# A Computer Model for Band Structure of One Dimensional Arbitrary Periodic Potential

*Self-study assignment submitted by*

**Avoy Jana**
*2023PHS7164*

*under the guidance of*

**Dr. Sankalpa Ghosh**

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**Master of Science**


**Dept. of Physics**
**Indian Institute of Technology Delhi**

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**Abstract**

The numerical matrix method [1] is the best approach for band solutions of arbitrary periodic potentials in arbitrary dimensions.[2] [3]. We aim to construct a computer model for some famous periodic potentials in one dimension.

## Keywords

Kroning Penney potential, Arbitrary periodic potential, Reduced zone scheme, Periodic zone scheme, Extended zone scheme

## 1 Introduction

The Kronig-Penney model is a simplified yet insightful quantum mechanical problem often used to study the behavior of electrons in one-dimensional crystal structures. It can be thought of in two ways: as an approximation to describe electrons moving in the periodic potential of a crystal, or as an extension of the potential-barrier problem to a chain of potential wells and barriers in one dimension. In this model, the particle (typically an electron) is confined within a series of potential wells or barriers. The model helps us understand the behavior of particles in periodic potentials and the formation of energy bands and band gaps, which are crucial in understanding the electronic properties of materials. Now smoothing each potential well and barrier by replacing the rectangle with famous potentials like periodic parabolic potential (PPP), inverted PP (IPPP), Gaussian potential (PGP), inverted GP (IPGP), linear potential (PLP), pseudo-Coulomb potential (PpCP), etc., we will study energy bands and band gaps and difference with Kroning Penney potential (KPP).

## 2 Formulation

We know for a one-dimensional square well with periodic boundary condition $\psi(x+a) = \psi(x)$ and the solutions that are plane wave states are given by,

$$\psi_p(x) = \sqrt{\frac{1}{a}} e^{i\frac{2\pi p}{a}x} \tag{1}$$

and energy eigenvalues are given by,

$$E_p = (2p)^2 \frac{\pi^2\hbar^2}{2ma^2} \tag{2}$$

where $p$ takes integer values, $p = ...., -2, -1, 0, 1, 2, .....$
Bloch's theorem states $\psi(x+a) = e^{ika}\psi(x)$ where $a$ is the unit cell length and k is the wave vector such that $-\pi < ka < \pi$.
Then modified wave functions and energy eigenvalues should be,

$$\phi_p(x) = e^{ikx}\psi_p(x) = \sqrt{\frac{1}{a}} e^{ikx} e^{i\frac{2\pi p}{a}x} \tag{3}$$

$$E_p^{(0)} = \frac{\pi^2\hbar^2}{2ma^2}\left(2p + \frac{ka}{\pi}\right)^2 \tag{4}$$

Now for any arbitrary potential $V(x)$, we want to write Hamiltonian matrix elements are given by,

$$\begin{aligned} & H_{pq} \\ & =< \phi_p(x)|(H_0 + V)|\phi_q x) > \\ & = \delta_{pq}E_p^{(0)} + H_{pq}^V \end{aligned} \tag{5}$$

where

$$\begin{aligned} & H_{pq}^V \\ & =< \phi_p(x)|V(x)|\phi_q(x) > \\ & = \frac{1}{a}\int e^{-ikx} e^{i\frac{-2\pi p}{a}x} V(x) e^{ikx} e^{i\frac{2\pi q}{a}x} dx \\ & = \frac{1}{a}\int e^{i\frac{2\pi(q-p)}{a}x} V(x) dx \end{aligned} \tag{6}$$

The problem is easily handled by making a convenient dimensionless form dividing Hamiltonian by infinite square-well ground state energy, $\epsilon_1^{(0)} = \frac{\pi^2\hbar^2}{2ma^2}$,

$$\begin{aligned} & h_{pq} \\ & = H_{pq}/\epsilon_1^{(0)} \\ & = \delta_{pq}\frac{E_p^{(0)}}{\epsilon_1^{(0)}} + \frac{H_{pq}^V}{\epsilon_1^{(0)}} \\ & = \delta_{pq}\left(2p + \frac{ka}{\pi}\right)^2 + \frac{1}{a}\int e^{i\frac{2\pi(q-p)}{a}x}\frac{V(x)}{\epsilon_1^{(0)}}dx \\ & = \delta_{pq}\left(2p + \frac{ka}{\pi}\right)^2 + \frac{1}{a}\int e^{i\frac{2\pi(q-p)}{a}x}v(x)dx \end{aligned} \tag{7}$$

Now we aim to find the dimensionless potential matrix elements for any arbitrary potential $V(x)$ given by,

$$h_{pq}^V = \frac{1}{a}\int e^{i\frac{2\pi(q-p)}{a}x}v(x)dx \tag{8}$$

# 3 Algorithm of the model

## 3.1 Create matrix structure

The dimensionless Hamiltonian matrix element, $h_{pq} = h_{pq}^T + h_{pq}^V$, and the matrix will be an order of $p \times q$. From the formulation, it is clear that $p$ and $q$ can take integer values $..., -3, -2, -1, 0, 1, 2, 3, ....$To diagonalize the matrix, we have to take a square matrix.
Taking a basis limit of $N'$, let's create a $N \times N$ Hamiltonian matrix for $N = 2N' + 1$.The structural form of the matrix looks like,

| (p,q) | 0 | -1 | 1 | -2 | 2 | .... | N' |
|---|---|---|---|---|---|---|---|
| 0 | (0,0) | (0,-1) | (0,1) | (0,-2) | (0,2) | .... | (0,N) |
| -1 | (-1,0) | (-1,-1) | (-1,1) | (-1,-2) | (-1,2) | .... | (-1,N') |
| 1 | (1,0) | (1,-1) | (1,1) | (1,-2) | (1,2) | .... | (1,N') |
| -2 | (-2,0) | (-2,-1) | (-2,1) | (-2,-2) | (-2,2) | .... | (-2,N') |
| 2 | (2,0) | (2,-1) | (2,1) | (2,-2) | (2,2) | .... | (2,N') |
| : | : | : | : | : | : | .... | : |
| N' | (N',0) | (N',-1) | (N',1) | (N',-2) | (N',2) | .... | (N',N') |

Table 1: Positional elements of Hamiltonian matrix

To create it, we aim to create a sequence array using $i(-1)^i$ for $i \in [0, N]$ and it is given by, sequence array $= (0, -1, 2-3, 4, -5, 6, ...., 2N')$ and the basis array can be created using $\sum_{j=0}^{j} i(-1)^i$ for $i, j \in [0, N]$ and it is given by, basis array $= (0, -1, 1, -2, 2, ...., N')$

## 3.2 Fill potential matrix elements

For having a null square matrix $h^0$ of order $(N \times N)$, we aim to fill potential matrix elements, as given by,

$$h_{pq}^V = \frac{1}{a}\int e^{i\frac{2\pi(q-p)}{a}x}v(x)dx \tag{9}$$

The integration limits will be decided according to the potential given. For example, for Kroning Penney potential, below we will see,

$$\begin{aligned} & v(x) \\ & \quad = 0 \text{ for } 0 < x < b \\ & \quad = \frac{V_0}{\epsilon_1^{(0)}} \text{ for } b < x < a \end{aligned} \tag{10}$$

Then the limits will be divided into two parts like $\int = \int_0^b + \int_b^a$.
The diagonal potential matrix elements are given by,

$$h_{pp}^V = \frac{1}{a}\int v(x)dx \tag{11}$$

The non-diagonal matrix elements are given by,

$$h_{pq}^V = \frac{1}{a}\int e^{i\frac{2\pi(q-p)}{a}x}v(x)dx \tag{12}$$

Now adding $h_{pp}^V$ and $h_{pq}^V$ to $h^0$, we have $h^V = h^0 + h_{pp}^V + h_{pq}^V$

### 3.3 Fill kinetic elements for a fixed k-value

We have to diagonalize $h$ repeatedly in the range $-\pi < ka < \pi$ to get a band structure solution. For a fixed k-value, the Hamiltonian matrix, $h = h^T + h^V$ where $h_{pq}^T = \delta_{pq}(2p + \frac{ka}{\pi})^2$ and if we diagonalize $h$, we will get $N$ eigenvalues corresponding to $N$ bands and we have to sort them.

### 3.4 Repeat diagonalization for all k-values

If we want to repeat diagonalization $n$ times, then we have $(n+1)$ number of k-values like,

| (band index,k-index) | $k_1$ | $k_2$ | $k_3$ | .... | $k_{n+1}$ |
|---|---|---|---|---|---|
| 1 | $E_{11}$ | $E_{12}$ | $E_{13}$ | .... | $E_{1n+1}$ |
| 2 | $E_{21}$ | $E_{22}$ | $E_{23}$ | .... | $E_{2n+1}$ |
| 1 | $E_{11}$ | $E_{12}$ | $E_{13}$ | .... | $E_{1n+1}$ |
| : | : | : | : | .... | : |
| N | $E_{N1}$ | $E_{N2}$ | $E_{N3}$ | .... | $E_{Nn+1}$ |

Table 2: All sorted energy eigenvalues

### 3.5 Plot

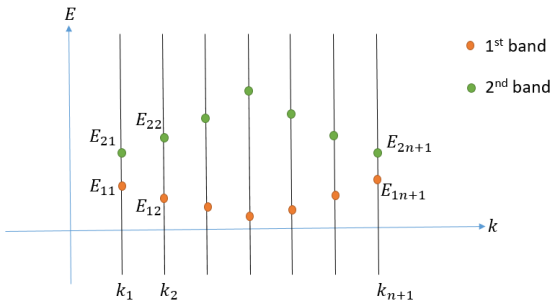



Figure 1: E-k plot

Actually, we aim to plot here $E/\epsilon_1^{(0)}$ versus $\frac{ka}{\pi}$ in the range $[-1, 1]$.

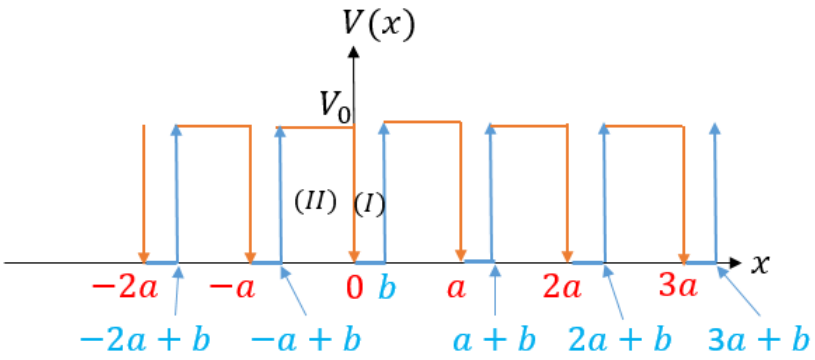
## 4 Arbitrary Periodic Potentials

### 4.1 Kroning Penney Potential

The motion of the electron in Kroning Penney potential given by,

$$V = V_0 \sum_{n=-\infty}^{n=+\infty} \Theta[x - (na + b)]\Theta[(n+1)a - x] \tag{13}$$

It is a periodic array of rectangular potential wells and barriers. The potential can be shown as




The potential can be written as for $n = 0$,

$$\begin{aligned} & V(x) \\ & = V_0(\Theta[x-b]\Theta[a-x]) \\ & = 0 \text{ for } 0 < x < b \\ & = V_0 \text{ for } b < x < a \end{aligned} \tag{14}$$

The dimensionless form of it,

$$\begin{aligned} & v(x) \\ & = \frac{V(x)}{\epsilon_1^{(0)}} \\ & = 0 \text{ for } 0 < x < b \\ & = \frac{V_0}{\frac{\pi^2\hbar^2}{2ma^2}} \text{ for } b < x < a \end{aligned} \tag{15}$$

Taking $a$ in $\mathring{\text{A}}$ and $V_0$ in $eV$, we have $\eta = \frac{V_0}{\epsilon_1^{(0)}} = 0.0103198 V_0 a^2$

Choosing a Python 3.0 language, our script will be like,

```
#packages
import numpy as np
import matplotlib.pyplot as plt
from scipy.integrate import quad

#basis limit
N_ = int(input('Basis limit: '))
N = 2*N_+1

#parameters
a = float(input('a in A: '))
V0=float(input('V0 in eV: '))
rho=float(input('b/a = rho: '))

b = rho * a
eta = 0.0103198 * V0 * (a ** 2)
fac = 10 ** (-10)

#sequence and basis array
seq_arr=np.array([i*(-1)**i for i in range(N)])
basis_arr=np.array([np.sum(seq_arr[:i+1]) for i in range(N)])
```

Taking the basis limit, $N_- = 2$, we have sequence array $[0, -1, 2, -3, 4]$ and basis array $[0, -1, 1, -2, 2]$ respectively.

```
#create a blank matrix
h = np.zeros((N, N))
```

The null matrix of $5 \times 5$ be like

$$\begin{matrix}[[0,0,0,0,0] \\ [0,0,0,0,0] \\ [0,0,0,0,0] \\ [0,0,0,0,0] \\ [0,0,0,0,0]\end{matrix} \tag{16}$$

```
#create potential elements in unit of eta
def f1(x):
    return 0
def f2(x):
    return 1
def g1(x,p,q):
    return np.exp(complex(0,1)*2*np.pi*(q-p)/(a*fac))*f1(x)
def g2(x,p,q):
    return np.exp(complex(0,1)*2*np.pi*(q-p)/(a*fac))*f2(x)

vpp=(1/(a*fac))*(quad(f1, 0*fac, b*fac)[0]+quad(f2,b*fac,a*fac)[0])
def vpq(p, q):
    return (1/(a*fac))*(quad(g1, 0*fac, b*fac, args=(p, q))[0]+quad(g2, b*fac, a*fac, args=(p, q))[0])
```

All the diagonal elements are the same and it's 0.5, non-diagonal elements are in parallel with diagonal from both sides same, and elements of two lines are different like $(2,1) = (1,2) = (3,2) = (2,3) = (4,3) = (3,4) = (5,4) = (4,5) = 0.4999999999949853$

```
#revised matrix elements and filling potential matrix
h_pot=np.copy(h)
for i in range(N):
    for j in range(N):
        if i==j:
            h_pot[i,j]=eta*vpp
        else:
            h_pot[i,j]=eta*vpq(i,j)
```

For taking $a = 1\mathring{A}$, $V_0 = 100eV$, $\rho = 0.5$, we have filled potential matrix,

$$\begin{bmatrix}
[0.5159899999999999, 0.5159899999948200, 0.5159899999793000, 0.5159899998855100, 0.5159899999172000] \\
[0.5159899999948200, 0.5159899999999999, 0.5159899999948200, 0.5159899999793000, 0.5159899998855100] \\
[0.5159899999793000, 0.5159899999948200, 0.5159899999999999, 0.5159899999948200, 0.5159899999793000] \\
[0.5159899998855100, 0.5159899999793000, 0.5159899999948200, 0.5159899999999999, 0.5159899999948200] \\
[0.5159899999172000, 0.5159899998855100, 0.5159899999793000, 0.5159899999948200, 0.5159899999999999]
\end{bmatrix} \tag{17}$$

```
#iterating for all k-values
iter_=int(input('Number of iterations: '))

E = np.zeros((N, iter_+1))

ka=np.linspace(-np.pi,np.pi,iter_+1)
```

For a specific k-value, there are 5 energy eigenvalues as for the Hamiltonian matrix of order $5 \times 5$. If we have $m$ number of k-values, then we need $m$ arrays, each of order 5 to take all the eigenvalues over iterations. It is insightful to take a k-value always zero, for that we have to take $m = 2n + 1$ where $2n$ is the total number of iterations and symbolically, we can call $n$ as half-number of iterations. Taking $n = 5$, we have 11 k-values, equally spaced in the range between $-\frac{\pi}{a}$ and $\frac{\pi}{a}$. Here we take ka-values for dimensionless, which are in the range between $-\pi$ and $\pi$ i.e. ka = [-3.14159265,-2.51327412,-1.88495559,-1.25663706,-0.62831853,0,0.62831853,1.25663706,1.88495559,2.51327412,3.14159265] and energy eigenvalues blank matrix,

$$\begin{bmatrix}
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0] \\
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0] \\
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0] \\
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0] \\
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0]
\end{bmatrix} \tag{18}$$

```
#filling kinetic energy elements for every k-values and finding eigenvalues array for every k-values and filling blank
↪  energy eigenvalues matrix
for i in range(iter_+1):
    h = np.copy(h_pot)
    for j in range(N):
        h[j, j] = h[j, j] + (2*basis_arr[j]+ka[i]/np.pi)**2
    E_eig = np.linalg.eigvalsh(h)
    E[:, i] = np.sort(np.real(E_eig))
```

After filling all the kinetic energy matrix elements for ka=0, we have a complete Hamiltonian matrix,

$$\begin{bmatrix}
[0.5159899999999999, 0.5159899999948200, 0.5159899999793000, 0.5159899998855100, 0.5159899999172000] \\
[0.5159899999948200, 4.5159900000000004, 0.5159899999948200, 0.5159899999793000, 0.5159899998855100] \\
[0.5159899999793000, 0.5159899999948200, 4.5159900000000004, 0.5159899999948200, 0.5159899999793000] \\
[0.5159899998855100, 0.5159899999793000, 0.5159899999948200, 16.515989999999986, 0.5159899999948200] \\
[0.5159899999172000, 0.5159899998855100, 0.5159899999793000, 0.5159899999948200, 16.515989999999986]
\end{bmatrix} \tag{19}$$

Its eigenvalues are [0.38184751,4,5.0405177,16,17.15758479] and for ka= $\pi$, the complete Hamiltonian matrix,

$$\begin{bmatrix}
[1.5159899999999999, 0.5159899999948200, 0.5159899999793000, 0.5159899998855100, 0.5159899999172000] \\
[0.5159899999948200, 1.5159899999999999, 0.5159899999948200, 0.5159899999793000, 0.5159899998855100] \\
[0.5159899999793000, 0.5159899999948200, 9.5159900000000004, 0.5159899999948200, 0.5159899999793000] \\
[0.5159899998855100, 0.5159899999793000, 0.5159899999948200, 9.5159900000000004, 0.5159899999948200] \\
[0.5159899999172000, 0.5159899998855100, 0.5159899999793000, 0.5159899999948200, 25.515989999999986]
\end{bmatrix} \tag{20}$$

Its eigenvalues are [ 1,1.8840402,9,10.11986826,25.57604154] and for these two ka-values, filled eigenvalues matrix will be,

$$\begin{bmatrix}
[0, 0, 0, 0, 0, 0.38184751, 0, 0, 0, 0, 1.00000] \\
[0, 0, 0, 0, 0, 4.0000000, 0, 0, 0, 0, 1.8840402] \\
[0, 0, 0, 0, 0, 5.0405177, 0, 0, 0, 0, 9.0000000] \\
[0, 0, 0, 0, 0, 16.000000, 0, 0, 0, 0, 10.11986826] \\
[0, 0, 0, 0, 0, 17.15758479, 0, 0, 0, 0, 25.57604154]
\end{bmatrix} \tag{21}$$

```
#plot
bands=int(input('Number of bands: '))
c_map=plt.cm.get_cmap('hsv',bands+1)
for i in range(bands):
    plt.plot(ka/np.pi, E[i],'.',color=c_map(i), markersize=4)
for x_coord in [-1,1]:
    plt.axvline(x=x_coord, color='black', linestyle='--', linewidth=0.5)
plt.xlabel('$Ka/\pi\ \ $$\longrightarrow$')
plt.ylabel('$E/E_1{(0)}\ \ $$\longrightarrow$')
plt.title('Band Structure in Reduced Zone Scheme (RZS) for KPP')
plt.show()
```

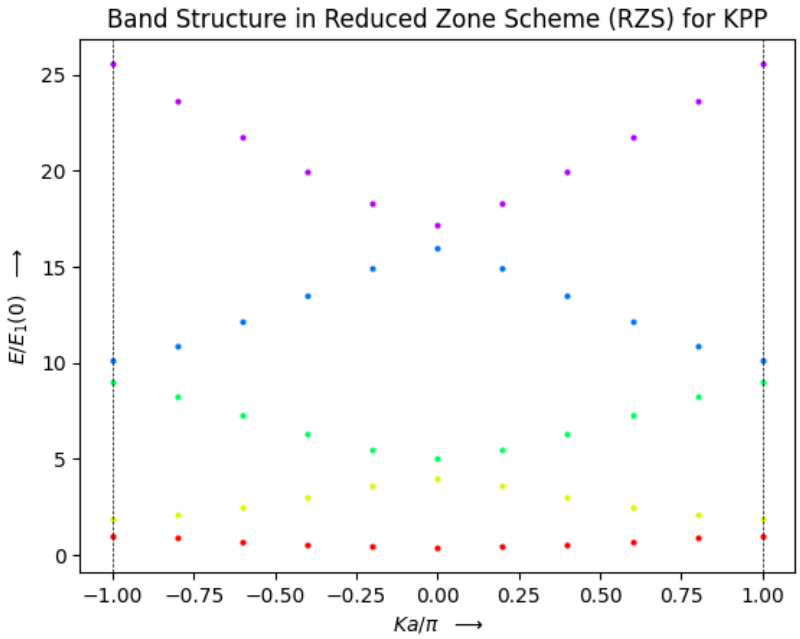



Figure 2: $a = 1\mathring{A}$, $\rho = 0.5$, $V_0 = 100eV$

Now we want to diagonalize h repeatedly in the range $-6\pi < ka < 6\pi$ to get a band structure solution in a periodic zone scheme (PZS) taking basis limit $N_- = 10$ and half-number of iterations=50,

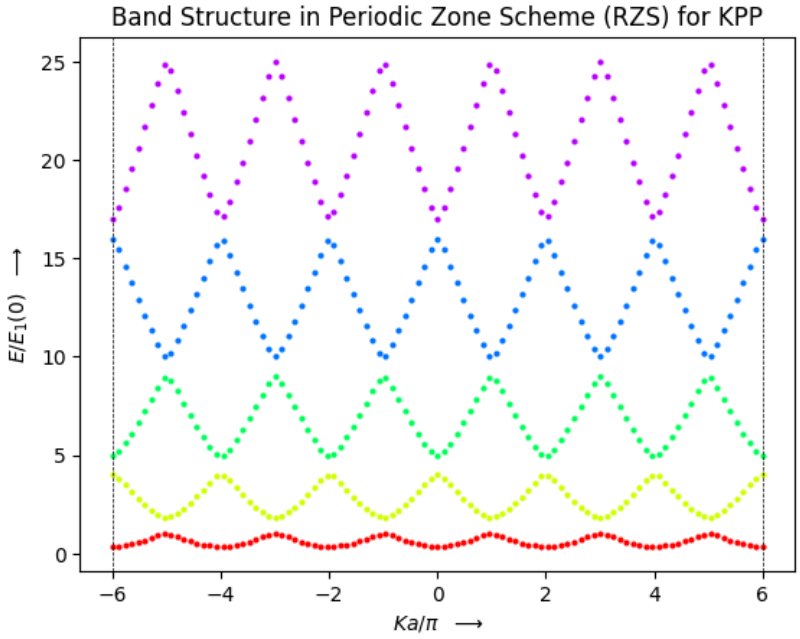



Figure 3: $a = 1\mathring{A}$, $\rho = 0.5$, $V_0 = 100eV$

Input taking:

Basis limit: It gives the matrix size, generally taken a value in the range 20 to 100 to get a more accurate result

a in A: It can generally be taken in order 1

V0 in eV: It can generally be taken in order $10^2$

b/a = rho: It is always less than 1, for zero, b=0
Number of iterations: It takes the number of k-values, more iterations, more points
Number of bands: It can take any value just below 2*(Basis limit)+1
Taking basis limit = 50, number of iterations = 100, and number of bands = 5, we have some outcomes.

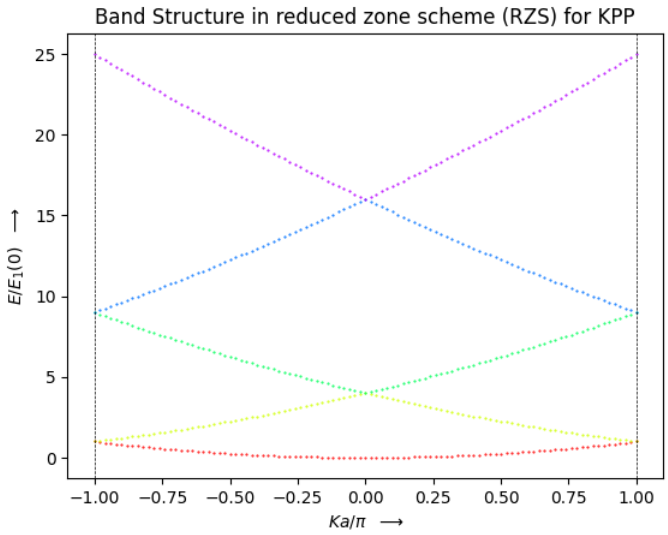



Figure 4: $a = 1\mathring{A}$, $\rho = 0$, $V_0 = 0eV$

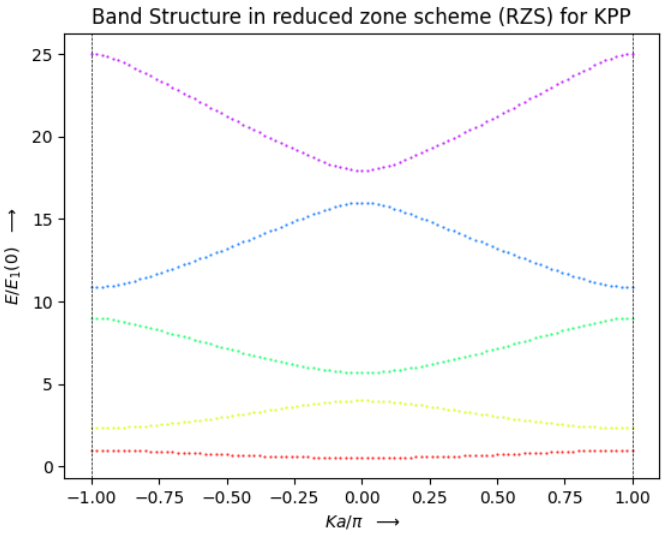



Figure 5: $a = 1\mathring{A}$, $\rho = 0$, $V_0 = 100eV$

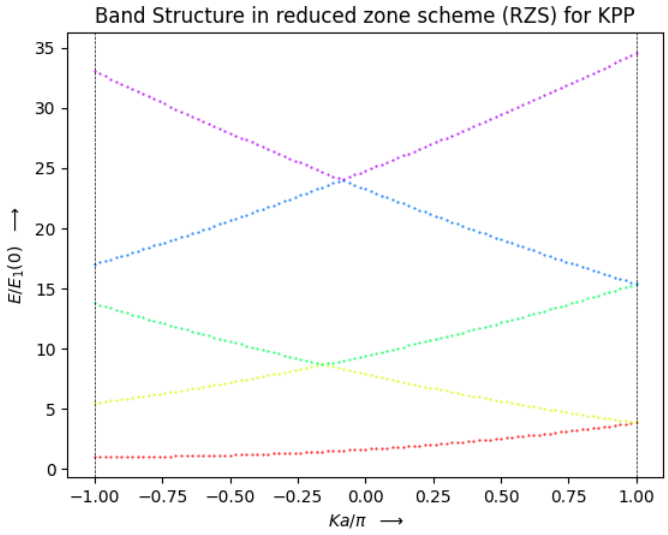



Figure 6: $a = 4\mathring{A}$, $\rho = 0.5$, $V_0 = 100eV$

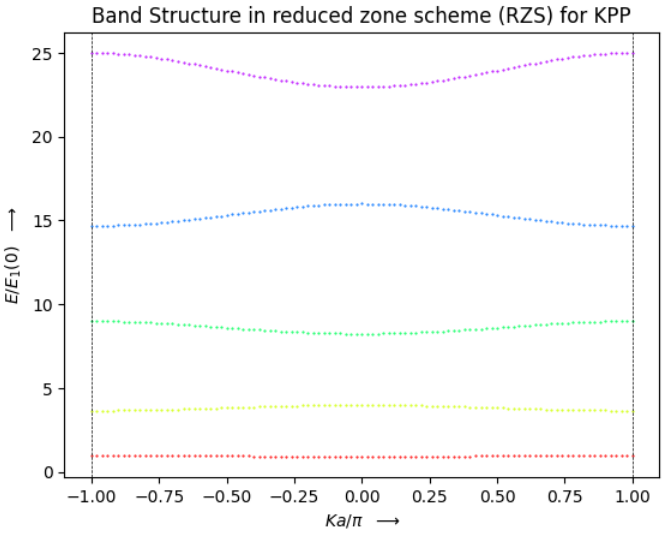



Figure 7: $a = 2\mathring{A}$, $\rho = 0.9$, $V_0 = 1000eV$

We want to diagonalize $h$ repeatedly in the range $-6\pi < ka < 6\pi$ to get a band structure solution in a periodic zone scheme.

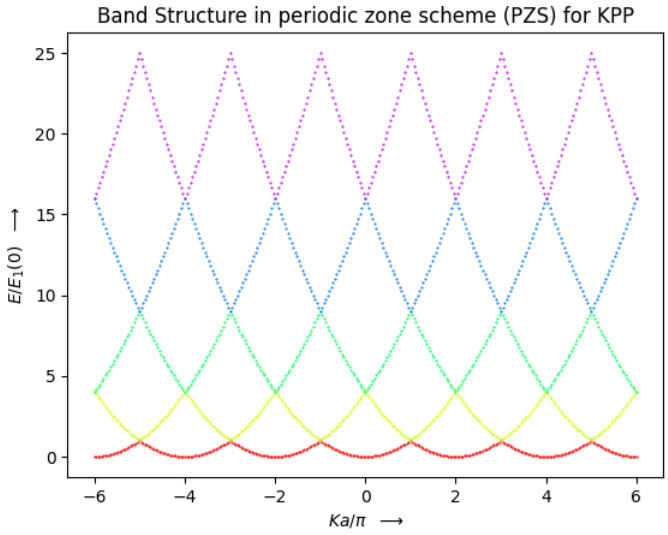



Figure 8: $a = 1\mathring{A}$, $\rho = 0$, $V_0 = 0eV$

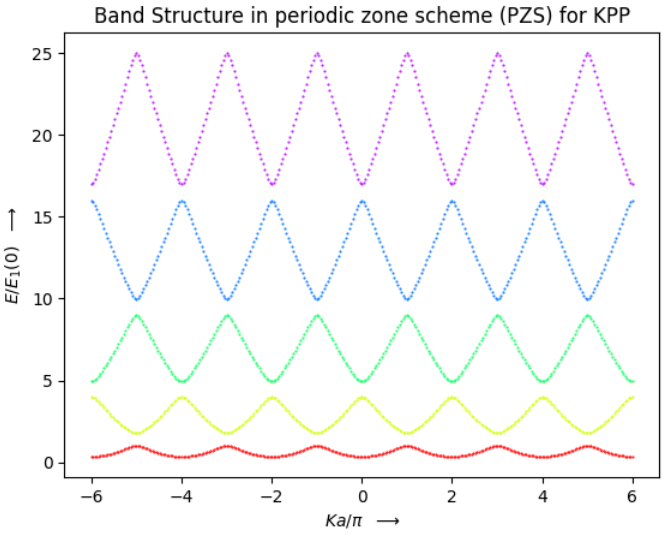



Figure 9: $a = 1\mathring{A}$, $\rho = 0.5$, $V_0 = 100eV$

For the extended zone scheme, we can add a script,

```
colors = ['r', 'y', 'c', 'b', 'm']

for i in range(iter_+1):
    x_values = ka[i] / np.pi
    y_values = E[:, i]

    for band, color in zip(range(1, bands+1), colors):
        plt.plot(x_values, np.where(((x_values >= -band) & (x_values <= -band+1)) |
                                    ((x_values >= band-1) & (x_values <= band)),
                                    y_values[band-1], np.nan), color+'.', markersize=1)

for x_coord in range(-bands, bands+1):
    plt.axvline(x=x_coord, color='black', linestyle='--', linewidth=0.1)

plt.xlabel('$Ka/\pi\ \ $$\longrightarrow$')
plt.ylabel('$E/E_1{(0)}\ \ $$\longrightarrow$')
plt.title('Band Structure in extended zone scheme (EZS) for KPP')
plt.show()
```

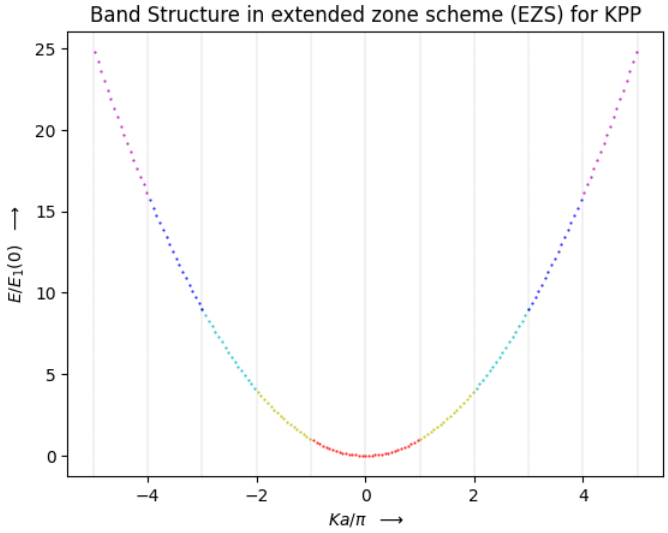



Figure 10: $a = 1\mathring{A}$, $\rho = 0$, $V_0 = 0eV$

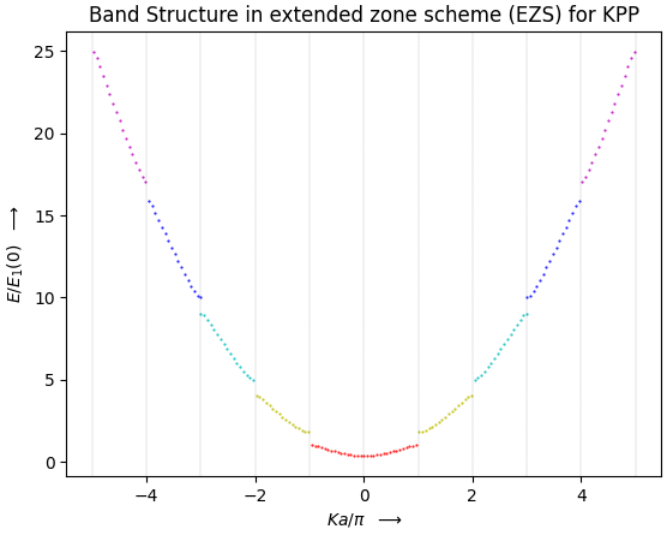
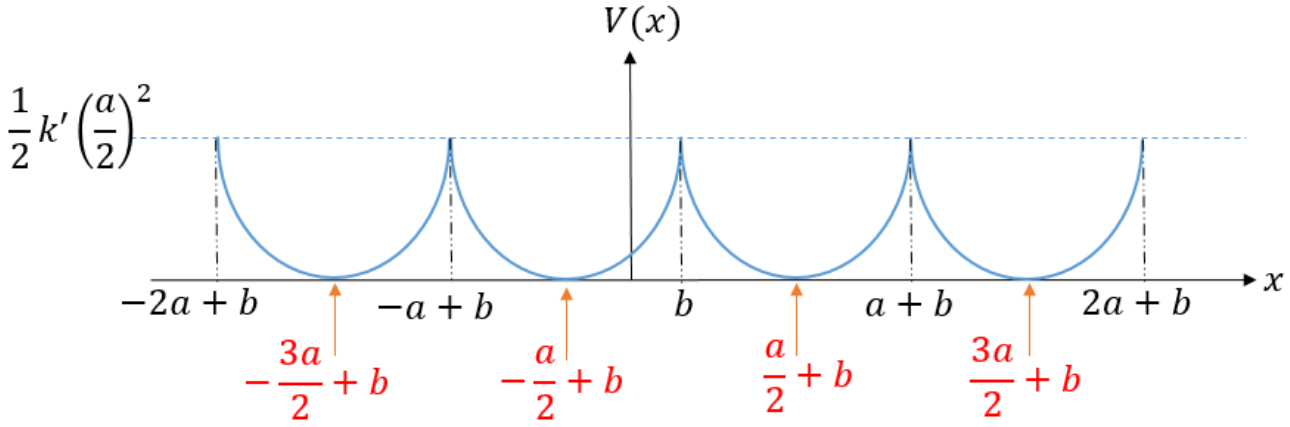



Figure 11: $a = 1\mathring{A}$, $\rho = 0.5$, $V_0 = 100eV$

## 4.2 Periodic parabolic potential (PPP) and Inverted PPP

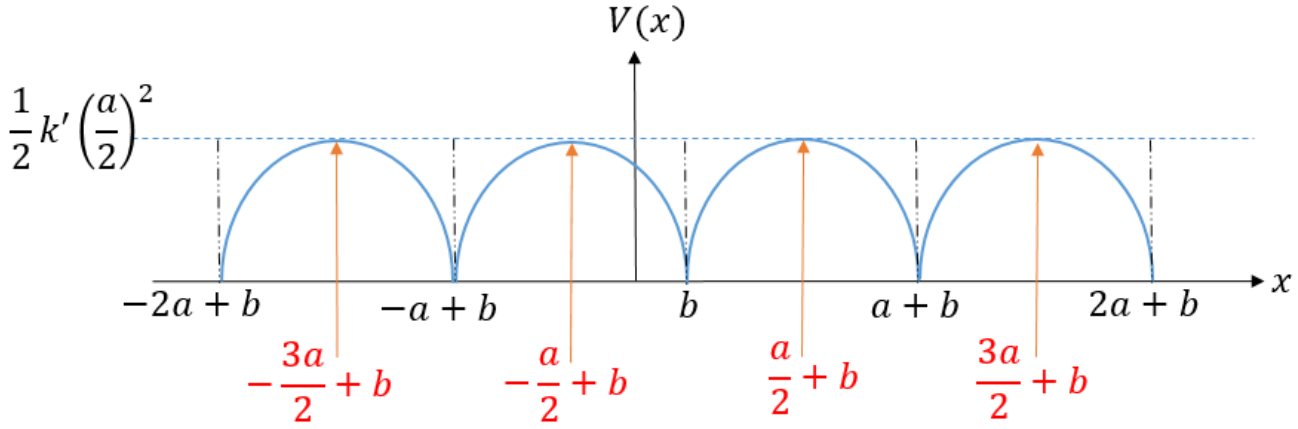
We can draw an asymmetric periodic parabolic potential with the analogy of asymmetric Kroning Penney potential well.




The origin of each parabola can be given by, $x = \frac{(2n-1)}{2}a + b$, and then the endpoints of each parabola can be written as $x = na + b$ and $x = (n-1)a + b$ and to restrict endpoints we will use Heaviside step function.
The potential can be written as,

$$V(x) = \sum_{n=-\infty}^{n=\infty} \frac{1}{2}k' \left(x - \left(\frac{(2n-1)}{2}a + b\right)\right)^2 [-\Theta[x - (na + b)] + \Theta[x - ((n-1)a + b)]] \tag{22}$$

The case of an inverted version of the previous one be like,




The potential can be written as,

$$V(x)=\sum_{n=-\infty}^{n=\infty}\frac{1}{2}k'\left[\left(\frac{a}{2}\right)^2-\left(x-\left(\frac{(2n-1)}{2}a+b\right)\right)^2\right][\Theta[x-(na+b)]-\Theta[x-((n-1)a+b)]] \tag{23}$$

Taking $n=1$, the parabolic and inverted parabolic potentials are,

$$\begin{aligned}&V_{PP}(x)\\&=\frac{1}{2}k'\left(x-\left(\frac{a}{2}+b\right)\right)^2[\Theta(x-b)-\Theta(x-(a+b))]\\&=\frac{1}{2}k'\left(x-\left(\frac{a}{2}+b\right)\right)^2\ \text{for } b<x<a+b\end{aligned} \tag{24}$$

$$\begin{aligned}&V_{IPP}(x)\\&=\frac{1}{2}k'\left[\left(\frac{a}{2}\right)^2-\left(x-\left(\frac{a}{2}+b\right)\right)^2\right][\Theta(x-b)-\Theta(x-(a+b))]\\&=\frac{1}{2}k'\left[\left(\frac{a}{2}\right)^2-\left(x-\left(\frac{a}{2}+b\right)\right)^2\right]\ \text{for } b<x<a+b\end{aligned} \tag{25}$$

Now we aim to get a dimensionless form of these potentials,

$$\begin{aligned}v_{PP}(x)&=\frac{V_{PP}(x)}{\epsilon_1^{(0)}}\\&=\frac{1}{2}\frac{k'}{\epsilon_1^{(0)}}\left(x-\frac{a}{2}-b\right)^2\\&=\frac{1}{2}\frac{m\omega^2a^2}{\epsilon_1^{(0)}}\left(\frac{x}{a}-\frac{1}{2}-\frac{b}{a}\right)^2\ \text{where } \omega^2=\frac{k'}{m}\\&=\frac{\pi^2}{4}\left(\frac{\hbar\omega}{\epsilon_1^{(0)}}\right)^2\left(\frac{x}{a}-\frac{1}{2}-\rho\right)^2\ \text{where } \rho=\frac{b}{a}\\&=\frac{\pi^2}{4}\gamma^2\left(\frac{x}{a}-\frac{1}{2}-\rho\right)^2\ \text{where } \gamma=\frac{\hbar\omega}{\epsilon_1^{(0)}}\end{aligned} \tag{26}$$

$$v_{IPP}(x)=\frac{\pi^2}{4}\gamma^2\left[\left(\frac{1}{2}\right)^2-\left(\frac{x}{a}-\frac{1}{2}-\rho\right)^2\right] \tag{27}$$

Taking $a$ in $\mathring{A}$ and $k'$ in $kN/m$, we have $\gamma = 0.582\sqrt{k'}a^2$ and here are some outcomes,

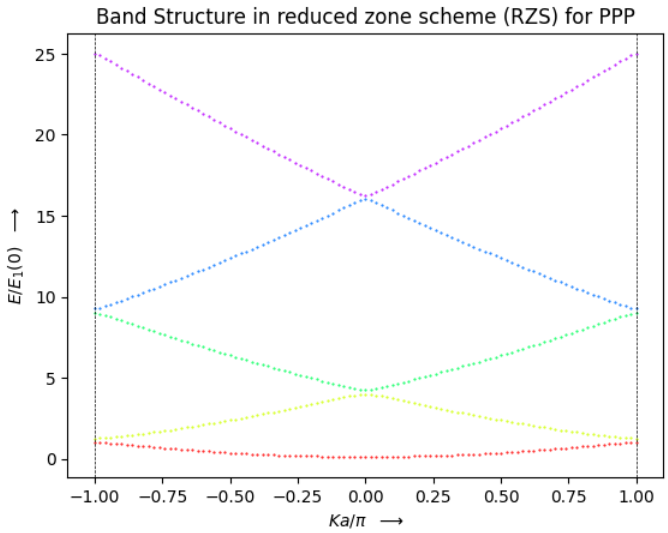



Figure 12: $\rho = 0$, $k' = 2kN/m$, $a = 1\mathring{A}$

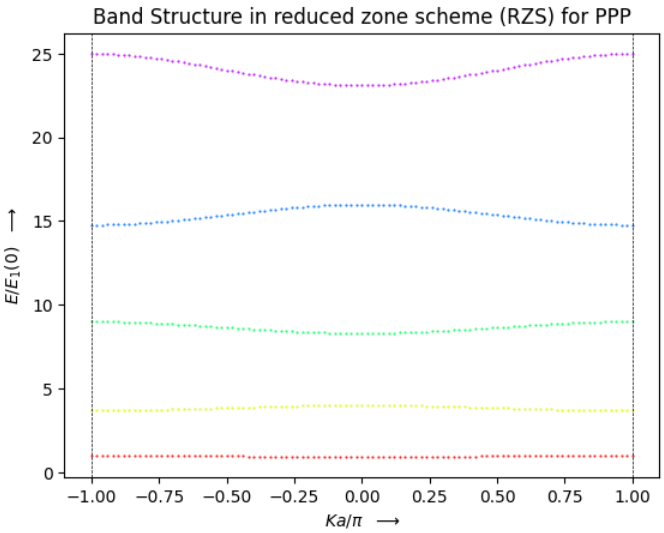



Figure 13: $\rho = 0.5$, $k' = 1kN/m$, $a = 2\mathring{A}$

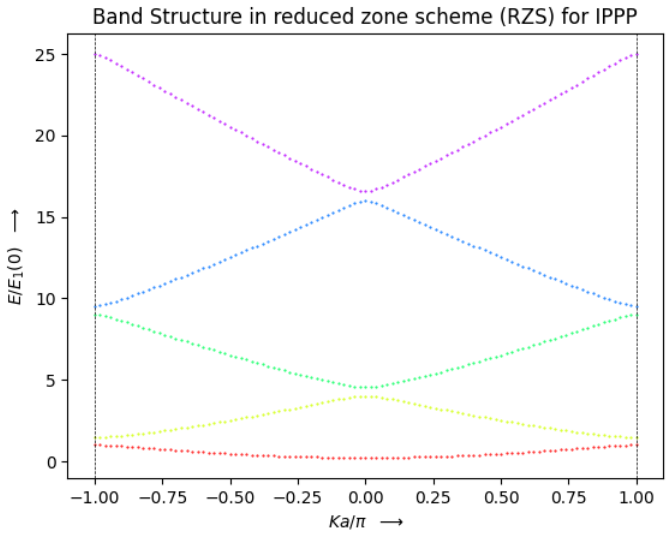



Figure 14: $\rho = 0$, $k' = 2kN/m$, $a = 1\mathring{A}$

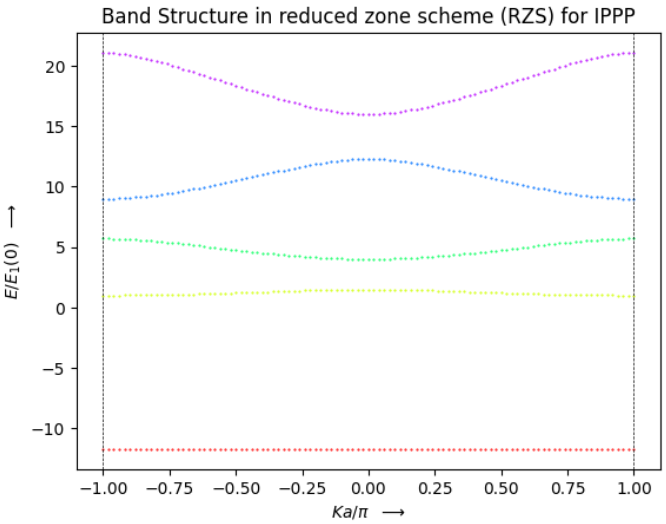
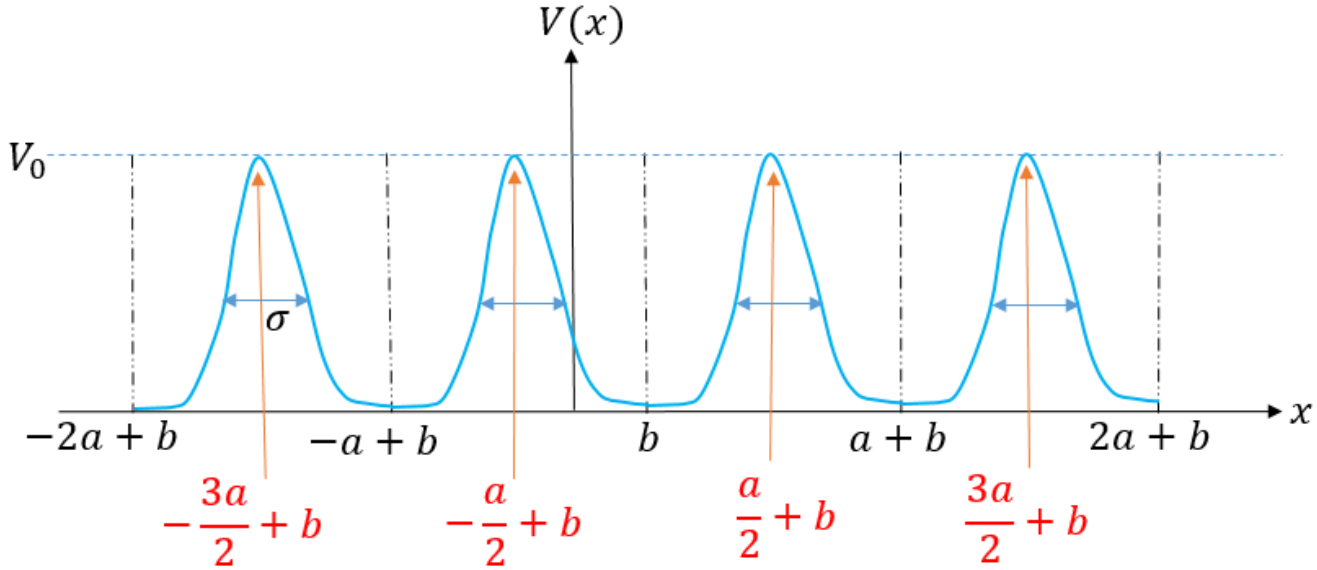



Figure 15: $\rho = 0.5$, $k' = 1kN/m$, $a = 2\mathring{A}$

## 4.3 Periodic Gaussian potential (PGP) and Inverted PGP

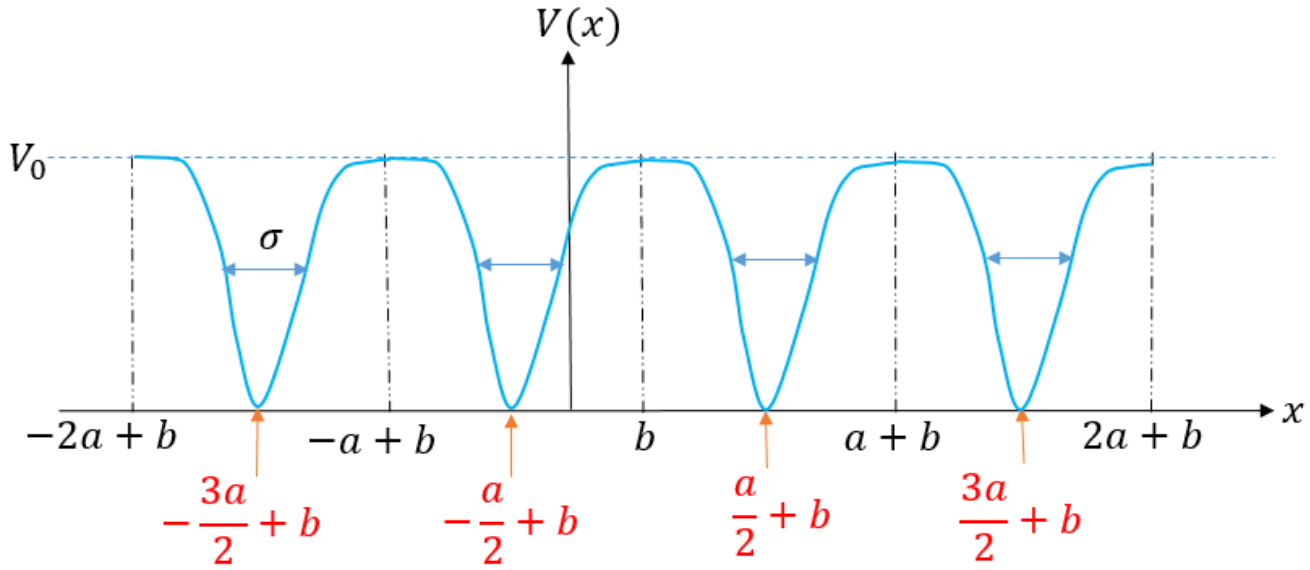
An asymmetric periodic Gaussian potential will be like



The origin of each Gaussian can be given by, $x = \mu = \frac{(2n-1)}{2}a + b$, and then the endpoints of each Gaussian can be written as $x = na + b$ and $x = (n-1)a + b$ and to restrict endpoints we will use Heaviside step function.
The potential can be written as,

$$V(x) = \sum_{n=-\infty}^{n=\infty} V_0 \exp\left[-\frac{\left(x - \left(\frac{(2n-1)}{2}a + b\right)\right)^2}{\sigma^2}\right][-\Theta[x - (na+b)] + \Theta[x - ((n-1)a+b)]] \tag{28}$$

The case of an inverted version of the previous one be like,




The potential can be written as,

$$V(x) = \sum_{n=-\infty}^{n=\infty} V_0 \left[1 - \exp\left[-\frac{\left(x - \left(\frac{(2n-1)}{2}a + b\right)\right)^2}{\sigma^2}\right]\right][-\Theta[x - (na+b)] + \Theta[x - ((n-1)a+b)]] \tag{29}$$

Taking $n = 1$, the Gaussian and inverted Gaussian potentials are,

$$\begin{aligned} &V_{GP}(x) \\ &\quad = V_0 \exp\left[-\frac{(x - (\frac{a}{2} + b))^2}{\sigma^2}\right][-\Theta[x - (a+b)] + \Theta[x - b]] \\ &\quad = V_0 \exp\left[-\frac{(x - (\frac{a}{2} + b))^2}{\sigma^2}\right] \text{ for } b < x < a + b \end{aligned} \tag{30}$$

$$\begin{aligned} &V_{IGP}(x) \\ &\quad = V_0 \left[1 - \exp\left[-\frac{(x - (\frac{a}{2} + b))^2}{\sigma^2}\right]\right][-\Theta[x - (a+b)] + \Theta[x - b]] \\ &\quad = V_0 \left[1 - \exp\left[-\frac{(x - (\frac{a}{2} + b))^2}{\sigma^2}\right]\right] \text{ for } b < x < a + b \end{aligned} \tag{31}$$

Now we aim to get a dimensionless form of these potentials,

$$\begin{aligned} v_{GP}(x) &= \frac{V_{GP}(x)}{\epsilon_1^{(0)}} \\ &= \frac{V_0}{\epsilon_1^{(0)}} \exp\left[-\left(\frac{a}{\sqrt{2}\sigma}\right)^2 \left(\frac{x}{a} - \frac{1}{2} - \rho\right)^2\right] \end{aligned} \tag{32}$$

$$v_{IGP}(x) = \frac{V_0}{\epsilon_1^{(0)}} \left[1 - \exp\left[-\left(\frac{a}{\sqrt{2}\sigma}\right)^2 \left(\frac{x}{a} - \frac{1}{2} - \rho\right)^2\right]\right] \tag{33}$$

Taking $a$ , $\sigma$ in $\mathring{\text{A}}$ and $V_0$ in $eV$, we have $\eta = \frac{V_0}{\epsilon_1^{(0)}} = 0.0103198 V_0 a^2$and here are some outcomes,

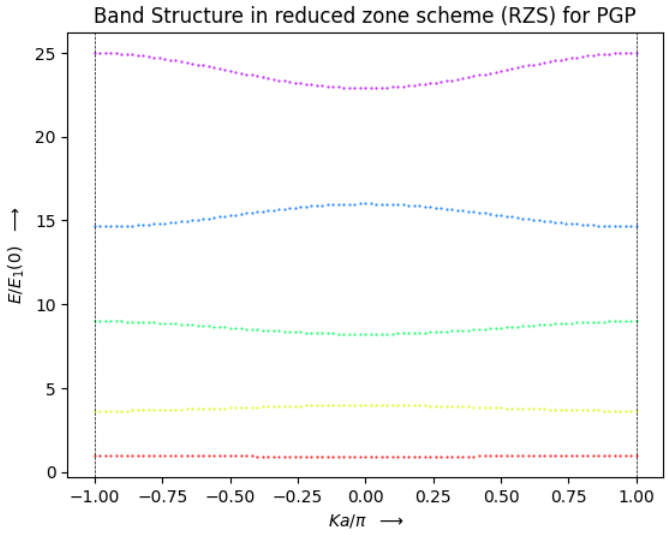



Figure 16: $\rho = 0.5$, $\sigma = 5\mathring{\text{A}}$, $a = 2\mathring{\text{A}}$, $V_0 = 100eV$

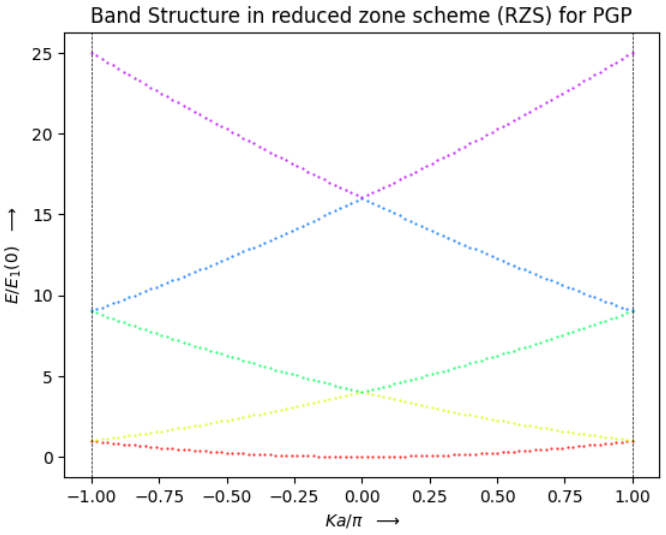



Figure 17: $\rho = 0$, $\sigma = 0.001\mathring{\text{A}}$, $a = 1\mathring{\text{A}}$, $V_0 = 1000eV$

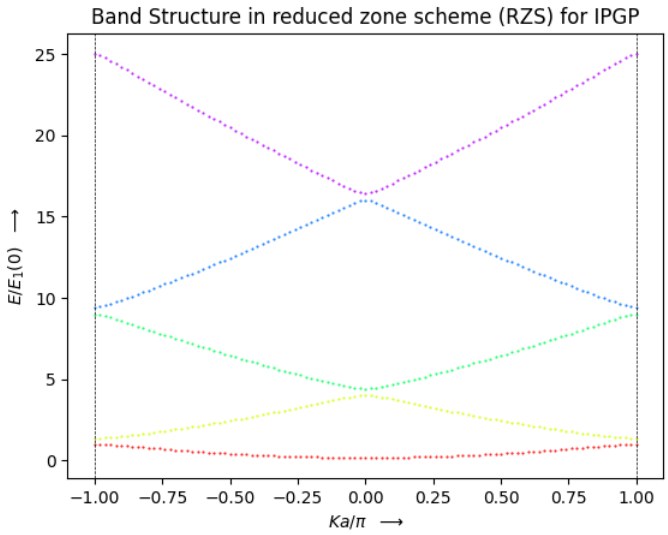



Figure 18: $\rho = 0.5$, $\sigma = 5\mathring{\text{A}}$, $a = 2\mathring{\text{A}}$, $V_0 = 100eV$

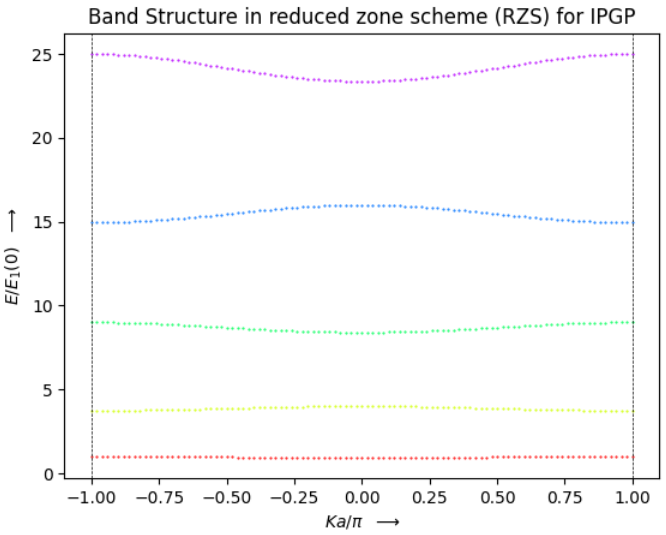
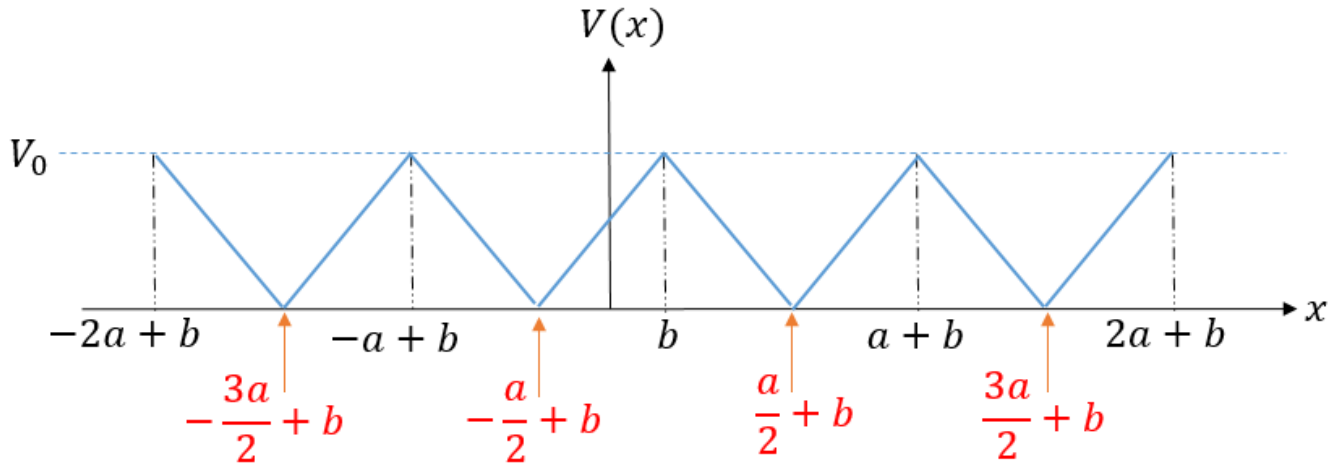



Figure 19: $\rho = 0$, $\sigma = 0.001\mathring{\text{A}}$, $a = 1\mathring{\text{A}}$, $V_0 = 1000eV$

## 4.4 Periodic linear potential (PLP)

An asymmetric periodic linear potential will be like




The zero-point of each V-shaped can be given by, $x = \frac{(2n-1)}{2}a + b$, and then the endpoints of each V-shaped can be written as $x = na + b$ and $x = (n-1)a + b$ and to restrict endpoints we will use Heaviside step function.
The potential can be written as,

$$V(x) = \sum_{n=-\infty}^{n=\infty} V_0 \left| \frac{x - ((n-1)a + b)}{\frac{a}{2}} - 1 \right| [-\Theta[x - (na + b)] + \Theta[x - ((n-1)a + b)]] \tag{34}$$

Taking $n = 1$, the linear potential will be,

$$\begin{aligned} V_{LP}(x) & \\ &= V_0 \left| \frac{x - b}{\frac{a}{2}} - 1 \right| [-\Theta[x - (a + b)] + \Theta[x - b]] \\ &= -V_0 \left( \frac{x - b}{\frac{a}{2}} - 1 \right) \text{ for } b < x < \frac{a}{2} + b \\ &= +V_0 \left( \frac{x - b}{\frac{a}{2}} - 1 \right) \text{ for } \frac{a}{2} + b < x < a + b \end{aligned} \tag{35}$$

Now we aim to get a dimensionless form of this potential,

$$\begin{aligned} v_{LP}(x) = & \frac{V_{LP}(x)}{\epsilon_1^{(0)}} \\ &= -\frac{V_0}{\epsilon_1^{(0)}} \left( 2\frac{x}{a} - 2\rho - 1 \right) \text{ for } b < x < \frac{a}{2} + b \text{ and } \rho = \frac{b}{a} \\ &= +\frac{V_0}{\epsilon_1^{(0)}} \left( 2\frac{x}{a} - 2\rho - 1 \right) \text{ for } \frac{a}{2} + b < x < a + b \end{aligned} \tag{36}$$

Taking $a$ in $\mathring{\text{A}}$ and $V_0$ in $eV$, we have $\eta = \frac{V_0}{\epsilon_1^{(0)}} = 0.0103198 V_0 a^2$ and here are some outcomes,

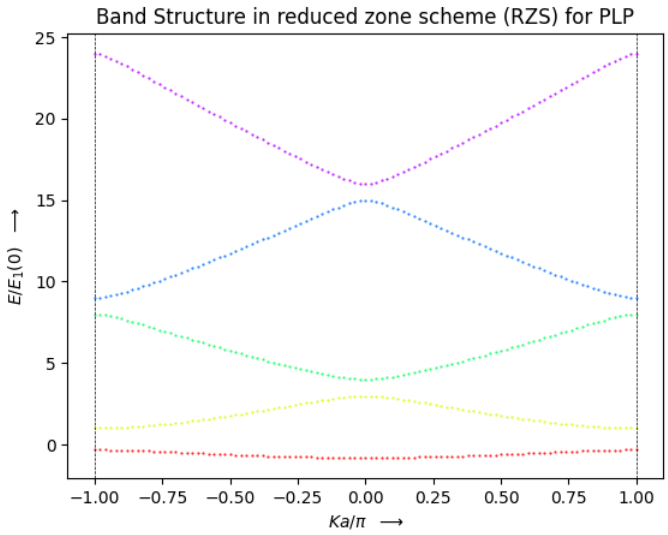



Figure 20: $\rho = 0.9$, $a = 1\mathring{\text{A}}$, $V_0 = 100eV$

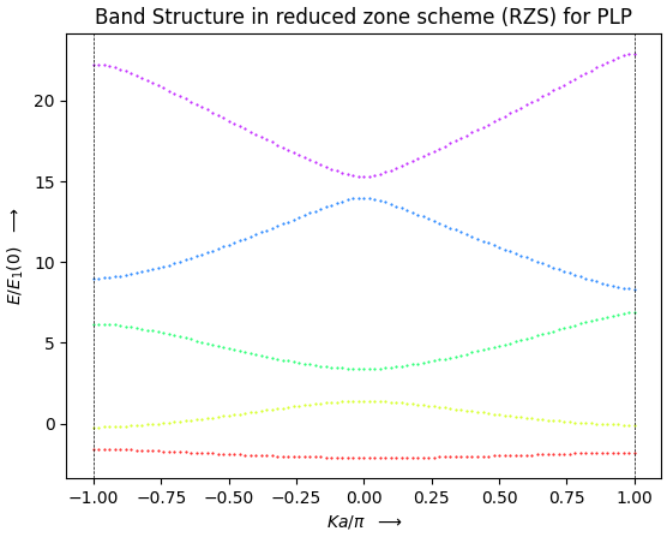
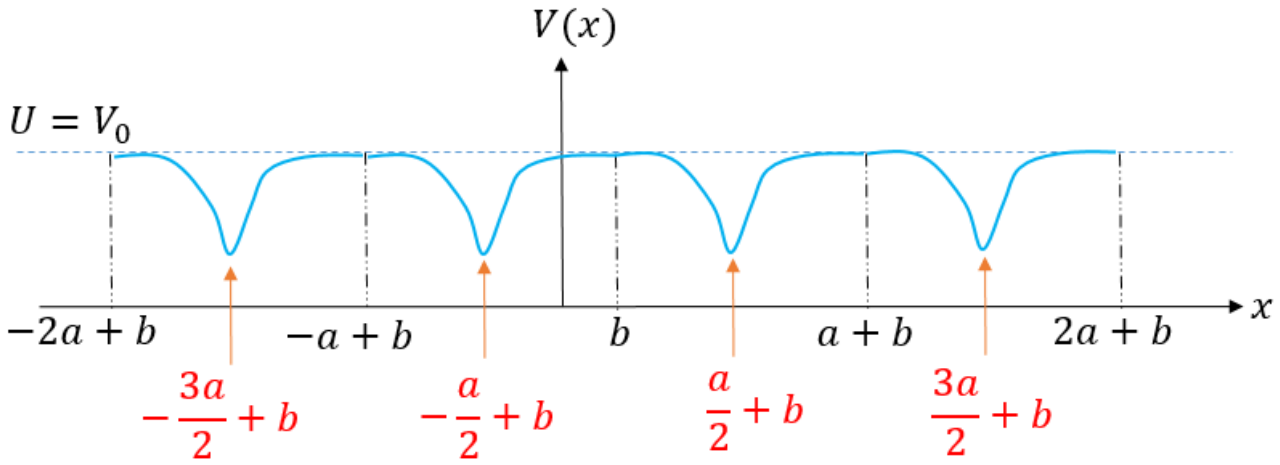



Figure 21: $\rho = 0$, $a = 3\mathring{\text{A}}$, $V_0 = 10eV$

## 4.5 Periodic pseudo-Coulomb potential (PpCP)

The so-called pseudo-Coulomb potential is given by $V'(x) = -\frac{A}{\sqrt{(x-\alpha)^2+\beta^2}}$ and the true Coulomb potential can recovered using $\beta = 0$. The parameter $\beta$ controls the depth of the wells. By shifting the potential, above the x-axis, it is given by, $V(x) = U - \frac{A}{\sqrt{(x-\alpha)^2+\beta^2}}$. An asymmetric periodic pseudo-Coulomb potential will be like




The potential can be written as,

$$V(x) = \sum_{n=-\infty}^{n=\infty} V_0 \left[1 - \frac{a}{\sqrt{(x - (\frac{(2n-1)}{2}a + b))^2 + \beta^2}}\right] [-\Theta[x - (na + b)] + \Theta[x - ((n-1)a + b)]] \tag{37}$$

Taking $n = 1$, the pseudo-Coulomb potential will be,

$$\begin{aligned} &V_{pCP}(x) \\ &\quad = V_0 \left[1 - \frac{a}{\sqrt{(x - \frac{a}{2} - b)^2 + \beta^2}}\right] [-\Theta[x - (a + b)] + \Theta[x - b]] \\ &\quad = V_0 \left[1 - \frac{a}{\sqrt{(x - \frac{a}{2} - b)^2 + \beta^2}}\right] \text{ for } b < x < a + b \end{aligned} \tag{38}$$

Now we aim to get a dimensionless form of these potentials,

$$\begin{aligned} v_{pCP}(x) &= \frac{V_{pCP}(x)}{\epsilon_1^{(0)}} \\ &= \eta \left(1 - \frac{1}{\sqrt{(\frac{x}{a} - \frac{1}{2} - \rho)^2 + (\frac{\beta}{a})^2}}\right) \end{aligned} \tag{39}$$

for $\eta = \frac{V_0}{\epsilon_1^{(0)}}$ and $\rho = \frac{b}{a}$ and taking $a$ and $\beta$ in $\mathring{A}$ and $V_0$ in $eV$, we have $\eta = \frac{V_0}{\epsilon_1^{(0)}} = 0.0103198 V_0 a^2$and here are some outcomes,

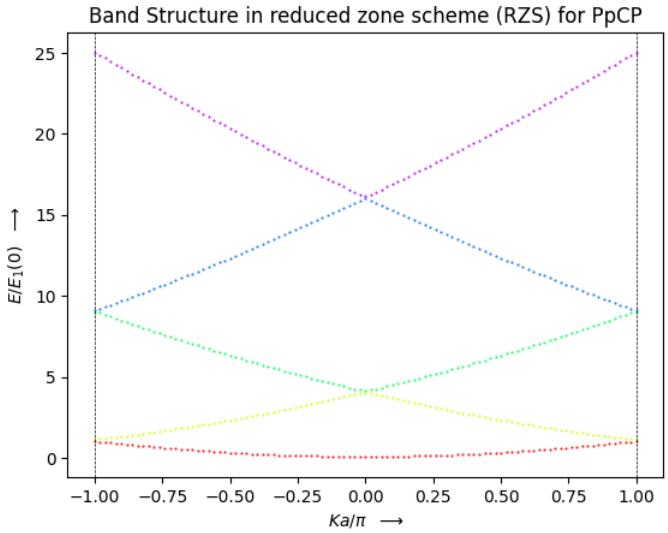



Figure 22: $\rho = 0$, $\beta = 1\mathring{A}$, $a = 1\mathring{A}$, $V_0 = 200eV$

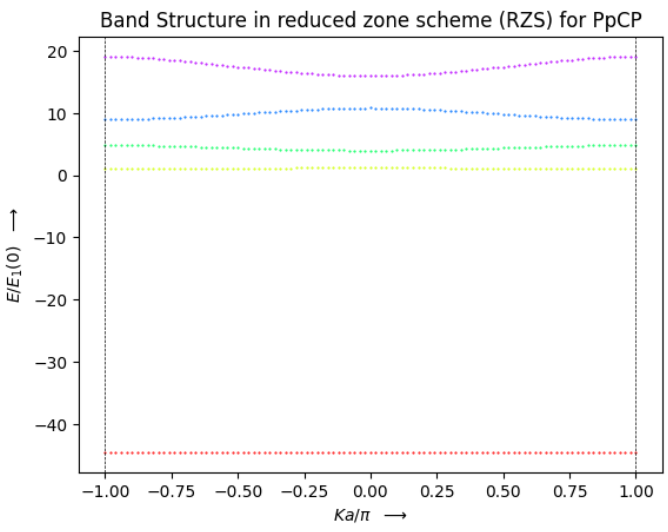



Figure 23: $\rho = 0.5$, $\sigma = 0.01\mathring{A}$, $a = 1\mathring{A}$, $V_0 = 100eV$

## Conclusion

We have completed the algorithm and code for a computer model to find band structure solutions of arbitrary one-dimensional periodic potentials. Similarly, we can extend this to two and three-dimensional cases and apply it to two and three-dimensional lattices. This extension will be more important for studying particles in periodic potentials.

## Acknowledgement

I express my heartfelt gratitude to my classmate Jishnu Patra (IIT Delhi) for his help in the design of the matrix structure, especially the sequence and basis array.

## Reference

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