# Evolution of Our Band Structure Understanding

by Dr. Colton, Physics 581 (last updated: Fall 2020)

**1. Actual band structure (for GaAs), from Yu & Cardona**

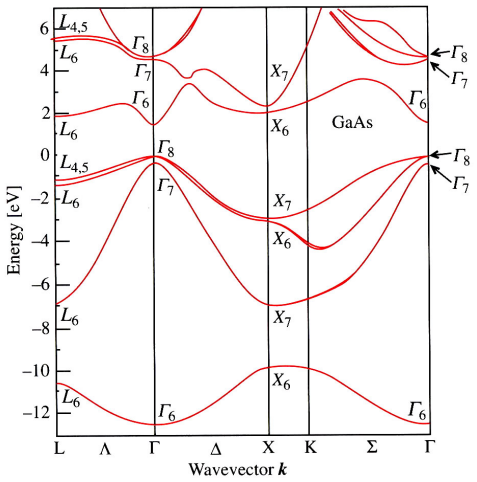



**Fig. 2.14.** Electronic band structure of GaAs calculated by the pseudopotential technique. [Ref.: Cohen and Chelikowsky, 1989.]

**2. Free electron model, from Kittel.**

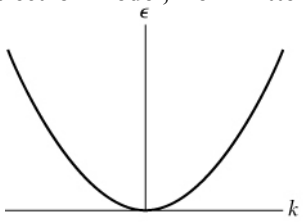



**Fig 7.2.** (a) Plot of energy $\varepsilon$ vs. wavevector $k$ for a free electron.

**3. Free electron model with periodicity of lattice, from Ibach & Lüth.**

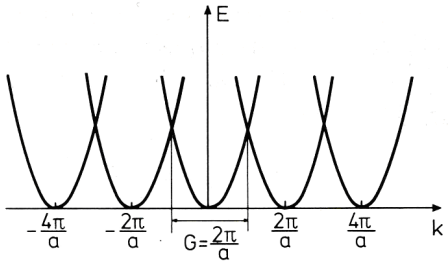
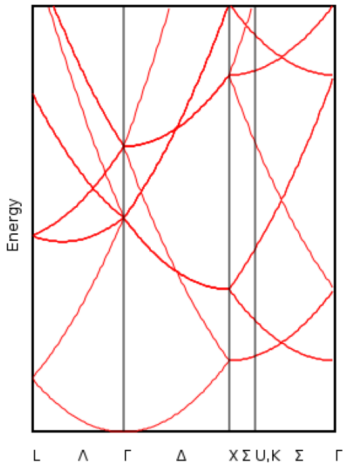


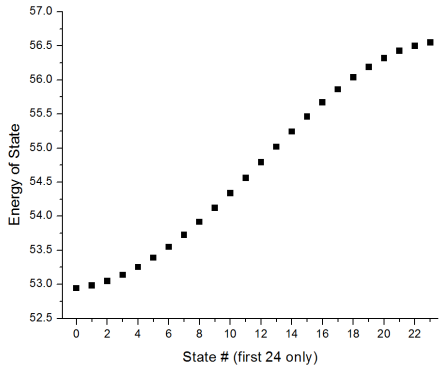

**Fig. 7.2.** The parabolic energy curves of a free electron in one dimension, periodically continued in reciprocal space. The periodicity in real space is $a$. This $E(\boldsymbol{k})$ dependence corresponds to a periodic lattice with a vanishing potential ("empty" lattice)

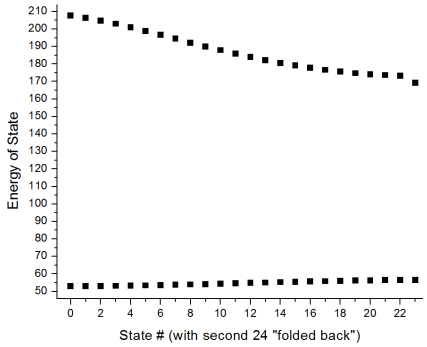
**4. Empty lattice model for fcc, from Wikipedia.**




Free electron bands in a FCC crystal structure.
http://en.wikipedia.org/wiki/Empty_lattice_approximation

**5. "24 deep wells" model, from Colton handout.**




**6. Kronig-Penney model, from Kittel.**

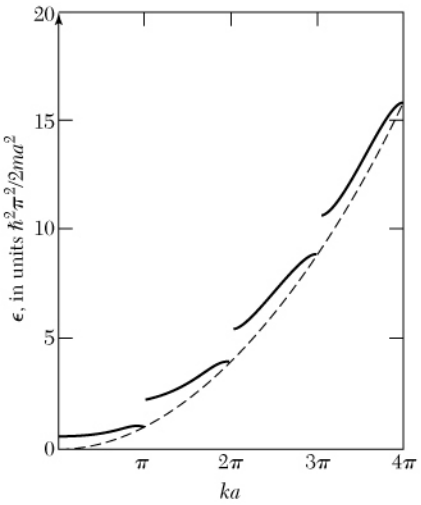
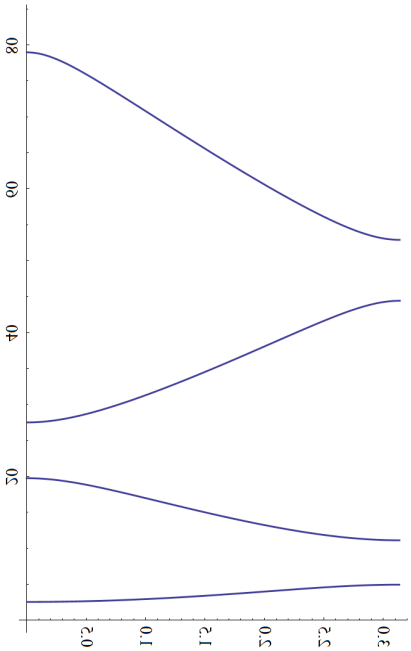



**Fig 7.6.** Plot of energy vs. wavenumber for the Kronig-Penney potential, with P = 3π/2. Notice the energy gaps at *ka* = π, 2π, 3π, ….

**7. Kronig-Penney model, folded back to 1st B.Z, from Colton HW problem.**



**Note**: The plot was produced with axes reversed. To recover usual x- and y-axes I rotated the image, then horizontally flipped it with an image editor.

## 8. Side note: wavefunctions via Bloch theorem, from Ibach & Lüth.

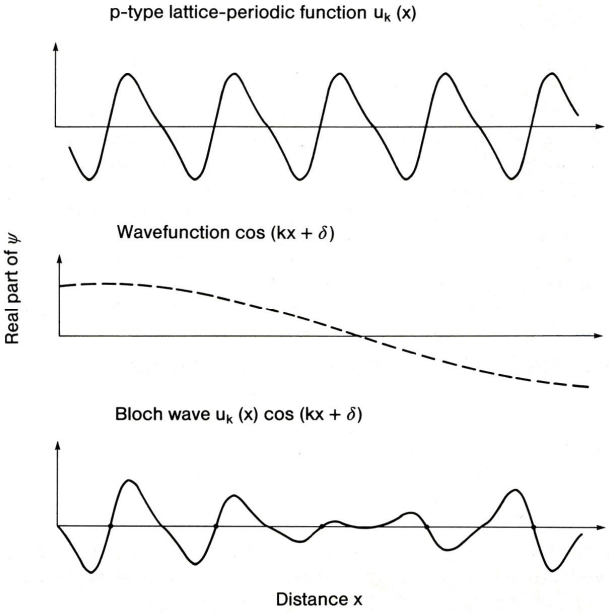



**Fig. 7.1.** Example of the construction of a Bloch wave $\psi_k(r) = u_k(r)e^{ik\cdot r}$ from a lattice-periodic function $u_k(r)$ with $p$-type bonding character and a plane wave

## 9. Side note, cont.: Approximate wavefunctions, results from Nearly Free Electron approximation and Central Equation, from Ibach & Lüth.

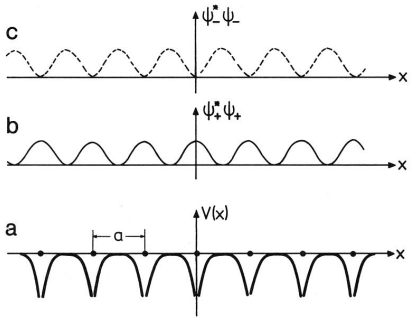



**Fig. 7.4.** **(a)** Qualitative form of the potential energy $V(x)$ of an electron in a one-dimensional lattice. The positions of the ion cores are indicated by the points with separation $a$ (lattice constant). **(b)** Probability density $\varrho_+ = \psi_+^* \psi_+$ for the standing wave produced by Bragg reflection at $k = \pm\pi/a$ (upper edge of band ① in Fig. 7.5). **(c)** Probability density $\varrho_- = \psi_-^* \psi_-$ for the standing wave at the lower edge of band ② (Fig. 7.5) at $k = \pm\pi/a$

## 10. Results of "Nearly Free Electron approximation" and Central Equation, from Ibach & Lüth.

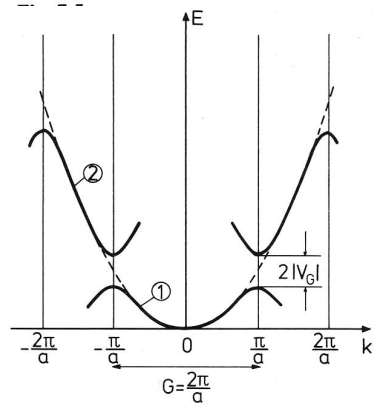



**Fig. 7.5.** Splitting of the energy parabola of the free electron (– – –) at the edges of the first Brillouin zone ($k = \pm\pi/a$ in the one-dimensional case). To a first approximation the gap is given by twice the corresponding Fourier coefficient $V_G$ of the potential. Periodic continuation over the whole of $k$-space gives rise to continuous bands ① and ② , shown here only in the vicinity of the original energy parabola

**11. Connection between Nearly Free Electron approx. and original free electron model, from Ibach & Lüth.**

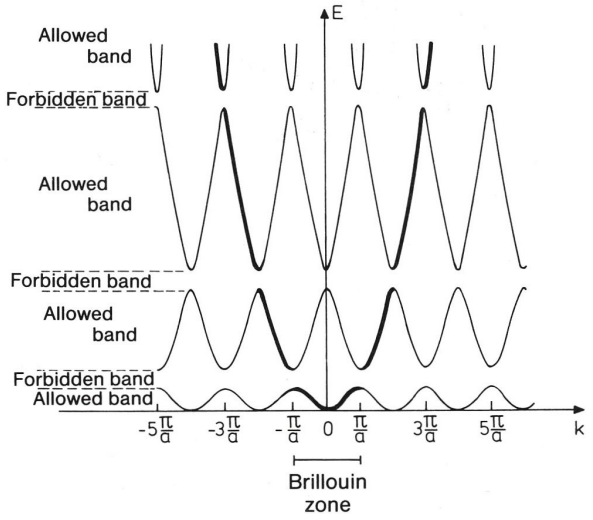



**Fig. 7.6.** Energy dispersion curves $E(k)$ for a one-dimensional lattice (lattice constant $a$) in the extended zone scheme. As can be seen, the quasi-free-electron approximation gives rise to forbidden and allowed energy regions due to the opening of band gaps, as shown in Fig. 7.5 (cf. the vanishing potential case of Fig. 7.2). The parts of the bands corresponding to the free-electron parabola are indicated by the thick lines

**12. Tight binding, qualitative picture. From Yu & Cardona, for Ge or GaAs.** Note: Middle section is like "Two Coulomb wells" from Colton handout, but with larger interaction between atoms.

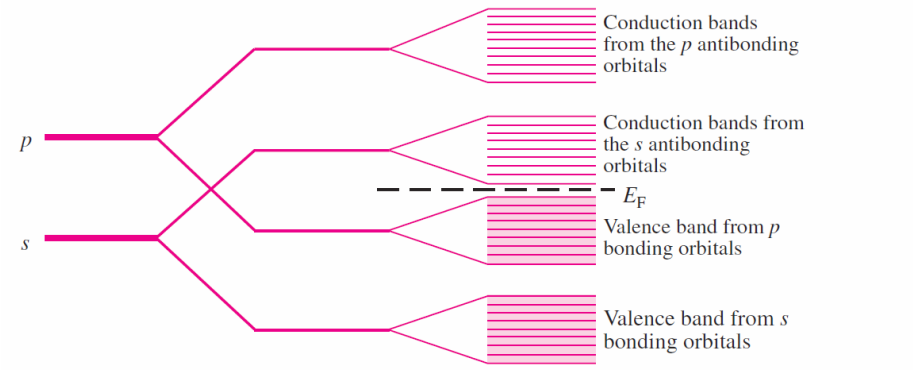



**Fig. 2.22.** Evolution of the atomic $s$ and $p$ orbitals into valence and conduction bands in a semiconductor. $E_F$ is the Fermi energy

**13. Tight binding, full calculation. Comparison with true bands and empty lattice approximation. From Yu & Cardona.** Note: "true bands" were done via a combination of another method and experimental input. Also, they call the empty lattice approximation both "free electron bands" (in figure) and "nearly free electron" model (in caption). That's not the same as what I called the "nearly free electron" model. (Yu & Cardona's name is not standard.)

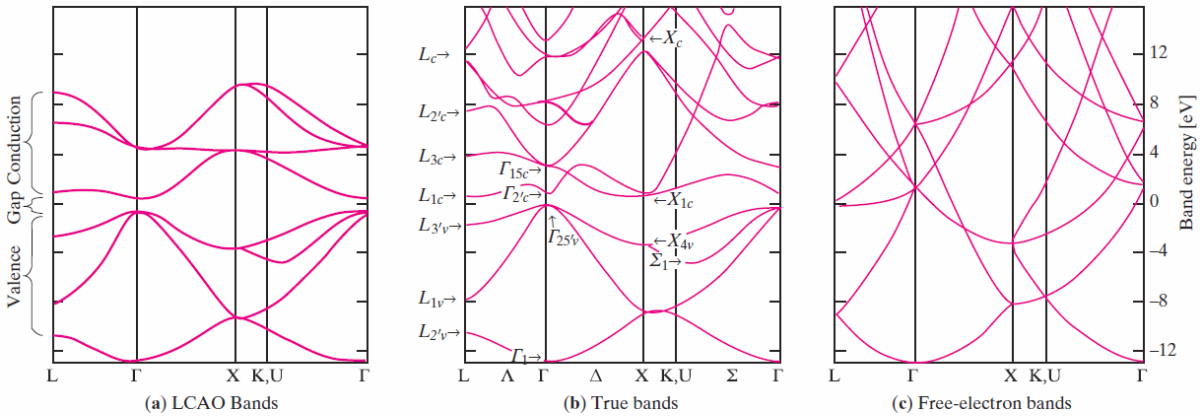



**Fig. 2.25.** A comparison between the band structure of Ge calculated by (**a**) the tight-binding method, (**b**) the empirical pseudopotential method, and (**c**) the nearly free electron model [Ref. 2.24, p. 79]