Python script for calculating the energy dispersion for triangular and Kagome lattice

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1 Equations used for triangular lattice

The following equations will be used for calculating the energy dispersion for the triangular lattice as show in Figure(1).

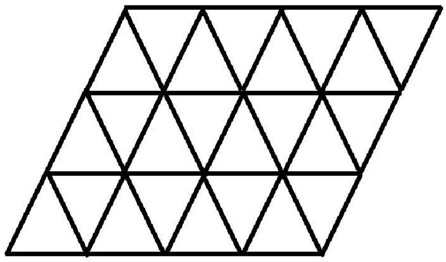


Figure 1: Structure of 2 dimensional triangular lattice

Firstly , we need to obtain the energy dispersion relation equations E_k for the triangular lattice. Note that for this lattice , it has 6 nearest neighbours in the tight-binding model whose equation is

$$E(\vec{k}) = \varepsilon + t \sum_{\text{nearest neighbour: } nn} e^{i\vec{k}\cdot\vec{R}_{nn}} \tag{1}$$

The position vectors for the 6 nearest neighbours are

$$\vec{\delta}_1 = \vec{a}_2 = \frac{a}{2}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix} \tag{2}$$

$$\vec{\delta}_2 = \vec{a}_1 = a\begin{pmatrix}1\\ 0\end{pmatrix} \tag{3}$$

$$\vec{\delta}_3 = \frac{a}{2}\begin{pmatrix}1\\ -\sqrt{3}\end{pmatrix} \tag{4}$$

$$\vec{\delta}_4 = \frac{a}{2}\begin{pmatrix}-1\\ -\sqrt{3}\end{pmatrix} = -\frac{a}{2}\begin{pmatrix}1\\ \sqrt{3}\end{pmatrix} \tag{5}$$

$$\vec{\delta}_5 = a\begin{pmatrix}-1\\ 0\end{pmatrix} = -a\begin{pmatrix}1\\ 0\end{pmatrix} \tag{6}$$

$$\vec{\delta}_6 = \frac{a}{2}\begin{pmatrix}-1\\ \sqrt{3}\end{pmatrix} = -\frac{a}{2}\begin{pmatrix}1\\ -\sqrt{3}\end{pmatrix} \tag{7}$$

Using these position vectors in the second term of the tight-binding equation, we can rewrite it into

$$\sum_{nn} e^{i\vec{k}\cdot\vec{R}_{nn}} = \sum_{\vec{\delta}_i} e^{i\vec{k}\cdot\delta_i} = 2\cos\left(\frac{a}{2}(k_x+\sqrt{3}k_y)\right) + 2\cos(ak_x) + 2\cos\left(\frac{a}{2}(k_x-\sqrt{3}k_y)\right) \tag{8}$$

The energy dispersion equation obtained from the tight-binding model can be written as

$$E(k_x,k_y) = \varepsilon - 2t\Big[\cos(k_x a) + \cos\Big(\frac{k_x a + \sqrt{3}k_y a}{2}\Big) + \cos\Big(\frac{k_x a - \sqrt{3}k_y a}{2}\Big)\Big] \tag{9}$$

The energy dispersion equation can be simplified as accordingly.

$$\begin{aligned}
E(k_x,k_y) &= \varepsilon-2t\Big[\cos(k_xa)+\cos\Big(\frac{k_xa+\sqrt{3}k_ya}{2}\Big)+\cos\Big(\frac{k_xa-\sqrt{3}k_ya}{2}\Big)\Big] && (10)\\
&\mid \quad \text{using identities } \cos(a+b)+\cos(a-b)=2\cos a\cos b \text{ and } \cos 2a = 2\cos^2 a-1 && (11)\\
&\mid \quad \text{we obtain } \cos\Big(\frac{k_xa+\sqrt{3}k_ya}{2}\Big)+\cos\Big(\frac{k_xa-\sqrt{3}k_ya}{2}\Big)=2\cos\Big(\frac{k_xa}{2}\Big)\cos\Big(\frac{\sqrt{3}k_ya}{2}\Big) && (12)\\
&= \varepsilon-2t\Big[\cos(k_xa)+2\cos\Big(\frac{k_xa}{2}\Big)\cos\Big(\frac{\sqrt{3}k_ya}{2}\Big)\Big] && (13)\\
&= \varepsilon-2t\Big[2\cos^2\Big(\frac{k_xa}{2}\Big)-1+2\cos\Big(\frac{k_xa}{2}\Big)\cos\Big(\frac{\sqrt{3}k_ya}{2}\Big)\Big] && (14)\\
&= \varepsilon+2t-2t\Big[2\cos^2\Big(\frac{k_xa}{2}\Big)+2\cos\Big(\frac{k_xa}{2}\Big)\cos\Big(\frac{\sqrt{3}k_ya}{2}\Big)\Big] && (15)\\
&= \varepsilon+2t-4t\cos\Big(\frac{k_xa}{2}\Big)\Big[\cos\Big(\frac{k_xa}{2}\Big)+\cos\Big(\frac{\sqrt{3}k_ya}{2}\Big)\Big] && (16)
\end{aligned}$$

Note that for the condition of $E(k_x=0,k_y=0)=0$, we obtain $\varepsilon=6t$. Hence, the equation can be written into

$$E(k_x,k_y)=8t-4t\cos\Big(\frac{k_xa}{2}\Big)\Big[\cos\Big(\frac{k_xa}{2}\Big)+\cos\Big(\frac{\sqrt{3}k_ya}{2}\Big)\Big] \tag{17}$$

2 Equations used for Kagome lattice

The following equations will be used for calculating the energy dispersion for the Kagome lattice in the case of spinless-fermions. The Kagome lattice is a 2 dimensional lattice with three-atomic basis as shown in Figure(2) with 3 sites denoted as A, B, and C.

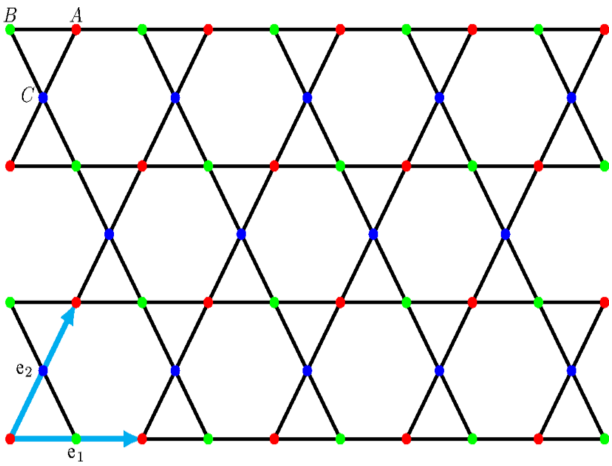


Figure 2: Structure of 2 dimensional Kagome lattice

The position vectors $\vec{\delta}_i$ for the 6 nearest neighbours for the Kagome lattice can be defined below using the basis vectors of $\vec{a}_1$ and $\vec{a}_2$

$$\begin{aligned}
\vec{a}_1 &= a\begin{pmatrix}1\\0\end{pmatrix} && (18)\\
\vec{a}_2 &= \frac{a}{2}\begin{pmatrix}1\\\sqrt{3}\end{pmatrix} && (19)\\
\vec{\delta}_1 &= \frac{a}{4}\begin{pmatrix}1\\\sqrt{3}\end{pmatrix} && (20)\\
\vec{\delta}_2 &= \frac{a}{4}\begin{pmatrix}1\\-\sqrt{3}\end{pmatrix} && (21)\\
\vec{\delta}_3 &= -\frac{a}{2}\begin{pmatrix}0\\1\end{pmatrix} && (22)\\
\vec{\delta}_4 &= -\frac{a}{4}\begin{pmatrix}1\\\sqrt{3}\end{pmatrix} && (23)
\end{aligned}$$

$$\vec{\delta}_5 = \frac{a}{4}\begin{pmatrix}-1\\ \sqrt{3}\end{pmatrix} \tag{24}$$

$$\vec{\delta}_6 = \frac{a}{2}\begin{pmatrix}0\\ 1\end{pmatrix} \tag{25}$$

Now we will recall the Hamiltonian of the tight-binding model given by the following equation.

$$H_{\mathrm{tb}} = -t\sum_{\langle ij\rangle}(c_i^\dagger c_j + \mathrm{h.c.}) \tag{26}$$

where h.c. stands for Hermitian conjugate. Using the Fourier transformation, given by the following equations below, we can transform the real space of the Hamiltonian to the momentum k-space.

$$c_j = \frac{1}{\sqrt{N}}\sum_{\vec{k}\in\text{Brillouin Zone:BZ}} e^{i\vec{k}\cdot\vec{R}_j}\, c_{\vec{k}} \tag{27}$$

$$c_j^\dagger = \frac{1}{\sqrt{N}}\sum_{\vec{k}\in\mathrm{BZ}} e^{-i\vec{k}\cdot\vec{R}_j}\, c_{\vec{k}}^\dagger \tag{28}$$

$$c_j^\dagger c_{j+\delta} = \frac{1}{N}\sum_{j,\delta}\sum_{\vec{k},\vec{q}} e^{i\vec{q}\cdot\vec{\delta}} e^{-i(\vec{k}-\vec{q})\cdot\vec{R}_j} c_{\vec{k}}^\dagger c_{\vec{q}} \tag{29}$$

$$= \sum_{\vec{k},\vec{q}} e^{i\vec{q}\cdot\vec{\delta}} \underbrace{\left(\frac{1}{N}\sum_j e^{-i(\vec{k}-\vec{q})\cdot\vec{R}_j}\right)}_{\delta_{\vec{k},\vec{q}}} c_{\vec{k}}^\dagger c_{\vec{q}} = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{\delta}} c_{\vec{k}}^\dagger c_{\vec{k}} \tag{30}$$

Simplifying the Hamiltonian, we obtain the following expression.

$$H_{\mathrm{tb}} = -t\sum_{\vec{k}}\Big[\Big(e^{\frac{ik_xa}{2}} + e^{-\frac{ik_xa}{2}}\Big)c_{\vec{k},A}^\dagger c_{\vec{k},B} + \Big(e^{i\left(\frac{k_xa}{4}+\frac{\sqrt{3}k_ya}{4}\right)} + e^{-i\left(\frac{k_xa}{4}+\frac{\sqrt{3}k_ya}{4}\right)}\Big)c_{\vec{k},A}^\dagger c_{\vec{k},C} \tag{31}$$

$$+\Big(e^{i\left(\frac{k_xa}{4}-\frac{\sqrt{3}k_ya}{4}\right)} + e^{-i\left(\frac{k_xa}{4}-\frac{\sqrt{3}k_ya}{4}\right)}\Big)c_{\vec{k},B}^\dagger c_{\vec{k},C} + \ldots + \mathrm{h.c.}\Big] \tag{32}$$

$$H_{\mathrm{tb}} = -t\sum_k\Big[2\cos\Big(\frac{k_xa}{2}\Big)\big[c_{\vec{k},A}^\dagger c_{\vec{k},B} + c_{\vec{k},B}^\dagger c_{\vec{k},A}\big] + 2\cos\Big(\frac{k_xa}{4}+\frac{\sqrt{3}k_ya}{4}\Big)\big[c_{\vec{k},A}^\dagger c_{\vec{k},C} + c_{\vec{k},C}^\dagger c_{\vec{k},A}\big] + \ldots \tag{33}$$

$$+2\cos\Big(\frac{k_xa}{4}-\frac{\sqrt{3}k_ya}{4}\Big)\big[c_{\vec{k},B}^\dagger c_{\vec{k},C} + c_{\vec{k},C}^\dagger c_{\vec{k},B}\big]\Big] \tag{34}$$

We are now able to write the Hamiltonian in terms of its matrix form, where $H(\vec{k})$ is known as the Bloch Hamiltonian.

$$H_{\mathrm{tb}} = \sum_{\vec{k}} \Psi^\dagger(\vec{k})H(\vec{k})\Psi(\vec{k}) \tag{35}$$

$$\Psi(\vec{k}) = c_{\vec{k},A}c_{\vec{k},B}c_{\vec{k},C} \tag{36}$$

Based on our previous calculations, we can obtain the Bloch Hamiltonian as follows.

$$H(\vec{k}) = -2t\begin{bmatrix} 0 & \cos\left(\frac{k_xa}{2}\right) & \cos\left(\frac{k_xa}{4}+\frac{\sqrt{3}k_ya}{4}\right)\\ \cos\left(\frac{k_xa}{2}\right) & 0 & \cos\left(\frac{k_xa}{4}-\frac{\sqrt{3}k_ya}{4}\right)\\ \cos\left(\frac{k_xa}{4}+\frac{\sqrt{3}k_ya}{4}\right) & \cos\left(\frac{k_xa}{4}-\frac{\sqrt{3}k_ya}{4}\right) & 0 \end{bmatrix} \tag{37}$$

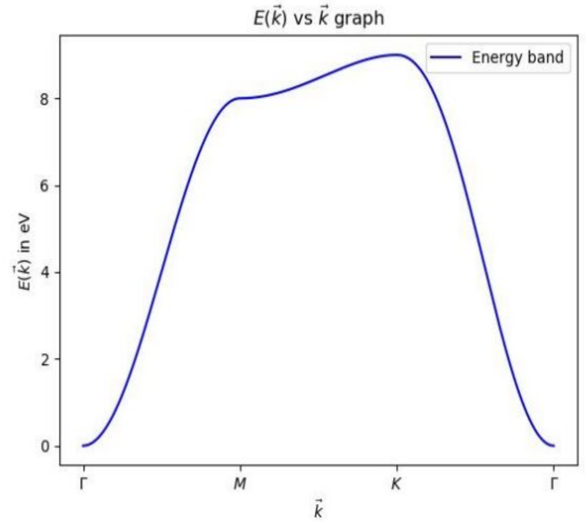
Solving the determinant of the Bloch Hamiltonian gives the energy dispersion equations for the Kagome lattice in the case of spinless fermions.

$$E^A = 2t \tag{38}$$

$$E^{B,C} = t\Big\{-1 \pm \sqrt{4\Big[\cos^2\Big(\frac{k_xa}{2}\Big) + \cos^2\Big(\frac{k_xa}{4}+\frac{\sqrt{3}k_ya}{4}\Big) + \cos^2\Big(\frac{k_xa}{4}-\frac{\sqrt{3}k_ya}{4}\Big)\Big] - 3}\Big\} \tag{39}$$

3 Result from Python script for triangular lattice

After running the Python script, we obtain the following graphs as shown in Figure(3). The graph on the left shows the electronic structure that would be measured using angle-resolved photo-emission (ARPES), showing its energy at the relevant critical points (Γ, M, K, Γ) on the Brillouin Zone. The graph on the right shows the energy dispersion graph in 2-dimensional momentum-space for the triangular lattice.



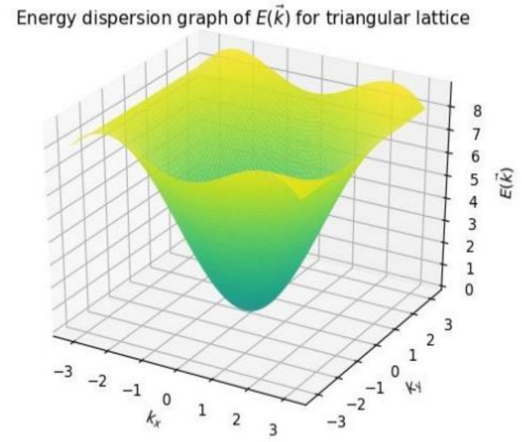
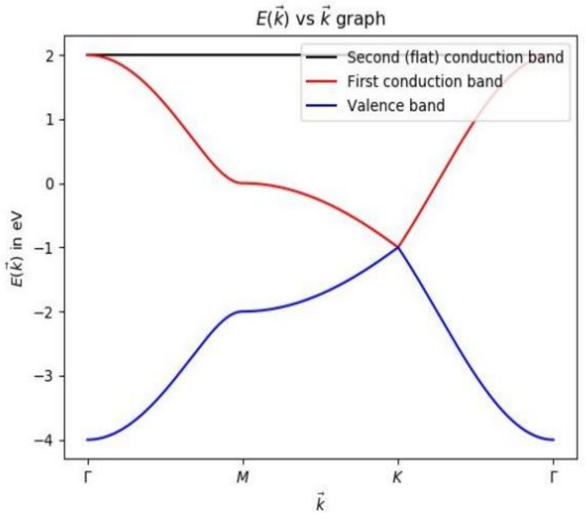


Figure 3: Results for triangular lattice

4 Result from Python script for Kagome lattice

After running the Python script, we obtain the following graphs as shown in Figure(4). The graph on the left shows the electronic structure that would be measured using angle-resolved photo-emission (ARPES), showing its energy at the relevant critical points (Γ, M, K, Γ) on the Brillouin Zone. The graph on the right shows the energy dispersion graph in 2-dimensional momentum-space for the Kagome lattice in the case of spinless fermions.



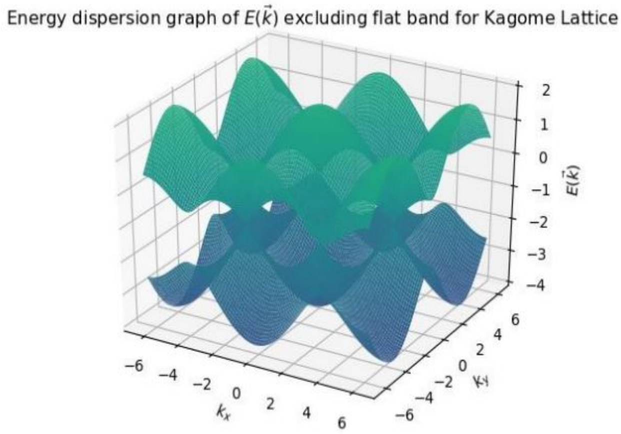


Figure 4: Results for Kagome lattice

Note that the results corresponds to a similar image found in Figure(5) obtained from Ghimire and Mazin [1].

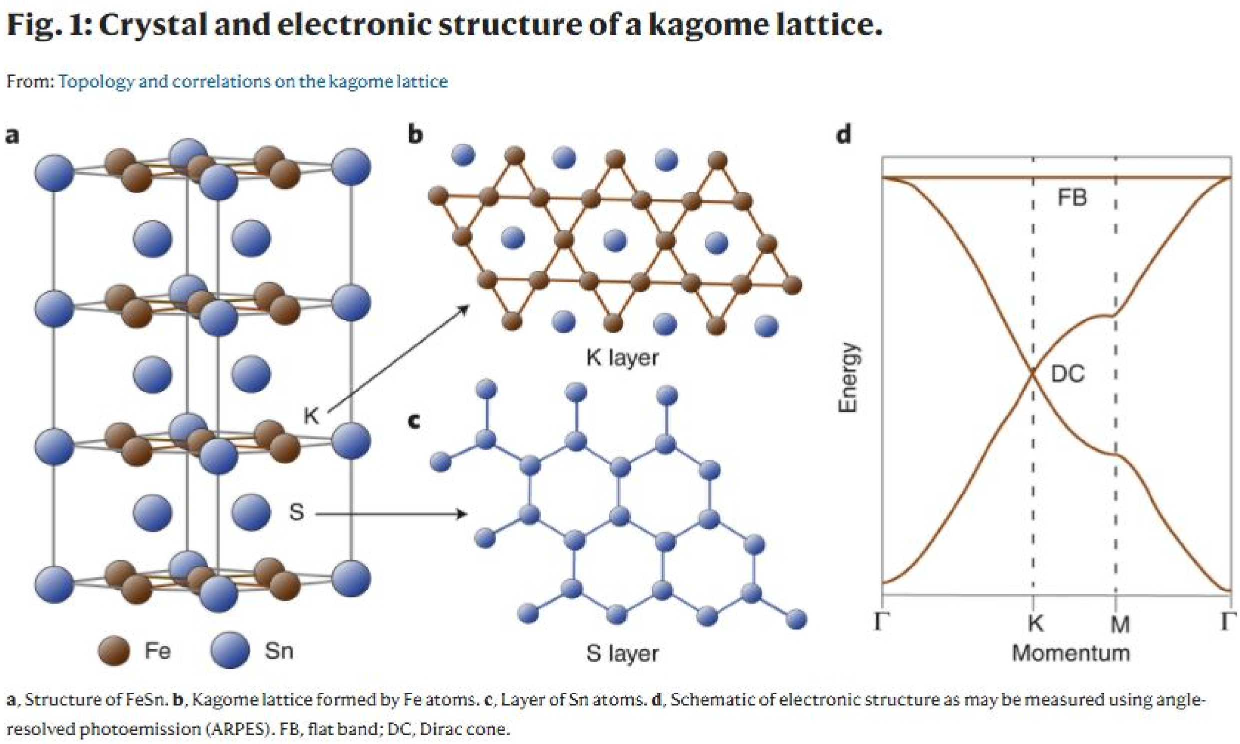


Figure 5: Crystal and electronic structure of a Kagome lattice [1]

5 Appendix

The image of a Japanese basket showing the Kagome pattern obtained from Wikipedia, as shown in Figure(6).

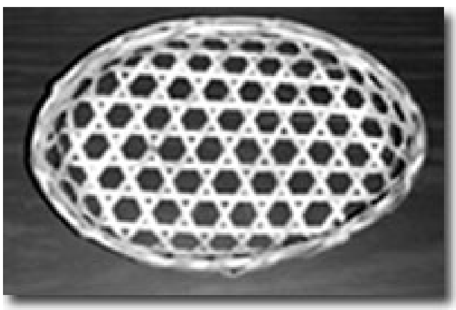


Figure 6: Japanese Kagome basket

This document is typed out using the LaTeX software. Please refer to the .tex attached in the GitHub repository.

References

1. Ghimire, N. J. & Mazin, I. I. Topology and correlations on the kagome lattice. *Nature Materials* **19,** 137–138 (2020).