ELEC4705 – Fall 2009

Tom Smy

LECTURE 7
Periodic Potentials

Contents

ELEC4705 – Fall 2009 1

Lecture 7. Periodic Potentials 1
7.1. 1D Crystal Potential 4
7.2. Kronig-Penny Model 8
7.3. Summery of Energies and Wavefunctions in Various Potentials 13

7.1. 1D Crystal Potential

In a crystal, electrons move in a potential $V(x)$ which is produced by regularly-spaced ion cores. A large number of materials are well described by regular atomic spacing and a periodic potential for a crystal lattice which is like a string of finite wells, as shown in figure 1 .

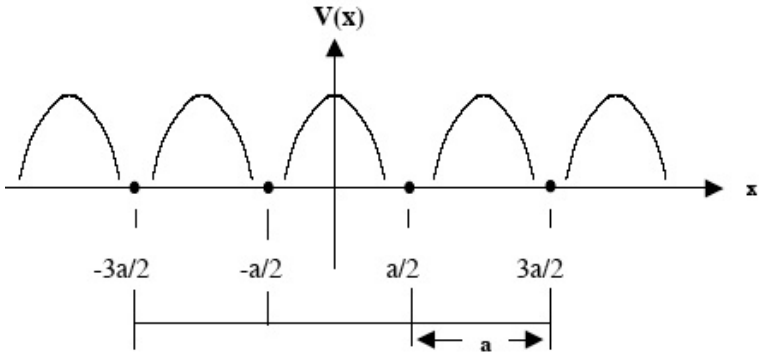

Figure 1. Crystal Potential a is the lattice constant

To analyze the electron behavior in such a crystal we need to solve the Schrodinger equation with a periodic $V(x)$ and obtain the wavefunction $\Psi(x)$. Due to periodic nature of $V(x)$, i.e. $V(x+a) = V(x)$ we are able to use the Fourier series techniques in which $V(x)$ is defined as a set of spatial frequencies G_n as below:

$$V(x) = \sum_{-\infty}^{\infty} V_G \, e^{jG_n x} \tag{7.1}$$

$$G_n = \frac{2\pi n}{a} \qquad n \; is \; an \; integer \tag{7.2}$$

$$V_G = \frac{1}{2\pi a} \int_0^a V(x) e^{-jG_n x} dx \tag{7.3}$$

Equation 7.1 is the complex Fourier representation of a periodic function.

The solution of a periodic version of a wave equation like the SCE is complicated, however, the basic formulation was worked out by Bloch and others. Using Bloch's theorem it can be shown the solution will be as the following form:

$$\Psi(x) = U(x) e^{ikx} \tag{7.4}$$

Where we have:

- A solution very similar to a plane wave for free electron.
- The primary difference is that in free electron case the amplitude is constant whereas with a periodic potential, the amplitude is a periodic function as well.

$$U(x+a) = U(x)$$

- The parameter k is again associated with the momentum of a quantum state in electron energy. A big difference is that it can be shown that unique k values lie only between $-\pi/a$ and π/a.
- $\Psi(k)$ is periodic over $2\pi/a$.

Now we will go over some special cases.

7.1.1. Free Electrons (V(x) = 0)

This is similar to what we solved before for a free electron, but we will force a periodic solution. The Bloch solution is as before a parabolic $E(k)$ as equation however the new solution is multivalued (Eq. 7.5) as is shown in figure 2.

$$E_k = \frac{\hbar^2(k+G_n)^2}{2m} \tag{7.5}$$

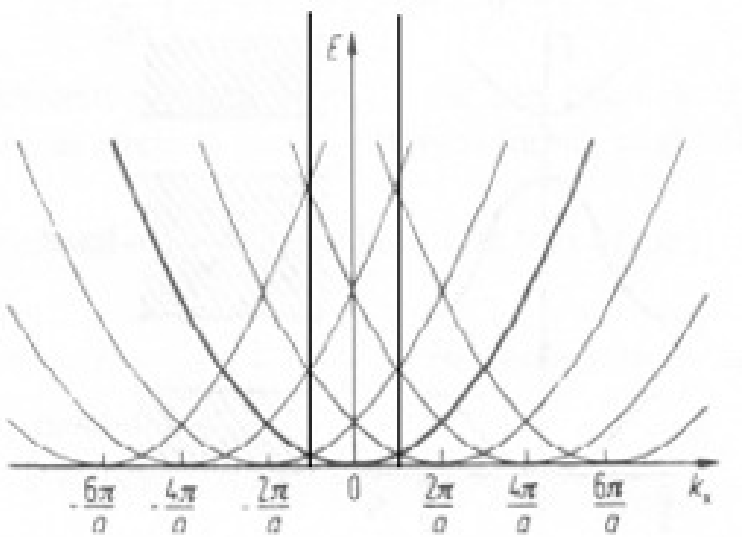

Figure 2. Parabolic energies for free electrons

In this solution there are set of solutions denoted by n where:

- Each n provides one parabola for $E(k)$.

- E is a periodic function of k with periodicity of $2\pi/a$.
- E is multi-valued function.
- E is unique only in the range $-\pi/a < k < \pi/a$

Due to the last point as shown in figure 3 we draw E only in region $-\pi/a < k < \pi/a$. This region is called 1^{st} *Brillouin zone* or if it is symmetrical (as in this case) only from 0 to π/a.

Periodic free electrons will therefore act very much like free electrons. One can form wave-packets form them and they will propagate in similar manner. However, the wavefunctions are limited to k values in the 1st Brillouin zone and we have multi allowed energies at a single momentum value.

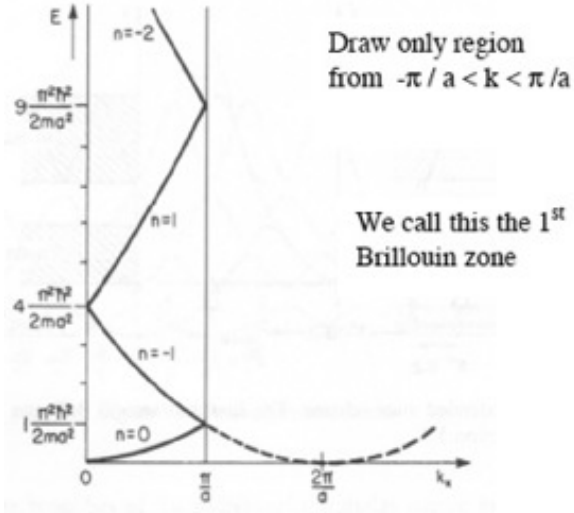

Figure 3. Energies in first brillouin zone

7.1.2. A Cosine Potential

The previous example was very artificial as the periodicity was forced – imposed mathematically but not physically present. A real situation has an actual periodic potential causing the perodicity in the wavefunction. A simple case when $V(x)$ is a cosine function as in figure 4 is a closer model for a crystal potential.

We have,

$$V(x) = 2V_0 \cos(\frac{2\pi x}{a}) = V_0 e^{2\pi jx/a} + V_0 e^{-2\pi jx/a} \tag{7.6}$$

It is difficult to generally solve the problem, but we can solve it for $k = \pi/a$ which is an edge of the brillouin zone. Suppose the wavefunction

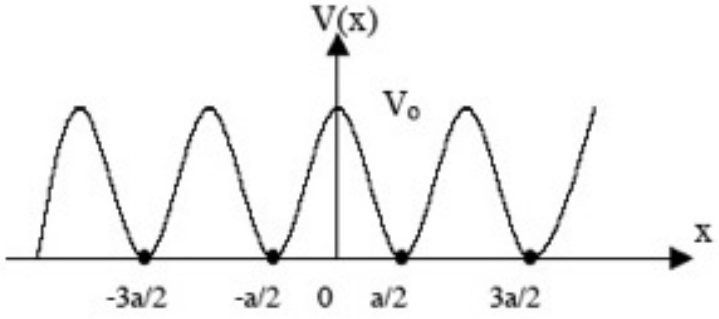

Figure 4. A Cosine Potential function

will be as:

$$\psi(x) = C_k e^{jkx} + C_{-k} e^{-jkx} = C_{\pi/a}\, e^{j\pi x/a} + C_{-\pi/a}\, e^{-j\pi x/a} \tag{7.7}$$

By substituting the wavefunction 7.7 in the Schrodinger equation we will have:

$$(\frac{\hbar^2\pi^2}{2ma^2} - E)C_{\pi/a} + V_0 C_{-\pi/a} = 0 \tag{7.8}$$

$$(\frac{\hbar^2\pi^2}{2ma^2} - E)C_{-\pi/a} + V_0 C_{\pi/a} = 0 \tag{7.9}$$

From equation 7.8 we have:

$$C_{-\pi/a} = -\frac{1}{V_0}(\frac{\hbar^2\pi^2}{2ma^2} - E)C_{\pi/a} \tag{7.10}$$

By substitution in equation 7.9 we get:

$$[-(\frac{\hbar^2\pi^2}{2ma^2} - E)^2\frac{1}{V_0} + V_0]C_{\pi/a} = 0 \tag{7.11}$$

Then to have $C_{\pi/a} \neq 0$ we must have $V_0^2 = (\frac{\hbar^2\pi^2}{2ma^2} - E)^2$ i.e.

$$E = \frac{\hbar^2\pi^2}{2ma^2} - V_0 \quad or \quad E = \frac{\hbar^2\pi^2}{2ma^2} + V_0 \tag{7.12}$$

So we see that for a cosine potential function, the energy levels split at the band edge ($k = \pi/a$) as is shown in figure 5. Away from the band edge the solution is close to parabolic and we have free electron like behavior.

> *Note: As a general principle, the presence of a periodic potential separates the electron energies into allowed bands separated by band gaps.*

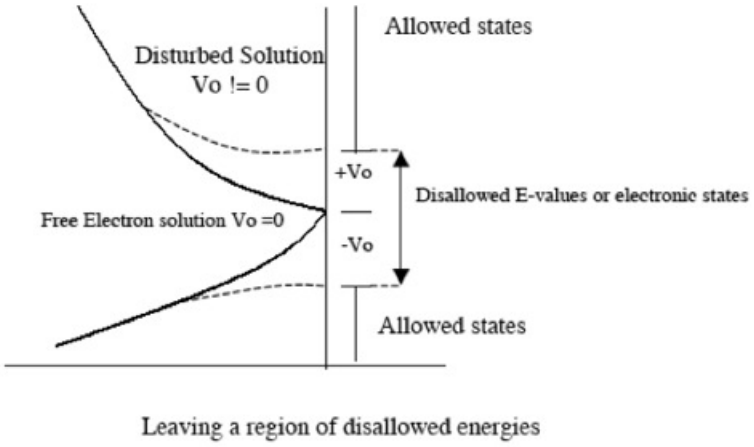

Figure 5. split of energy levels at the band edge

Figure6 shows a less detailed plot of allowed states of E. This way of representing band diagram as function of space is often called the "band structure". We collapse all the detailed branch information into just the availability of an energy state and plot the allowable energy bands as a function of position.

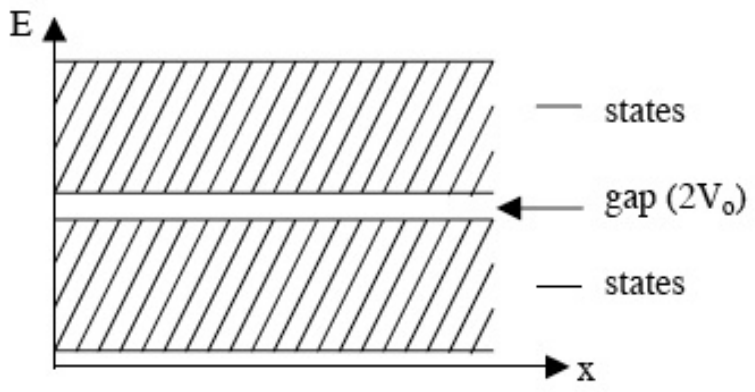

Figure 6. split of energy levels at the band edge

7.2. Kronig-Penny Model

A more realistic model for a metal or semiconductor crystal is a periodic array of square wells. We can analyze this case in a similar manner as we did the finite well and it will also produce the band structure.

Consider the following idealized crystal potential as shown in figure 7 and assume $E < V_0$:

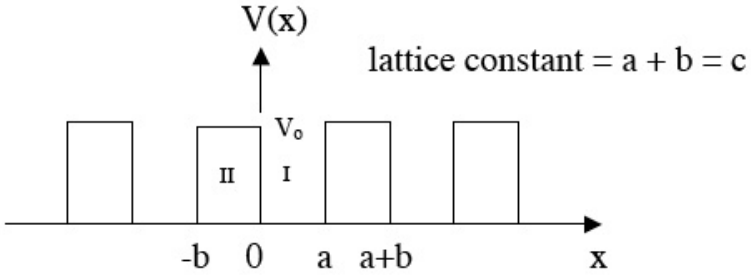

Figure 7. Idealized crystal potential, Krong-Penny Model

(a) Region $0 \leq x \leq a$:

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}E\Psi = 0 \tag{7.13}$$

(b) Region $-b \leq x \leq 0$:

$$\frac{d^2\Psi}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\Psi = 0 \tag{7.14}$$

As we said before using Bloch's theorem the solution will be as the following form:

$$\Psi(x) = U(x)e^{ikx} \tag{7.15}$$

substituting equation 7.15 into equations 7.13 and 7.14 we see that the function $U(x)$ must satisfy equations 7.16 and 7.17.

$$\frac{d^2u_1}{dx^2} + 2jk\frac{du_1}{dx} - (k^2 - \alpha^2)u_1 = 0 \qquad 0 \leq x \leq a \tag{7.16}$$

$$\frac{d^2u_2}{dx^2} + 2jk\frac{du_2}{dx} - (k^2 - \gamma^2)u_2 = 0 \qquad -b \leq x \leq 0 \tag{7.17}$$

Notes:

- Where $u_1(x)$ and $u_2(x)$ represent the value of $U(X)$ respectively in the region I and II in figure 7.
- $\gamma = \sqrt{2m(V_0 - E)}/\hbar$
- $\alpha = \sqrt{2mE}/\hbar$

From equation 7.16 and 7.17 we have the solution as

$$u_1(x) = Ae^{j(\alpha-k)x} + Be^{-j(\alpha+k)x} \tag{7.18}$$

$$u_2(x) = Ce^{j(\gamma+jk)x} + De^{-j(\gamma-jk)x} \tag{7.19}$$

Notes:

- The solution is periodic.
- The barrier has a limited thickness.
- The solution does not continue decaying to zero.
- We have tunneling between the wells.
- Using the boundary conditions and the fact that the wavefunction and its first derivative must be continuous, we are able to find the coefficients, A, B, C and D as below.

(a) at $x = 0$

$$u_1(0) = u_2(0) = 0$$
$$du_1(0)/dx = du_2(0)/dx$$

which leads to equations 7.20 and 7.21

$$A + B = C + D \tag{7.20}$$
$$Aj(\alpha - k) - Bj(\alpha + k) = C(\gamma + jk) + D(\gamma - jk) \tag{7.21}$$

(b) Boundaries ar $x = a$ and $x = -b$

$$u_1(0) = u_2(a+b) = 0 \text{ or } u_1(a) = u_2(-b)$$
$$du_1(a)/dx = du_2(-b)/dx$$

which leads to equations 7.22 and 7.23

$$Ae^{j(\alpha-k)a} + Be^{-j(\alpha+k)a} = Ce^{(\gamma+jk)b} + De^{-(\gamma-jk)b} \tag{7.22}$$

$$Aj(\alpha-k)e^{j(\alpha-k)a} - Bj(\alpha+k)e^{-j(\alpha+k)a} = \tag{7.23}$$
$$-C(\gamma+jk)e^{(\gamma+jk)b} + D(\gamma-jk)e^{-(\gamma-jk)b}$$

The set of equations 7.20 -7.23 has a non trivial solution only if

$$\frac{\gamma^2-\alpha^2}{2\gamma\alpha}\sin(\alpha a)\sinh(\gamma b) + \cos(\alpha a)\cosh(\gamma b) = cos(k(a+b)) \tag{7.24}$$

Now this is still a little hard to analyse so we simplify it further.

7.2.1. Special case – Delta Function Potential

We consider the Delta Function Potential case. Where we have $b \longrightarrow 0$ and $V_0 \longrightarrow \infty$ while $V_0 \cdot b = const.$ as shown in figure 8
Let $P = (maV_0b)/\hbar^2$ then the equation 7.25 we will be as:

$$\frac{P}{\alpha a}\sin(\alpha a) + \cos(\alpha a) = \cos(ka) \tag{7.25}$$

which can be solved graphically. As an example we solve it for $P = 3\pi/2$ which corresponds to a high barrier. The left hand side (term1:

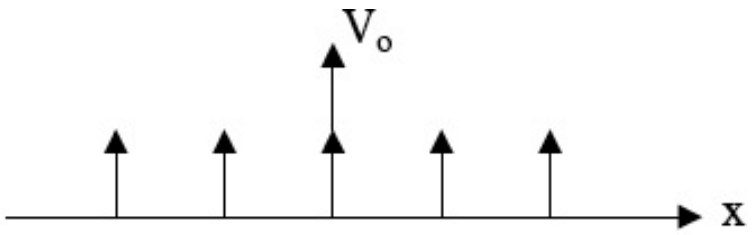

Figure 8. Delta Function Potential

$\frac{P}{\alpha a}\sin(\alpha a) + \cos(\alpha a))$ is plotted as a function of αa in figure 9.

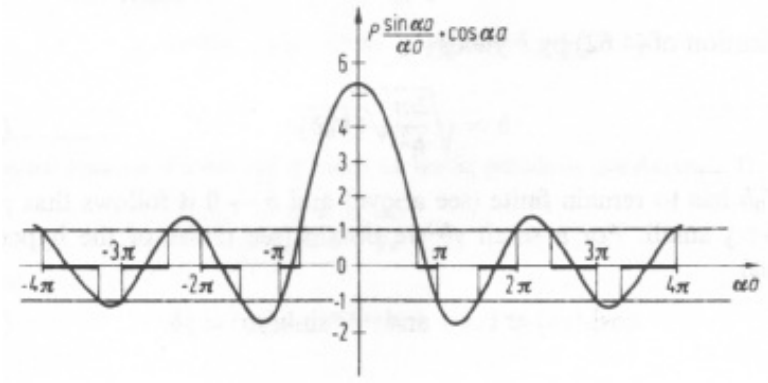

Figure 9. left hand side of equation 7.25

The right hand side of equation 7.25 is a *cosine* function which limits the value of left hand side (term1) between $+1$ and -1, i.e.

$$\frac{P}{\alpha a}\sin(\alpha a) + \cos(\alpha a) \leq |1| \tag{7.26}$$

Since αa is a function of the energy, this limitation means that the electrons can only occupy certain allowed energy states ($E = \hbar^2\alpha^2/2m$). The disallowed region of energy is call the energy gap and again can be plotted in energy band diagram(see figure 10).

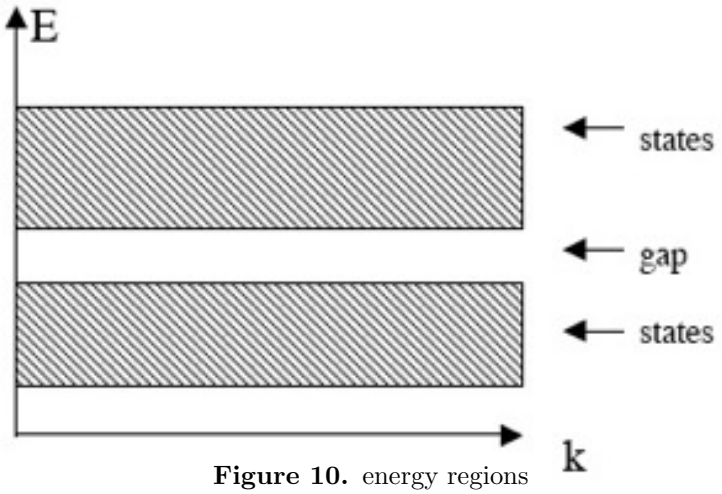

Figure 10. energy regions

7.3. Summery of Energies and Wavefunctions in Various Potentials

7.3.1. Isolated Potential Well

- Only discrete energies (E)are allowed.
- Wavefunction are standing waves.

See figure 11.

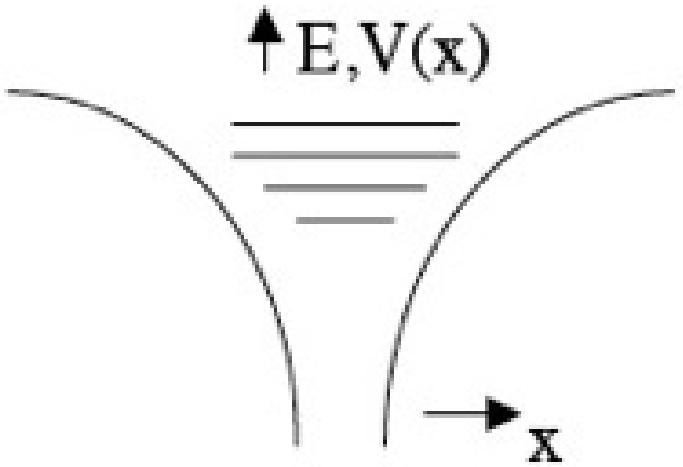

Figure 11. an electron in an isolated potential well

7.3.2. Free Electrons

- The wavefunctions are plane waves as
$$\Psi(x) = Ce^{jkx} \qquad \Psi(x,t) = Ce^{j(kx-wt)}$$
- E versus k is a parabolic function $E = \hbar^2 k^2/2m$ as shown in figure 14. Therefore all the energies are allowed.

7.3.3. Periodic Potential

- Ability of electrons to tunnel between barrier walls spreads out the discrete energy levels seen for isolated wells into bands
- Only a number of bands of energies are allowed.
- The value of k is restricted i.e. $-\pi/a \leq k \leq \pi/a$
- The wavefunctions are Bloch waves as below. Which in fact are modulated traveling waves
$$\Psi_{n,k}(x) = U_{n,k}e^{jkx} \qquad \Psi_{n,k}(x,t) = U_{n,k}e^{j(kx-wt)}$$
- Wavefunctions act like free electrons.

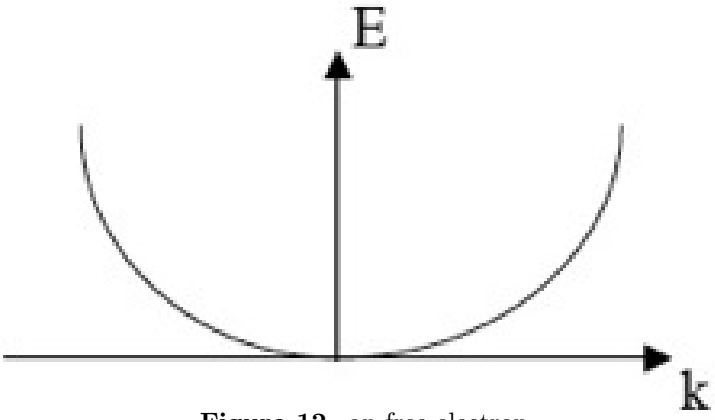

Figure 12. an free electron

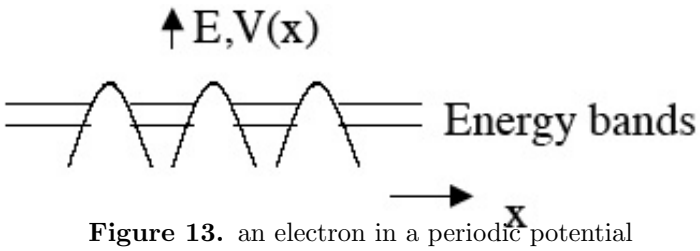

Figure 13. an electron in a periodic potential

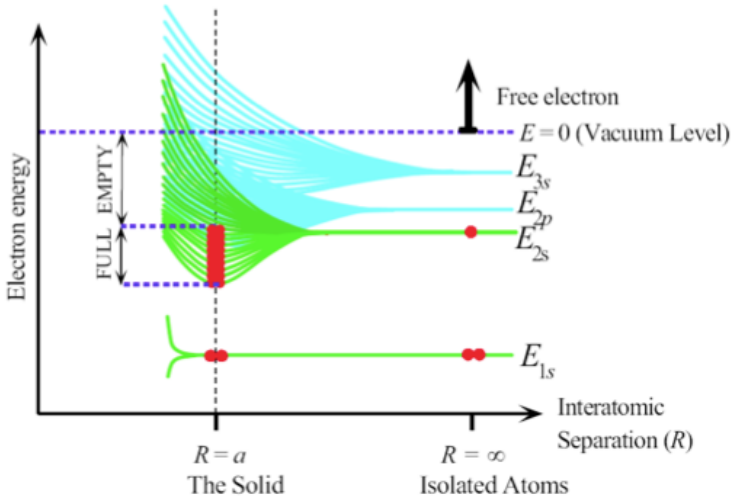

Figure 14. The transition from a gas to solid

- As atoms coalesce into a solid the individual atomic levels split into bands.
- The energy diagram is shown in figure 15.

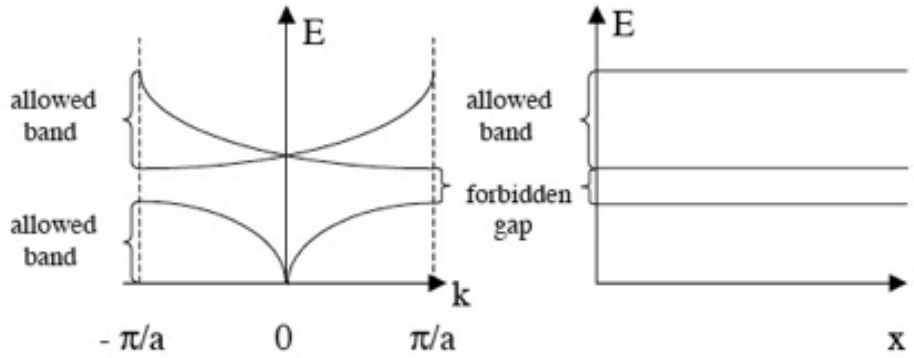

Figure 15. Simplified Energy Diagram

7.3.4. General Results from the Kroning-Penny model

- For stronger potential barriers between wells, the energy bands are narrower and more spaced. This corresponds to crystals in which electrons are tightly bond to ion cores, and wave functions do not overlap much with adjacent cores.
- For weaker potential barrier between wells, energy bands are wider and less spaced. This is typically situation for metals with weak bond electrons e.g. alkali metals. Here the *nearly free* electron model works well