Homework7

March 12, 2019

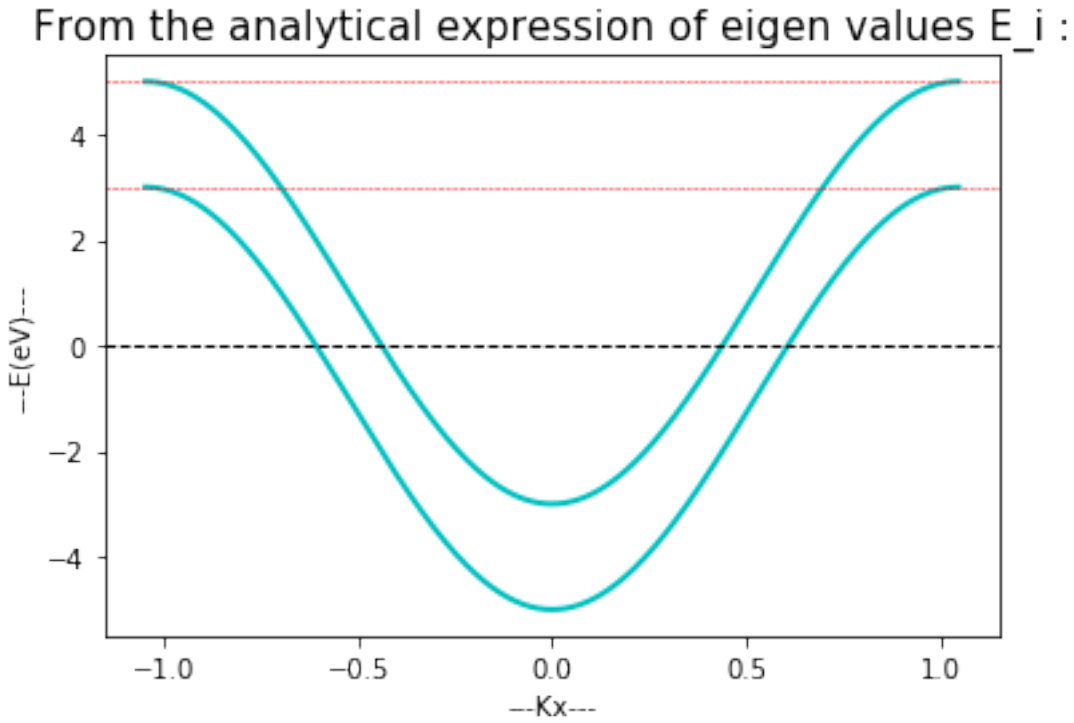
1 Srivani :Homework 7

1.1 Problem 1. Band structure of two coupled linear chain of atoms separated by an horizontal interatomic distance of 3 angstroms.

1.1.1 a) Obtain the Hamiltonian and the eigenenergies analytically when one considers in-plane horizontal hopping t0 = -2 eV and interchain vertical hopping terms or t1 = 1 eV.

Hamiltonian and eigen enrgies analytically:

In [3]:



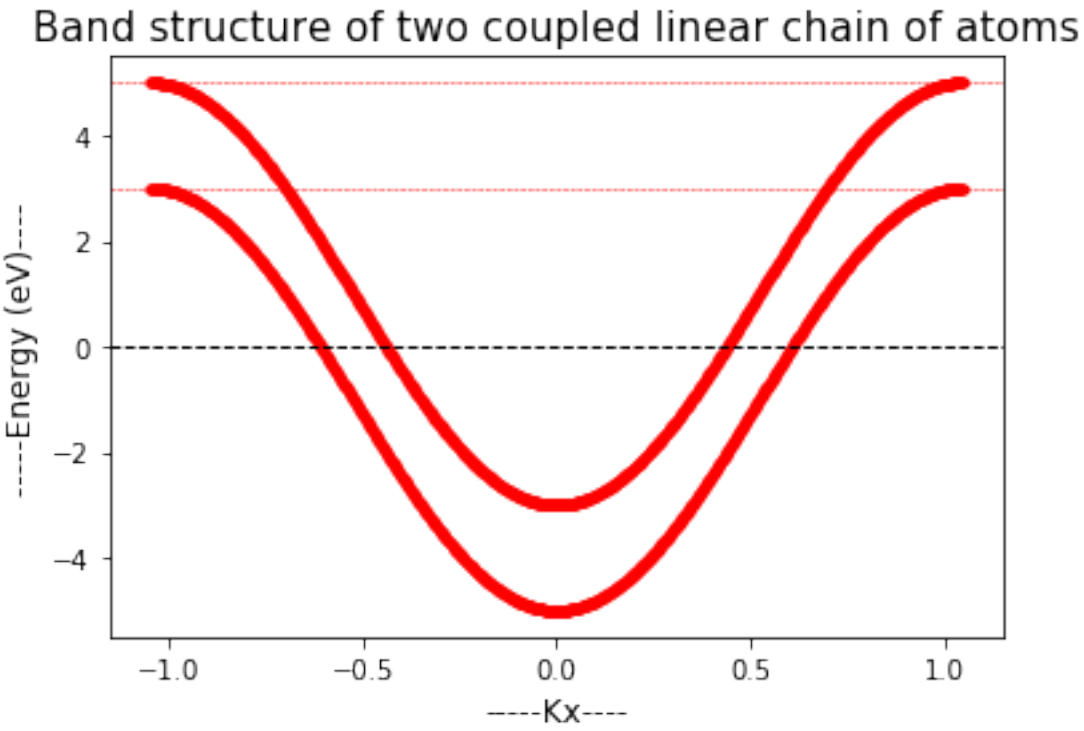
Hamiltonian and eigen enrgies Numerically:

In [2]:

```
[[ 4. -1.]
 [-1.  4.]]
```

1.1.2 b) Plot the band structure.

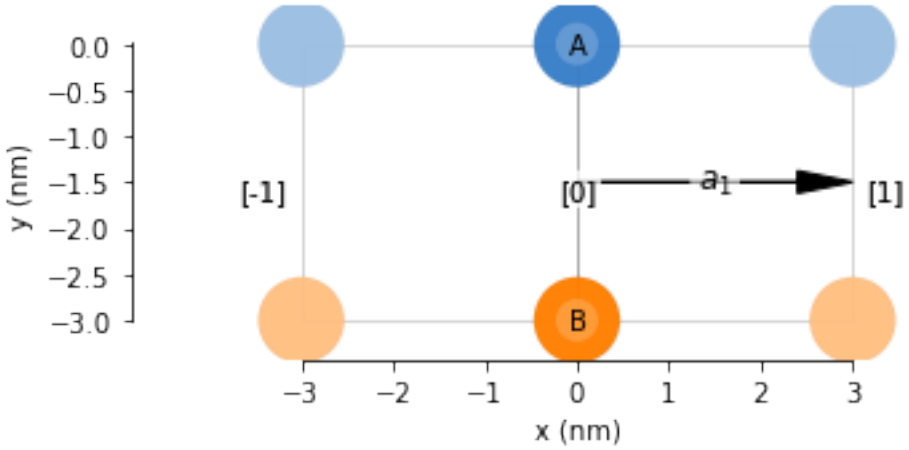
In [29]:

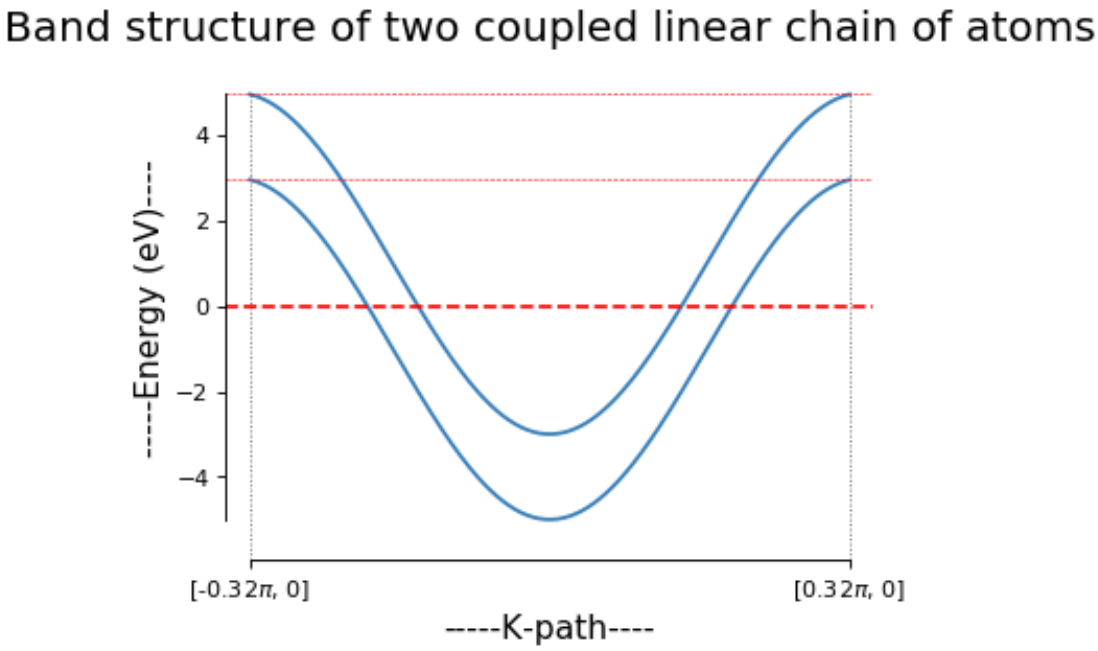


1.1.3 c) Solve the problem using pybinding.

In [30]:

Out[30]: <matplotlib.lines.Line2D at 0x7f898acef0b8>





1.2 2. Band structure of two coupled staggered linear chain of atoms

1.2.1 a) Obtain the Hamiltonian when one considers in-plane horizontal hopping term of t0 = -2 eV and interchain vertical hopping terms or t1 = 1 eV. The site potentials for blue and orange have respectively VA = -1 eV and VB = 1 eV.

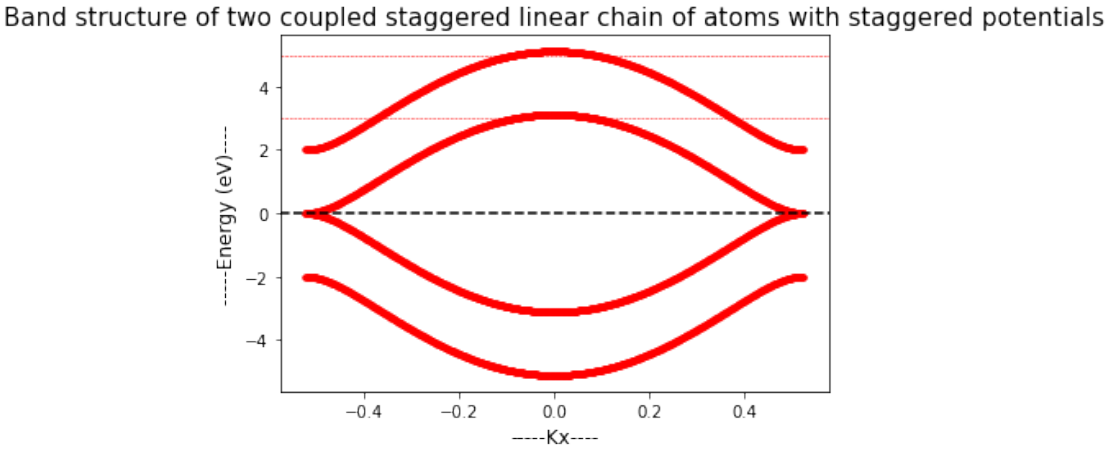
In [9]:

```
[[-1.  4. -1.  0.]
 [ 4.  1.  0. -1.]
```

```
[-1.  0. -1.  4.]
[ 0. -1.  4.  1.]]
```

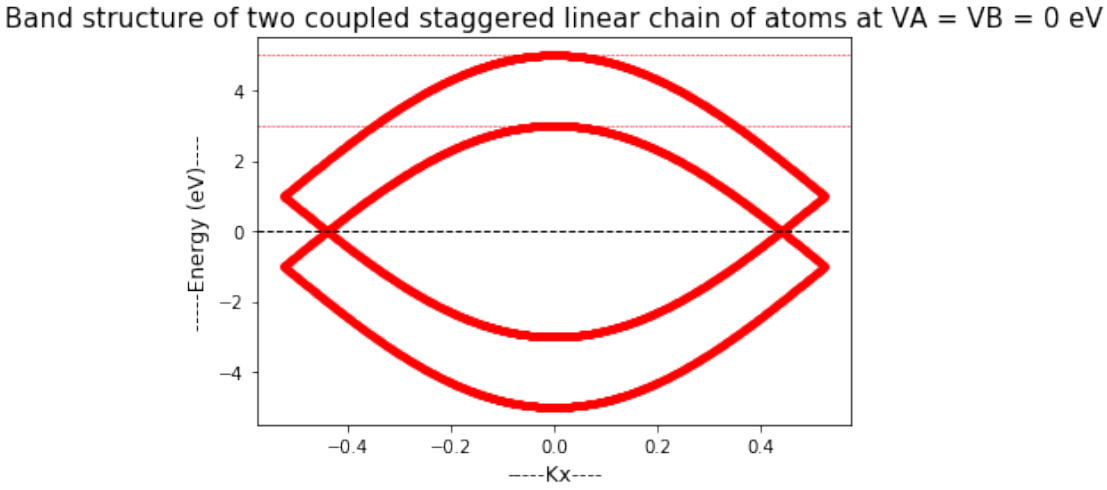
1.3 b) Plot the band structure

In [10]:



1.3.1 if VA =VB =0

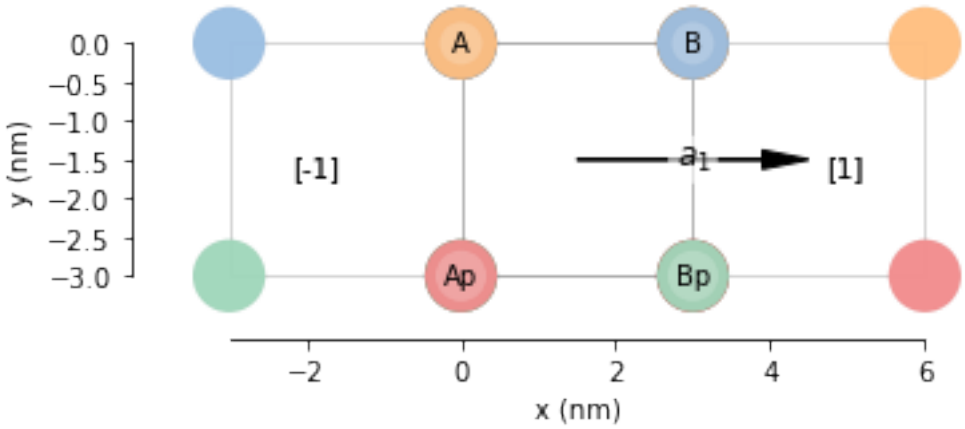
In [11]:



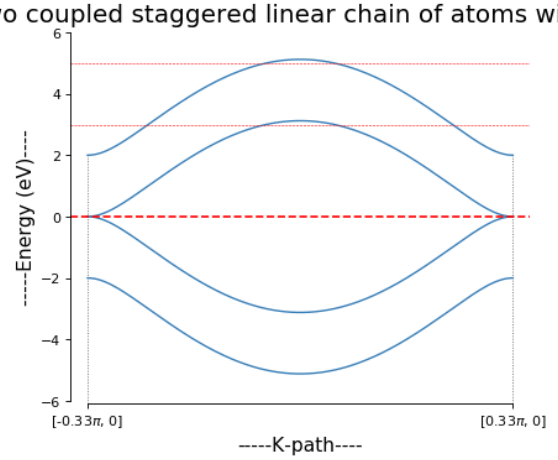
1.4 c) Solve the problem using pybinding.

In [28]:

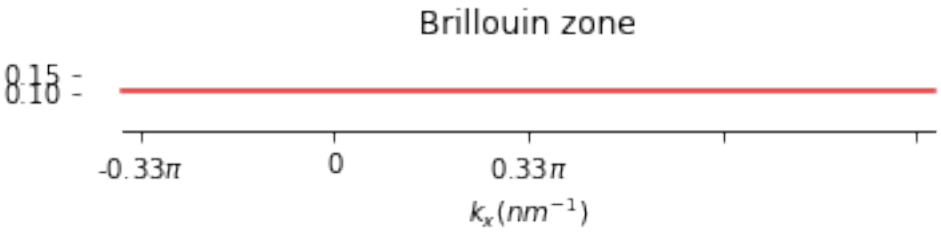
Out[28]: Text(0.5,1,'Band structure of two coupled staggered linear chain of atoms with stagge



Band structure of two coupled staggered linear chain of atoms with staggered potentials



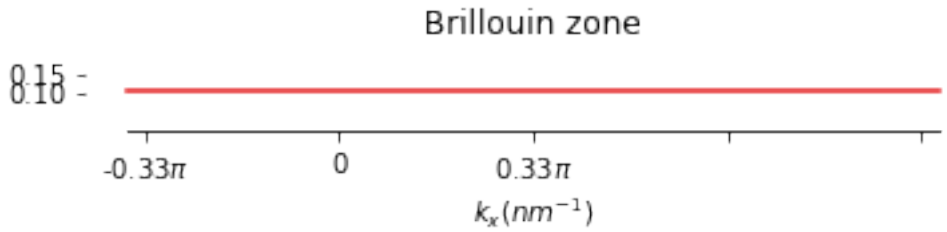
In [29]:
```
lattice.plot_brillouin_zone()
plt.title("Brillouin zone")
plt.show()
```



In [2]:

Out[2]: Text(0.5,1,'Band structure of two coupled staggered linear chain of atoms at VA = VB =

In [3]:
```
lattice.plot_brillouin_zone()
plt.title("Brillouin zone")
plt.show()
```



1.4.1 What happened to its Brillouin zone with respect to the non-staggered case? what if VA = VB= 0