

Electronic Band Structure of Graphene and Kagome Lattice

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Abstract

The electronic band structure of a material can give us valuable information regarding the properties of it in the real world. It can also help in designing new materials with desired characteristics. There are many methods to obtain the band structure of a material but one of the fastest and simplest ways to get a qualitative understanding of the band structure is the Tight Binding method. We can get the E-k dependence and then fit the parameters according to observed data or data obtained from other calculations. In this paper, the tight binding method is applied to find the band structures of Honeycomb and Kagome lattices. First the basis vectors are established and then the problem is solved using the method. Finally a matrix is obtained which is solved using a program. Then the obtained relation is plotted using Python. This analysis for Kagome lattice reveals the presence of a flat band which is of quite significance in future research.

1 Graphene (Honeycomb Lattice)

Graphene is a structure made of Carbon atoms arranged in a 2 Dimensional Honeycomb Lattice. It is obvious that there are two types of sites in the structure, A and B. We use the first quantization tight binding method at both the sites to obtain the Hamiltonian and then to find the energy dispersion relation.

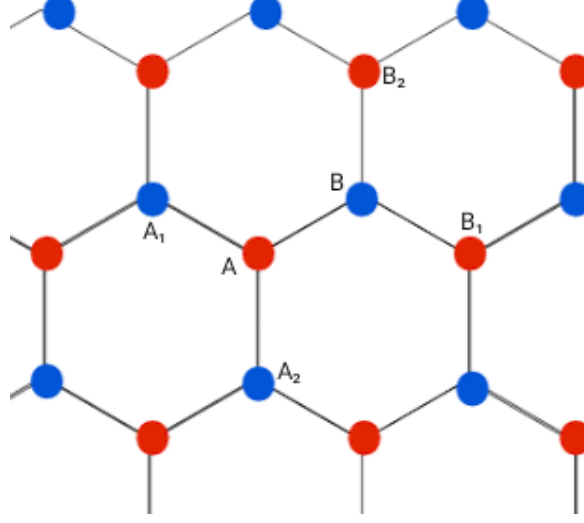


Fig. 1 Honeycomb Lattice Structure

$$\begin{aligned}\vec{AB} = \vec{a}_1 &= \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \quad \vec{AA_1} = \vec{a}_2 = \left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \quad \vec{AA_2} = \vec{a}_3 = (0, -1) \\ \vec{BB_1} = \vec{b}_1 &= -\vec{a}_2, \quad \vec{BB_2} = \vec{b}_2 = -\vec{a}_3, \quad \vec{BA} = \vec{b}_3 = -\vec{a}_1\end{aligned}$$

The self-energies for the atomic orbitals are the same since the atoms are taken to be of the same species.

$$E_0^A = E_0^B = E_0$$

Applying the tight binding method for site A [1] [3],

$$E_0^A C_{\vec{r}_m}^A - t \sum_{\vec{r}_n} C_{\vec{r}_n}^B [\delta_{\vec{r}_n, \vec{r}_m + \vec{a}_1} + \delta_{\vec{r}_n, \vec{r}_m + \vec{a}_2} + \delta_{\vec{r}_n, \vec{r}_m + \vec{a}_3}] = E C_{\vec{r}_m}^A$$

Inserting the Bloch wavefunctions

$$\begin{aligned}C_{\vec{r}}^A &= \alpha e^{i\vec{k} \cdot \vec{r}}, \quad C_{\vec{r}}^B = \beta e^{i\vec{k} \cdot \vec{r}} \\ \Rightarrow (E_0 - E)\alpha - t\beta [e^{i\vec{k} \cdot \vec{a}_1} + e^{i\vec{k} \cdot \vec{a}_2} + e^{i\vec{k} \cdot \vec{a}_3}] &= 0 \\ \Rightarrow (E_0 - E)\alpha - t\beta \left[e^{i(\frac{\sqrt{3}k_x}{2} + \frac{k_y}{2})} + e^{i(\frac{-\sqrt{3}k_x}{2} + \frac{k_y}{2})} + e^{i(-k_y)} \right] &= 0\end{aligned}$$

Similarly, for site B

$$\Rightarrow (E_0 - E)\beta - t\alpha \left[e^{-i(\frac{\sqrt{3}k_x}{2} + \frac{k_y}{2})} + e^{-i(\frac{-\sqrt{3}k_x}{2} + \frac{k_y}{2})} + e^{-i(-k_y)} \right] = 0$$

This gives rise to a Homogeneous Linear equation of the form $DX=0$

$$\begin{bmatrix} E_0 - E & -t \left[e^{i(\frac{\sqrt{3}k_x}{2} + \frac{k_y}{2})} + e^{i(\frac{-\sqrt{3}k_x}{2} + \frac{k_y}{2})} + e^{i(-k_y)} \right] \\ -t \left[e^{-i(\frac{\sqrt{3}k_x}{2} + \frac{k_y}{2})} + e^{-i(\frac{-\sqrt{3}k_x}{2} + \frac{k_y}{2})} + e^{-i(-k_y)} \right] & E_0 - E \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

For a non-trivial solution, $\det(D)=0$. Putting $\det(D)=0$ gives a quadratic equation in E and solving it using Mathematica [2], we get,

$$E = E_0 \pm \sqrt{1 + 4\cos^2\left(\frac{\sqrt{3}k_x}{2}\right) + 4\cos\left(\frac{\sqrt{3}k_x}{2}\right)\cos\left(\frac{3k_y}{2}\right)}$$

Plotting this relation, we get

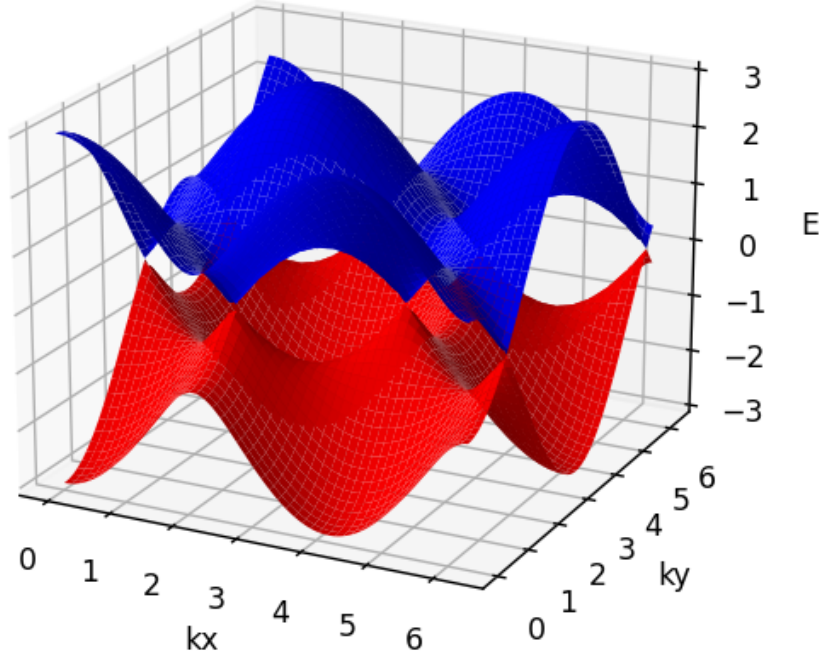


Fig. 2 Graphene Band Structure in 3D

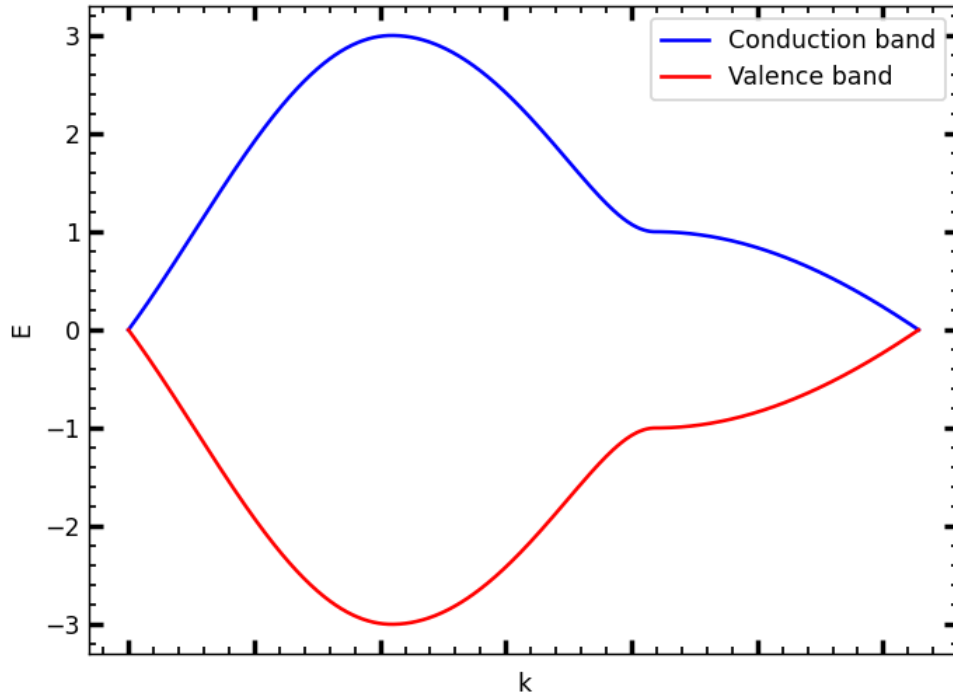


Fig. 3 Graphene Band Structure in 2D

2 Kagome Lattice Tight Binding

Kagome lattice structure is a two dimensional structure where a single site is removed from a triangular lattice structure at repeated positions. It forms a star like pattern where every site has four neighbours. There are three distinct points in the lattice named A, B and C. Using the tight binding model like in the case of graphene for sites A, b and C, we get the energy dispersion relation.

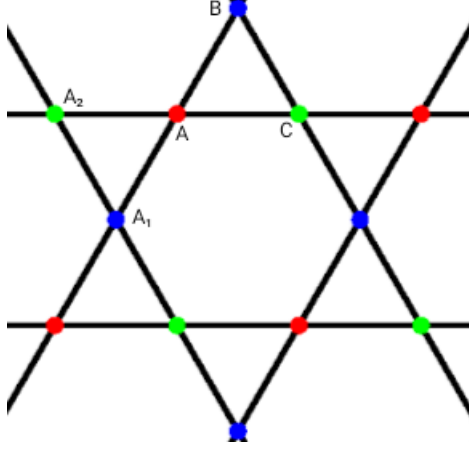


Fig. 4 Kagome Lattice Structure

$$\begin{aligned}\vec{AC} = \vec{v}_1 = (1, 0), \quad \vec{AB} = \vec{v}_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \quad \vec{v}_3 = \vec{v}_2 - \vec{v}_1 = \left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \\ \vec{AC} = \vec{a}_1 = \vec{v}_1, \quad \vec{AA}_1 = \vec{a}_2 = -\vec{v}_2, \quad \vec{AA}_2 = \vec{a}_3 = -\vec{v}_1, \quad \vec{AB} = \vec{a}_4 = \vec{v}_2\end{aligned}$$

The self-energies for the atomic orbitals are the same since the atoms are taken to be of the same species.

$$E_0^A = E_0^B = E_0^C = E_0$$

Applying the tight binding method for site A [1]

$$\begin{aligned}E_0^A C_{\vec{r}_m}^A - t \sum_{\vec{r}_n} C_{\vec{r}_n}^C [\delta_{\vec{r}_n, \vec{r}_m + \vec{a}_1} + \delta_{\vec{r}_n, \vec{r}_m + \vec{a}_3}] - t \sum_{\vec{r}_n} C_{\vec{r}_n}^B [\delta_{\vec{r}_n, \vec{r}_m + \vec{a}_2} + \delta_{\vec{r}_n, \vec{r}_m + \vec{a}_4}] = EC_{\vec{r}_m}^A \\ \Rightarrow E_0^A C_{\vec{r}_m}^A - t [C_{\vec{r}_n, \vec{r}_m + \vec{a}_1}^C + C_{\vec{r}_n, \vec{r}_m + \vec{a}_3}^C] - t [C_{\vec{r}_n, \vec{r}_m + \vec{a}_2}^B + C_{\vec{r}_n, \vec{r}_m + \vec{a}_4}^B] = EC_{\vec{r}_m}\end{aligned}$$

Putting in the Bloch wavefunctions given below in the equation

$$C_{\vec{r}}^A = \alpha e^{i\vec{k} \cdot \vec{r}}, \quad C_{\vec{r}}^B = \beta e^{i\vec{k} \cdot \vec{r}}, \quad C_{\vec{r}}^C = \gamma e^{i\vec{k} \cdot \vec{r}}$$

We get,

$$\begin{aligned}(E_0 - E)\alpha - t\gamma [e^{i\vec{k} \cdot \vec{a}_1} + e^{i\vec{k} \cdot \vec{a}_3}] - t\beta [e^{i\vec{k} \cdot \vec{a}_2} + e^{i\vec{k} \cdot \vec{a}_4}] = 0 \\ \vec{k} \cdot \vec{v}_1 = k_x = \theta_1, \quad \vec{k} \cdot \vec{v}_2 = \frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} = \theta_2, \quad \vec{k} \cdot \vec{v}_3 = -\frac{k_x}{2} + \frac{\sqrt{3}k_y}{2} = \theta_3 \\ \alpha(E_0 - E) + \gamma(-2t\cos\theta_1) + \beta(-2t\cos\theta_2) = 0\end{aligned}$$

Similarly for sites B and C,

$$\beta(E_0 - E) + \gamma(-2t\cos\theta_3) + \alpha(-2t\cos\theta_2) = 0$$

$$\gamma(E_0 - E) + \alpha(-2t\cos\theta_1) + \beta(-2t\cos\theta_3) = 0$$

This system of three linear equations for variables α , β and γ can be written in the matrix notation as

$$\begin{bmatrix} E_0 - E & -2t\cos\theta_2 & -2t\cos\theta_1 \\ -2t\cos\theta_2 & E_0 - E & -2t\cos\theta_3 \\ -2t\cos\theta_1 & -2t\cos\theta_3 & E_0 - E \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

This is a homogeneous linear equation of the form $DX=O$. For a non-trivial solution we need the determinant of D to be zero. Therefore putting $\det(D)=0$, we get a cubic equation in E . Solving it [2] and simplifying using the relation between θ_1 , θ_2 and θ_3 we get

$$E = 2t$$

$$E = -t \left[1 \pm \sqrt{4(\cos^2\theta_1 + \cos^2\theta_2 + \cos^2\theta_3) - 3} \right]$$

Plotting it gives the following band structure

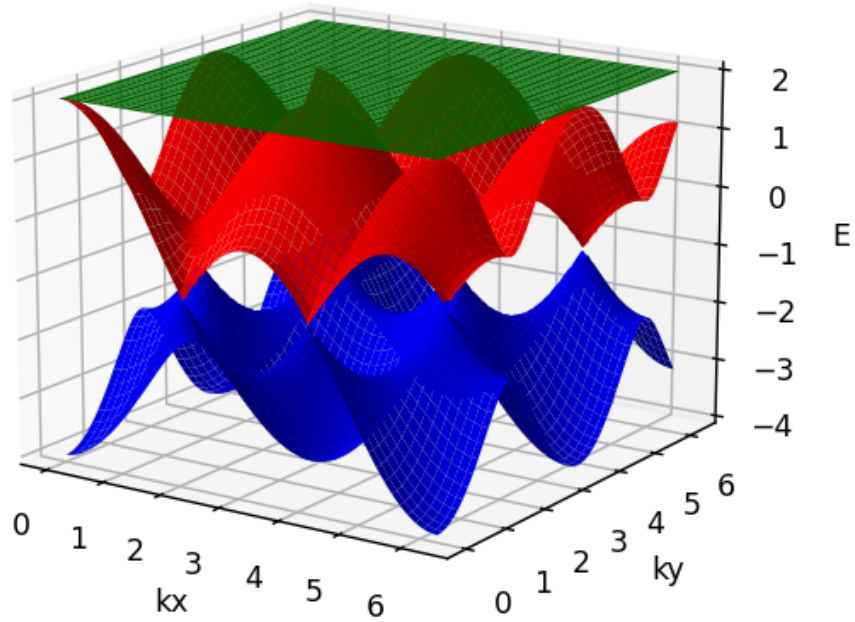


Fig. 5 Kagome Lattice Band Structure

3 Conclusion

We have seen the tight binding models for Honeycomb and Kagome lattices. Two bands were obtained for the Graphene lattice and they were plotted. The flat band obtained for the Kagome lattice is of great significance because electrons in the flat band are not momentum dependent for the energies i.e. they have constant energy at all point of the k-space. This means that the effective mass becomes infinite which leads to exotic material properties.

References

- [1] N. W. Ashcroft and N. D. Mermin. *Solid State Physics*. Holt-Saunders, 1976.
- [2] Wolfram Research, Inc. Mathematica, Version 13.1. Champaign, IL, 2022.
- [3] J. C. Slater and G. F. Koster. Simplified lcao method for the periodic potential problem. *Phys. Rev.*, 94:1498–1524, Jun 1954.