به نامِ خدا

دانش‌گاهِ صنعتی‌ِ اصفهان ـ دانش‌کده‌ی فیزیک

تصاویر فصل ۱۱

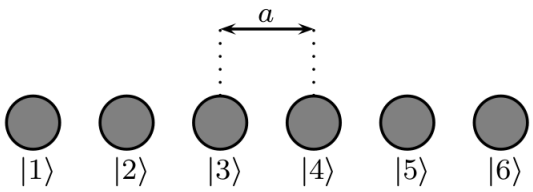

Fig. 11.1 The tight binding chain. There is one orbital on each atom, and electrons are allowed to hop from one atom to the neighboring atom.

[1] As 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.

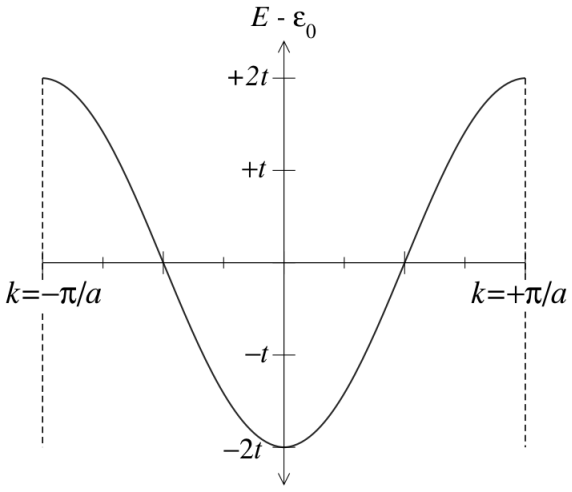

Fig. 11.2 Dispersion of the tight binding chain. Energy is plotted versus wavevector in the first Brillouin zone.

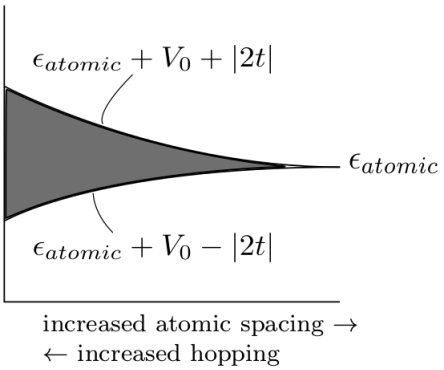

Fig. 11.3 Caricature of the dependence of bandwidth on interatomic spacing. On the far right there is no hopping and the energy of every state in the band is ϵ_0. As hopping increases (towards the left) the energies of states in the band spread out. At each value of hopping there are eigenstates with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

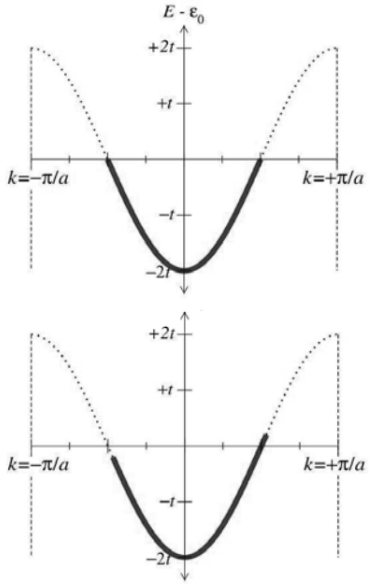

Fig. 11.4 Top: If each atom has valence 1, then the band is half-filled. The states that are shaded are filled with both up and down spin electrons. The Fermi surface is the boundary between the filled and unfilled states. **Bottom:** When a small electric field is applied, at only a small cost of energy,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

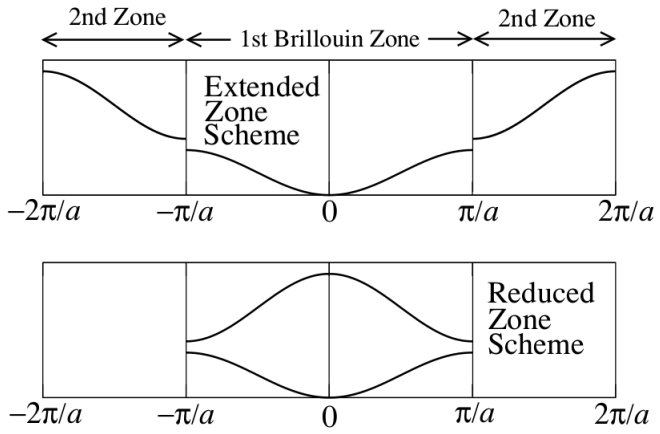

Fig. 11.5 Diatomic tight binding dispersion in one dimension. **Bottom:** Reduced zone scheme. **Top:** Extended zone scheme. Note that in obtaining the extended zone scheme from the reduced zone scheme, one simply translates pieces of the dispersion curve by appropriate reciprocal lattice vectors.

[10]Each atom actually has an infinite

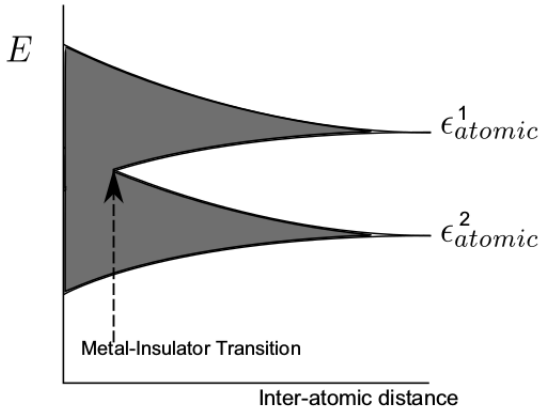

Fig. 11.6 Caricature of bands for a two-band model as a function of interatomic spacing. In the atomic limit, the orbitals have energies ϵ^1_{atomic} and ϵ^2_{atomic}. If the system has valence two per unit cell, then in the atomic limit the lower orbital is filled and the upper orbital is empty. When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

- Solving the tight-binding Schroedinger equation for electron waves is very similar to solving Newton's equations for vibrational (phonon) waves. The structure of the reciprocal lattice and the Brillouin zone remains the same.
- We obtain energy bands where energy eigenstates exist, and gaps between bands.
- Zero hopping is the atomic limit. As hopping increases, atomic orbitals spread into bands.

- Energies are parabolic in k near bottom of band—like free electrons, but with a modified effective mass.
- A filled band with a gap to the next band is an insulator (a *band* insulator), a partially filled band has a Fermi surface and is a metal.
- Whether a band is filled depends on the valence of the atoms.
- As we found for phonons, gaps open at Brillouin zone boundaries. Group velocities are also zero at zone boundaries.
