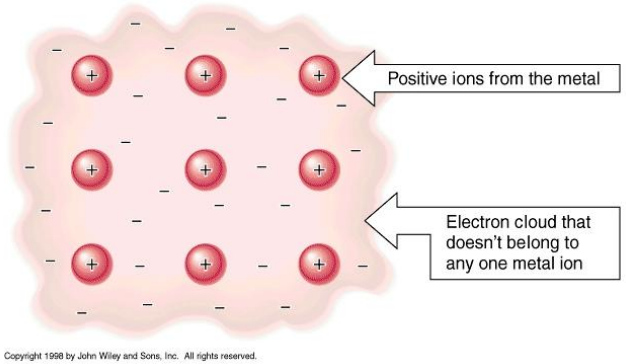
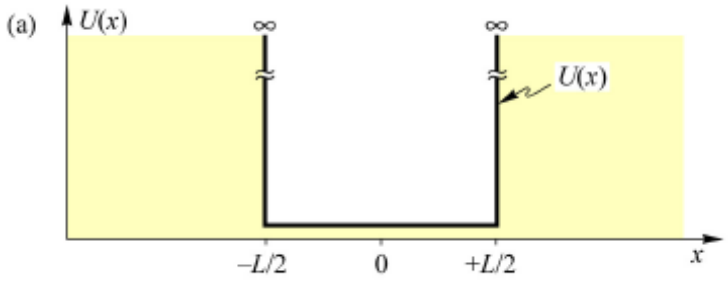
ECE 162B
January 24th - Lecture 6

Supplementary Notes: Band Theory of Solids 1

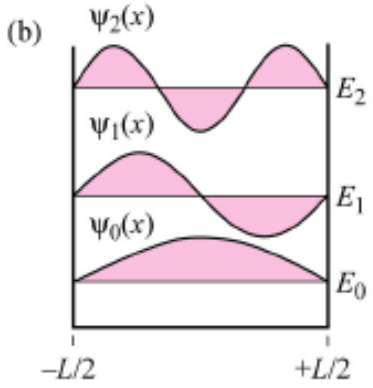
Free Electron Model

1. Atoms contribute valence electrons which are completely free and bound by the edges of the material
2. Electrons have no interaction with the lattice
3. Electrons are described by wave functions
4. Electrons obey the Pauli exclusion





$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi = E\psi$$



$$\psi(\vec{r}) = A\,e^{i\vec{k}\cdot\vec{r}}$$

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

Density of States

- Density of States - describes the number of available states per unit energy per unit volume

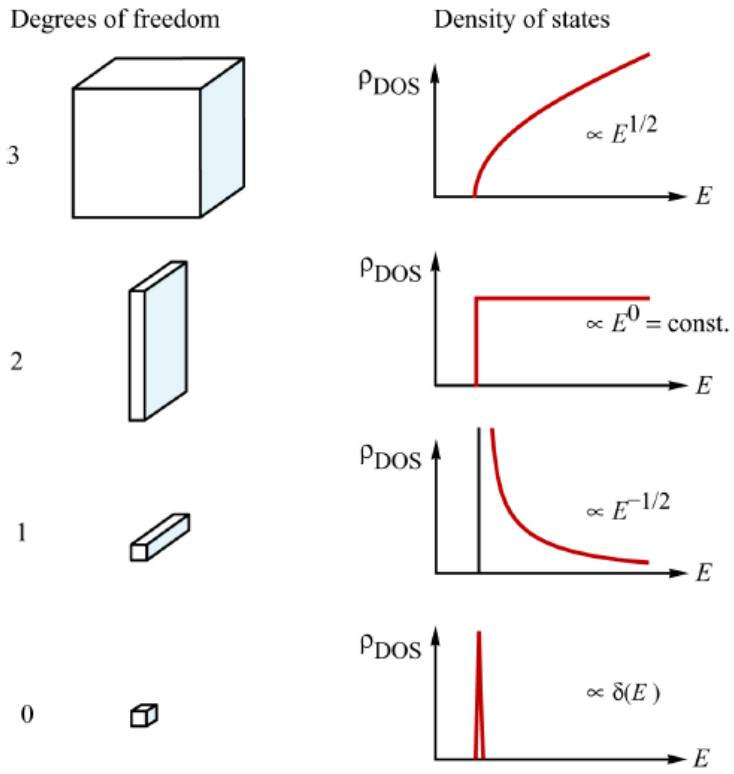


Fig. 12.7. Electronic density of states of semiconductors with 3, 2, 1, and 0 degrees of freedom for electron propagation. Systems with 2, 1, and 0 degrees of freedom are referred to as quantum wells, quantum wires, and quantum boxes, respectively.

Fermi–Dirac Distribution

- Fermi-Dirac Distribution - describes the probability that an available state is filled

$$f_{\mathrm{F}}(E) = \left[1 + \exp\left(\frac{E - E_{\mathrm{F}}}{kT}\right)\right]^{-1}$$

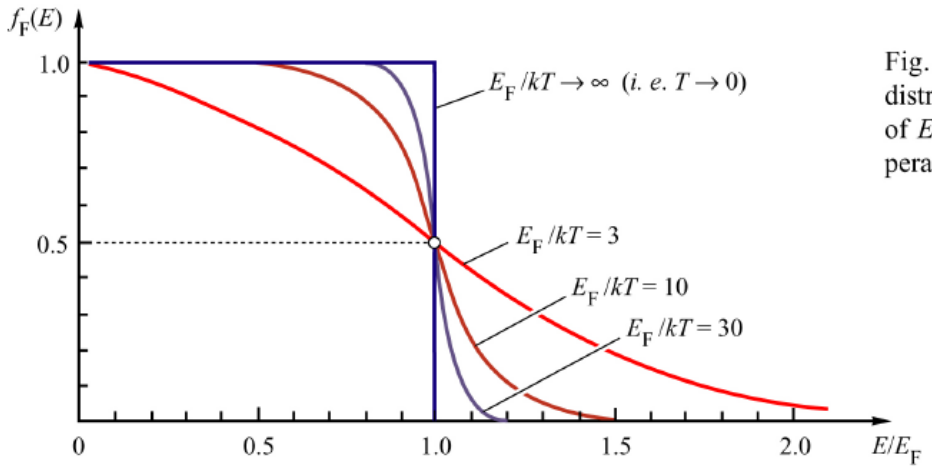


Fig. 13.4. Fermi–Dirac distribution as a function of E/E_{F} for different temperatures.

Free Electron Model Successes and Failures

- Insights:
  - Discrete set of energies (density of states)
  - Fermi-Dirac distribution
  - Heat capacity

- Fails to Describe:
  - Electrical conductivity
  - The distinction between metals, semimetals, semiconductors, and insulators
  - Positive values of Hall coefficient

$\Rightarrow$ Introduce interaction with lattice ions

Nearly Free Electron Model

Three common approaches:

1. Kronig-Penney Model – Solution to Schrodinger equation in a periodic potential
2. Ziman Model – Bragg reflection from the crystal lattice
3. Feynman Model – Energy splitting of atoms brought close to each other

Results:

- Allowed energy states are distributed in bands
- Structure of allowed energy bands distinguishes between metals, semimetals, insulators, and semiconductors
- Electrons exhibit an effective mass, m*
- Electrons can behave as if they have positive or negative charges

Periodic Potential and Bloch's Theorem

- We need the solution to Schrodinger equation in a periodic potential
- Assumption: wave functions will not deviate significantly from those of the free electron model (slightly perturbation)

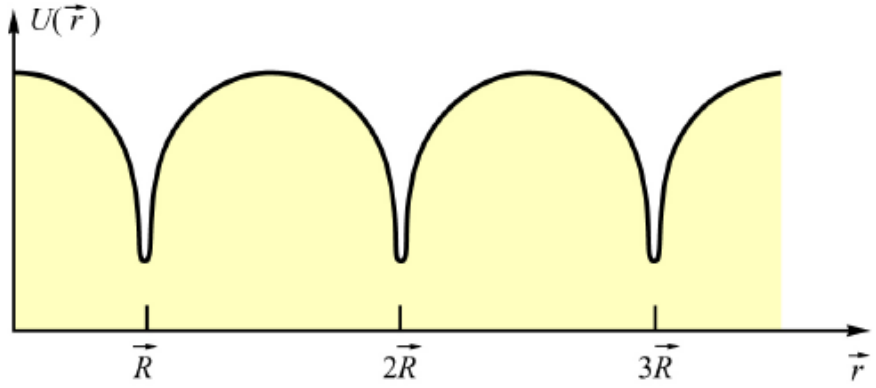


Fig. 8.1 Schematic illustration of a one-dimensional periodic potential caused by equally spaced atoms in a crystal lattice. The potential is periodic with period $\vec{R}$, that is $U(\vec{r}) = U(\vec{r} + \vec{R})$.

- Bloch showed the wave functions are of the form:

$$\psi_{nk}(\vec{r}) = u_{nk}\, e^{i\vec{k}\cdot\vec{r}}$$

$$u_{nk}(\vec{r}) = u_{nk}(\vec{r} + \vec{R}) = u_{nk}(\vec{r} + 2\vec{R}) = \cdots$$

Kronig-Penney Model

- Simplified 1-D periodic potential consisting of finite potential wells will yield:
  - allowed energy bands
  - forbidden energy gaps
  - dispersion relation

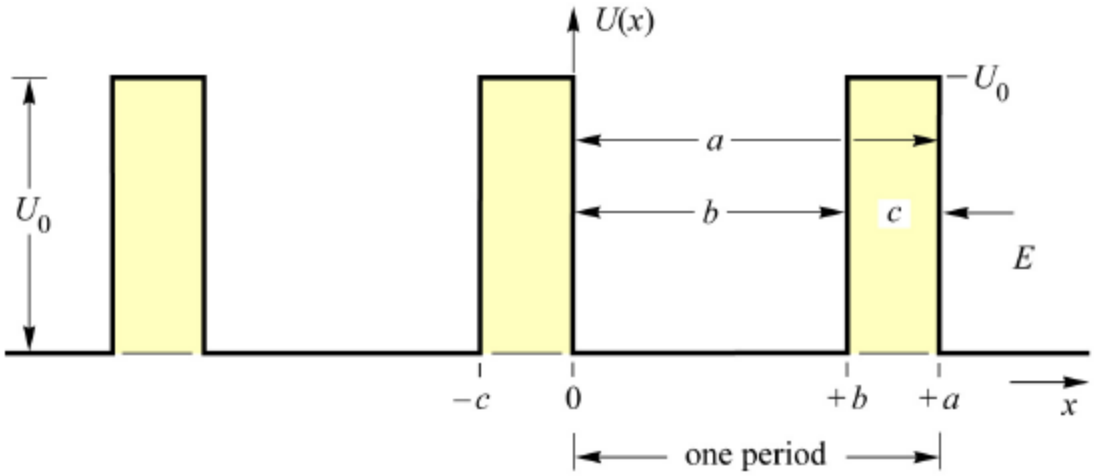


Fig. 8.2. Periodic square well potential used for the Kronig-Penney calculation. The height of the barriers is U_0 and the electron energy is denoted as E.

- See class notes for outline of solution to Schrodinger equation with this potential

Result: Band Structure of 1-D Lattice

Condition arising from solution to Schrodinger equation:

$$\frac{\beta^2 - \alpha^2}{2\,\alpha\,\beta}\sinh(\beta\,c)\,\sin(\alpha\,b) + \cosh(\beta\,c)\,\cos(\alpha\,b) = \cos(k\,a)$$

$$\alpha^2 = 2\,m\,E/\hbar^2 \qquad \beta^2 = 2\,m\,(U_0 - E)/\hbar^2$$

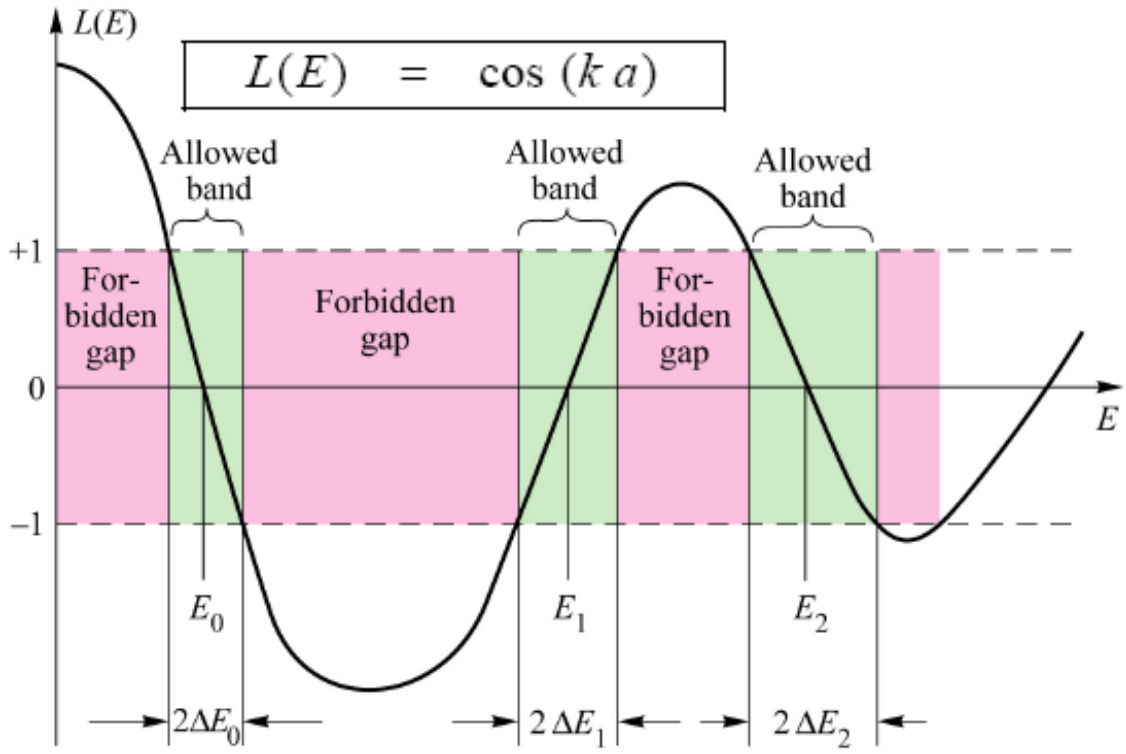


Fig. 8.3 Band structure of a one-dimensional lattice. The function $L(E)$ defines the allowed bands and the forbidden gaps of the lattice. The allowed bands have a center energy of E_n and an energetic width of $2\Delta E_n$. With increasing energy the allowed bands become wider and the forbidden gaps narrower.

E vs. k - Dispersion Relation

- Kronig-Penney model also yields the dispersion relation (see class notes)

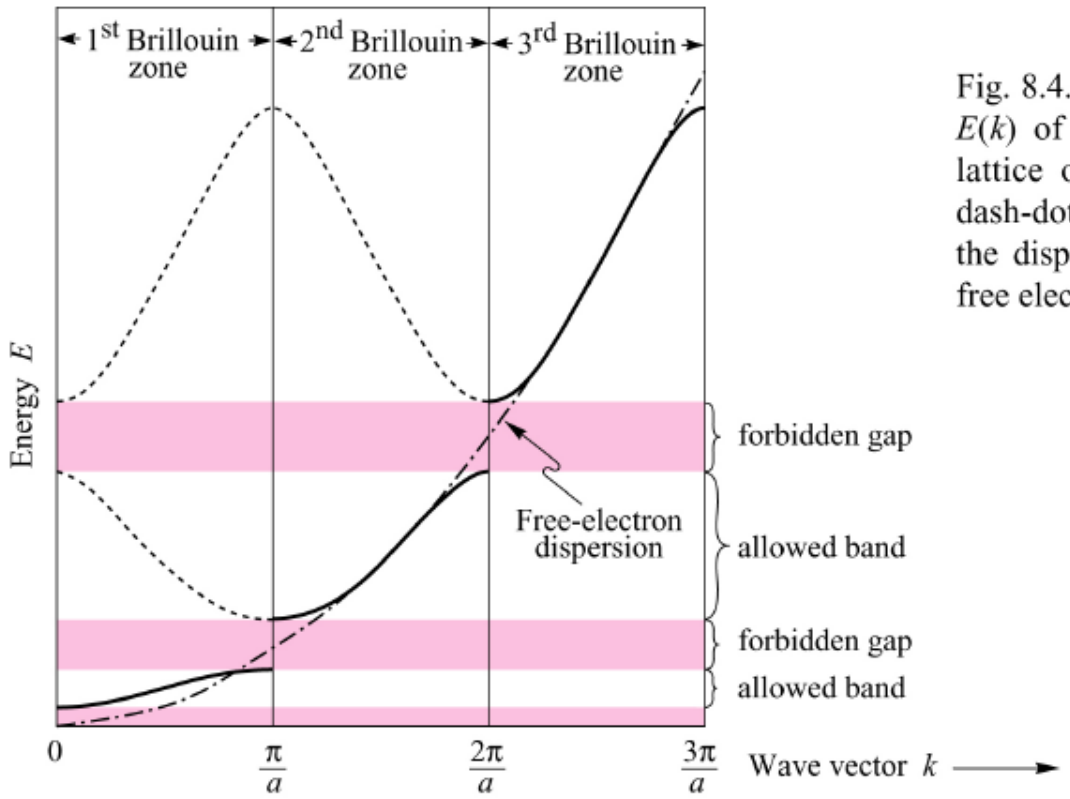
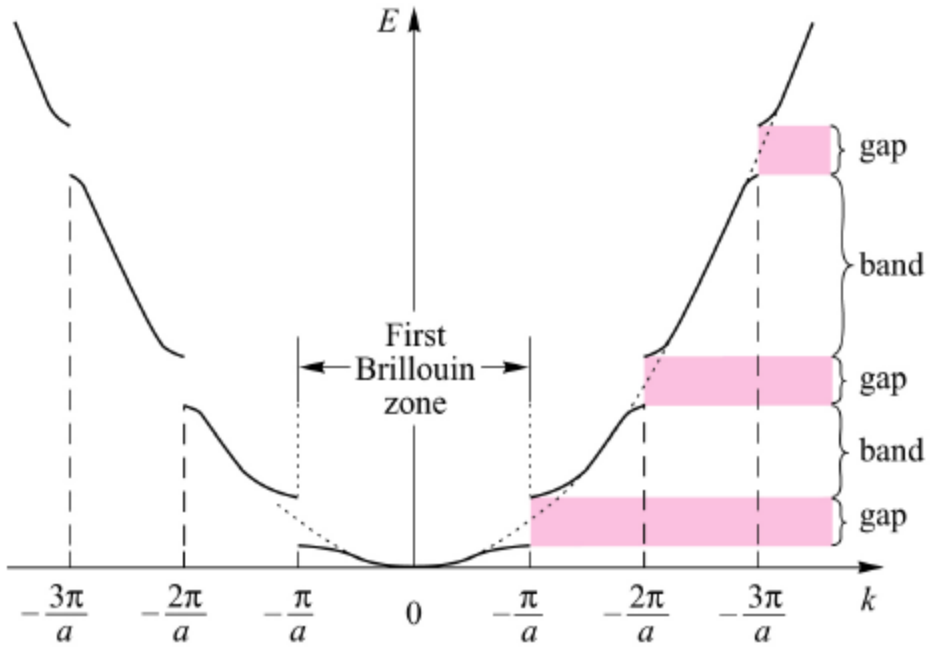


Fig. 8.4. Dispersion relation $E(k)$ of a one-dimensional lattice of a period a. The dash-dotted line represents the dispersion relation of a free electron.

E vs. k - Dispersion Relation

- Significant deviations from the free electron parabolic curve only exist at Brillouin zone boundaries



$$2a = n\lambda$$ Bragg condition!

Semiconductor Band Structure

- 3-D: dispersion relation depends on propagation direction since the atomic structure and hence the periodic potential depend on the electron propagation direction

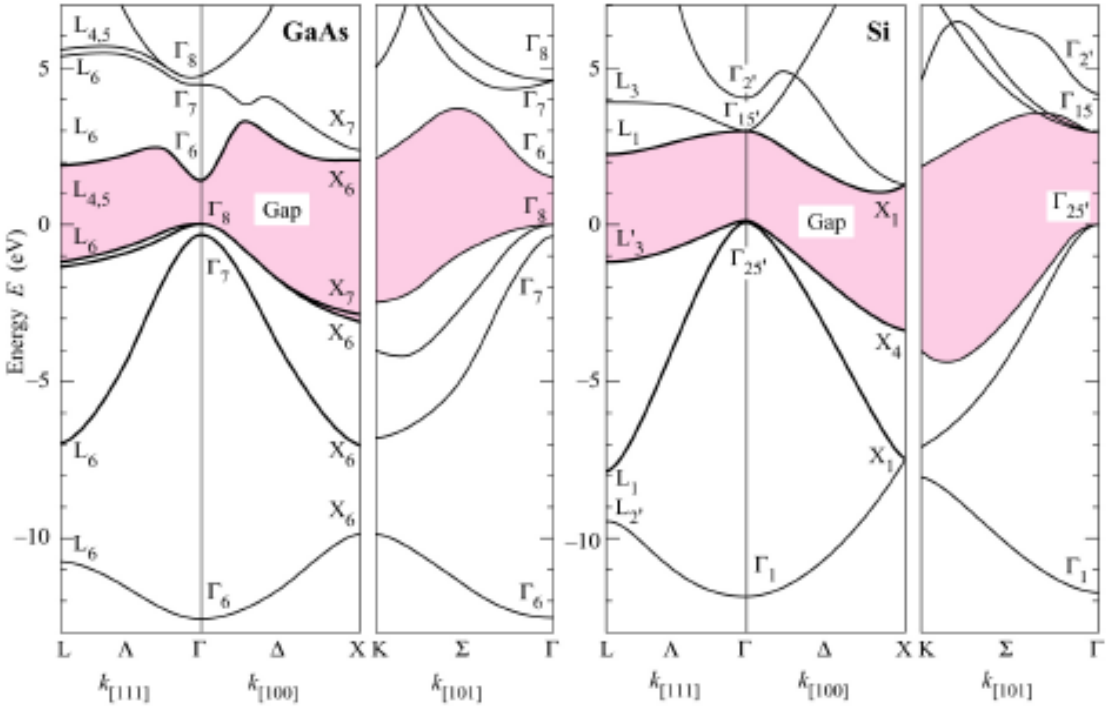


Fig. 8.6 Dispersion relation (band structure) for electrons and holes in the conduction and valence band within the first Brillouin zone for GaAs and Si.

Energy Gap vs. Lattice Constant

- In general, as bond length gets smaller the energy gap increases