Periodic potentials - Kronig-Penney model

Electrons in a lattice see a periodic potential due to the presence of the atoms, which is of the form shown in Figure 1.

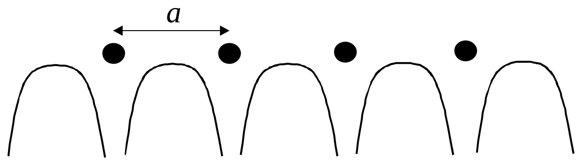


Figure 1. Periodic potential in a one-dimensional lattice.

As will be shown shortly, this periodic potential will open gaps in the dispersion relation, i.e. it will impose limits on the allowed energies. To simplify the problem, we will assume that the width of the potential energy term goes to zero, i.e. we represent them as δ-functions (see Fig. 2):

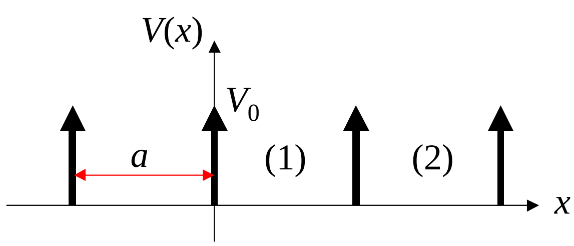


Figure 2. Periodic δ-function potentials (a simplified model to the one from Figure 1).

We can express mathematically this potential energy term *V(x)* as:

$$V(x) = V_0 \sum_{n=-\infty}^{\infty} \delta(x - na) \quad .$$

In region (1), the wavefunction is given by:

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx} \text{ , where } k = \sqrt{\frac{2mE}{\hbar^2}} \quad .$$

To connect this wavefunction to the one in region (2), we will use the so-called **Bloch theorem**, which states that for a periodic potentials, the solutions to the TISE are of the following form:

$$\psi(x) = u(x)e^{iKx} \quad ,$$

where $u(x)$ is the Bloch periodic part that has the periodicity of the lattice, i.e. $u(x+a)$=u(x), and the exponential term is the plane-wave component. Using Bloch theorem, we have:

$$\left.\begin{array}{l}\psi(0)=u(0)\\ \psi(a)=u(a)e^{ika}\end{array}\right\}\rightarrow\frac{\psi(a)}{\psi(0)}=\frac{u(a)e^{iKa}}{u(0)}=e^{iKa}\rightarrow\psi(a)=\psi(0)e^{iKa}$$

Therefore, we can write the wavefunction in region (2) in terms of the one in region (1) using Bloch theorem, to get:

$$\psi_2(x)=\psi_1(x-a)e^{iKa}=\left[Ae^{ik(x-a)}+Be^{-ik(x-a)}\right]e^{iKa}\quad .$$

We also know that for a wavefunction to be a proper function, it must satisfy the continuity requirement, i.e.

$$\psi_1(a)=\psi_2(a)\ ,$$

which gives:

$$(A+B)e^{iKa}=Ae^{ika}+Be^{-ika}\rightarrow A\left(e^{iKa}-e^{ika}\right)=B\left(e^{-ika}-e^{iKa}\right)\quad . \qquad (1)$$

The continuity of the first derivative is not satisfied when $V(x)$ is a δ-function. This can be shown directly from the 1D TISE,

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

If this equation is integrated in the neighborhood of $x=a$, we get:

$$\begin{aligned}\int_{x=a-\delta}^{x=a+\delta}\frac{d}{dx}\left(\frac{d\psi}{dx}\right)dx&=\left.\frac{d\psi}{dx}\right|_{x=a+\delta}-\left.\frac{d\psi}{dx}\right|_{x=a-\delta}\\&=\frac{2m}{\hbar^2}\int_{x=a-\delta}^{x=a+\delta}\left[V_0\delta(x-a)-E\right]\psi_2(x)dx\xrightarrow{\delta\rightarrow 0}\frac{2m}{\hbar^2}V_0\psi_2(a)\end{aligned}$$

Using the expression for $\psi_2(a)$, we arrive at a second equation that is relating coefficients A and B:

$$\left[ike^{iKa}-ike^{ika}-\frac{2mV_0}{\hbar^2}e^{iKa}\right]A=\left[ike^{iKa}-ike^{-ika}+\frac{2mV_0}{\hbar^2}e^{iKa}\right]B\quad . \qquad (2)$$

Dividing equations (1) and (2) and rearranging the terms leads to the following final expression:

$$\cos(Ka)=\frac{2mV_0}{\hbar^2}\frac{\sin(ka)}{ka}+\cos(ka)\quad .$$

Let's consider the limiting cases of the above equation first:

(a) Free particle

In this case, $V_0=0$, which gives

$$\cos(Ka)=\cos(ka)\rightarrow K=k=\sqrt{\frac{2mE}{\hbar^2}}\rightarrow E=\frac{\hbar^2K^2}{2m}\quad .$$

We recovered the free-particle dispersion relation, in which there is no limit on the allowed particle energy.

(b) Infinite potential well

For the infinite potential well case, we have $V_0 \to \infty$, which implies:

$$\sin(ka) = 0 \to ka = n\pi \to E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 \ .$$

We have recovered the expression for the energy levels in an infinite potential well.

(c) General solution

Consider now the general solution, which is repeated below for convenience:

$$\cos(Ka) = \frac{2mV_0}{\hbar^2}\frac{\sin(ka)}{ka} + \cos(ka) \ . \qquad (3)$$

The LHS is bounded in the region [-1,1], which imposes limits on the allowed values of *k*. This, in turn, means that the energy and the wavevector of a particle in a periodic potential do not satisfy the free-particle dispersion relation. This observation is graphically illustrated in Figure 3:

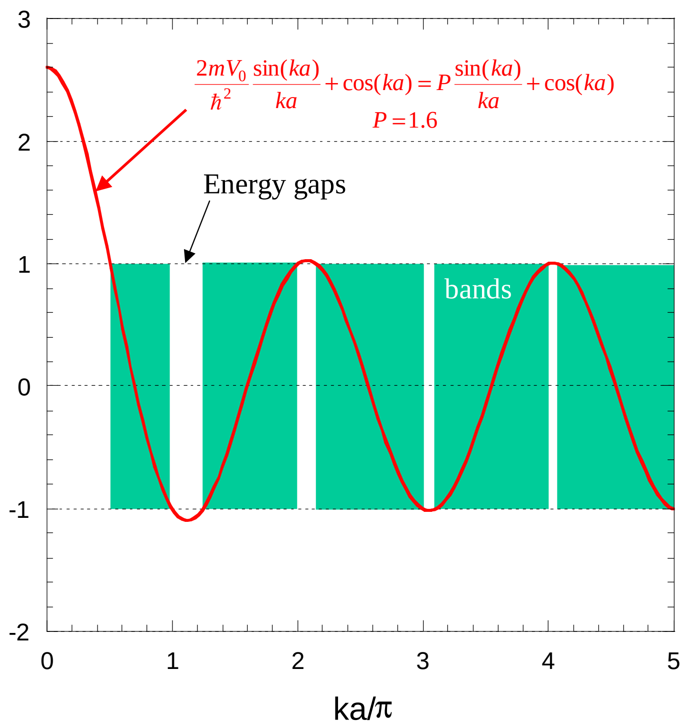
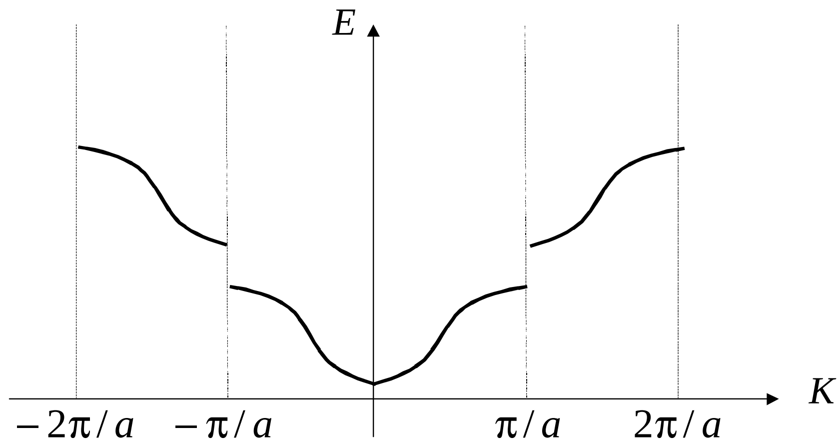
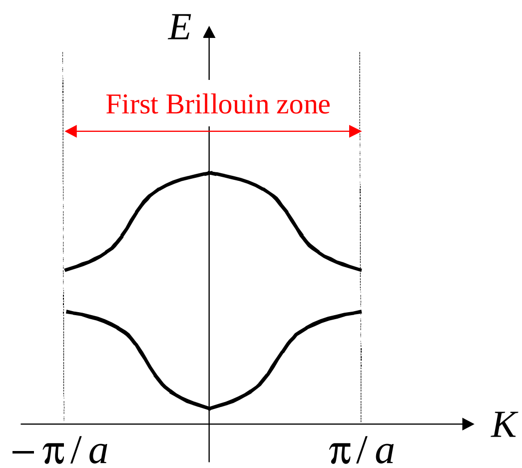


Figure 3. Graphical representation of the real solutions of equation (3).

As it is clear from the figure, the periodic potential introduces gaps in the free particle dispersion relation. If one starts from the other extreme (with infinite well, that has discrete energy levels), then we can say that the interactions between the wells lift the degeneracy of the energy levels and broaden them into bands. This can rather easily be demonstrated on a two-well problem, which was given as a homework problem last year (see the web-site to get to the solution of this problem). The dispersion relation for a particle in a periodic potential is shown in Figure 4.



(a)



(b)

Figure 4. Dispersion relation for a particle in a periodic potential. (a) expanded zone scheme. (b) reduced zone scheme, also known as the First Brillouin zone.