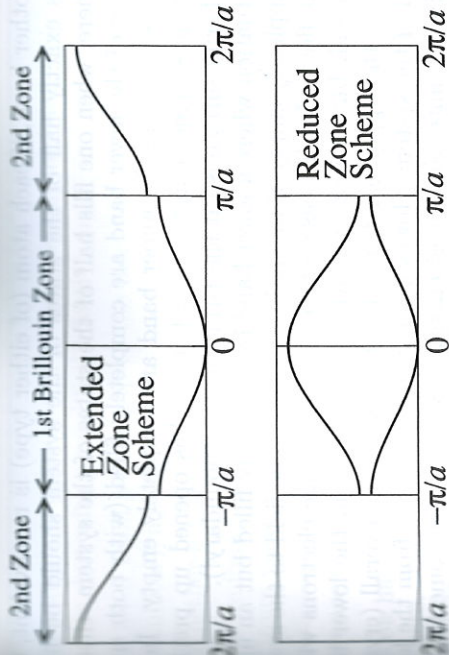
It is crucial in this picture that there is a Fermi surface—the point where the shaded meets the unshaded region. If a small electric field is applied to the system, it only costs a very small amount of energy to shift the Fermi surface as shown in the bottom of Fig. 11.4, populating a few k -states moving right and depopulating some k -states moving left. In other words, the state of the system responds by changing a small bit and a current is induced. As such, this system is a *metal* in that it conducts electricity. Indeed, crystals of atoms that are monovalent are very frequently metals!

On the other hand, if each atom in our model were di-valent (donate two electrons to the band) then the band would be entirely full of electrons. In fact, it does not matter if we think about this as being a full band where every k -state $|k\rangle$ is filled with two electrons (one up and one down), or a filled band where every site $|n\rangle$ is filled—these two statements describe the same multi-electron wavefunction. In fact, there is a single unique wavefunction that describes this completely filled band.

In the case of the filled band, were one to apply a small electric field to this system, the system cannot respond at all. There is simply no freedom to repopulate the occupation of k -states because every state is already filled. Thus we conclude an important principle.

Principle: A filled band carries no current.⁹

Thus our example of a divalent tight-binding model is an insulator (this type of insulator is known as a *band insulator*). Indeed, many systems of divalent atoms are insulators (although in a moment we will discuss how divalent atoms can also form metals).



11.4 Multiple Bands

In the tight binding chain considered in this chapter, we considered only the case where there is a single atom in the unit cell and a single orbital per atom. However, more generally we might consider a case where we have multiple orbitals per unit cell.

One possibility is to consider one atom per unit cell, but several orbitals per atom.¹⁰ Analogous to what we found for the tight binding model having only one orbital per atom, when the atoms are very far apart, one has only the atomic orbitals on each atom. However, as the atoms are moved closer together, the orbitals merge together and the energies spread to form bands.¹¹ Analogous to Fig. 11.3 we have shown how this occurs for the two band case in Fig. 11.6.

A very similar situation occurs when we have two atoms per unit cell but only one orbital per atom (see Exercises 11.2 and 11.4.) The general result will be quite analogous to what we found for vibrations of a diatomic chain in Chapter 10.

In Fig. 11.5 we show the spectrum of a tight-binding model with two different atoms per unit cell—each having a single orbital. We have shown results here in both the reduced and extended zone schemes.

As for the case of vibrations, we see that there are now two possible energy eigenstates at each value of k . In the language of electrons, we say that there are two bands (we do not use the words "acoustic" and "optical" for electrons, but the idea is similar). Note that there is a gap between the two bands where there are simply no energy eigenstates.

Let us think for a second about what might result in this situation where there are two atoms per unit cell and one orbital per atom. If each atom (of either type) were divalent, then the two electrons donated per atom would completely fill the single orbital on each atom. In this case, both bands would be completely filled with both spin-up and spin-down electrons.

Fig. 11.5 Diatomic tight binding dispersion in one dimension. **Bottom:** Reduced zone scheme. **Top:** Extended zone scheme. Note that in obtaining the extended zone scheme from the reduced zone scheme, one simply translates pieces of the dispersion curve by appropriate reciprocal lattice vectors.

¹⁰Each atom actually has an infinite number of orbitals to be considered at higher and higher energy. But only a small number of them are filled, and within our level of approximation we can only consider very few of them.

¹¹This picture of atomic orbitals in the weak hopping limit merging together to form bands does not depend on the fact that the crystal of atoms is ordered. Glasses and amorphous solids can have this sort of band structure as well!

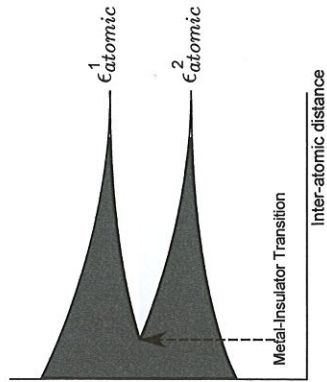


Fig. 11.6 Caricature of bands for a two-band model as a function of inter-atomic spacing. In the atomic limit, the orbitals have energies ϵ^1_{atomic} and ϵ^2_{atomic} . If the system has valence two per unit cell, then in the atomic limit the lower orbital is filled and the upper orbital is empty. When the atoms are pushed together, the lower band remains filled, and the upper band remains empty, until the bands start to overlap, whereupon we have two bands both partially filled, which becomes a metal.

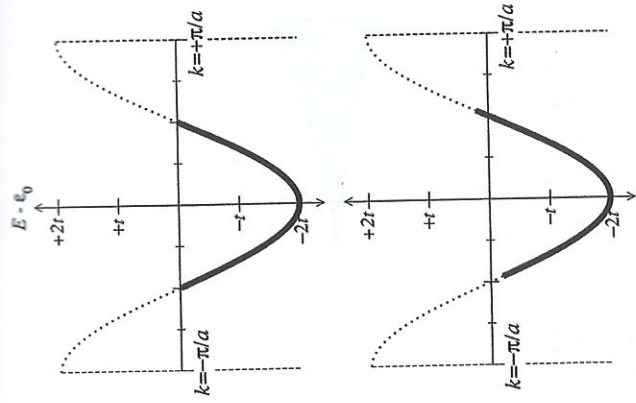


Fig. 11.4 Top: If each atom has valence 1, then the band is half-filled. The states that are shaded are filled with both up and down spin electrons. The Fermi surface is the boundary between the filled and unfilled states. **Bottom:** When a small electric field is applied, at only a small cost of energy, the Fermi sea can shift slightly (moving a few electrons from the right side to the left side) thus allowing current to flow.

⁹In one dimension this principle is absolutely correct. In higher dimensions, it is sometimes possible to have Hall effect current (but not longitudinal current) from bands that are entirely filled. While this situation, a so-called "Chern band", is of great current research interest, it is far beyond the scope of this book. As such, I'd recommend ignoring this unusual possibility and just viewing the principle as being *almost* always true for most practical situations.

momentum is defined only modulo $2\pi/a$). However, so long as we stay at very small k , then there is no need to worry about the periodicity of k which occurs. Nonetheless, we should keep in mind that if electrons scatter off of other electrons, or off of phonons, it is crystal momentum that is conserved (see the discussion in Section 9.4).

11.3 Introduction to Electrons Filling Bands

We now imagine that our tight binding model is actually made up of atoms and each atom "donates" one electron into the band (i.e., the atom has *valence* one). Since there are N possible k -states in the band and electrons are fermions, you might guess that this would precisely fill the band. However, there are two possible spin states for an electron at each k , so in fact, this then only half-fills the band. This is depicted in the top of Fig. 11.4. The filled states (shaded) in this picture are filled with both up and down spins.

It is crucial in this picture that there is a Fermi surface—the point where the shaded meets the unshaded region. If a small electric field is applied to the system, it only costs a very small amount of energy to shift the Fermi surface as shown in the bottom of Fig. 11.4, populating a few k -states moving right and depopulating some k -states moving left. In other words, the state of the system responds by changing a small bit and a current is induced. As such, this system is a *metal* in that it conducts electricity. Indeed, crystals of atoms that are monovalent are very frequently metals!

On the other hand, if each atom in our model were di-valent (donates two electrons to the band) then the band would be entirely full of electrons. In fact, it does not matter if we think about this as being a full band where every k -state $|k\rangle$ is filled with two electrons (one up and one down), or a filled band where every site $|n\rangle$ is filled—these two statements describe the same multi-electron wavefunction. In fact, there is a single unique wavefunction that describes this completely filled band. In the case of the filled band, were one to apply a small electric field to this system, the system cannot respond at all. There is simply no freedom to repopulate the occupation of k -states because every state is already filled. Thus we conclude an important principle.

Principle: A filled band carries no current.⁹

Thus our example of a divalent tightbinding model is an insulator (this type of insulator is known as a *band insulator*). Indeed, many systems of divalent atoms are insulators (although in a moment we will discuss how divalent atoms can also form metals).



11.4 Mult

in the tight binding... the case where the... per atom. However... have multiple orbi... One possibility... total per atom... model having only... part, one has on... atoms are moved... energies spread to... low this occurs k... A very similar... but only one... general result will... a diatomic chain... In Fig. 11.5 we... different atoms p... down results her... As for the case... energy eigenstate... say that there ar... "optical" for elec... between the two... Let us think f... where there are t... atom (of either t... both bands woul... electrons.