

1 Exercise 1 - Kronig-Penney Model

a. Analytical solution of the model

Solution: For this problem we need to solve the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right) \phi_{nk}(x) = E_{nk} \phi_{nk}(x). \quad (1)$$

If $V(x)$ is a periodic potential we don't have to solve the problem for all space, since Bloch theorem tells us that the solutions will be the product of plane waves and a periodic function with the same periodicity as the potential. Assuming that $V_1 < E < V_2$ we will have (once solved it is easy to extend this result)

$$\phi_{nk}(x) = \begin{cases} Ae^{iKx} + Be^{-iKx}, & 0 < x < b, \\ Ce^{Qx} + De^{-Qx}, & -a < x < 0. \end{cases} \quad (2)$$

With

$$K = \sqrt{\frac{2m(E - V_1)}{\hbar^2}}, \quad (3)$$

$$Q = \sqrt{\frac{2m(V_2 - E)}{\hbar^2}}. \quad (4)$$

By Bloch theorem, we know that

$$\phi_{nk}(b < x < b + a) = \phi_{nk}(-a < x < 0)e^{ik(b+a)}. \quad (5)$$

Moreover, we know that the solution must be continuous. This imposes boundary conditions at $x = 0$, and $x = b$. When $x = 0$ both solutions will look like this

$$A + B = C + D \quad (6)$$

$$iK(A - B) = Q(C - D) \quad (7)$$

At $x = b$, using the condition in eq. 5 we will have $\phi(-a)e^{ik(b+a)} = \phi(b)$, and a condition for the derivatives $\phi'(-a)e^{ik(b+a)} = \phi'(b)$ we have

$$Ae^{iKb} + Be^{-iKb} = (Ce^{-Qa} + De^{Qa})e^{ik(b+a)} \quad (8)$$

$$iK(Ae^{iKb} + Be^{-iKb}) = Q(Ce^{-Qa} - De^{Qa})e^{ik(b+a)} \quad (9)$$

Solving this four equation simultaneously leads us to ask for this determinant to be zero

$$\begin{vmatrix} 1 & 1 & -1 & -1 \\ iK & -iK & -Q & Q \\ e^{iKb} & e^{-iKb} & -e^{-Qa}e^{ik(b+a)} & -e^{Qa}e^{ik(b+a)} \\ iKe^{iKb} & -iKe^{-iKb} & -Qe^{-Qa}e^{ik(b+a)} & Qe^{Qa}e^{ik(b+a)} \end{vmatrix} = 0. \quad (10)$$

When we solve this determinant (by Mathematica) we get the following result

$$\left(\frac{Q^2 - K^2}{2QK}\right) \sinh(Qa) \sin(Kb) + \cosh(Qa) \cos(Kb) = \cos(k(b+a)). \quad (11)$$

We can introduce extra simplifications by taking the limit $b \rightarrow 0$ and $V_2 \rightarrow \infty$. While keeping $Q^2ba/2 = P$ constant. This means particularly that $Q \gg K$, and $Qa \ll 1$. So, we will have

$$f(Kb) = \frac{P}{Kb} \sin(Kb) + \cos(Kb) = \cos(kb). \quad (12)$$

Here we can see clearly that the only allowed solutions are the ones with $-1 \leq f(Kb) \leq 1$

Not all arguments fulfill this condition, as we can see in fig. 1

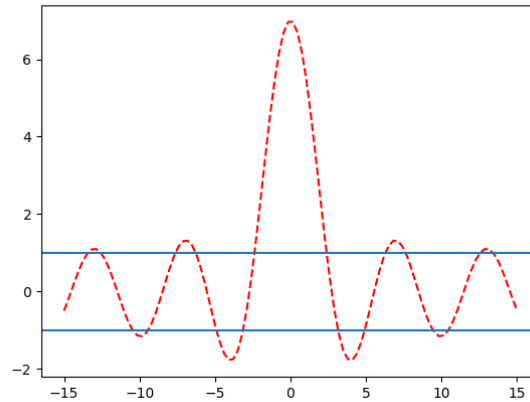


Figure 1: Plot of the qualitative behavior of eq. 11.

If we find the roots of eq. 11 numerically we will find the band structure displayed in fig. 2

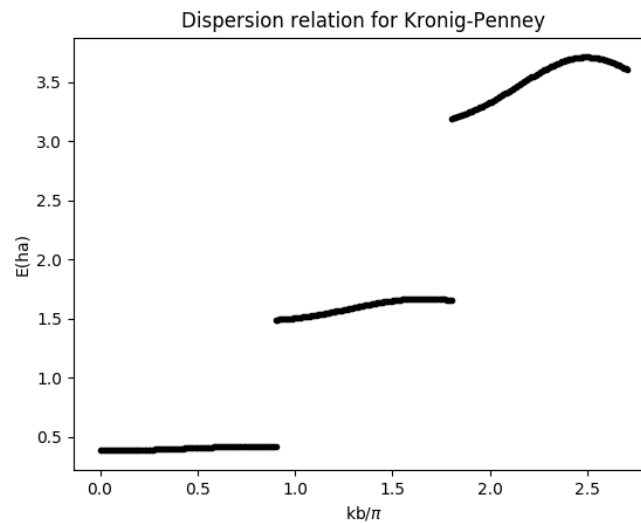


Figure 2: Band structure of the given material.

Finally we can have an idea of the density of states just by counting and displaying the histogram showed in fig. 3

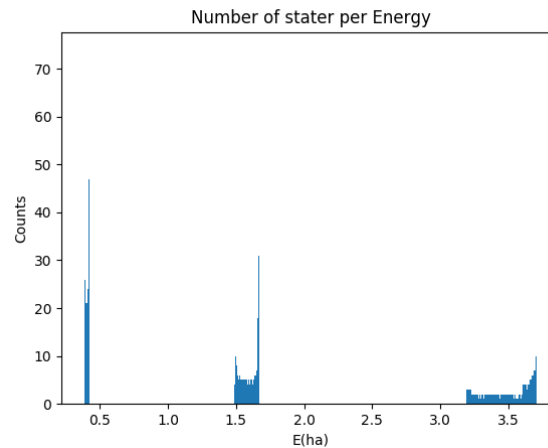


Figure 3: Number of solutions for k as function of E .

Here we can see that we have more states close to the gaps that in the middle section of the bands.

But I'm missing the Fermi energy in both plots, the reason is the following. In the model of Kronig-Penney there is no statement concerning the position of the Fermi level, for more information read https://www.springer.com/cda/content/document/cda_downloaddocument/9783319197630-c2.pdf?SGWID=0-0-45-1514427-p177405762

I do not add the codes because adding them does not add anything new to the discussion, but they can be found here <https://github.com/UriAceves/QuantumTheoryofMaterialsHW/tree/master/HW06>

2 Exercise 2 - Kronig-Penney Model (Numerical)

a. Numerical solution

Solution: In order to simplify my calculations I'm going to set my periodic potential as follows

$$U(x) = A \sum_s \delta(x - sa), \quad s \in \mathbb{Z} \quad (13)$$

where A is a constant and a is the lattice parameter. We approximate this potential by spiked functions as we can see in fig. 4

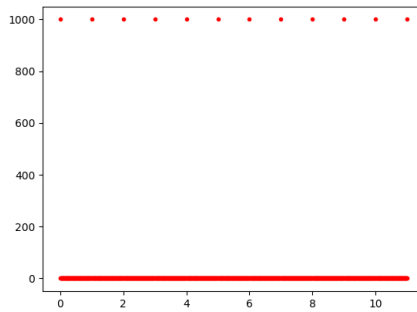
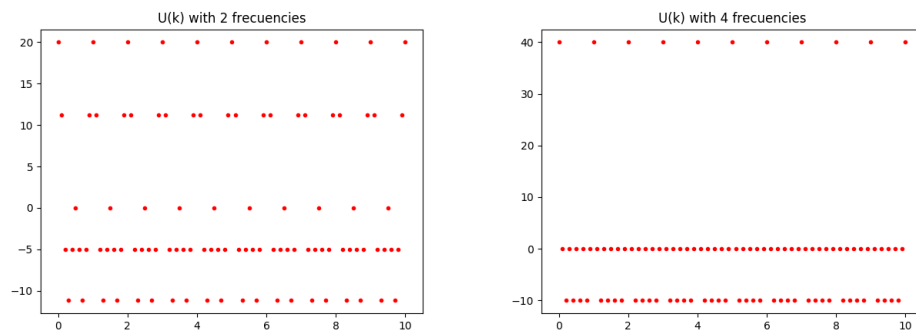


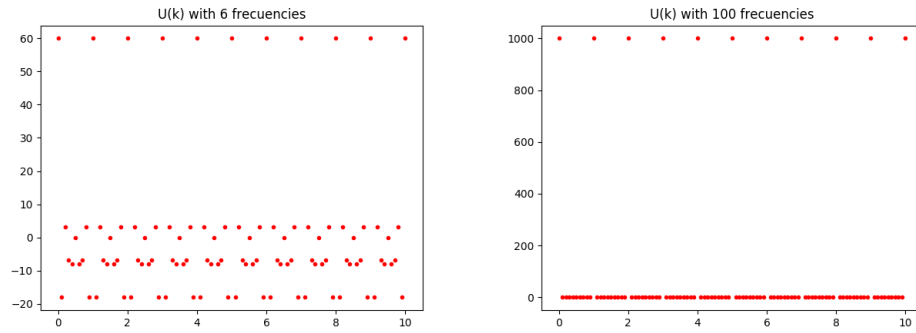
Figure 4: Qualitative behavior of delta function potential

Hence, if we calculate the fourier coefficients of $U(x)$ we will have

$$\begin{aligned}
 U_G &= \frac{1}{a} \int_{-a/2}^{a/2} dx U(x) e^{-iGx}, \\
 &= \frac{1}{a} \int_{-a/2}^{a/2} dx \sum_s A \delta(x - sa) e^{-iGx}, \\
 &= \frac{1}{a} \int_{-a/2}^{a/2} dx A \delta(x) e^{-iGx}, \\
 &= \frac{A}{a}.
 \end{aligned} \tag{14}$$

To go from the second to the third line we used the fact that $s \in \mathbb{Z}$ and $\delta(x - sa)$ is non-zero just when $s = 0$, for $x \in [-a/2, a/2]$. In fig. 5 we can see the reconstruction of the initial delta potential using the Fourier components U_G . As we can see the more frequencies we add the more accurate our reconstruction is.



Figure 5: $U(k)$ using 2, 4, 6, and 100 frequencies.

The final step is to actually know what is the system of equations we are going to solve numerically, for this matter we deal with the following calculations. The wave equation of an electron in a crystal is (See Kittel)

$$\left(\frac{1}{2m} p^2 + \sum_G U_G e^{iGx} \right) \psi(x) = \epsilon \psi(x). \quad (15)$$

Now, assuming our solution is of the form

$$\psi = \sum_k C(k) e^{ikx}, \quad (16)$$

and plugging this equation into eq. 15 the wave equation changes to

$$\sum_k \frac{\hbar^2}{2m} k^2 C(k) e^{ikx} + \sum_G \sum_k U_G C(k) e^{iGx} = \epsilon \sum_k C(k) e^{ikx}. \quad (17)$$

All Fourier components must have the same coefficient on both sides if the equation. This leads us to the central equation

$$(\lambda_k - \epsilon) C(k) + \sum_G U_G C(k - G) = 0, \quad (18)$$

where

$$\lambda_k = \frac{\hbar^2 k^2}{2m}. \quad (19)$$

Solving this equation we find the following solutions (using similar parameters to the first exercise)

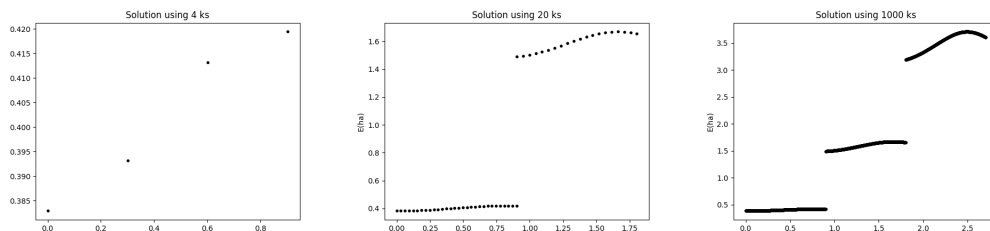


Figure 6: $U(k)$ using 2, 4, 6, and 100 frequencies.

If we use more k values we obviously get more energies, and therefore our bands are more populated. The band-gap is determined by the lattice factors. This changes if we modify for example the lattice parameter.

Our solutions on this section look similar to the analytical solutions, even though we started with a delta-like potential and therefore were solving a different equation. If we pay attention that equation is actually our eq. 12. Analytically we solved eq. 11. But at the end, they yielded similar results.