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Band dispersion, velocity and effective mass of electrons in Kagome lattice

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Abstract. Kagome materials haven been one of the recent research hotspots, which cause many important phenomena such as ferromagnetism and superconductivity. The present study analyzes the electronic structure properties of Kagome materials, which reveals that the energy band structure is effectively regulated by the electron hopping term and that its flat band properties will disappear when the hopping terms cannot cancel each other. Meanwhile, it is also found that the effective mass and velocity of electrons are significantly dependent on the energy band structure. The results would help us better understand the properties of Kagome materials and contribute to their industrial applications.

Keywords: Kagome lattice, energy band theory, electrons

1. Introduction

Electron motion is central to the properties and dynamics of solids, on which the electron energy band structure has a decisive influence. It defines the relationship between the energy and momentum of electrons; and traditionally, the electrons of a solid can be approximated as if there were free electrons of different effective masses. The energy band theory has laid the theoretical foundation for electronic devices. For example, due to the gapless Dirac band structure, graphene has special electronic properties, including high carrier mobility [1], ultrafast optical response [2] and its electrocatalytic activity toward small biomolecules (hydrogen peroxide, dopamine, etc.), [3] which are suitable for making electrochemical biosensors. The energy band theory has also led to the birth of modern information technology. The nitrogen vacancy (NV) center serves as another good example [4]. Because the electron structure makes the coherence time of NV center to reach the millisecond scale, it is considered as a very promising quantum computer system which has been used for the measurement of NMR signals of organic materials [5].

In recent years, the discovery of flat bands (FB) structures has attracted much attention [6-8]. As the kinetic energy of electrons is quenched in FB, Coulomb interactions become crucial, giving rise to various exotic many-body states such as ferromagnetic, superconducting, and Wiener crystals [9]. As a typical FB system, Kagome materials [10-13] have become emerging research topics, which have many interesting properties such as the fractional quantum Hall effect at high temperatures [14].

In this study, we explore the band structure and corresponding velocity and effective mass in Kagome materials and reveal the electronic structure properties of Kagome materials. It is found that the energy

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band structure is effectively regulated by the electron hopping term, and that its flat-band properties will disappear when the hopping terms cannot cancel each other. In addition, we also find that the effective mass and velocity of electrons are significantly regulated by the energy band structure, where the larger energy slope corresponding to the higher electron velocity and the smaller effective mass.

2. Method

The electron hopping on a general Kagome lattice can be written as:

$$H_{hop} = \sum_{i,j,a,b} t_{ia,jb}\, c_{i,a}^{\dagger} c_{j,b} \tag{1}$$

Where *i* and *j* are the indexes of unit cells, *a* and *b* label different orbitals of one unit cell, and $\{t_{ia,jb}\}$ are the hopping matrix elements.

The energy band of states ε_{nk} can be obtained by solving the eigenvalue problem of h_k where $h_k = \sum_{k,a,b} c_{k,a}^{\dagger} h_{ab}(k) c_{k,b}$ is based on the Bloch theorem.

For the FB in Kagome lattice, the bands can be dispersion less, i.e., ε_{nk} = const. Typically the nontrivial FB requires the net hopping disappear in the whole lattice, namely, the destructive interference.

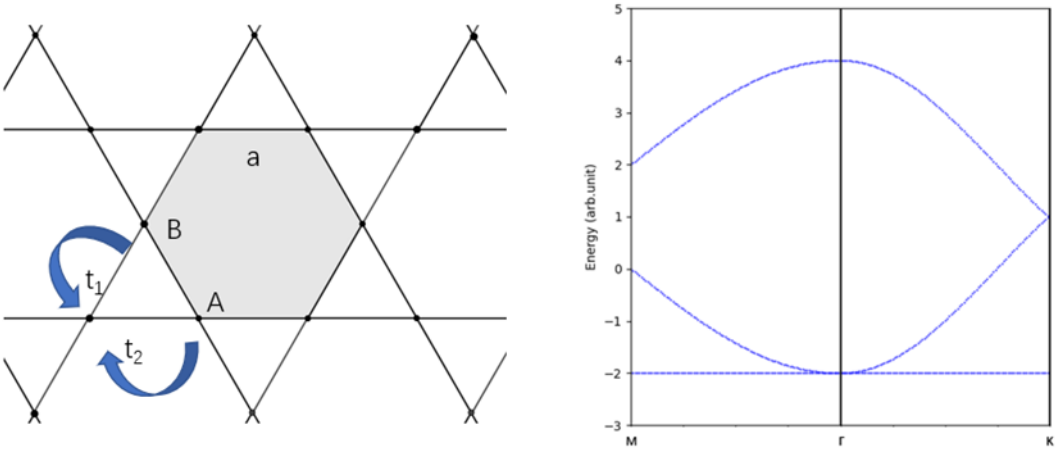

Figure 1. (a) A localized eigenstate of the FB and the destructive interference. (b) Band structure from Eq. (3).

Here we consider a two-dimensional Kagome lattice, which has the honeycomb lattice combined with split-angle triangles (Figure. 1(a)). Within a cell, there are three unequal loci A, B, and C. We consider a single orbit on each locus, i.e., *a, b* = A, B, C, with respect to Eq. (1), and set an equal jump amplitude *t* for all nearest neighbor (NN) bonds. The Bloch Hamiltonian is then [15]

$$h(k) = \begin{pmatrix} 0 & 2tcosk_1 & 2tcosk_2 \\ 2tcosk_1 & 0 & 2tcosk_3 \\ 2tcosk_2 & 2tcosk_3 & 0 \end{pmatrix} \tag{2}$$

$h(k)$ produces a completely destructive interference, making the *n*th band dispersion-free. This statement makes us wander if the FB can be impacted by the unequal *t*. In order to investigate this, we apply the new Hamiltonian

$$h'(k) = \begin{pmatrix} 0 & 2t_1cosk_1 & 2t_2cosk_2 \\ 2t_1cosk_1 & 0 & 2t_2cosk_3 \\ 2t_1cosk_2 & 2t_2cosk_3 & 0 \end{pmatrix} \tag{3}$$

and study the dependence of band dispersion on the different intensity of t_1 *and* t_2.

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3. Result

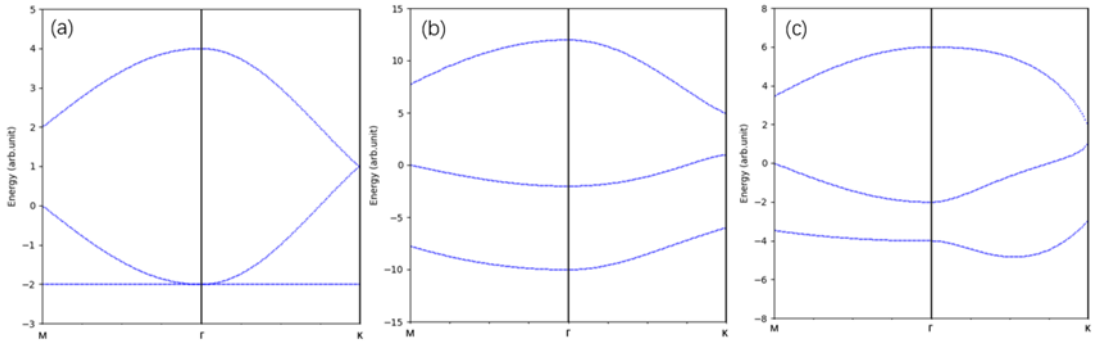

Figure2. Band dispersion of Kagome lattice with t_1=t_2=1 (a), t_1=1, t_2=-3 (b), t_1=1, t_2=5 (c).

The three lines in Figure 2(a) show the energy band dispersion of Kagome lattice along M-Γ-K with t_1=t_2=1. For the first normal energy band, from M to Γ, the energy grows and the growth becomes progressively smaller. At the point Γ, the maximum value is reached. From Γ to K, the energy decreases and the decrease becomes progressively larger, reaching a minimum at the point K. Overall, the total amount of energy decreases from M to K. The second band is symmetric with the first curve about Energy=1. The band dispersion descends slowly and then rises slowly to form a downward concave curve. In particular, the FB shows a perfectly straight line because the net hopping vanishes and interferes with phase extinction throughout the lattice, creating a localization of the electron real space.

The three lines in Figure 2(b) show the energy band dispersion of Kagome lattice along M-Γ-K with t_1=1, t_2=-3. The three lines in Figure 2(c) show the energy band dispersion of Kagome lattice along M-Γ-K with t_1=1, t_2=5. In both figures, there is no longer a FB presence. In the interval M-Γ-K, the three energy bands no longer intersect. The trend of the original two normal bands remains the same. The original FB now becomes approximately a downward convex curve. Thus, the electron has the corresponding speed and effective mass.

From the above description and images, it can be concluded that the strength of the hopping of electrons can significantly affect the transport properties of electrons, such as the effective mass and speed of electrons.

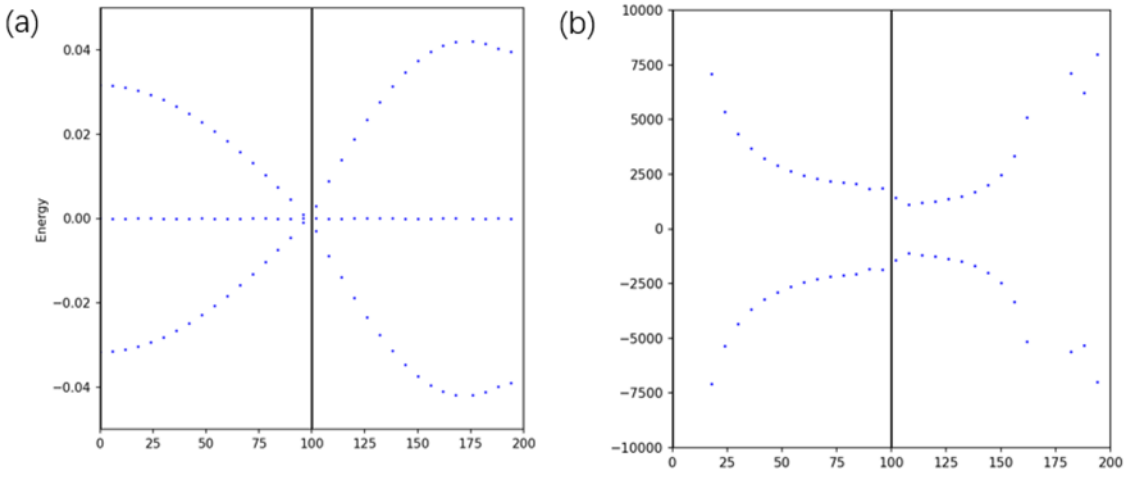

Figure 3. Velocity (a) and effective mass (b) of electrons in Kagome lattice with t_1=t_2=1.

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The three lines in Figure 3, represent the electron velocity and effective mass corresponding to the band structure of Kagome lattice with $t_1=t_2=1$. In Figure 3(a), for the normal bands, the two energy band curves are symmetrical. One of them drops first from M to K and reaches a minimum near the K point; and then the energy rises. The other one is the opposite, with rising velocity first and a small decrease in energy near the K point. The FB in the middle means that the velocity of this electron is zero. In Figure 3(b), for the normal bands, the two energy bands are also symmetric. One of them has a decreasing trend from M to Γ. In contrast, from Γ to K, it has an upward trend with increasing amplitude and reaches the maximum at the point K. The other curve presupposes the opposite.

In contrast, the dispersion relation of FB completely disappears, which leads to its electron velocity always being zero. The electron mass is therefore infinite. The results show that the disappearance of the energy band curvature due to the interference phase extinction greatly affects the electron transport properties.

4. Conclusion

By studying the electronic structure properties of Kagome materials, it is found that their energy band structure is effectively regulated by the hopping term of electrons, and that their flat band properties will disappear when the hopping terms cannot cancel each other. Besides, we also discover that the effective mass and speed of electrons have a significant relationship with the energy band structure. Therefore, it can be concluded that the strength of the hopping of electrons can significantly affect the transport properties of electrons, such as the effective mass and speed of electrons. These results may help us better understand the physical properties and contribute to industrial applications of Kagome materials.

5. Reference

[1] Tian, J., Katsounaros, A., Smith, D., & Hao, Y. (2015). Graphene field-effect transistor model with improved carrier mobility analysis. IEEE Transactions on Electron Devices, 62(10), 3433-3440.

[2] Li, W. et al., (2014). Ultrafast all-optical graphene modulator. Nano letters, 14(2), 955-959.

[3] Shao, Y., Wang, J., Wu, H., Liu, J., Aksay, I. A., & Lin, Y. (2010). Graphene based electrochemical sensors and biosensors: a review. Electroanalysis: An International Journal Devoted to Fundamental and Practical Aspects of Electroanalysis, 22(10), 1027-1036.

[4] Acosta, V.M., & Hemmer, P.R. (2013). Nitrogen-vacancy centers: Physics and applications. Mrs Bulletin, 38, 127-130.

[5] Staudacher, T. et al., (2013). Nuclear magnetic resonance spectroscopy on a (5-nanometer) 3 sample volume. Science, 339(6119), 561-563.

[6] Slot, M. R. et al., (2017). Experimental realization and characterization of an electronic Lieb lattice. Nature Physics, 13(7), 672–676. https://doi.org/10.1038/nphys4105

[7] Tristan H. Harder, Oleg A. Egorov, Johannes Beierlein, Philipp Gagel, Johannes Michl, Monika Emmerling, Christian Schneider, Ulf Peschel, Sven Höfling, & Sebastian Klembt. (2020), Exciton-polaritons in flatland: Controlling flatband properties in a Lieb lattice, Phys. Rev. B 102, 121302(R)

[8] Wu, F., Lovorn, T., & MacDonald, A. H. (2017). Topological Exciton Bands in Moiré Heterojunctions. Physical review letters, 118(14), 147401.

[9] Mielke, A. (1991). Ferromagnetism in the Hubbard model on line graphs and further considerations. Journal of Physics A: Mathematical and General, 24(14), 3311.

[10] H.-M. Guo & M. Franz. (2009). Topological insulator on the kagome lattice. Topological insulator on the kagome lattice.

[11] Jiang, W., Ni, X., & Liu, F. (2021). Exotic Topological Bands and Quantum States in Metal-Organic and Covalent-Organic Frameworks. Accounts of chemical research, 54(2), 416–426.

[12] Lin, Z., Choi, J. H., Zhang, Q., Qin, W., Yi, S., Wang, P., Li, L., Wang, Y., Zhang, H., Sun, Z., Wei, L., Zhang, S., Guo, T., Lu, Q., Cho, J. H., Zeng, C., & Zhang, Z. (2018). Flatbands and

DOI: 10.54254/2753-8818/5/20230283

Emergent Ferromagnetic Ordering in Fe_3Sn_2 Kagome Lattices. Physical review letters, 121(9), 096401.

[13] Kang, M. et al., (2020). Dirac fermions and flat bands in the ideal kagome metal FeSn. Nature materials, 19(2), 163–169.

[14] Liu, H., Sethi, G., Sheng, D. N., Zhou, Y., Sun, J. T., Meng, S., & Liu, F. (2022). High-temperature fractional quantum Hall state in the Floquet kagome flat band. Physical Review B, 105(16), L161108.

[15] Liu, Zheng, Liu, Feng, Wu, Yong-Shi (2014) Exotic electronic states in the world of flat bands: From theory to material. Chinese Physics B, 23. 77308pp.