

Band Structure of 2D Kagome Lattice

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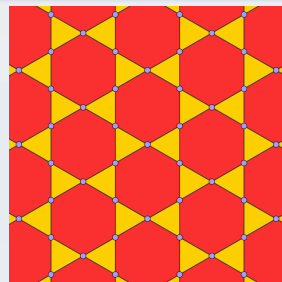
INTRODUCTION

What is Kagome? — The Trihexagonal

Coined by Kôdi Husimi

The kagome lattice first appeared in a paper by Kôdi Husimi's assistant Ichirô Shôji [1]. Satisfying the $p6m$ symmetry.

- Six-fold rotation about hexagon centers
- Multiple mirror reflection lines
- Triangular and hexagonal sublattice symmetries
- Combined rotation-reflection ($C_6\sigma$) operations

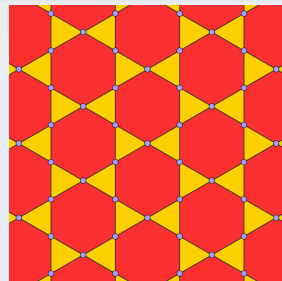


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Outlook

- Discovering new Kagome materials
- Kagome quantum spin liquid and superconducting behaviors
- Kagome topological properties

Lattice Structure

Three type of sites

- Marked as A (blue), B (red), and C (green), respectively
- Hops' magnitude between different types of sites is different

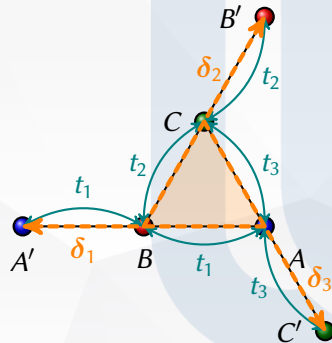
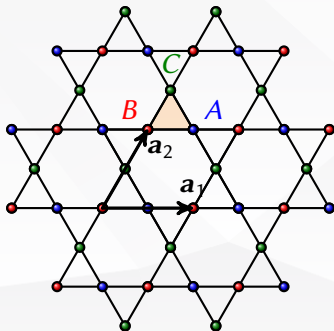


Figure. Top view of the Kagome Lattice and tight-binding model with NN hopping



METHODOLOGY

Model Hamiltonian

Tight-binding model in second quantization [2]

Consider the nearest-neighbor (NN) hopping

$$\mathcal{H} = - \sum_{\mathbf{r}} [t_1(\hat{a}_{\mathbf{r}}^\dagger \hat{b}_{\mathbf{r}} + \hat{b}_{\mathbf{r}}^\dagger \hat{a}_{\mathbf{r}+\delta_1}) + t_2(\hat{b}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}} + \hat{c}_{\mathbf{r}}^\dagger \hat{b}_{\mathbf{r}+\delta_2}) + t_3(\hat{c}_{\mathbf{r}}^\dagger \hat{a}_{\mathbf{r}} + \hat{a}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}+\delta_3})] + \text{H.c.} \quad (1)$$

The operators $\hat{a}_{\mathbf{r}}$ ($\hat{a}_{\mathbf{r}}^\dagger$), $\hat{b}_{\mathbf{r}}$ ($\hat{b}_{\mathbf{r}}^\dagger$), $\hat{c}_{\mathbf{r}}$ ($\hat{c}_{\mathbf{r}}^\dagger$) stands for annihilating (or creating) an electron at site \mathbf{r} .

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Uniform labels via Fourier transformation

Raising an extra phase factor for the annihilation/creation operators of the NN sites

$$\hat{o}_{\mathbf{r}+\delta_i} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot (\mathbf{r}+\delta_i)} \hat{o}_{\mathbf{k}}, \quad \hat{o}_{\mathbf{r}+\delta_i}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot (\mathbf{r}+\delta_i)} \hat{o}_{\mathbf{k}}^\dagger$$

Operators $\hat{o} = \{\hat{a}, \hat{b}, \hat{c}\}$.

Dispersion Relation

Diagonalized Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \tilde{\mathcal{H}} \Psi_{\mathbf{k}} = \sum_{\mathbf{k}} \begin{pmatrix} \hat{a}_{\mathbf{k}}^{\dagger} \\ \hat{b}_{\mathbf{k}}^{\dagger} \\ \hat{c}_{\mathbf{k}}^{\dagger} \end{pmatrix}^T \begin{pmatrix} 0 & -t_1(1 + e^{-i\mathbf{k} \cdot \delta_1}) & -t_3(1 + e^{+i\mathbf{k} \cdot \delta_3}) \\ -t_1(1 + e^{+i\mathbf{k} \cdot \delta_1}) & 0 & -t_2(1 + e^{-i\mathbf{k} \cdot \delta_2}) \\ -t_3(1 + e^{-i\mathbf{k} \cdot \delta_3}) & -t_2(1 + e^{+i\mathbf{k} \cdot \delta_2}) & 0 \end{pmatrix} \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \\ \hat{c}_{\mathbf{k}} \end{pmatrix} \quad (2)$$

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Eigen Equation

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

$$E^3 - 2E \sum_i^3 t_i^2 (1 + \cos(\mathbf{k} \cdot \boldsymbol{\delta}_i)) + 4t_1 t_2 t_3 \left[1 + \sum_i^3 \cos(\mathbf{k} \cdot \boldsymbol{\delta}_i) \right] = 0 \quad (3)$$

This is a universal result.

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Cubic eigen equation \Rightarrow Three energy bands = Two dispersive bands + One flat band



RESULT DISCUSSION

Band Structure

Trivial case

Simply taking $t_1 = t_2 = t_3 = t$

$$E_{\pm} = t \left[-1 \pm \sqrt{3 + 2 \sum_i^3 \cos(\mathbf{k} \cdot \boldsymbol{\delta}_i)} \right], \quad E_{\text{flat}} = 2t \quad (4)$$

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Numerical plotting

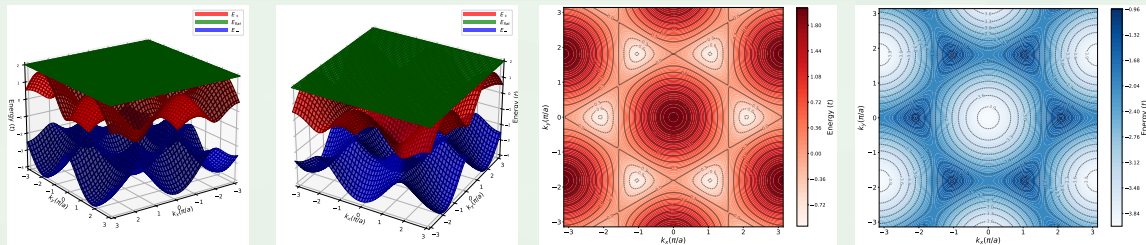


Figure. 3D/2D Band structure for NN hopping under different perspectives plotted by Python

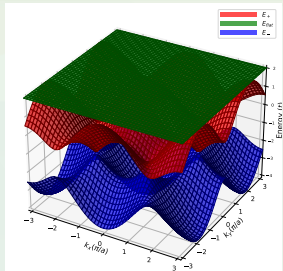
Dirac Point

At the Dirac point

Taking $K = \frac{2\pi}{a} \left(0, \frac{1}{\sqrt{3}}\right)$

$$E_+ = 2t = E_{\text{flat}}, \quad E_- = -4t$$

Implies that E_{flat} and E_+ are tangent at four K -points, which can be seen in the right figure.



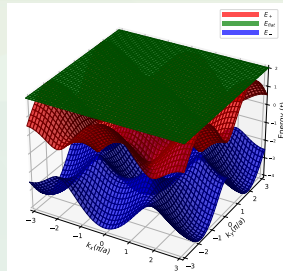
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Near the Dirac point

Taking $\mathbf{k} = \mathbf{b}_2 + \mathbf{q}$ with $|\mathbf{q}| \ll 1$

$$E_+ = t \left(2 - \frac{4}{3} \pi^2 |\mathbf{q}|^2 \right), \quad E_- = t \left(-4 + \frac{4}{3} \pi^2 |\mathbf{q}|^2 \right)$$

Indicates that the dispersive bands around the Dirac points are parabolic.



ADVANCED STUDY

An Extra NNN or NNNN Hopping

The Hamiltonian with the NNN or NNNN hopping term

$$\mathcal{H}' = \mathcal{H}_{\text{NN}}(t'_i) + \mathcal{H}_{\text{NNN/NNNN}}(t''_i) \quad (5)$$

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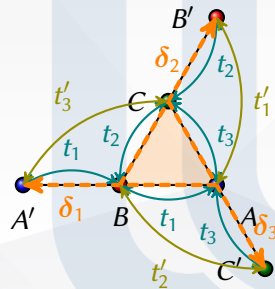


Figure. Graph for NN and NNN hopping

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with the corresponding diagonalized ones

$$\begin{aligned} \mathcal{H}_{\text{NNN}} &= - \sum_{\mathbf{r}} [t'_1 (\hat{a}_{\mathbf{r}}^\dagger \hat{b}_{\mathbf{r}+\delta_2} + \hat{b}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}+\delta_3} + \hat{c}_{\mathbf{r}}^\dagger \hat{a}_{\mathbf{r}+\delta_1})] + \text{H.c.} \\ &= \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \begin{pmatrix} 0 & -t'_1 e^{+i\mathbf{k} \cdot \delta_2} & -t'_1 e^{-i\mathbf{k} \cdot \delta_1} \\ -t'_1 e^{-i\mathbf{k} \cdot \delta_2} & 0 & -t'_2 e^{+i\mathbf{k} \cdot \delta_3} \\ -t'_3 e^{+i\mathbf{k} \cdot \delta_1} & -t'_2 e^{-i\mathbf{k} \cdot \delta_3} & 0 \end{pmatrix} \Psi_{\mathbf{k}} \quad (6) \end{aligned}$$

$$\begin{aligned} \mathcal{H}_{\text{NNNN}} &= - \sum_{\mathbf{r}} [t''_1 \hat{a}_{\mathbf{r}}^\dagger \hat{a}_{\mathbf{r}+\delta_1} + t''_2 \hat{b}_{\mathbf{r}}^\dagger \hat{b}_{\mathbf{r}+\delta_2} + t''_3 \hat{c}_{\mathbf{r}}^\dagger \hat{c}_{\mathbf{r}+\delta_3}] + \text{H.c.} \\ &= \begin{pmatrix} -2t''_1 \cos(\mathbf{k} \cdot \delta_1) & & \\ & -2t''_2 \cos(\mathbf{k} \cdot \delta_2) & \\ & & -2t''_3 \cos(\mathbf{k} \cdot \delta_3) \end{pmatrix} \quad (7) \end{aligned}$$

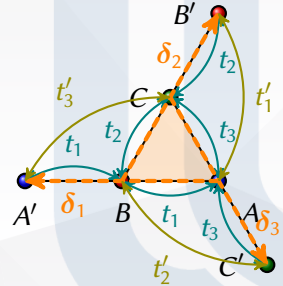


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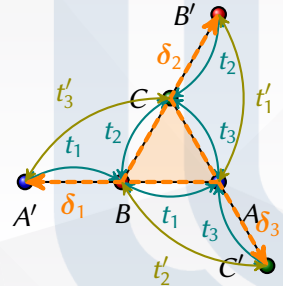


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Interesting, $\mathcal{H}_{\text{NNNN}}$ is a diagonal matrix. Energy bands can be obtained from $\det(\tilde{\mathcal{H}} - E\mathbb{1}) = 0$.

Bibliography I

- [1] WIKIPEDIA. *Trihexagonal tiling*. Available online at: https://en.wikipedia.org/wiki/Trihexagonal_tiling. 2025.
- [2] Tianyu Liu. “Strain-induced pseudomagnetic field and quantum oscillations in kagome crystals”. In: *Phys. Rev. B* 102 (4 July 2020), p. 045151. doi: 10.1103/PhysRevB.102.045151. URL: <https://link.aps.org/doi/10.1103/PhysRevB.102.045151>.
- [3] H.-M. Guo and M. Franz. “Topological insulator on the kagome lattice”. In: *Phys. Rev. B* 80 (11 Sept. 2009), p. 113102. doi: 10.1103/PhysRevB.80.113102. URL: <https://link.aps.org/doi/10.1103/PhysRevB.80.113102>.



Thanks for Listening! Any Questions?
