به نامِ خدا

دانش‌گاهِ صنعتیِ اصفهان ـ دانش‌کده‌یِ فیزیک

تصاویر فصل ۱۵

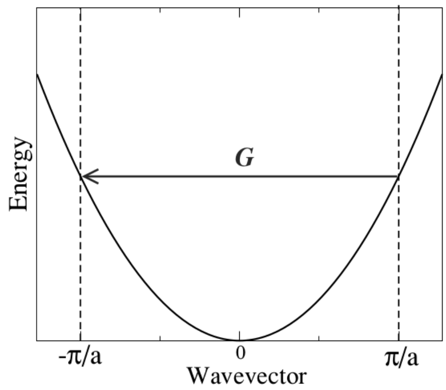

Fig. 15.1 Scattering from Brillouin zone boundary to Brillouin zone boundary. The states at the two zone boundaries are separated by a reciprocal lattice vector **G** and have the same energy. This situation leads to a divergence in perturbation theory, Eq. 15.2, because when the two energies match, the denominator is zero.

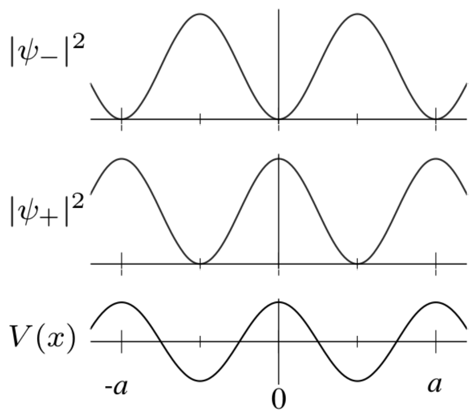

Fig. 15.2 Structure of wavefunctions at the Brillouin zone boundary. The higher-energy eigenstate ψ_+ has its density concentrated near the maxima of the potential V, whereas the lower-energy eigenstate ψ_- has its density concentrated near the minima of V.

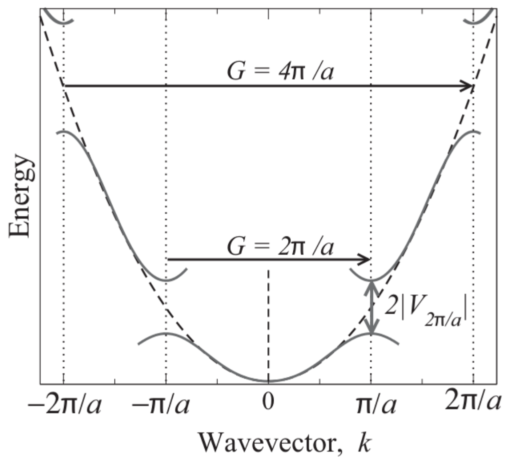

Fig. 15.3 Dispersion of a nearly free electron model. In the nearly free electron model, gaps open up at the Brillouin zone boundaries in an otherwise parabolic spectrum. Compare this to what we found for the tight binding model in Fig. 11.5.

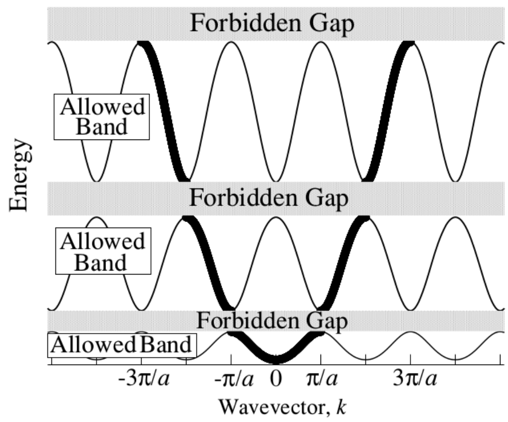

Fig. 15.4 Dispersion of a nearly free electron model. Same as Fig. 15.3, but plotted in repeated zone scheme. This is equivalent to the reduced zone scheme but the equivalent zones are repeated. Forbidden bands are marked where there are no eigenstates. The similarity to the free electron parabolic spectrum is emphasized.

- When electrons are exposed to a periodic potential, gaps arise in their dispersion relation at the Brillouin zone boundary. (The dispersion is quadratic approaching a zone boundary.)
- Thus the electronic spectrum breaks into bands, with forbidden energy gaps between the bands. In the nearly free electron model, the gaps are proportional to the periodic potential $|V_{\mathbf{G}}|$.
- Bloch's theorem guarantees that all eigenstates are some periodic function times a plane wave. In repeated zone scheme the wavevector (the *crystal momentum*) can always be taken in the first Brillouin zone.