

Outline

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1. Central Equation for Periodic Systems

In general, for a periodic potential

$$V(x) = \sum_G V_G e^{iGx}$$

the Schrödinger equation becomes the following Central Equation

$$\frac{\hbar^2}{2m} k^2 C_k + \sum_G V_G C_{k-G} = E C_k$$

This is really a set of infinite equations for every possible shift in the index k . Practically this means solving an eigenvalue problem for a large $n \times n$ matrix.

The larger we make this matrix, the more precise our calculations will be.

E.g.

Consider the following periodic potential with lattice constant a :

$$V(x) = 2W \cos\left(\frac{4\pi x}{a}\right)$$

Draw the first three bands using a 1X1, 2X2, and 3X3 matrix approximation.

Rewriting $V(x) = 2W \cos\left(\frac{4\pi x}{a}\right) = W(e^{i2gx} + e^{-i2gx})$

where $g = \frac{2\pi}{a}$

For a 1X1 approximation:

$$\frac{\hbar^2}{2m} k^2 C_k = E C_k$$

This just says

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

For a 2X2 approximation:

$$\begin{bmatrix} \frac{\hbar^2}{2m} k^2 & 0 \\ 0 & \frac{\hbar^2}{2m} (k+G)^2 \end{bmatrix} \begin{bmatrix} C_k \\ C_{k+G} \end{bmatrix} = E \begin{bmatrix} C_k \\ C_{k+G} \end{bmatrix}$$

$$\det \begin{vmatrix} \frac{\hbar^2}{2m} k^2 - E & 0 \\ 0 & \frac{\hbar^2}{2m} (k+G)^2 - E \end{vmatrix} = 0$$

$$\left(\frac{\hbar^2}{2m} k^2 - E\right) \left(\frac{\hbar^2}{2m} (k+G)^2 - E\right) = 0$$

$$E(k) = \frac{\hbar^2}{2m} k^2 \text{ or } E(k) = \frac{\hbar^2}{2m} (k + G)^2$$

For a 3X3 approximation:

$$\begin{bmatrix} \frac{\hbar^2}{2m} (k - G)^2 & 0 & W \\ 0 & \frac{\hbar^2}{2m} k^2 & 0 \\ W & 0 & \frac{\hbar^2}{2m} (k + G)^2 \end{bmatrix} \begin{bmatrix} C_{k-G} \\ C_k \\ C_{k+G} \end{bmatrix} = E \begin{bmatrix} C_{k-G} \\ C_k \\ C_{k+G} \end{bmatrix}$$

$$\det \begin{vmatrix} \frac{\hbar^2}{2m} (k - G)^2 - E & 0 & W \\ 0 & \frac{\hbar^2}{2m} k^2 - E & 0 \\ W & 0 & \frac{\hbar^2}{2m} (k + G)^2 - E \end{vmatrix} = 0$$

$$\left(\frac{\hbar^2}{2m} (k - G)^2 - E \right) \left(\frac{\hbar^2}{2m} k^2 - E \right) \left(\frac{\hbar^2}{2m} (k + G)^2 - E \right) - W^2 \left(\frac{\hbar^2}{2m} k^2 - E \right) = 0$$

An obvious eigenvalue is

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

This again is just the free electron energy bands.

Expanding and solving for the other eigenenergies:

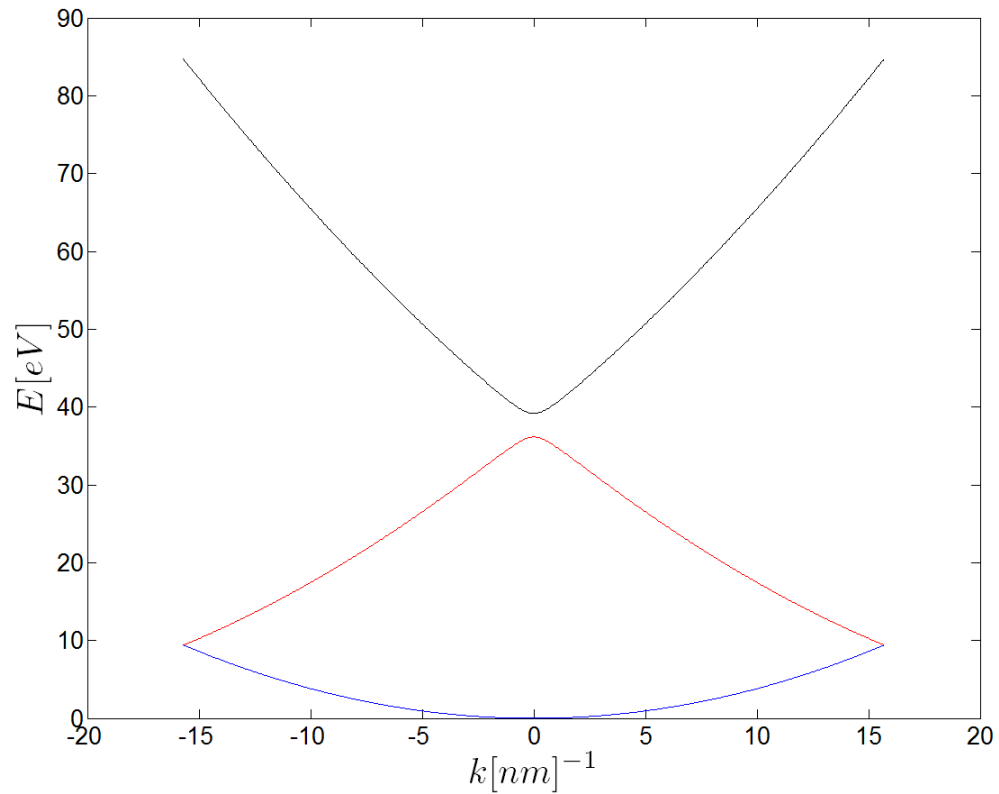
$$\left(\left(\frac{\hbar^2}{2m} \right)^2 (k + G)^2 (k - G)^2 - E \frac{\hbar^2}{2m} ((k + G)^2 + (k - G)^2) + E^2 - W^2 \right) = 0$$

$$\left(\left(\frac{\hbar^2}{2m} \right)^2 (k^2 - G^2)^2 - W^2 - E \frac{\hbar^2}{2m} 2(k^2 + G^2) + E^2 \right) = 0$$

Using the quadratic formula:

$$E = \frac{\hbar^2}{2m} (k^2 + G^2) \pm \sqrt{\left(\frac{\hbar^2}{2m} (k^2 + G^2) \right)^2 - \left(\left(\frac{\hbar^2}{2m} \right)^2 (k^2 - G^2)^2 - W^2 \right)}$$

Plotting this as a function of k with $a = 0.2$ nm and $W = 1.5$ eV along with the lower band for the other eigenenergy.



2. Band Diagrams

a. General Properties

In general, band diagrams are plots of the energy of the electron versus k , where k is the reciprocal space wave number. Since bands are periodic, they are plotted within the first Brillouin zone $-\pi/a$ to π/a . Each band represents an increase in the electron's energy, with the difference in the bands representing the minimum energy required for an electron to be excited to that higher band state. The electron has two important properties at a given point on the band diagram.

Group Velocity

$$\vec{v}_g = \frac{1}{\hbar} \vec{\nabla}_k E$$

Effective Mass

$$m_e^* = \frac{\hbar^2}{\frac{\partial^2 E_c}{\partial k^2}}$$

b. Material Examples

Ge	$E_g = 0.66$ eV (indirect)
GaAs	$E_g = 1.43$ eV (direct)
Si	$E_g = 1.14$ eV (indirect)
GaN	$E_g = 3.4$ eV (direct)
Diamond	$E_g = 5.4$ eV (indirect)

Note that indirect band gaps require a coupling of a phonon transfer in addition to a photon for an electron transition to an excited state to occur if the energy of the photon is less than the direct band gap but greater than the indirect band gap.

c. Born-Von Karman Boundary Conditions

Considering a periodic system to behave as an infinite lattice, one can equivocally consider the first atom of the lattice interacting periodically with the last atom of the finite chain with length L . This results in the following considering Bloch theorem:

$$\begin{aligned}u_k(x + R) &= e^{ikR}u_k(x) \\u_k(x + L) &= u_k(x) = e^{ikL}u_k(x) \\e^{ikL} &= 1 \\k &= \frac{2\pi}{L}n\end{aligned}$$

This means the total number of states in the system (considering spin) is as follows:

$$N = 2 \frac{\text{Length of Entire Brillouin Zone}}{\text{Length of Between Two Atoms}} = 2 \frac{\left(\frac{2\pi}{a}\right)}{\left(\frac{2\pi}{L}\right)} = 2 \frac{L}{a}$$

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3.024 Electronic, Optical and Magnetic Properties of Materials
Spring 2013

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