Run on Google Colab View on Github

Imports

In [1]:
```python
import numpy as np
import matplotlib.pyplot as plt
from sympy import *
```

Defining a Function to get the energy corresponding to a given K.

In [2]:
```python
def give_energy(K, h=1, m=1):
    """
    This function calculates the energy of a particle in a potential
    field.
    """
    return (h**2*K**2)/(2*m)

give_energy = np.vectorize(give_energy)
```

Solution

Defining the Matrix

The final matrix, that we get is:

$$M = \begin{bmatrix} \frac{\hbar^2K^2}{2m} - E & V_{\frac{-2\pi}{a}} & V_{\frac{2\pi}{a}} \\ V_{\frac{2\pi}{a}} & \frac{\hbar^2(K+\frac{2\pi}{a})^2}{2m} - E & V_{\frac{4\pi}{a}} \\ V_{\frac{-2\pi}{a}} & V_{\frac{-4\pi}{a}} & \frac{\hbar^2(K-\frac{2\pi}{a})^2}{2m} - E \end{bmatrix}$$

We need to diagonalize this, namely, we need to find E such that

$$det(M) = 0$$

In [3]:
```python
#Setting the variables
E = Symbol('E')
Vp = Symbol('V', complex=True)
Vm = Vp.conjugate()
Vpp = Symbol('Vp', complex=True)
Vmm = Vpp.conjugate()
E0 = Symbol('E0')
Ep = Symbol('Ep')
Em = Symbol('Em')
```

In [4]:
```python
#Creating the matrix
mat = Matrix([[E0-E, Vm, Vp], [Vm, Ep-E, Vpp], [Vp, Vmm, Em-E]])
mat
```

Out[4]:

$$\begin{bmatrix} -E + E_0 & \overline{V} & V \\ \overline{V} & -E + Ep & Vp \\ V & \overline{Vp} & -E + Em \end{bmatrix}$$

Here for simplicity, I have used:

$$E_0 = \frac{\hbar^2K^2}{2a^2}$$

$$E_p = \frac{\hbar^2(K + \frac{2\pi}{a})^2}{2a^2}$$

$$E_m = \frac{\hbar^2(K - \frac{2\pi}{a})^2}{2a^2}$$

$$V = V_{\frac{-2\pi}{a}}$$

$$\bar{V} = V_{\frac{2\pi}{a}}$$

$$V_p = V_{\frac{4\pi}{a}}$$

$$\bar{V}_p = V_{\frac{-4\pi}{a}}$$

Solving for E

If I solve the equation symbolically for E, I'll get a HUGE expression for E. To make the expression smaller, I'll set the values of V and V_P to be equal to 1.

In [5]:
```python
#Getting the determinant
eq = mat.det()
#Substituting Vp = Vpp =1 to simplify the equation
eq = eq.subs(Vp, 1)
eq = eq.subs(Vpp, 1)
eq
```

Out[5]:

$$-E^3 + E^2E_0 + E^2Em + E^2Ep - EE_0Em - EE_0Ep - EEmEp + 3E + E_0EmEp - E_0 - Em - Ep + 2$$

Now, I need to solve for E in terms of E_0, E_M and E_P.

In [6]:
```python
Es = solve(eq, E)
len(Es)
```

Out[6]: 3

Since the equation was third order, we should get three different solutions of E. As we can see from the output of the above cell, `len(Es)` is indeed 3. Let's see what these three solutions are:

First Solution

In [7]:
```python
E1 = Es[0]
E1
```

Out[7]:

$$\frac{E_0}{3} + \frac{Em}{3} + \frac{Ep}{3} - \frac{-3E_0Em - 3E_0Ep - 3EmEp + (-E_0 - Em - Ep)^2 + 9}{3\sqrt[3]{-\frac{27E_0EmEp}{2} + \frac{27E_0}{2} + \frac{27Em}{2} + \frac{27Ep}{2} + \frac{\sqrt{-4\left(-3E_0Em-3E_0Ep-3EmEp+(-E_0-Em-Ep)^2+9\right)^3 + \left(-27E_0EmEp+27E_0+27Em+27Ep-(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)+2(-E_0-Em-Ep)^3-54\right)^2}}{2} - \frac{(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)}{2} + (-E_0 - Em - Ep)^3 - 27}} - \frac{\sqrt[3]{-\frac{27E_0EmEp}{2} + \frac{27E_0}{2} + \frac{27Em}{2} + \frac{27Ep}{2} + \frac{\sqrt{-4\left(-3E_0Em-3E_0Ep-3EmEp+(-E_0-Em-Ep)^2+9\right)^3 + \left(-27E_0EmEp+27E_0+27Em+27Ep-(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)+2(-E_0-Em-Ep)^3-54\right)^2}}{2} - \frac{(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)}{2} + (-E_0 - Em - Ep)^3 - 27}}{3}$$

Second Solution

In [8]:
```python
E2 = Es[1]
E2
```

Out[8]:

$$\frac{E_0}{3} + \frac{Em}{3} + \frac{Ep}{3} - \frac{-3E_0Em - 3E_0Ep - 3EmEp + (-E_0 - Em - Ep)^2 + 9}{3\left(-\frac{1}{2} - \frac{\sqrt{3}i}{2}\right)\sqrt[3]{-\frac{27E_0EmEp}{2} + \frac{27E_0}{2} + \frac{27Em}{2} + \frac{27Ep}{2} + \frac{\sqrt{-4\left(-3E_0Em-3E_0Ep-3EmEp+(-E_0-Em-Ep)^2+9\right)^3 + \left(-27E_0EmEp+27E_0+27Em+27Ep-(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)+2(-E_0-Em-Ep)^3-54\right)^2}}{2} - \frac{(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)}{2} + (-E_0 - Em - Ep)^3 - 27}} - \frac{\left(-\frac{1}{2} - \frac{\sqrt{3}i}{2}\right)\sqrt[3]{-\frac{27E_0EmEp}{2} + \frac{27E_0}{2} + \frac{27Em}{2} + \frac{27Ep}{2} + \frac{\sqrt{-4\left(-3E_0Em-3E_0Ep-3EmEp+(-E_0-Em-Ep)^2+9\right)^3 + \left(-27E_0EmEp+27E_0+27Em+27Ep-(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)+2(-E_0-Em-Ep)^3-54\right)^2}}{2} - \frac{(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)}{2} + (-E_0 - Em - Ep)^3 - 27}}{3}$$

Third Solution

In [9]:
```python
E3  = Es[2]
E3
```

Out[9]:

$$\frac{E_0}{3} + \frac{Em}{3} + \frac{Ep}{3} - \frac{-3E_0Em - 3E_0Ep - 3EmEp + (-E_0 - Em - Ep)^2 + 9}{3\left(-\frac{1}{2} + \frac{\sqrt{3}i}{2}\right)\sqrt[3]{-\frac{27E_0EmEp}{2} + \frac{27E_0}{2} + \frac{27Em}{2} + \frac{27Ep}{2} + \frac{\sqrt{-4\left(-3E_0Em-3E_0Ep-3EmEp+(-E_0-Em-Ep)^2+9\right)^3 + \left(-27E_0EmEp+27E_0+27Em+27Ep-(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)+2(-E_0-Em-Ep)^3-54\right)^2}}{2} - \frac{(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)}{2} + (-E_0 - Em - Ep)^3 - 27}} - \frac{\left(-\frac{1}{2} + \frac{\sqrt{3}i}{2}\right)\sqrt[3]{-\frac{27E_0EmEp}{2} + \frac{27E_0}{2} + \frac{27Em}{2} + \frac{27Ep}{2} + \frac{\sqrt{-4\left(-3E_0Em-3E_0Ep-3EmEp+(-E_0-Em-Ep)^2+9\right)^3 + \left(-27E_0EmEp+27E_0+27Em+27Ep-(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)+2(-E_0-Em-Ep)^3-54\right)^2}}{2} - \frac{(-9E_0-9Em-9Ep)(E_0Em+E_0Ep+EmEp-3)}{2} + (-E_0 - Em - Ep)^3 - 27}}{3}$$

The solutions are still quite big and complex. The reason behind this is that `sympy` is not very good at simplifying expressions.

Plotting the Energy Curves

Final step is evaluating the energy of the system by substituting the values of E_P, E_M and E_0 into the equation. We already have a function `give_energy` that returns the energy E, given k, m and a. By default, $m = a = 1$. We'll use this defualt values. However, we can easily pass m and a as arguments to the function to change the default values.

In [10]:
```python
def substitute(E, K, **kwargs):
    """
    Takes one value of E and returns numerical value of E after making all the substit
    for a specific K value
    """
    #Substituing E0
    E_num = E.subs(E0, give_energy(K=K, **kwargs))
    #Substituing Ep which is nothing but E0 with K= K + G and as G = 2*pi, so K = K +
    E_num = E_num.subs(Ep, give_energy(K=K+2*np.pi, **kwargs))
    #Substituing Em which is nothing but E0 with K= K - G and as G = 2*pi, so K = K -
    E_num = E_num.subs(Em, give_energy(K=K-2*np.pi, **kwargs))
    E_num = E_num.evalf()
    #Sometimes, we are getting a complex number, with very small imaginary part(ususa
    #because of the precision of the computer. So, we are removing the imaginary part
    E_num = E_num.subs(I, 0)
    return E_num

#Finally, we'll make the function a vectorized function
substitute = np.vectorize(substitute)
```

Let's do a sanity check!

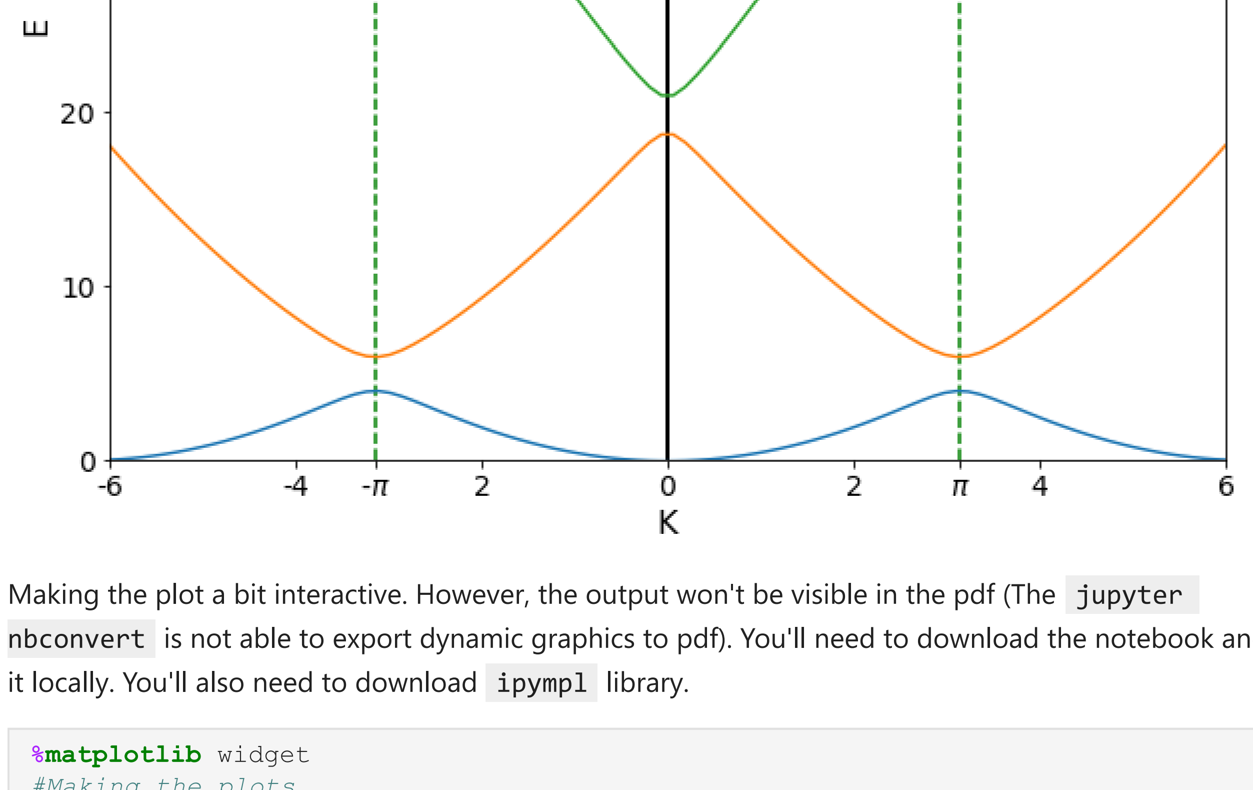
In [11]:
```python
display(substitute(E1, 0.5))
display(substitute(E2, 0.5))
display(substitute(E3, 0.5))
display(substitute(E1, np.pi))
display(substitute(E2, np.pi))
display(substitute(E3, np.pi))
```

```
array(0.0265444478729320, dtype=object)
array(16.6090607554717, dtype=object)
array(23.2178124010128, dtype=object)
array(3.93480220054468, dtype=object)
array(5.88289503360872, dtype=object)
array(44.4651269718381, dtype=object)
```

So, it is working. Let's plot them.

In [12]:
```python
#Defining K values
K = np.linspace(-2*np.pi, 2*np.pi, 100)

#Getting the values of energies
Ev1 = substitute(E1, K)
Ev2 = substitute(E2, K)
Ev3 = substitute(E3, K)
```

In [13]:
```python
%matplotlib inline

#Setting Figure Size
plt.figure(figsize=(10,8))

#Plotting the three energies
plt.plot(K, Ev1, label='E1')
plt.plot(K, Ev2, label='E2')
plt.plot(K, Ev3, label='E3')

#Making three vertical lines, one for x=0, ie. y-axis
#and two for x=pi, and x= -pi

plt.vlines(0,0,85, color='black', linewidth=2)
plt.vlines(np.pi,0,85, color='green', linestyle='dashed')
plt.vlines(-np.pi,0,85, color='green', linestyle='dashed')

#Setting the x and y labels and title
plt.xlabel('K', fontsize=16)
plt.ylabel('E', fontsize=16)
plt.title('Energy levels of electron in periodic potential', fontsize=16)

#Setting the xlimit and ylimit
plt.xlim(-6,6)
plt.ylim(0,50)

#Modifying the xticks and making the ticks larger
plt.xticks([-6,-4, -np.pi,-2, 0, 2, np.pi, 4,6],
     ['-6','-4','-$\pi$','2','0', '2', '$\pi$' ,'4','6'],
     fontsize=14)
plt.yticks(fontsize=14)

#Placing the legends
plt.legend();
```



Making the plot a bit interactive. However, the output won't be visible in the pdf (The `jupyter nbconvert` is not able to export dynamic graphics to pdf). You'll need to download the notebook and run it locally. You'll also need to download `ipympl` library.

In [14]:
```python
%matplotlib widget
#Making the plots
plt.plot(K, Ev1, label='E1')
plt.plot(K, Ev2, label='E2')
plt.plot(K, Ev3, label='E3')
plt.vlines(0,0,85, color='black', linewidth=2)
plt.vlines(np.pi,0,85, color='green', linestyle='dashed')
plt.vlines(-np.pi,0,85, color='green', linestyle='dashed')
plt.xlabel('K', fontsize=16)
plt.ylabel('E', fontsize=16)
plt.xlim(-6,6)
plt.xticks([-6,-4, -np.pi,-2, 0, 2, np.pi, 4,6],
     ['-6','-4','-$\pi$','2','0', '2', '$\pi$' ,'4','6'],
     fontsize=14)
plt.title('Energy levels of a particle in periodic potential', fontsize=14)
plt.yticks(fontsize=14)
plt.ylim(0,50)
plt.legend();
```