Band Structure of 2D Kagome Lattice: Tight-Binding Analysis with Nearest and Next-Nearest Neighbor Hopping

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Abstract

This article studies the Kagome lattice's electronic structure using a tight-binding approach. Deriving the dispersion relation for nearest-neighbor hopping reveals two dispersive bands and one flat band, which has been visualized through 3D/2D plots. Additionally, this article analyzes the band next-nearest-neighbor hopping, discussing how additional terms modify the band structure.

Keywords: Kagome lattice, Tight-binding model, Dispersion relation, Geometric frustration, Second quantization

I. INTRODUCTION

A. Background

The kagome lattice was coined by Japanese physicist Kôdi Husimi, and first appeared in a 1951 paper by his assistant Ichirō Shōji [1]. It has emerged as a paradigmatic platform for studying geometric frustration due to its unique combination of cornersharing triangles. This geometric arrangement naturally leads to competing interactions and degenerate ground states, making it an ideal system for investigating exotic quantum phases such as quantum spin liquids, which evade conventional magnetic ordering even at absolute zero temperature.

The lattice's inherent frustration arises from the impossibility of simultaneously minimizing all pairwise interactions in antiferromagnetically coupled Ising spins on triangular units.

Recent years have witnessed renewed interest in Kagome materials driven by experimental discoveries of real materials with Kagome-like structures, such as Herbertsmithite ($ZnCu_3(OH)_6Cl_2$), which exhibits signatures of quantum spin liquid behavior, and AV_3Sb_5 (A = K, Rb, Cs) compounds that display unconventional superconductivity and charge density wave orders.

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B. Lattice Structure

Different from the two types of sites in honeycomb lattice, the Kagome lattice has 3 types of sites, A (blue), B (red), and C (green), respectively.

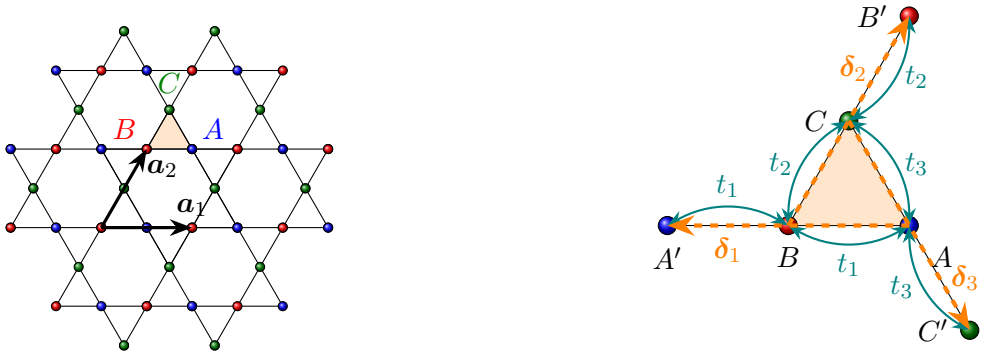

FIG. 1: Top view of the Kagome Lattice and tight-binding model with NN hopping

The three sites in the unit cell form a regular triangle, which is shaded in Fig. 1. The primitive vectors and reciprocal (Honeycomb, not shown in the article) vectors are

$$\boldsymbol{a}_1 = a(2,0), \quad \boldsymbol{a}_2 = a(1,\sqrt{3}); \quad \boldsymbol{b}_1 = \frac{2\pi}{a}\left(0, \frac{1}{\sqrt{3}}\right), \quad \boldsymbol{b}_2 = \frac{2\pi}{a}\left(\frac{1}{2}, -\frac{1}{2\sqrt{3}}\right). \tag{1.1}$$

Simply taking the unit cell located at $\boldsymbol{r}$. Then, each site in the unit cell has 2 NN hoppings, pointing out by the lattice vectors

$$\boldsymbol{\delta}_1 = a(-2,0), \quad \boldsymbol{\delta}_2 = a(1,\sqrt{3}), \quad \boldsymbol{\delta}_3 = a(1,-\sqrt{3}), \tag{1.2}$$

where a is the lattice constant, the distance between any two NN lattices.

II. MODEL HAMILTONIAN

In this model, consider the nearest-neighbor (NN) hopping with different hopping magnitude t_1, t_2, and t_3. The Hamiltonian illustrates the tight-binding model in terms of second quantization [2]

$$\mathcal{H} = -\sum_{\boldsymbol{r}} [t_1(\hat{a}^\dagger_{\boldsymbol{r}}\hat{b}_{\boldsymbol{r}} + \hat{b}^\dagger_{\boldsymbol{r}}\hat{a}_{\boldsymbol{r}+\boldsymbol{\delta}_1}) + t_2(\hat{b}^\dagger_{\boldsymbol{r}}\hat{c}_{\boldsymbol{r}} + \hat{c}^\dagger_{\boldsymbol{r}}\hat{b}_{\boldsymbol{r}+\boldsymbol{\delta}_2}) + t_3(\hat{c}^\dagger_{\boldsymbol{r}}\hat{a}_{\boldsymbol{r}} + \hat{a}^\dagger_{\boldsymbol{r}}\hat{c}_{\boldsymbol{r}+\boldsymbol{\delta}_3})] + \text{H.c.} \tag{2.1}$$

Assume there are N A-, B-, and C- type sites in total. Applying the Fourier transformation to the Fermion operators

$$\hat{a}_{\boldsymbol{r}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,\hat{a}_{\boldsymbol{k}}, \qquad \hat{b}_{\boldsymbol{r}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,\hat{b}_{\boldsymbol{k}}, \qquad \hat{c}_{\boldsymbol{r}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\,\hat{c}_{\boldsymbol{k}},$$

$$\hat{a}_{\boldsymbol{r}+\boldsymbol{\delta}_1} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{\delta}_1)}\,\hat{a}_{\boldsymbol{k}}, \quad \hat{b}_{\boldsymbol{r}+\boldsymbol{\delta}_2} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{\delta}_2)}\,\hat{b}_{\boldsymbol{k}}, \quad \hat{c}_{\boldsymbol{r}+\boldsymbol{\delta}_3} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{\delta}_3)}\,\hat{c}_{\boldsymbol{k}}.$$

Similar for their Hermite conjugates

$$\hat{a}^\dagger_{\boldsymbol{r}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\,\hat{a}^\dagger_{\boldsymbol{k}}, \qquad \hat{b}^\dagger_{\boldsymbol{r}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\,\hat{b}^\dagger_{\boldsymbol{k}}, \qquad \hat{c}^\dagger_{\boldsymbol{r}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\,\hat{c}^\dagger_{\boldsymbol{k}},$$

$$\hat{a}^\dagger_{\boldsymbol{r}+\boldsymbol{\delta}_1} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{\delta}_1)}\,\hat{a}^\dagger_{\boldsymbol{k}},\ \hat{b}^\dagger_{\boldsymbol{r}+\boldsymbol{\delta}_2} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{\delta}_2)}\,\hat{b}^\dagger_{\boldsymbol{k}},\ \hat{c}^\dagger_{\boldsymbol{r}+\boldsymbol{\delta}_3} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}+\boldsymbol{\delta}_3)}\,\hat{c}^\dagger_{\boldsymbol{k}}.$$

Substituting the transformed operators into the Hamiltonian (2.1)

$$\begin{aligned}\mathcal{H} &= -\sum_{\boldsymbol{k}}[t_1(1+\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1})\hat{a}^\dagger_{\boldsymbol{k}}\hat{b}_{\boldsymbol{k}} + t_2(1+\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_2})\hat{b}^\dagger_{\boldsymbol{k}}\hat{c}_{\boldsymbol{k}} + t_3(1+\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_3})\hat{c}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}] + \text{H.c.} \\ &= -\sum_{\boldsymbol{k}}[\tilde{t}_1\hat{a}^\dagger_{\boldsymbol{k}}\hat{b}_{\boldsymbol{k}} + \tilde{t}_2\hat{b}^\dagger_{\boldsymbol{k}}\hat{c}_{\boldsymbol{k}} + \tilde{t}_3\hat{c}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}] + \text{H.c.}\end{aligned}$$

Here $\tilde{t}_i$ are used for simplification, and the identity

$$\sum_{A,B,C} \mathrm{e}^{\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} = N\delta_{\boldsymbol{k}',\boldsymbol{k}}$$

is applied.

III. DISPERSION RELATION

Diagonalizing the Hamiltonian first. The Hamiltonian can be written as

$$\mathcal{H} = \sum_{\boldsymbol{k}} \Psi^\dagger_{\boldsymbol{k}}\tilde{\mathcal{H}}\Psi_{\boldsymbol{k}} = \sum_{\boldsymbol{k}} \begin{pmatrix}\hat{a}^\dagger_{\boldsymbol{k}} & \hat{b}^\dagger_{\boldsymbol{k}} & \hat{c}^\dagger_{\boldsymbol{k}}\end{pmatrix} \begin{pmatrix} 0 & -\tilde{t}_1 & -\tilde{t}^*_3 \\ -\tilde{t}^*_1 & 0 & -\tilde{t}_2 \\ -\tilde{t}_3 & -\tilde{t}^*_2 & 0 \end{pmatrix} \begin{pmatrix}\hat{a}_{\boldsymbol{k}} \\ \hat{b}_{\boldsymbol{k}} \\ \hat{c}_{\boldsymbol{k}}\end{pmatrix}, \tag{3.1}$$

it is naturally that all diagonal elements of $\tilde{\mathcal{H}}$ are zero since there is not exist the elements like $\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}$ in the transformed Hamiltonian. The diagonalized Hamiltonian (3.1) can be determined by comparing

$$\mathcal{H} = \sum_{\boldsymbol{k}} \begin{pmatrix}\hat{a}^\dagger_{\boldsymbol{k}} & \hat{b}^\dagger_{\boldsymbol{k}} & \hat{c}^\dagger_{\boldsymbol{k}}\end{pmatrix} \begin{pmatrix} -H_{11} & -H_{12} & -H_{13} \\ -H_{21} & -H_{22} & -H_{23} \\ -H_{31} & -H_{32} & -H_{33} \end{pmatrix} \begin{pmatrix}\hat{a}_{\boldsymbol{k}} \\ \hat{b}_{\boldsymbol{k}} \\ \hat{c}_{\boldsymbol{k}}\end{pmatrix}$$

with the transformed Hamiltonian.

From the eigenequation $\det(\tilde{\mathcal{H}} - E\mathbb{1}) = 0$, one can obtain a cubic polynomial in E

$$E^3 - E(|\tilde{t}_1|^2 + |\tilde{t}_2|^2 + |\tilde{t}_3|^2) + \tilde{t}_1\tilde{t}_2\tilde{t}_3 + \tilde{t}^*_1\tilde{t}^*_2\tilde{t}^*_3 = 0. \tag{3.2}$$

Expanding $|\tilde{t}_1|^2$

$$|\tilde{t}_1|^2 = \tilde{t}_1\tilde{t}^*_1 = t_1^2(1+\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1})(1+\mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1}) = t_1^2[2+2\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_1)].$$

Similarly for $|\tilde{t}_2|^2$ and $|\tilde{t}_3|^2$

$$|\tilde{t}_2|^2 = t_2^2[2 + 2\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_2)], \quad |\tilde{t}_3|^2 = t_3^2[2 + 2\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_3)].$$

Expanding $\tilde{t}_1\tilde{t}_2\tilde{t}_3$

$$\begin{aligned}\tilde{t}_1\tilde{t}_2\tilde{t}_3 = t_1t_2t_3[1 &+ \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1} + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_2} + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_3} \\ &+ \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{\delta}_2+\boldsymbol{\delta}_3)} + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_3)} + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_2)} + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_2+\boldsymbol{\delta}_3)}].\end{aligned}$$

Similarly for the conjugate

$$\begin{aligned}\tilde{t}_1^*\tilde{t}_2^*\tilde{t}_3^* = t_1t_2t_3[1 &+ \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1} + \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_2} + \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_3} \\ &+ \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{\delta}_2+\boldsymbol{\delta}_3)} + \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_3)} + \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_2)} + \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_2+\boldsymbol{\delta}_3)}].\end{aligned}$$

Combining the two terms

$$\begin{aligned}\tilde{t}_1\tilde{t}_2\tilde{t}_3 + \tilde{t}_1^*\tilde{t}_2^*\tilde{t}_3^* &= t_1t_2t_3[2 + 2\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_1) + 2\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_2) + 2\cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_3) \\ &\quad + 2\cos(\boldsymbol{k}\cdot(\boldsymbol{\delta}_2+\boldsymbol{\delta}_3)) + 2\cos(\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_3)) + 2\cos(\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_2)) \\ &\quad + 2\cos(\boldsymbol{k}\cdot(\boldsymbol{\delta}_1+\boldsymbol{\delta}_2+\boldsymbol{\delta}_3))] \\ &= 4t_1t_2t_3[1 + \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_1) + \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_2) + \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_3)],\end{aligned}$$

where $\boldsymbol{\delta}_i + \boldsymbol{\delta}_j = -\epsilon_{ijk}\boldsymbol{\delta}_k$, $\sum_i \boldsymbol{\delta}_i = 0$ is used from (1.2).

Then, substituting these terms into the dispersion relation (3.2)

$$E^3 - 2E\sum_i^3 t_i^2(1 + \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_i)) + 4t_1t_2t_3\left[1 + \sum_i^3 \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_i)\right] = 0. \tag{3.3}$$

This is a universal result.

IV. RESULT DISCUSSION

Simply taking $t_1 = t_2 = t_3 = t$, then the dispersion relation (3.3) becomes

$$E^3 - 2Et^2\left[3 + \sum_i^3 \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_i)\right] + 4t^3\left[1 + \sum_i^3 \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_i)\right] = 0. \tag{4.1}$$

By using the solution of the cubic equation, there are three solutions for (4.1)

$$E_+ = t\left[-1 + \sqrt{3 + 2\textstyle\sum_i^3 \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_i)}\right], \tag{4.2a}$$

$$E_- = t\left[-1 - \sqrt{3 + 2\textstyle\sum_i^3 \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_i)}\right], \tag{4.2b}$$

$$E_{\text{flat}} = 2t, \tag{4.2c}$$

i.e., two dispersive bands (4.2a) and (4.2b), and one flat band (4.2c).

A. Band Structure

Python is used to plot its band structure. The hopping magnitude t is taken as 1. Fig. 2 shows the energy band structure for the two dispersive bands and the one flat band.

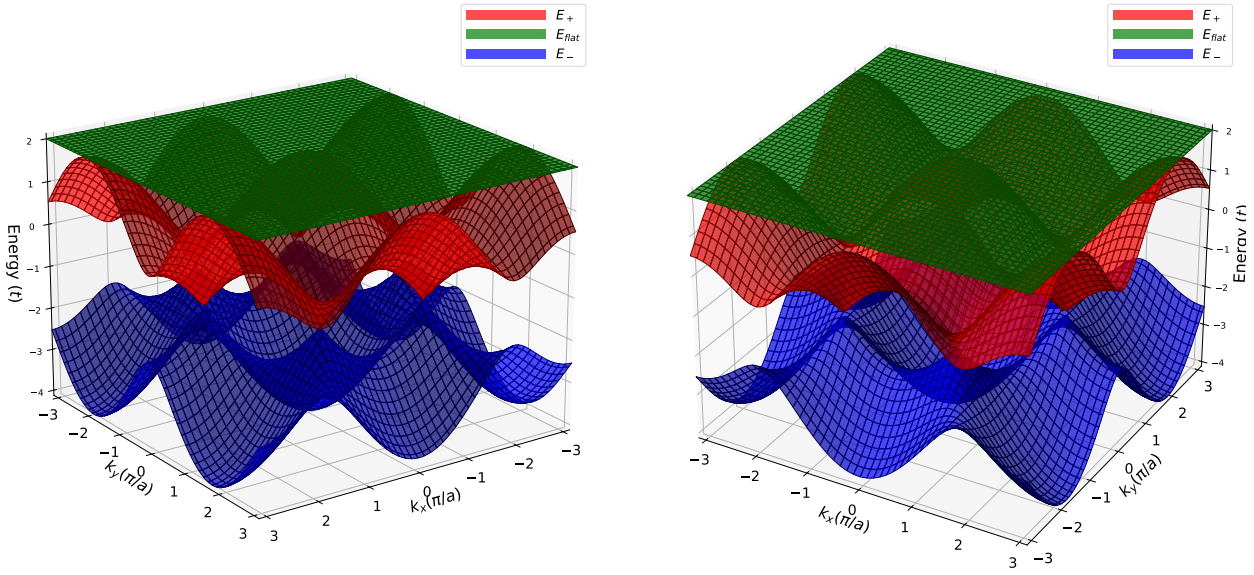

FIG. 2: 3D band structure for NN hopping under different perspectives

In momentum space, Fig. 3 demonstrates the contours for the two dispersive bands in the k_x-k_y plane.

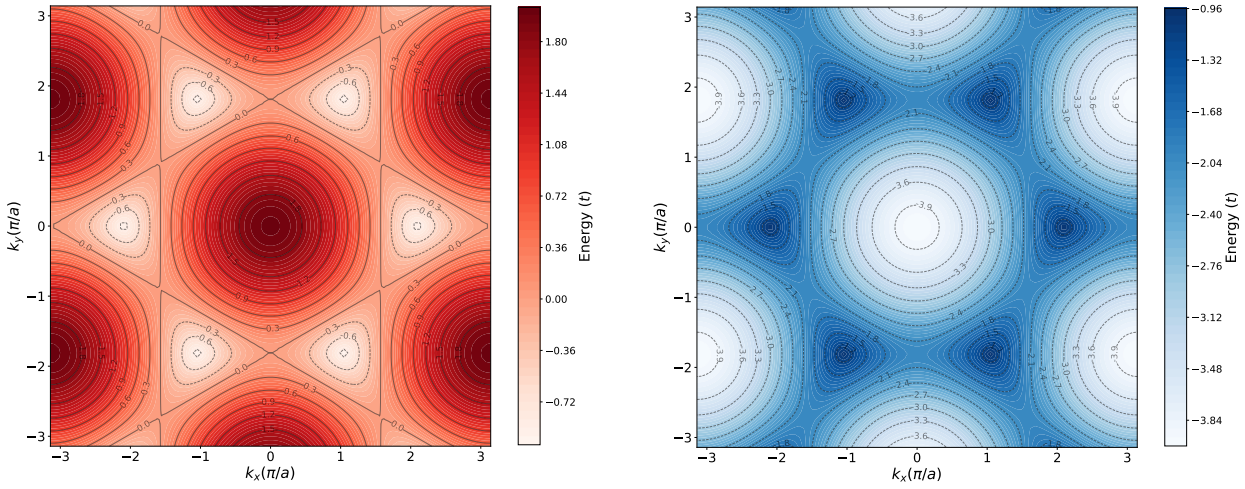

FIG. 3: 2D band structure for the two dispersive bands

B. Properties around the Dirac Point

Taking the simplest K-point: $\frac{2\pi}{a}\left(0, \frac{1}{\sqrt{3}}\right)$. At this point, this dispersion relation becomes

$$E_+ = t[-1 \pm \sqrt{3 + 2(\cos(0) + \cos(2\pi) + \cos(-2\pi))}] = 2t = E_{\text{flat}}, \quad E_- = -4t,$$

which is implied in Fig. 2: E_{flat} and E_+ are tangent at four K-points.

Sightly taking $\boldsymbol{k} = \boldsymbol{b}_2 + \boldsymbol{q}$ with $|\boldsymbol{q}| \ll 1$, then, the dispersion relation becomes

$$E_+ = t[-1 + \sqrt{3 + 2(3 - 12\pi^2|\boldsymbol{q}|^2)}] = t\left(2 - \frac{4}{3}\pi^2|\boldsymbol{q}^2|\right), \quad E_- = t\left(-4 + \frac{4}{3}\pi^2|\boldsymbol{q}|^2\right),$$

which indicates that the dispersive bands around the Dirac points are parabolic.

V. ADVANCED STUDY: THE NEXT-NEAREST NEIGHBOR HOPPING TERM

Assume the hopping magnitude between the NNN t_i', just add the NNN hopping in the right part of Fig. 1 is enough, since all the NNN and NN hopping can be covered by simply splicing each unit, as shown in Fig. 4

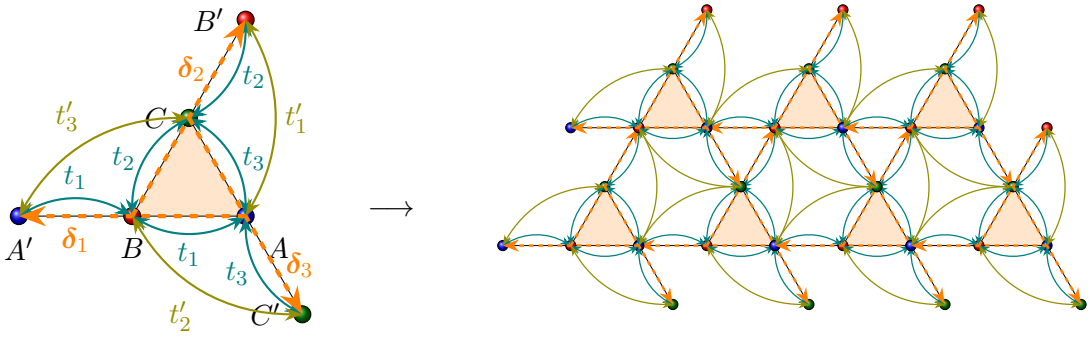

FIG. 4: TB model with NN and NNN hopping

The total Hamiltonian can be separated into two terms: The NN (Nearest neighbor) one and the NNN (Next-Nearest Neighbor) one

$$\mathcal{H}' = \mathcal{H}_{\text{NN}} + \mathcal{H}_{\text{NNN}}. \tag{5.1}$$

The NN term has already given in (2.1), similarly, the NNN term can be expressed as [3]

$$\begin{aligned}\mathcal{H}_{\text{NNN}} &= -\sum_{\boldsymbol{r}}[t_1'(\hat{a}_{\boldsymbol{r}}^\dagger \hat{b}_{\boldsymbol{r}+\boldsymbol{\delta}_2} + \hat{b}_{\boldsymbol{r}}^\dagger \hat{c}_{\boldsymbol{r}+\boldsymbol{\delta}_3} + \hat{c}_{\boldsymbol{r}}^\dagger \hat{a}_{\boldsymbol{r}+\boldsymbol{\delta}_1})] + \text{H.c.} \\ &= \sum_{\boldsymbol{k}} \Psi_{\boldsymbol{k}}^\dagger \begin{pmatrix} 0 & -t_1' \, \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_2} & -t_3' \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1} \\ -t_1' \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_2} & 0 & -t_2' \, \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_3} \\ -t_3' \, \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1} & -t_2' \, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_3} & 0 \end{pmatrix} \Psi_{\boldsymbol{k}} = \sum_{\boldsymbol{k}} \Psi_{\boldsymbol{k}}^\dagger \begin{pmatrix} 0 & -\tilde{t}_1' & -\tilde{t}_3'^* \\ -\tilde{t}_1'^* & 0 & -\tilde{t}_2' \\ -\tilde{t}_3' & -\tilde{t}_2'^* & 0 \end{pmatrix} \Psi_{\boldsymbol{k}}. \end{aligned} \tag{5.2}$$

Similarly to the NN case, let $\det(\tilde{\mathcal{H}}' - E\mathbb{1}) = 0$, we will obtain a very long equation of the dispersion relation. For simplification, sightly taking $t_1' = t_2' = t_3' = t'$, then

$$E^3 - 3E|t + t'|^2 + (\tilde{t} + \tilde{t}')^3 + (\tilde{t}^* + \tilde{t}'^*)^3 = 0, \tag{5.3}$$

and the energy band can be plotted from this equation.

It is interesting that the diagonal of the transformed Hamiltonian is always zero in the NN and NNN cases. So, if we further consider a farther NNN hopping (actually, it is NNNN hopping) instead of the NNN hopping right now, then taking the hopping magnitude between A and A' is t_1'', B and B' is t_2'', C and C' is t_3''. Finally, an extra term will be raised in the total Hamiltonian

$$\mathcal{H}_{\text{NNNN}} = -\sum_{\boldsymbol{r}}[t_1''\hat{a}_{\boldsymbol{r}}^\dagger \hat{a}_{\boldsymbol{r}+\boldsymbol{\delta}_1} + t_2''\hat{b}_{\boldsymbol{r}}^\dagger \hat{b}_{\boldsymbol{r}+\boldsymbol{\delta}_2} + t_3''\hat{c}_{\boldsymbol{r}}^\dagger \hat{c}_{\boldsymbol{r}+\boldsymbol{\delta}_3}] + \text{H.c.}, \tag{5.4}$$

and the Hamiltonian matrix in momentum space becomes

$$\tilde{\mathcal{H}}' = \begin{pmatrix} -2t_1'' \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_1) & -t_1(1 + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1}) & -t_2(1 + \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_2}) \\ -t_1(1 + \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_1}) & -2t_2'' \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_2) & -t_3(1 + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_3}) \\ -t_2(1 + \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_2}) & -t_3(1 + \mathrm{e}^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\delta}_3}) & -2t_3'' \cos(\boldsymbol{k}\cdot\boldsymbol{\delta}_3) \end{pmatrix}. \tag{5.5}$$

One can obtain the dispersion relation via $\det(\tilde{\mathcal{H}}' - E\mathbb{1}) = 0$.

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