Lecture 7

Reading Material

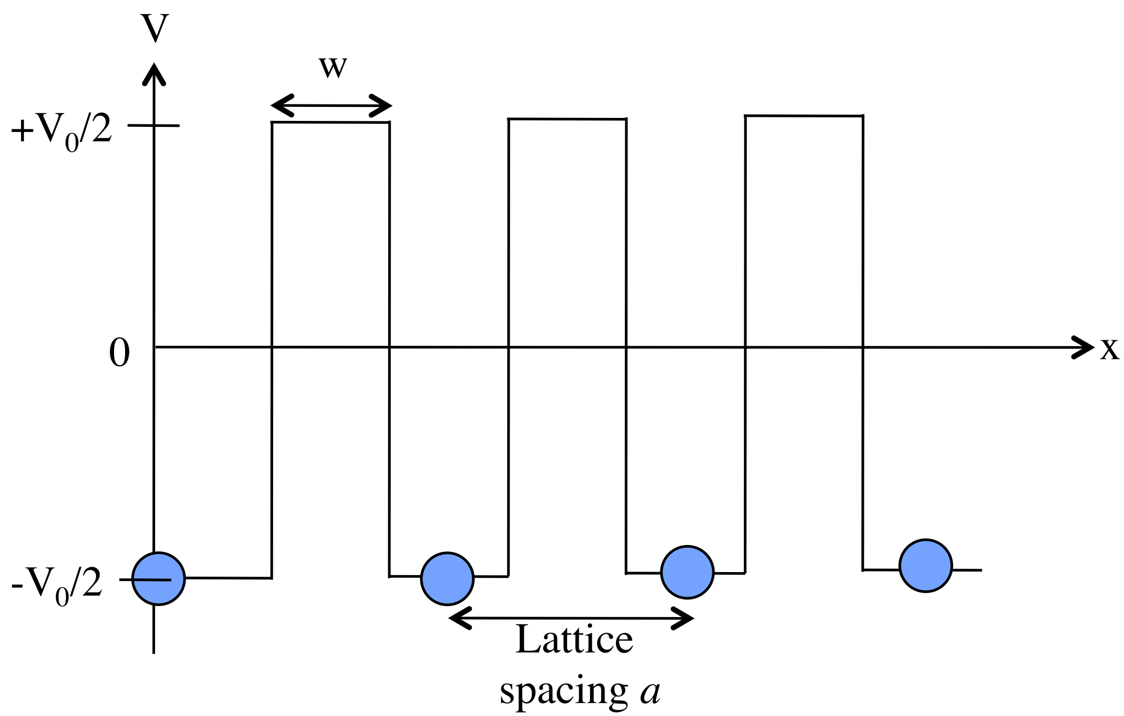
Reading:

Finish Chapter 6 Solymar and Walsh

Chapter 7 Solymar and Walsh

The Kronig-Penney Model

- Consider first the one dimensional case which has the following features
  - The potential has the same period as the lattice
  - The potential is lower near the lattice ions and higher in between the lattice ions.



The Kronig-Penney Model

- Now consider the time dependent Schrodinger equation and lets insert our model for the potential as a function of x (for the one dimensional case)

$$\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\left[E-V(x)\right]\psi=0$$

- Solving for the two cases $V(x) = +V_0/2$ and $V(x) = -V_0/2$ separately (piecewise linear) and matching the solutions at the boundaries (continuity), assume the wave-functions have the form (called a Bloch mode which we will look at later)

$$\psi_k = u_k(x)e^{ikx}$$

- Next lecture we will solve this solution and look at the Ziman and Feynman models and introduce the effective mass.

The Kronig-Penney Model

- A solution to the TISE (Time Independent Schrodinger Equation) if momentum (k) and energy (E) satisfy the following equality

$$\cos(ka) = P\frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a)$$

$$P = \frac{ma}{\hbar^2}V_0\omega$$

$$\alpha = \frac{1}{\hbar}\sqrt{2mE}$$

- We will see that P and alpha has physical interpretations

The Kronig-Penney Model

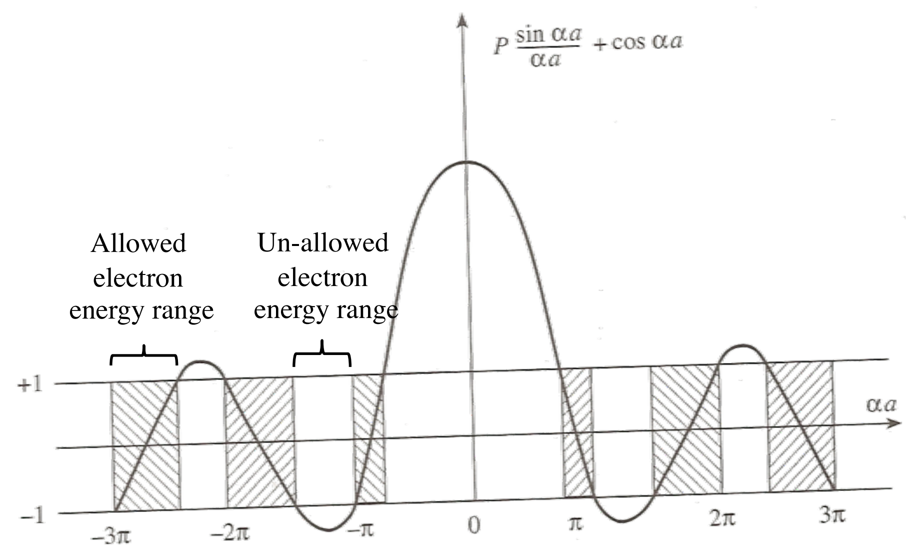
- If we plot the right side as a function of αa

$$P\frac{\sin(\alpha a)}{\alpha a}+\cos(\alpha a)$$

- We see that it is periodic and the height of the main and side lobes are a function of P
- The left hand side of the equation oscillates between +1 and -1 as a function of αa

$$\cos(ka)$$

- The equality is satisfied in the shaded regions in the picture to the right.
- The important result is that the shaded regions are discrete and there are regions where the left and right hand sides are not equal
  - Shaded regions are where electrons may have energy
  - Un-shaded regions are where electrons may not have energy
  - Shaded regions are the allowed energy bands
  - Un-shaded regions are the forbidden energy bands



The Kronig-Penney Model

- Note that as we vary P, the height and therefore the slopes of the oscillating curve change.
- As P is increased the slope of the right hand side increases within the [-1,+1] region and the forbidden bands increase width and allowed bands decrease in width
- Lets look at some limits in P to understand its physical significance
  - (i) $P \to \infty$

    $$\sin(\alpha a) \to 0$$

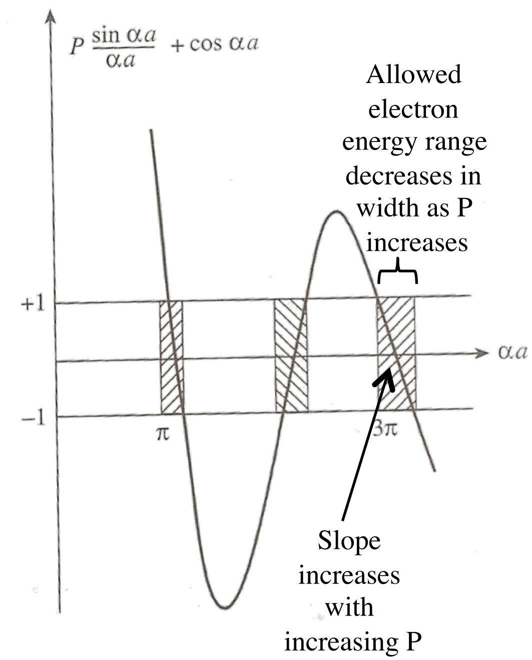
    $$E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2$$

    Which is the energy level of a potential well of width a. P is like the height of the potential barrier, infinite in this case, and each electron is confined independent to each other
  - (ii) $P \to 0$

    $$\cos(\alpha a) = \cos(ka)$$

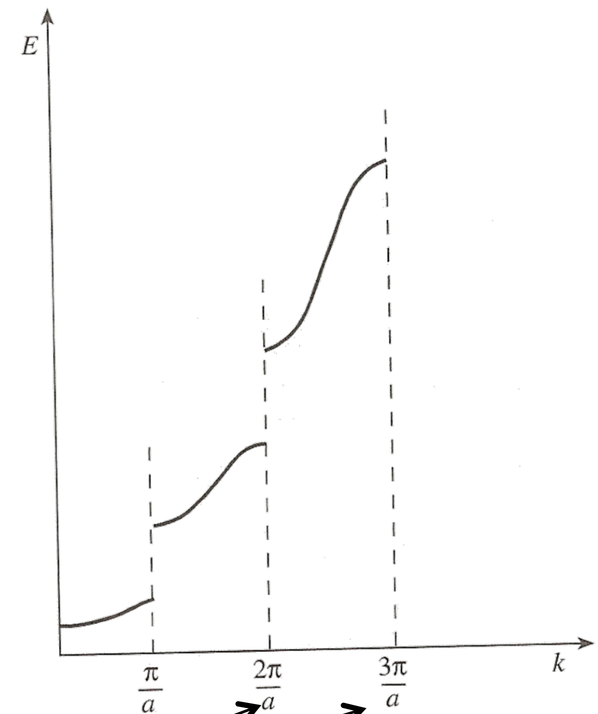
    $$E = \frac{\pi^2 \hbar^2}{2m}$$

    Which is the energy level of a free electron. P is then indicative of a zero height barrier and the electrons are not confined.



The Kronig-Penney Model

- At the boundary of each allowed band where cos(ka) = ±1, the momentum takes on discrete values and there is a discontinuity in energy at these boundaries as shown in the figure below.



$$k = \frac{n\pi}{a},\ n = 1,2,3\ldots$$

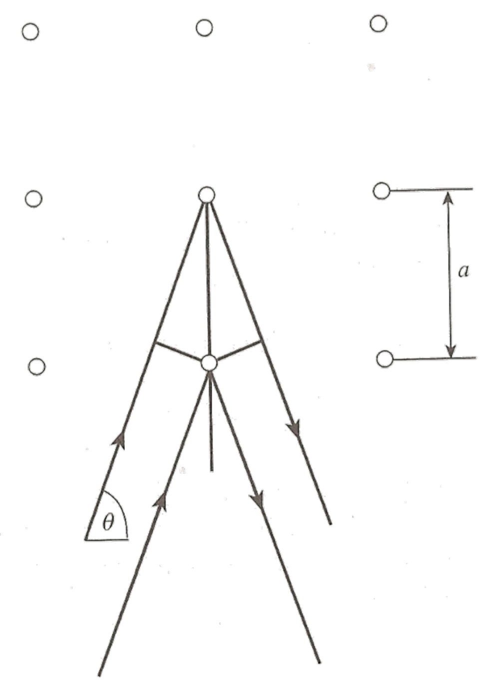
The Ziman Model

- Assume a lattice of ions, with period a, as show in the figure to the right and consider the wave aspect of the electron.
- We can model the electron as a ***propagating plane wave***. A plane wave by definition extends to infinity in all directions of equal phase and propagates in a direction normal to the plane of constant phase.
- A unity amplitude plane wave propagating in the x-direction with propagation constant k can be written as

$$\psi_k = e^{ikx}$$

- When the plane is incident on the lattice of ions (or any scattering structures), there are conditions of transmission and reflection that lead to ***constructive and destructive interference***.
- Bragg Reflection is the condition where the waves are incident at some angle θ, where the waves reflected off each row of the lattice add up constructively (in-phase) at the reflection angle θ such that for a wavelength λ (the electron wavelength in this case), the following condition holds

$$n\lambda = 2a\sin\theta,\ \text{n} = 1,2,3\ldots$$



The Ziman Model

- The electron wave being completely reflected by the lattice is the same thing as saying that the electron is not able (allowed) to propagate through the lattice, which is the same condition as having an energy in the forbidden energy band.
- The reflected wave function in the one dimensional case (x-direction) is written as

$$\psi_{-k} = e^{-ikx}$$

- And the total wave for the one dimensional case (easily extended to the 2D and 3D cases) is written as

$$\begin{aligned}\psi_{\pm k} &= \frac{1}{\sqrt{2}}\left(e^{ikx} \pm e^{-ikx}\right)\\ &= \sqrt{2}\begin{pmatrix}\cos kx\\ i\sin kx\end{pmatrix}\end{aligned}$$

- Electrons that have energies at this wave function can be found by integrating the the potential (*V(x)*), weighted by the wave function probability over space

$$\begin{aligned}V_{\pm} &= \frac{1}{L}\int \left|\psi_{\pm k}\right|^2 V(x)\,dx\\ &= \frac{1}{L}\int \begin{pmatrix}2\cos^2 kx\\ 2\sin^2 kx\end{pmatrix} V(x)\,dx\end{aligned}$$

The Ziman Model

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

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

$$= \frac{1}{a}\int_0^a \begin{pmatrix} 1+\cos 2kx \\ 1-\cos 2kx \end{pmatrix} V(x)\,dx$$

$$= \pm\frac{1}{a}\int_0^a \cos 2kx V(x)\,dx$$

$$= \pm V_n$$

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

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

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

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