Simulation of the Kronig-Penny Model

Bijin Joseph (182361). Hetanshu Bharadiya (182343)

18th April 2021

Abstract

In this Project we use the solved and simplified solution of the Schrodinger's equation for the Kronig-Penny model to plot the Energy diagrams. We change the value of the potential barrier and observe the changes in the graphs, especially the band diagram

Kronig-Penny Model, Band gap, Periodic potential

1 Introduction

It has been a long motive of physicists to understand metals and to know how we could exploit their peculiar properties. On studying their properties, we have come across some unexpected results and theories and we required different models to explain them. Physicist including Albert Einstein had tried and developed models to understand the heat capacity of metals and their relation with temperature and there have been models like the classical theory, Einstein's model, the Kronig-Penney model (KP), etc. The KP model has been really successful in explaining the specific heat of metals and it's based on the assumption that the potentials are a periodic square wave and the solution of this model is obtained from Schrodinger's equation (SE). According to quantum free electron theory of metals, a conduction electron in a metal experiences constant (or zero) potential and free to move inside the crystal but will not come out of the metal because an infinite potential exists at the surface. This theory successfully explains electrical conductivity, specific heat, thermionic emission, paramagnetism etc.However, this theory fails to explain many other physical properties, for example, it fails to explain the difference

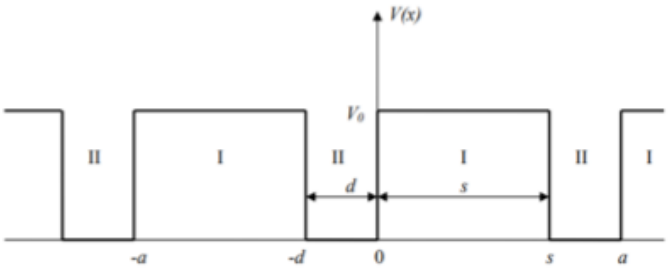
between conductors, insulators and semiconductors, positive Hall coefficient of metals and lower conductivity of divalent metals than monovalent metals. This problem was tackled by considering the positive ions to produce periodic potentials, through which the electron moves. It is not easy to solve Schrödinger's equation with these potentials.

So, Kronig and Penney approximated these potentials inside the crystal to the shape of rectangular steps as shown in the figure. This model is called the Kronig-Penney model of potentials.

2 Discussion

2.1 Theory

The KP model is a single-electron problem. The electron moves in a one-dimensional crystal of length L. The periodic potential that the electrons experience in the crystal lattice is approximated by the following periodic function. For the sinusoidal type of potential inside the crystal the Schrodinger equation is not easily traceable. Hence, Kronig and Penney introduced a simpler model for the shape of the potential variation. The potential inside the crystal is approximated to the shape of the rectangular step.



The regions denoted II correspond to the positively charged ions of the crystal lattice. The regions denoted I represent the empty spaces between the ions. It is the choice of this oversimplified potential that makes an analytical solution possible. The lattice parameter is a = d + s. The KP potential is defined by three parameters, e.g., V0, a, and d. The choice of zero on the energy axis has no influence on the physics of the problem. The single-electron problem is described by the Schrödinger equation (considering boundary condition) is given below:

$$\frac{d^2\Psi}{dx^2} + \alpha^2\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} - \beta^2\Psi = 0$$

The solution to this is

$$\boxed{\Psi = u_k(x)exp(ikx)}$$

The above equation is a bit complicated to solve numerically as it involves solving of a 4*4 eigenvectors and eigenvalues determinant. We shall consider the direct solution to the equation.

$$\frac{\beta^2 - \alpha^2}{\alpha\beta} sinh\beta\alpha \;\; sin\alpha a + cosh\beta b \;\; cos\beta b = cosk(a+b)$$

The above equation was wisefully simplified by Kronieg and penney by assuming that V0 is such large that it tends to infinity while 'b' is so small that it tends to 0, but V0*b remains finite.

$$\boxed{p\frac{sin\alpha}{\alpha a} + cos\alpha a = coska}$$

Here, $P = \frac{mV_o ab}{\hbar^2}$ and is a measure of the strength with which electrons in a crystal are attracted to the ions on the crystal lattice sites.

2.2 Algorithm

- Initially define a value for P and also keep an αK range.
- By taking the values, to obtain the above mentioned reduced function.
- We can plot this graph.
- By extracting ranges of -1 to 1 from this graph, we can obtain the k values by just taking the inverse of the cos values corresponding to these values.
- Now by replicating the above point in the opposite direction, we can get the observed energy gap graph.

2.3 Code

```
import numpy as np
import matplotlib.pylab as plt
```

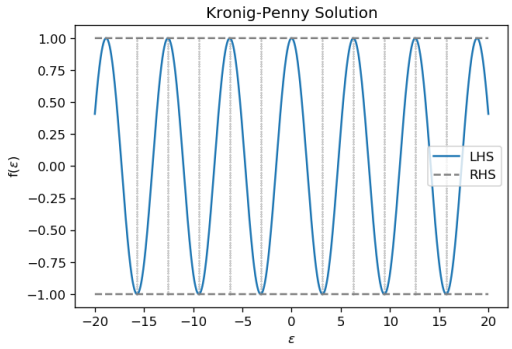
```
def KPM_Soln(p,eps_range):


    #Kronig-Penny Solution (LHS)
    def KPM_p(g, p):
        return p*(np.sin(g)/g) + np.cos(g)

    #Define epsilon space to plot
    g = np.linspace(-1*eps_range ,eps_range,200000)
    f_eps = KPM_p(g,p)
    #Define epsilon space to plot for energy gap plot
    g1 = np.linspace(0 ,eps_range,200000)
    f_eps1 = KPM_p(g1,p)

    return g, f_eps, g1, f_eps1

def Eband_KP(epslist,f_eps): #outputs energy band data

    k=[]
    bandlist=[]
    Eps=[]
    epsbuildlist=[]
    for i in range(len(f_eps)-1):
       #To get the energy values between 1 and -1
       if 1 >= f_eps[i] >= -1:
           bandlist.append(f_eps[i])
           epsbuildlist.append(epslist[i])
           #To get the end points of the values
           if (1 < f_eps[i+1] or  -1 > f_eps[i+1]):
               k.append(bandlist)
               Eps.append(epsbuildlist)
               bandlist=[]
               epsbuildlist=[]
    #To get the K values
    for i in range(len(k)):
        k[i]=np.arccos(k[i])/np.pi #dividing by pi has the effect of normalisation
        #Replicating the graph
        if i % 2 == 0:
            Eps[i]=np.concatenate((Eps[i][::-1],Eps[i][::1]))
            k[i]=np.concatenate((-1*np.array(k[i],dtype=float)[::-1],k[i][::1]))
        else:
            k[i]=np.concatenate((k[i][::1],-1*np.array(k[i],dtype=float)[::-1]))
            Eps[i]=np.concatenate((Eps[i][::1],Eps[i][::-1]))

    return k, Eps
```

```


eps_range = 20 #range of enrgy values
p= 3*np.pi.    #p value
epslist, f_eps, epslist1, f_eps1 = KPM_Soln(p, eps_range)
k, eps  = Eband_KP(epslist1, f_eps1)

#k values to plot for the RHS Solution
klist=np.linspace(-eps_range,eps_range,200000)
k_min=klist*0-1
k_max=klist*0+1

#Plot Kronig-Penny Solution
plt.figure(1,dpi=120)
plt.title("Kronig-Penny Solution")
plt.xlabel("$\epsilon$")
plt.ylabel("f($\epsilon$)")
#plt.ylim(-5,5)
plt.plot(epslist,f_eps,label="LHS")
plt.plot(klist,k_min, linestyle="dashed",color="grey",label="RHS")
plt.plot(klist,k_max, linestyle="dashed",color="grey")
plt.legend()
y = np.linspace(-1,1, 100)
g = [y*0-5*np.pi,y*0-4*np.pi,y*0-3*np.pi, y*0-2*np.pi, y*0-1*np.pi, y*0+1*np.pi, y*0+2*np.pi, y*0+3*np.pi, y*0+4*np.pi, y*0+5*np.pi]
```

```
for i in range(10):
    plt.scatter(g[i], y,color = 'grey', s= 0.10 )
plt.figure(2,dpi=120)
plt.title("Kronig-Penny Energy Bands")
plt.xlabel(r'k / ${\pi}$')
plt.ylabel("$\epsilon$")
for i in range(len(k)):
    plt.plot(k[i],eps[i])
```

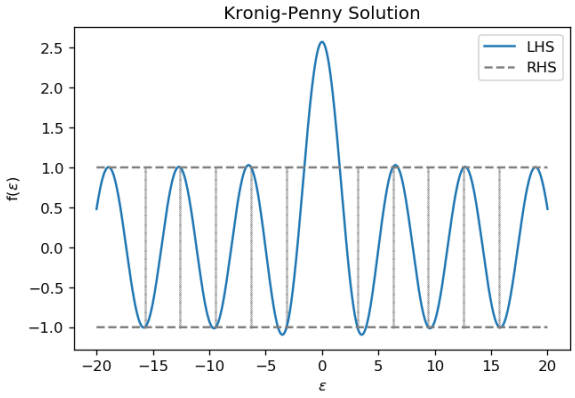
2.4 Result

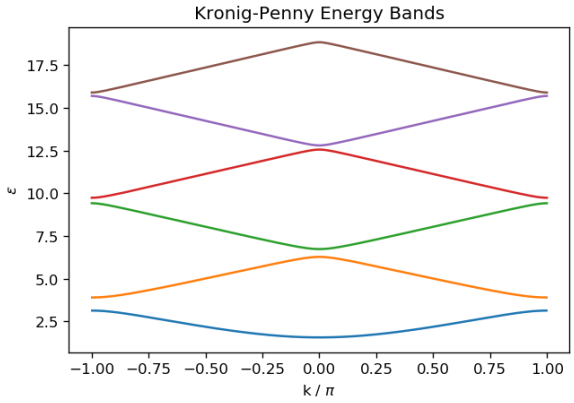
For p = 0



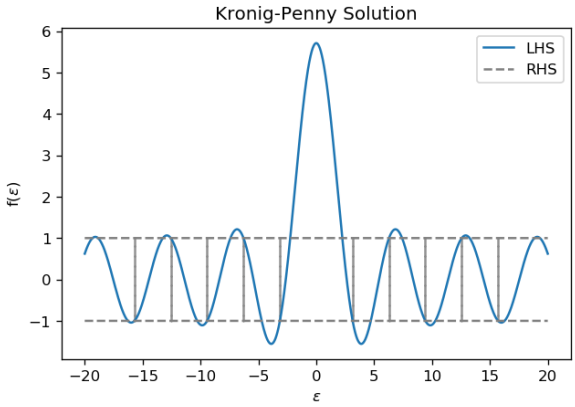
No E vs K graph because the particle is free

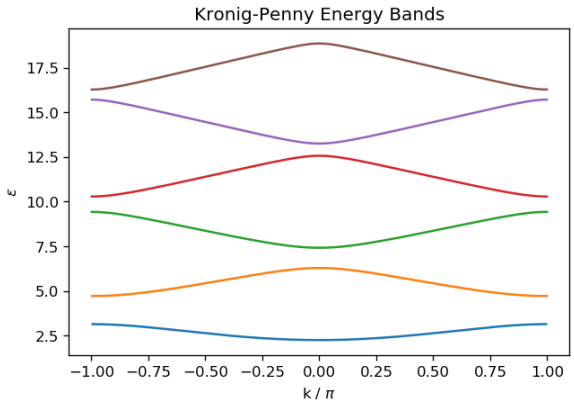
For p = $\frac{\pi}{2}$



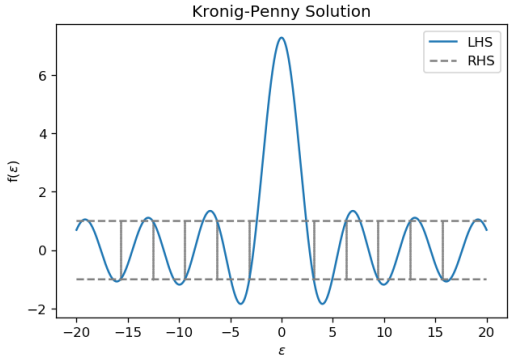


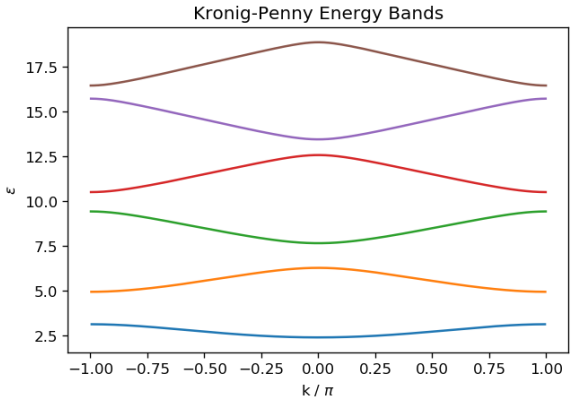
For p = 1.5 π



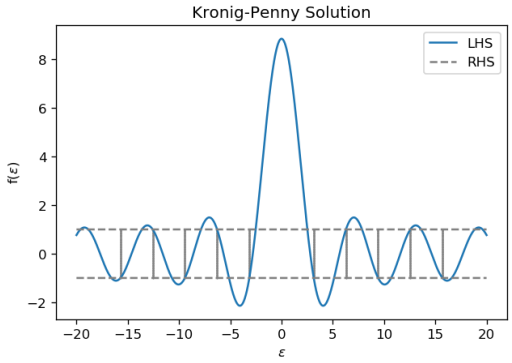


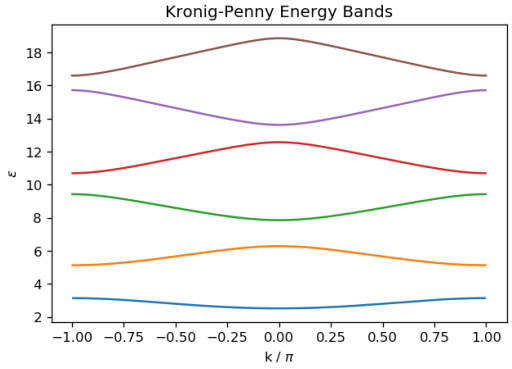
For p = 2 π



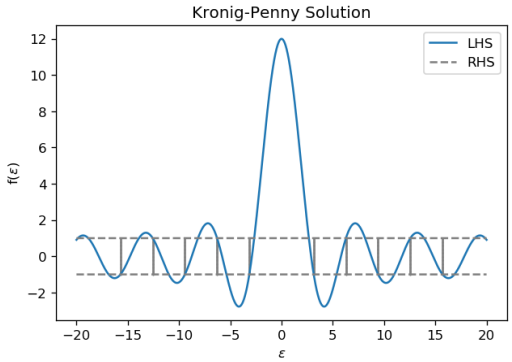


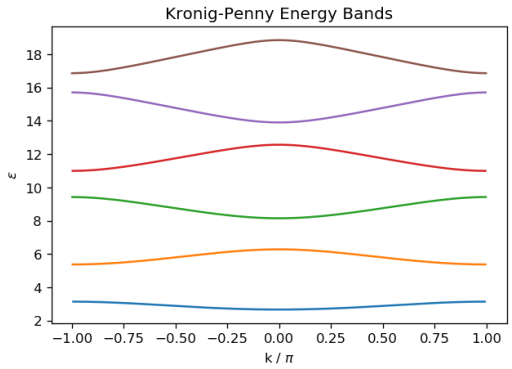
For p = 5 $\frac{\pi}{2}$



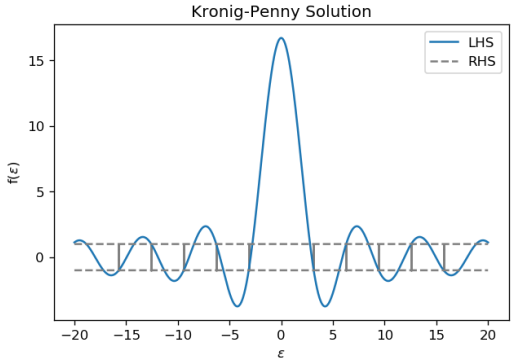


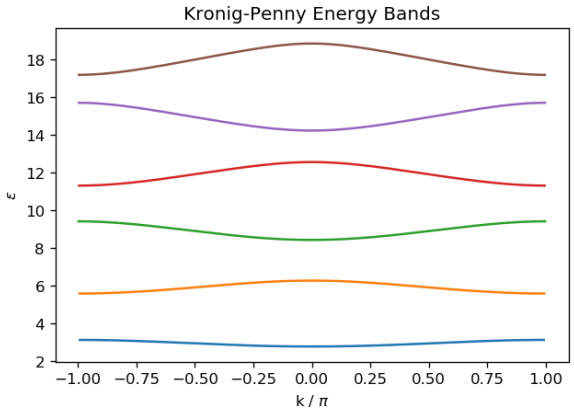
For p = 7 $\frac{\pi}{2}$



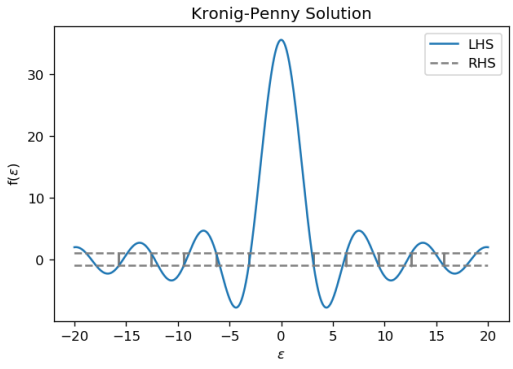


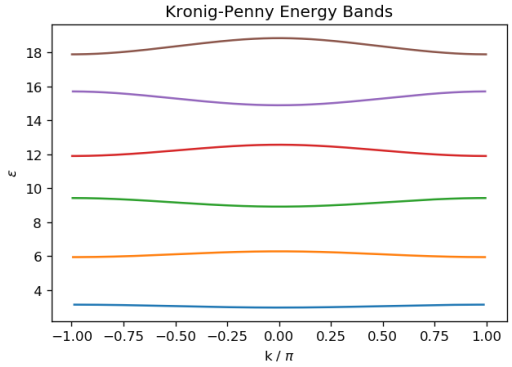
For p = 10 $\frac{\pi}{2}$





For p = 11




Kronig-Penny Energy Bands
18
16
14
12
10
8
6
4
ε
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
k / π

3 Conclusion

From the results that we got, we can see that as P increases, that is the potential barrier increases the allowed band decreases and the energy graph or the forbidden zone increases. This can be further visualised from the E vs K graph that we have plotted

4 Acknowledgment

First and foremost we would like to thank the physics department of St. Xaviers College, Mumbai, for giving us this opportunity to perform this project which has helped us to learn more and understand theory better. We specifically thank Professor Radhekrishna Dubey for approving this project and for being with us throughout this project to help us and guide us whenever it was required.

References

[1] S.O Pillai "Solid State Physics"

[2] Sören Kahl ("http://yclept.ucdavis.edu/course/215b.W17/Kronig-Penney$_R app-3.pdf$"