Homework1_Nepal

January 21, 2019

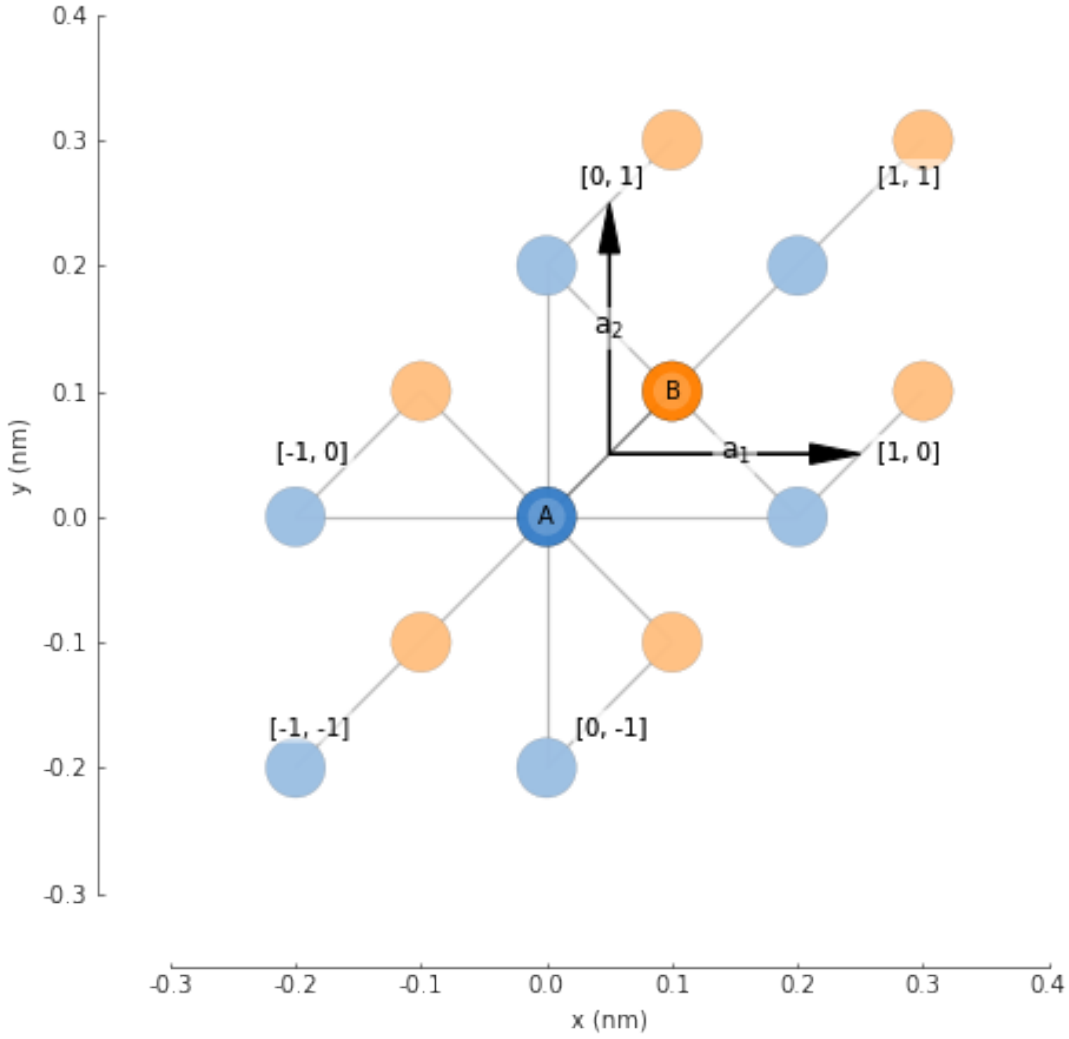
1 Problem 1:

Modify the square lattice given in pybinding notebook by adding a second B basis atom displaced at an arbitrary b = (b x , b y) of your choice. Define the A B hopping term to be t′ = 2. Represent graphically the resulting lattice.

In [1]:
```
import pybinding as pb
import numpy as np
import matplotlib.pyplot as plt
pb.pltutils.use_style()
```

In [3]:
```
import pybinding as pb
d =0.2                  # [nm] unit cell length
t1=2                    # [eV] hopping energy
t=1
a=0.1
bx=a
by=a
# create a simple 2D lattice with vectors a1 and a2
lattice = pb.Lattice(a1=[d, 0], a2=[0, d])
lattice.add_sublattices(
    ('A',[0, 0]),              # add an atom called 'A' at position [0, 0]
    ('B',[bx,by]),

)

lattice.add_hoppings(
#(relative_index, from_sublattice, to_sublattice, energy)
     ([0, 0],'A','B',t1),
     ([0, 1],'A','A',t ),
     ([1, 0],'A','A',t ),
     ([1, 0],'B','A',t1),
     ([0, 1],'B','A',t1),
     ([1, 1],'B','A',t1),
    #([-1,1],'B','A',t1)
)
```

```
In [4]: plt.figure(figsize=(8,8))
        lattice.plot()          # plot the lattice that was just constructed
        plt.show()              # standard matplotlib show() function
```

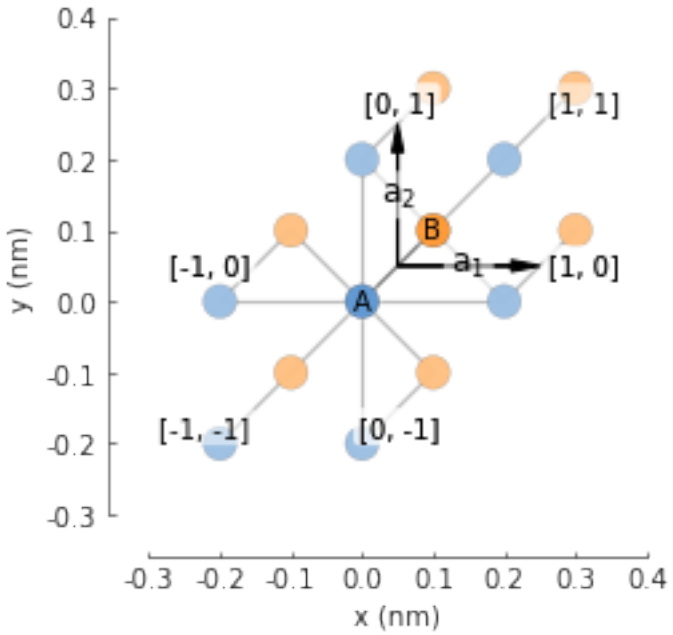


2 Problem 2:

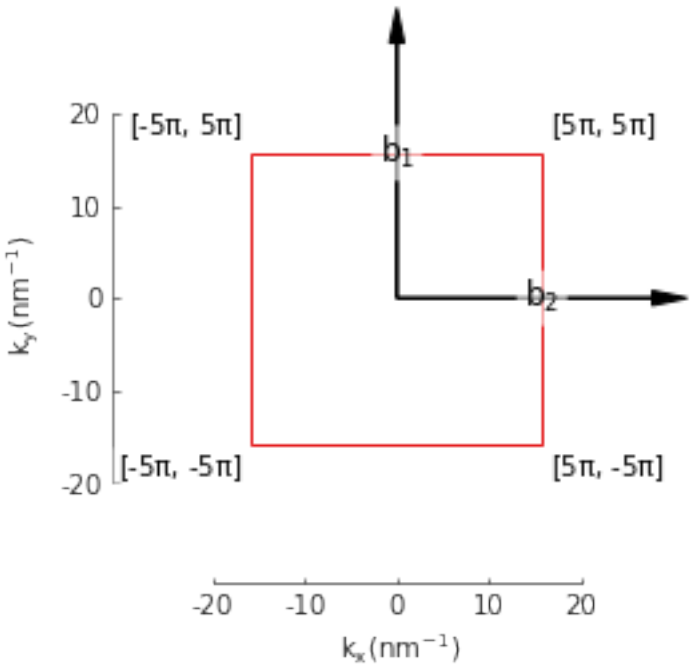
Write a short function to generate a square lattice with an arbitrary basis atom B whose relative position with respect to A can be defined at input. Plot the resulting lattices for two arbitrary choices of b.

```
In [79]: from math import sqrt

         def square_lattice(bx,by):
```

```
    d =0.2  # [nm] unit cell length
    t1=2    # [eV] hopping energy
# create a simple 2D lattice with vectors a1 and a2
    lat= pb.Lattice(a1=[d, 0], a2=[0, d])
    lat.add_sublattices(
    ('A',[0, 0]),   # add an atom called 'A' at position [0, 0]
    ('B',[bx,by]),
    )

    lat.add_hoppings(
#(relative_index, from_sublattice, to_sublattice, energy)
    ([0, 0],'A','B',t1),
    ([0, 1],'A','A',t ),
    ([1, 0],'A','A',t ),
    ([1, 0],'B','A',t1),
    ([0, 1],'B','A',t1),
    ([1, 1],'B','A',t1),
    #([-1,1],'B','A',t1)
    )
    return lat
a=0.1
lattice = square_lattice(bx=a,by=a)
lattice.plot()
plt.show()
```



In [80]: `lattice.plot_brillouin_zone()`



3 Problem 3:

What are the definitions of a reciprocal lattice and a Brillouin zone? Write down the formulas that relate the lattice vectors with the corresponding reciprocal lattice. Calculate the area of the Brillouin zone of the square lattice in Problem 1.

4 Reciprocal Lattice:

The set of all wave vectors K that yield plane waves with the periodicity of a given Bravais lattice is known as its reciprocal lattice.

5 Brillouin Zone:

The wigner sitz cell of the reciprocal space is called the Brillouin Zone.We can define it as the set of points in k space that can be reached from the origin without crossing any Bragg plane.The second Brillouin zone is the set of points that can be reached from the first zone by crossing only one Bragg plane.

Analytically, K belongs to the reciprocal lattice of a Bravais lattice of points R, provided that the relation

$$e^{i\vec{K}.(\vec{R+r})} = e^{i\vec{K}.\vec{r}}$$

Here the R is lattice periodicity.

$$e^{i\vec{K}.\vec{R}} = 1$$

For all R in the Bravais lattice.
Let

$$\vec{a}_1, \vec{a}_2, \vec{a}_3$$

be a set of primitive vectors, then the reciprocal lattice can be generated by the three primitive vectors:
Here

$$\vec{b}_1, \vec{b}_2, \vec{b}_3$$

are reciprocal lattice vector:-

$$\vec{b}_1 = 2\pi \frac{(\vec{a}_2 \times \vec{a}_3)}{(\vec{a}_1.\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{(\vec{a}_3 \times \vec{a}_1)}{(\vec{a}_1.\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 = 2\pi \frac{(\vec{a}_1 \times \vec{a}_2)}{(\vec{a}_1.\vec{a}_2 \times \vec{a}_3)}$$

6 Brillouin Zone Area:

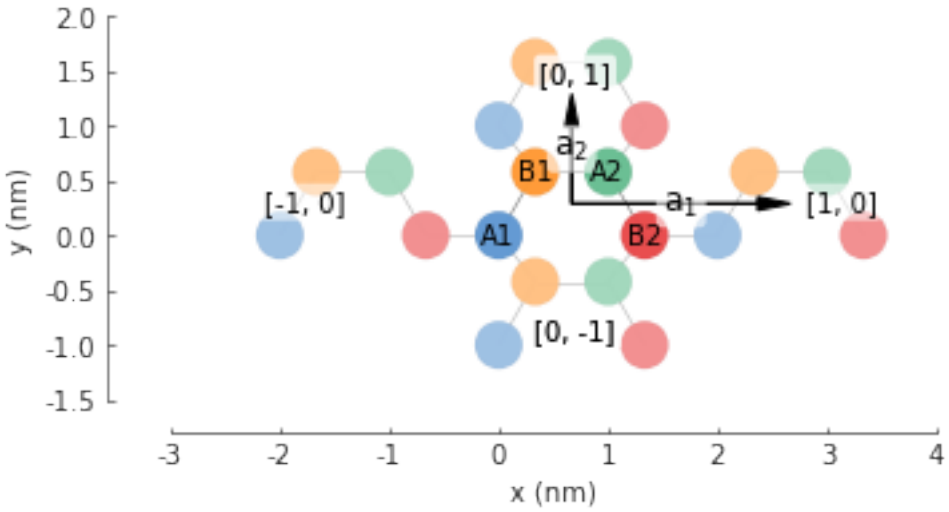
$$4\pi^2$$

7 Problem 4:

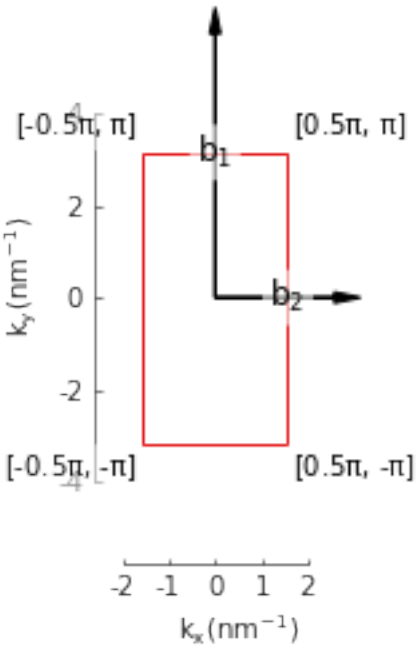
Modify the following example code provided in the python notebook such that it generates automatically the lattice vector of a rectangular lattice with lattice vectors $a_1 = (2, 0)$ and $a_2 = (0, 1)$ with and without a basis atom B. Illustrate the resulting lattice and the associated Brillouin zone.

```
In [77]: import pybinding as pb
         import matplotlib.pyplot as plt
         from math import sqrt

         def monolayer_graphene():
             a=2/3              # [nm] unit cell length

             t=1                # [eV] nearest neighbour hopping

             lat=pb.Lattice(a1=[3*a, 0],
                            a2=[0,(3/2)*a])

             lat.add_sublattices(('A1',[0,0]),
                                 ('B1',[0.5*a,a*(sqrt(3))/2]),
                                 ('A2',[(3/2)*a,a*(sqrt(3))/2]),
                                 ('B2',[2*a,0])
                                )
             lat.add_hoppings(
```

```
            # inside the main cell
             ([0, 0],'A1','B1',t),
             ([0, 0],'B1','A2',t),
             ([0, 0],'A2','B2',t),
            # between neighboring cell
             ([0,-1],'A1','B1' ,t),
             ([1, 0],'B2','A1' ,t),
             ([0,-1],'B2','A2' ,t)
        )
        return lat

lattice=monolayer_graphene()
lattice.plot()
plt.show()
```



In [73]: `lattice.plot_brillouin_zone()`


[-0.5π, π]
[0.5π, π]
b1
b2
[-0.5π, -π]
[0.5π, -π]
4
2
0
-2
-4
ky(nm−1)
-2 -1 0 1 2
kx(nm−1)