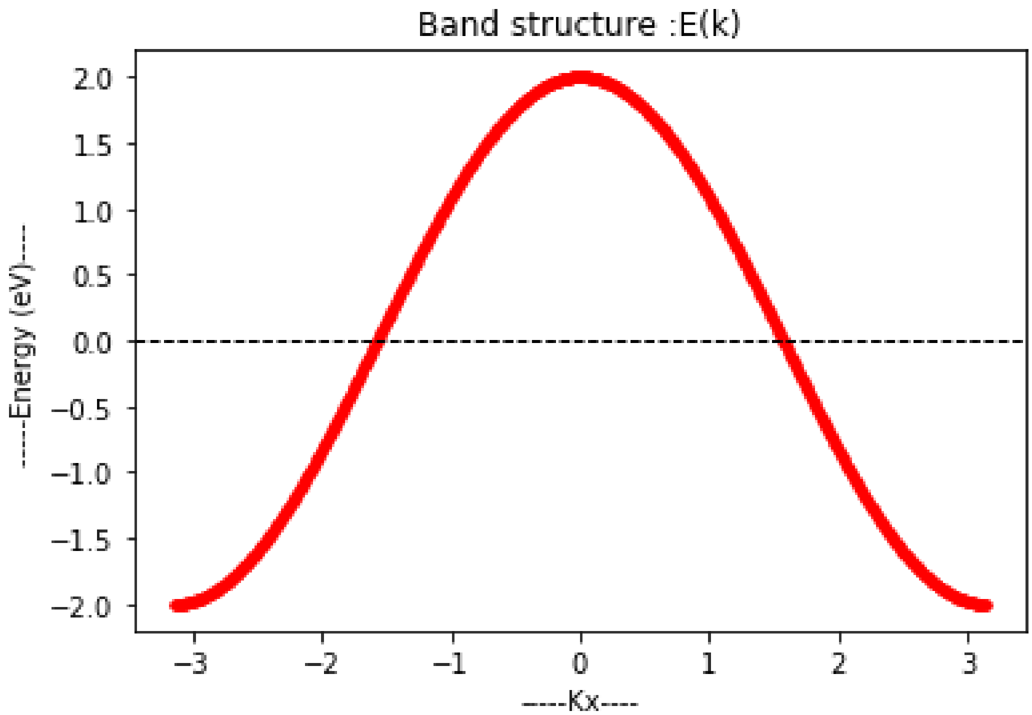
Homework4

July 2, 2018

1 Band structure

1.0.1 Problem.1 : Band structure of a linear chain of atoms

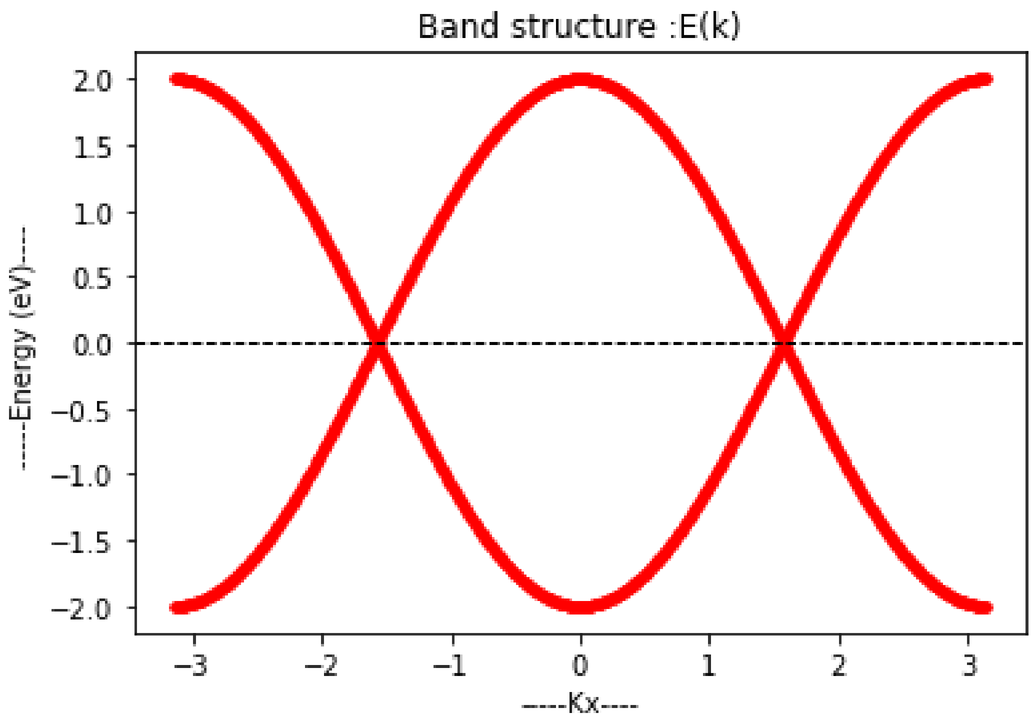
```
In [112]: import numpy as np
          from numpy import linalg as LA
          import matplotlib.pyplot as plt

          Eo = 0 #eV
          t = 1 #eV
          d = 1 #unit distance

          d1 = d
          d2 = -d

          k = np.linspace(-np.pi,np.pi, 1000)
          Ev = []

          for i in range(1000):
              kx = k[i]
              f = 2*np.cos(kx*d)#np.exp(1j*kx*d1)+ np.exp(1j*kx*d2)
              H = t*f
              Ev.append(H)

          #print(Ev)
          plt.plot(k,Ev,'.-r')
          plt.axhline(y=0.0, color='k', linestyle='--', linewidth=1.0)
          plt.xlabel('-----Kx----')
          plt.ylabel('-----Energy (eV)----')
          plt.title('Band structure :E(k)')
          plt.show()
```



1.0.2 Problem.2 : Band structure of a linear chain of atoms using a unit cell with twice its size

In [110]:
```
import numpy as np
from numpy import linalg as LA
import matplotlib.pyplot as plt

Eo = 0 #eV
t = 1 #eV
d = 1 #unit distance

d1 = d
d2 = -d

k = np.linspace(-np.pi,np.pi, 1000)
Ev = []

for i in range(1000):
    kx = k[i]
    f = 2*np.cos(kx*d)#np.exp(1j*kx*d1)+ np.exp(1j*kx*d2)
    H = np.array([[Eo,t*f],[t*np.conjugate(f),Eo]])
    #print('Hamiltonian =',H)
    w, v = LA.eig(H)
    #print('Eigen values =',w)
```

```
    Ev.append(w)

#print(Ev)
plt.plot(k,Ev,'.-r')
plt.axhline(y=0.0, color='k', linestyle='--', linewidth=1.0)
plt.xlabel('-----Kx----')
plt.ylabel('-----Energy (eV)----')
plt.title('Band structure :E(k)')
#plt.ylim([-0.5 ,0.5])
plt.show()
```



1.0.3 Problem3. Band structure of a linear chain of atoms using a unit cell with twice its size with VA = -1 eV and VB = 1 eV

```
In [111]: import numpy as np
          from numpy import linalg as LA
          import matplotlib.pyplot as plt

          EA = -1 #eV
          EB = 1
          t = 1 #eV
          d = 1 #unit distance

          d1 = d
```

```python
d2 = -d

k = np.linspace(-np.pi,np.pi, 1000)
Ev = []

for i in range(1000):
    kx = k[i]
    f = 2*np.cos(kx*d)#np.exp(1j*kx*d1)+ np.exp(1j*kx*d2)
    H = np.array([[EA,t*f],[t*np.conjugate(f),EB]])
    #print('Hamiltonian =',H)
    w, v = LA.eig(H)
    #print('Eigen values =',w)
    Ev.append(w)

#print(Ev)
plt.plot(k,Ev,'.-r')
plt.axhline(y=0.0, color='k', linestyle='--', linewidth=1.0)
plt.xlabel('-----Kx----')
plt.ylabel('-----Energy (eV)----')
plt.title('Band structure :E(k)')
plt.show()
```