Homework_2-DispersionRelation

April 22, 2019

1 Visualization of quadratic and honeycomb lattice dispersion relations in tight-binding model

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt

import sys
sys.path.insert(0, "./")
```

In [2]:
```
from dispersion import quadratic_lattice_calculator, graphene_dispersion_calculator
from density_calculator import DensityOfStatesCalculator
```

1.1 Quadratic lattice

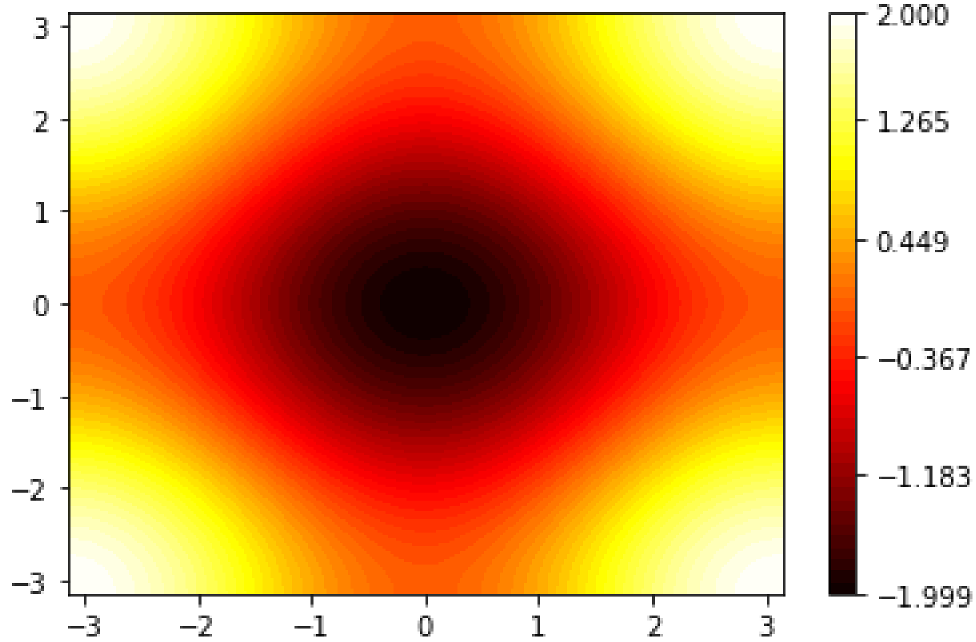
Quadratic lattice dispersion relation:
$\epsilon_{\vec{k}} = \epsilon_0 - 2t \cdot (\cos(k_x a_x) + \cos(k_y a_y))$
Where ϵ_0 is ground level energy at given site and $-t$ is hopping energy for nearest neighbours.

In [3]:
```
disp = quadratic_lattice_calculator()
```

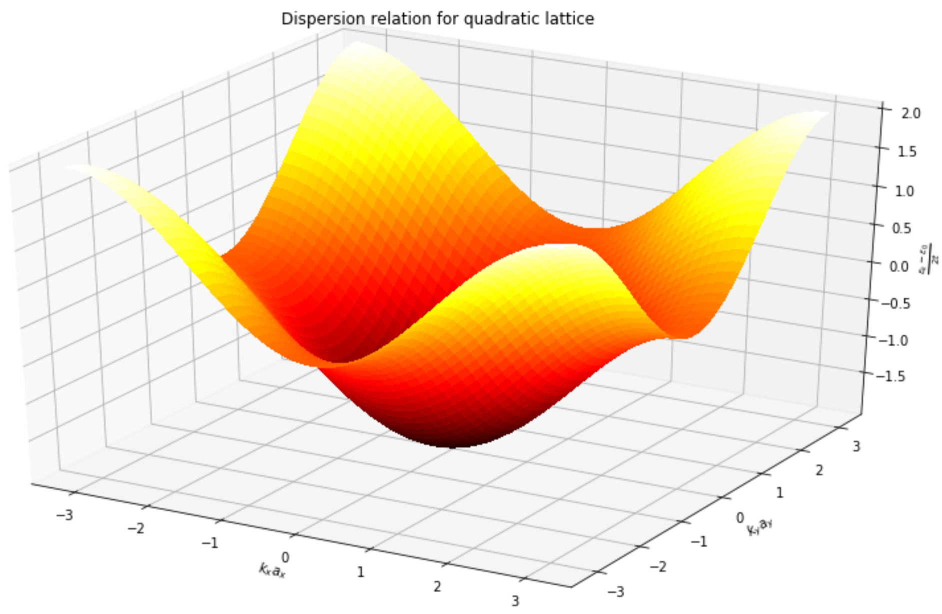
In [4]:
```
no_of_grid_points = 100
grid = np.array([np.linspace(-np.pi, np.pi, no_of_grid_points), np.linspace(-np.pi, np
```

In [5]:
```
calc = DensityOfStatesCalculator(disp, grid)
```

In [6]:
```
fig, ax = calc.get_2d_contourf_plot()


#fig
```




```
In [7]: fig, ax = calc.get_3d_plot()

        fig.set_figheight(9)
        fig.set_figwidth(15)

        ax.set_title("Dispersion relation for quadratic lattice")

        ax.set_zlabel(r"$\frac{\epsilon_k - \epsilon_0}{2t}$")
        ax.set_ylabel(r"$k_y a_y$")
        ax.set_xlabel(r"$k_x a_x$")

        #fig

Out[7]: Text(0.5, 0, '$k_x a_x$')
```



1.2 Honeycomb lattice (graphene)

Quadratic lattice dispersion relation:

$\epsilon_{\vec{k}} = \pm t \cdot |\sum_i e^{i\vec{k}\cdot\vec{\delta}_i}|$

Where ϵ_0 is ground level energy at given site and $-t$ is hopping energy for nearest neighbours.

Vectors $\vec{\delta}_1$, $\vec{\delta}_2$, $\vec{\delta}_3$ describe lattice:

$\vec{\delta}_1 = a_0(\frac{1}{2}, \frac{\sqrt{3}}{2})$

$\vec{\delta}_2 = a_0(\frac{1}{2}, -\frac{\sqrt{3}}{2})$

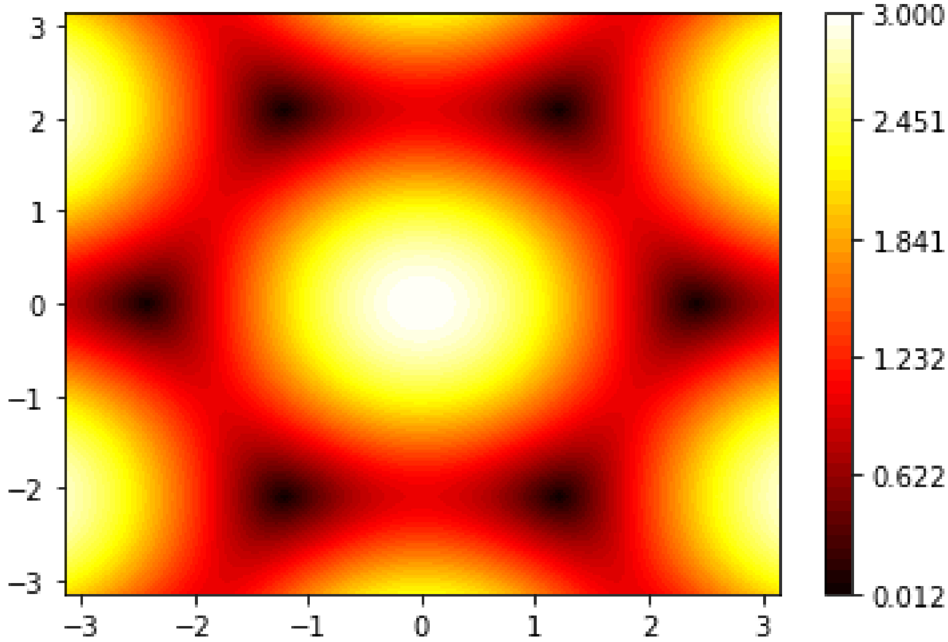
$\vec{\delta}_3 = a_0(-\frac{1}{2}, 0)$

In [8]:
```
disp = graphene_dispersion_calculator()
```

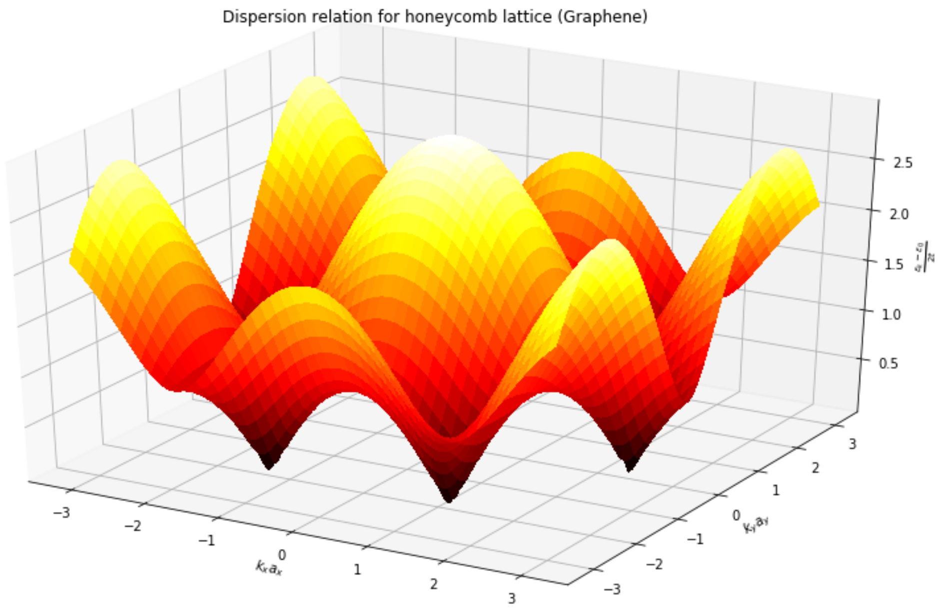
In [9]:
```
no_of_grid_points = 200
grid = np.array([np.linspace(-np.pi, np.pi, no_of_grid_points), np.linspace(-np.pi, np
```

In [10]:
```
calc = DensityOfStatesCalculator(disp, grid)
```

In [11]:
```
fig, ax = calc.get_2d_contourf_plot()
#fig
```




```
In [12]: fig, ax = calc.get_3d_plot()

         fig.set_figheight(9)
         fig.set_figwidth(15)

         ax.set_title("Dispersion relation for honeycomb lattice (Graphene)")

         ax.set_zlabel(r"$\frac{\epsilon_k - \epsilon_0}{2t}$")
         ax.set_ylabel(r"$k_y a_y$")
         ax.set_xlabel(r"$k_x a_x$")

Out[12]: Text(0.5, 0, '$k_x a_x$')
```


Dispersion relation for honeycomb lattice (Graphene)
−3
−2
−1
0
1
2
3
$k_x a_x$
$k_y a_y$
0.5
1.0
1.5
2.0
2.5

In [ ]: