



Lecture 8

Reading Material



Reading:

Finish Chapter 7 Solymar and Walsh

The Ziman Model

- Assuming the same potential as in the Kronig-Penney Model with $2w=a$

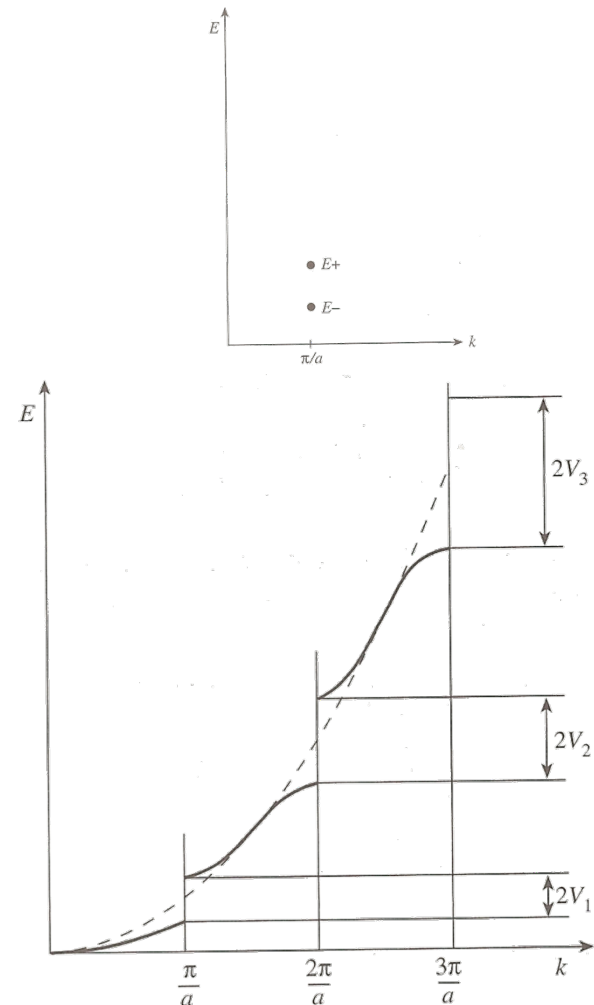
$$\begin{aligned}
 V_{\pm} &= \frac{1}{a} \int_0^a \begin{pmatrix} 2\cos^2 kx \\ 2\sin^2 kx \end{pmatrix} V(x) dx \\
 &= \frac{1}{a} \int_0^a \begin{pmatrix} 1 + \cos 2kx \\ 1 - \cos 2kx \end{pmatrix} V(x) dx \\
 &= \pm \frac{1}{a} \int_0^a \cos 2kx V(x) dx \\
 &= \pm V_n
 \end{aligned}$$

- The kinetic energies of the wave functions are the same and the total energy is the sum of the kinetic and potential energies

$$E_{\pm} = \frac{\hbar^2 k^2}{2m} \pm V_n$$

$$E_{+} = \frac{\hbar^2 k^2}{2m} + V_1$$

$$E_{-} = \frac{\hbar^2 k^2}{2m} - V$$



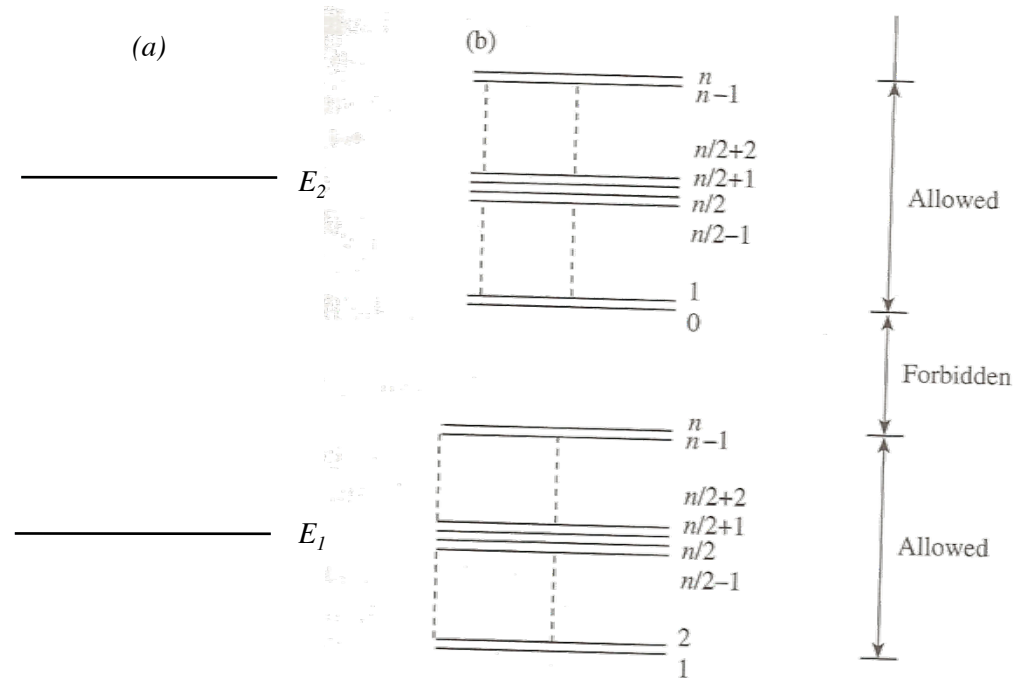
The Feynman Model



- Combines mathematical and physical pictures
- Draws on the coupled mode approach to describe covalent bonds
- Recall that we saw for two interacting atoms, that the energy level splits into two levels, one below the independent atom energy level and one above the independent atom energy level.
- What happens when we bring a collection (possible many) of atoms together?

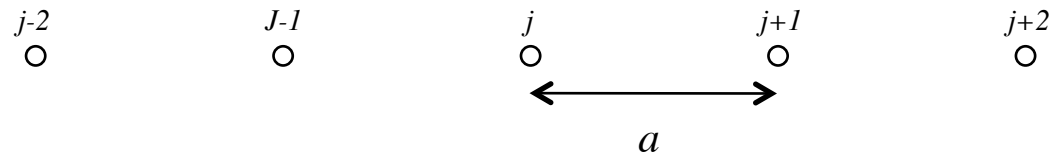
The Feynman Model

- We could expect that extending the model from two interacting atoms to n interacting atoms, that the energy levels would split n -times
- Figure (a) to the right shows the discrete energy levels, E_1 and E_2 , for each of n atoms far apart from each other (non-interacting)
- As the atoms are brought within interaction distance of each other, the energy levels split as shown in (b)
- We refer to the grouping of allowed energy levels as “Bands” and the forbidden energy levels as “Gaps”



The Feynman Model

- Consider a one-dimensional array of atoms, separated by lattice constant a , with atom j by default in energy state level E_1 .



- Consider only electron interaction between neighboring atoms
 - The electron from atom j has a finite probability of jumping to either atom $j+1$ or atom $j-1$ as we saw from our example with two nuclei and one shared electron.
- The coupled differential equation for atom j with the nearest neighbor assumption can be written as we did in the two atom case using the uncoupled energy E_1 and coupling coefficient (assuming symmetry) A

$$i\hbar \frac{d\omega_j}{dt} = E_1 \omega_j - A \omega_{j-1} - A \omega_{j+1}$$

The Feynman Model

- Assuming a time varying solution for ω_j of the form $\omega_j = K_j e^{-iEt/\hbar}$ we can rewrite the coupled DE for atom j as

$$EK_j = E_1 K_j - A(K_{j-1} + K_{j+1})$$

- Writing the amplitude as a function of their lattice position (x-coordinate) we end up with the difference equation

$$EK(x_j) = E_1 K(x_j) - A(K(x_j + a) + K(x_j - a))$$

- Solving the difference equation assuming the solution $K(x_j) = e^{ikx_j}$ results in E

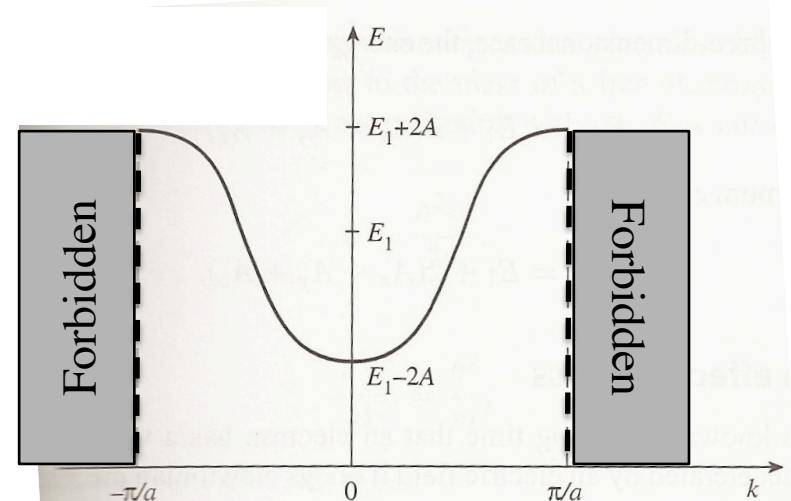
$$Ee^{ikx_j} = E_1 e^{ikx_j} - A(e^{ik(x_j+a)} + e^{ik(x_j-a)})$$

$$= E_1 e^{ikx_j} - Ae^{ikx_j} (e^{ika} + e^{-ika})$$

$$= e^{ikx_j} (E_1 - A(e^{ika} + e^{-ika}))$$

$$E = (E_1 - A(e^{ika} + e^{-ika}))$$

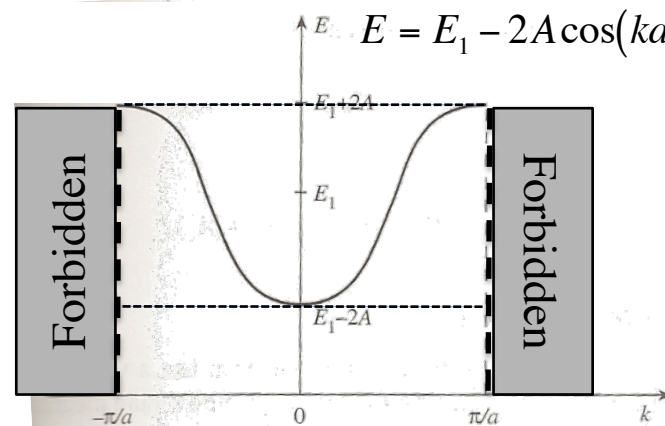
$$E = E_1 - 2A \cos(ka)$$



The Feynman Model

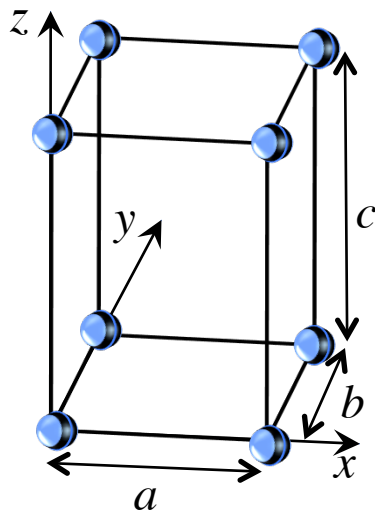
- Notice that we still see the property of allowed energy bands (between E_1+2A and E_1-2A) and forbidden bands outside this range. The energy band now take on the E vs. k shape of a sinusoid which looks like a parabolic function around the minimum point.
- Remember that there are still other energy bands as we have seen in the other models. We can obtain these relationships simply by replacing the index for the isolated atom

$$E = E_1 - 2A \cos(ka)$$



3D Extension of The Feynman Model

- We can simply extend the Feynman Model to three dimensions (not as easily done for the other models we looked at)



$$i\hbar \frac{\partial \omega(x, y, z, t)}{\partial t} = E_1 \omega(x, y, z, t) \\ - A_x \omega(x + a, y, z, t) - A_x \omega(x - a, y, z, t) \\ - A_y \omega(x, y + b, z, t) - A_y \omega(x, y - b, z, t) \\ - A_z \omega(x, y, z + c, t) - A_z \omega(x, y, z - c, t)$$

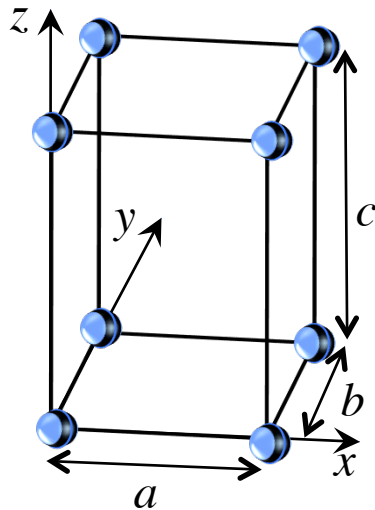
- With solution

$$\omega(x, y, z, t) = e^{-iEt/\hbar} e^{i[k_x x + k_y y + k_z z]}$$

$$E = E_1 - 2A_x \cos(k_x a) - 2A_y \cos(k_y b) - 2A_z \cos(k_z c)$$

3D Extension of The Feynman Model

- This yields the minimum and maximum energy bands in 3-dimensions to be



$$E = E_1 - 2A_x \cos(k_x a) - 2A_y \cos(k_y b) - 2A_z \cos(k_z c)$$

$$E_{\min} = E_1 - 2(A_x + A_y + A_z)$$

$$E_{\max} = E_1 + 2(A_x + A_y + A_z)$$

Effective Mass



- We know that the electron has a defined mass in a vacuum
- What happens to the electron mass in a crystal? It can't be the same because of interaction with field potentials and other atoms and particles
- We call this mass inside a specific crystalline structure (in a direction of motion) the “*effective mass*”

Effective Mass

- Using the quantum mechanical model for the velocity of the electron (which depends on the actual E vs. k curve)

$$v_g = \frac{1}{\hbar} \frac{\partial E}{\partial k}$$

- The classical work done by a particle traveling in an applied force qF_e a distance $v_g dt$ is

$$dE = qF_e v_g dt = qF_e \frac{1}{\hbar} \frac{\partial E}{\partial k} dt$$

- The acceleration of the particle is given by

$$a = \frac{dv_g}{dt} = \frac{1}{\hbar} \frac{d}{dt} \left(\frac{\partial E}{\partial k} \right) = \frac{1}{\hbar} \frac{d^2 E}{dt^2} \frac{dk}{dt}$$

Effective Mass

- Solving for dk/dt

$$dE = qF_e \frac{1}{\hbar} \frac{\partial E}{\partial k} dt$$

$$\frac{dk}{dt} = \frac{qF_e}{\hbar}$$

- And inserting into the equation for acceleration

$$\begin{aligned} \frac{dv_g}{dt} &= \frac{1}{\hbar} \frac{d^2 E}{dt^2} \frac{dk}{dt} = \frac{1}{\hbar} \frac{d^2 E}{dt^2} \frac{qF_e}{\hbar} \\ &= \frac{qF_e}{\hbar^2} \frac{d^2 E}{dt^2} \end{aligned}$$

Effective Mass



- Comparing the last result with the classical form of acceleration for a free particle

$$\frac{m dv}{dt} q F_e$$

- We can now define the effective mass

$$m^* \frac{dv}{dt} = m^* \frac{q F_e}{\hbar^2} \frac{d^2 E}{dt^2}$$

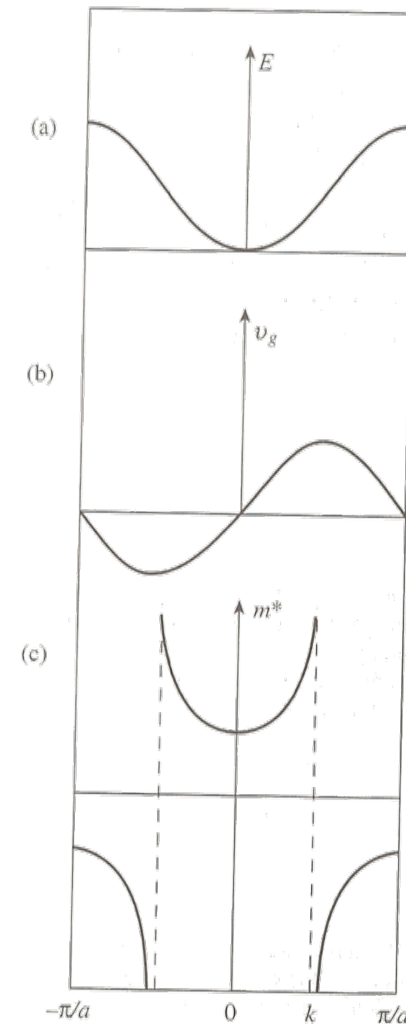
$$m^* = \hbar^2 \left(\frac{\partial^2 E}{\partial k^2} \right)^{-1}$$

Effective Mass

- In a one dimensional lattice, the effective mass can be written as

$$\begin{aligned}
 m^* &= \hbar^2 \left(\frac{\partial^2 E}{\partial k^2} \right)^{-1} \\
 &= \hbar^2 \left(\frac{\partial^2 (E_1 - 2A \cos(ka))}{\partial k^2} \right)^{-1} \\
 &= \frac{\hbar^2}{2Aa^2} \sec(ka)
 \end{aligned}$$

- Plots of E vs. v_g and m^* are shown to the right. Note that as an electron is moved from rest to higher and higher velocities its mass increases, reaching infinite mass at $k=\pi/2a$



Effective Mass

- For a 3D crystal, we can extend these results to propagation in x, y or z

$$\begin{pmatrix} m_x^* \\ m_y^* \\ m_z^* \end{pmatrix} = \begin{pmatrix} \frac{\hbar^2}{2A_x a^2} \sec(k_x a) \\ \frac{\hbar^2}{2A_y a^2} \sec(k_y b) \\ \frac{\hbar^2}{2A_z a^2} \sec(k_z c) \end{pmatrix}$$

- An even in arbitrary directions, e.g. the xy plane

$$m_{xy}^* = \hbar^2 \left(\frac{\partial^2 E}{\partial k_x \partial k_y} \right)^{-1}$$