The Basic Electronic and Topological Properties in Graphene and Kagome Lattices

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ABSTRACT

Graphene is one of the most important 2-D materials which is extensively studied by many researchers. As the line graph of graphene, kagome lattices also have impressive properties. This paper introduce the basic tight-binding method to calculate energy bands of these two lattices and further lead to the Berry curvature which imply the topological properties. This simple work is not novel enough to be paid attention to but really a great approach to modern physical research.

KEYWORDS: graphene, kagome lattice, tight-binding model, Berry curvature

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1 Introduction

The properties of Graphene and Kagome Lattices has been meticulously researched by previous works[2]. We exam the energy bands by the tight-binding model and observe the exists of Dirac Point which imply the massless conductive electron. On the contrary, its line graph, known as kagome lattices whose structure look like traditional Japanese baskets as called, shows another extreme properties with infinity mass. We compare the different symmetry of these two lattice and clarify the difference by topological properties. The discussion in external magnet field is also been included.

The paper is organized as follows: Section 2 discuss the Tight-Binding Model. Section 3 and 4 calculate the band structure of Graphene and Kagome. Section 5 introduce the Berry curvature and discuss the symmetry of two lattices by Berry curvature.

2 The Tight-Binding Model

It's hard to solve the original Schrödinger Equation without any approach. The tight-binding model(TB) based on the one electron approximation and consider the next nearest and farther sites are higher-order perturbation which can be neglected in the most of problems.

The TB wave function is the linear combine of Bloch sum.[3]

$$\begin{aligned}\varphi_i(\mathbf{k},\mathbf{r}) &= \sum_i c_i\phi_i(\mathbf{k},\mathbf{r}) \\ \phi_i(\mathbf{k},\mathbf{r}) &= \frac{1}{\sqrt{N}}\sum_{\mathbf{t_n}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t_n}}\psi(\mathbf{r}-\mathbf{t_n})\end{aligned} \tag{2.1}$$

, where ψ is the atomic orbital and i represents different orbitals. The TB hopping hamiltonian takes:

$$\mathcal{H}_{ij} = E_i\delta_{ij} + \sum_{\mathbf{t_I}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t_I}} \int \psi_i^*(\mathbf{r})V_a(\mathbf{r}-\mathbf{t_I})\psi_j(\mathbf{r}-\mathbf{t_I}) \tag{2.2}$$

, where V_a is the atom potential.

3 Graphene

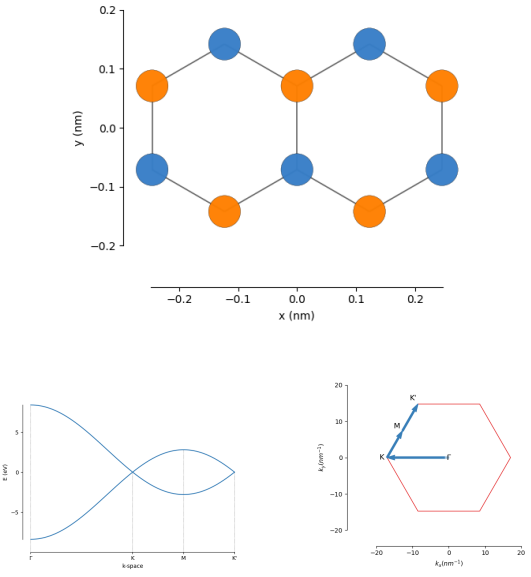

Figure 1: The two site of Graphene are characterized by orange and blue **Top:** The Structure of Graphene. **Bottom Left:** The energy bands structure of graphene, notice that the two bands touched at K and K′. **Bottom Right:** The First BZ of Graphene and the blue line represents the path of energy bands .

Apply the TB model, we have the energy bands of graphene is

$$E = \pm\sqrt{1 + 4\cos^2\frac{k_x a}{2} + 4\cos\frac{k_x a}{2}\sin\frac{k_y a}{2}} \quad (3.1)$$

The two bands degeneracy at K and K$'$. Taylor series shows that near this two points the energy bands takes:

$$E = v_F\hbar|k| \quad (3.2)$$

so the effectve mass of electron vanish

$$m^* = \hbar/\frac{\partial^2 E}{\partial k} \quad (3.3)$$

4 Kagome

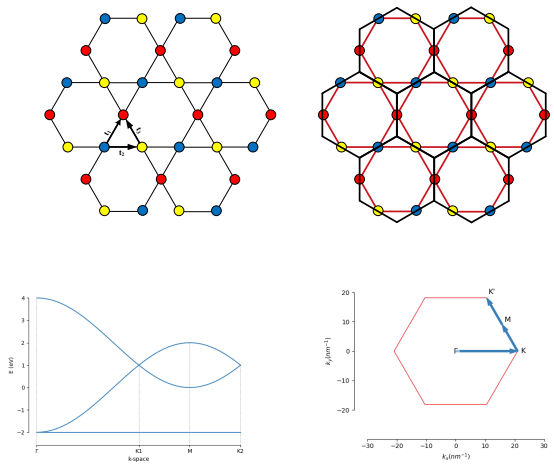

Figure 2: The three site of Graphene are characterized by orange, blue, and Green **Top Left:** The Structure of Kagome lattices. **Top Right:** If we exchange the vertex and edge, we got kagome. **Bottom Left:** The energy bands structure of kagome, notice that the two bands also touched at K1 and K2. and the lower bands is flat. **Bottom Right:** The First BZ of Graphene and the blue line represents the path of energy bands .

Apply the TB model, The Hamiltonian

$$\begin{bmatrix} 0 & 2\cos(\frac{k_x a}{2}) & 2\cos(\frac{k_x a}{4} + \frac{\sqrt{3}k_y a}{4}) \\ \dagger & 0 & 2\cos(-\frac{k_x a}{4} + \frac{\sqrt{3}k_y a}{4}) \\ \dagger & \dagger & 0 \end{bmatrix} \quad (4.1)$$

† represent the complex conjugate of corresponding position

we have the energy bands of kagome is

$$\begin{cases} E_1 = -2 \\ E_{2/3} = 1 \pm \sqrt{3 + 2\cos k_x + 4\cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}} \end{cases} \quad (4.2)$$

The flat bands is in which we are interested. In graph theory, the kagome lattice is the line graph of honeycomb lattice which means that we change the edge of origin graph into vertex. Figure **??** shows this relation. Due to some theories of graph, we can guarantee that if a lattice is the line graph of the other, there are flat bands in it energy band structure. As a typical example, we have introduced the kagome lattice.

And the effectve mass of electron at flat bands is infinity since $\frac{\partial^2 E}{\partial k^2}$ vanish

$$m^* = \hbar/\frac{\partial^2 E}{\partial k^2} \quad (4.3)$$

5 Berry Curvature

The Berry Curvature is defined by the geometric Berry phase which was introduced by Berry in 1984[1]

The Berry Phase was defined by

$$\begin{aligned} \gamma_n(C) &:= i\oint \langle\phi_n(r;\mathbf{R})\,|\,\nabla_{\mathbf{R}}\phi_n(r;\mathbf{R})\rangle\cdot d\mathbf{R} \\ &:= \oint A_n(\mathbf{R})d\mathbf{R} \end{aligned} \quad (5.1)$$

, where $A_n(\mathbf{R})$ is Berry connection, roughly use Stokes' Theorem we define:

$$B_n(\mathbf{R}) := \nabla_{\mathbf{R}} \times A_n(\mathbf{R}) \quad (5.2)$$

or equivalence form:

$$\begin{aligned} B_n(R) = -\Im\sum_{m(\neq n)} &\frac{\langle\phi_n(r;\mathbf{R})\,|\,\nabla_{\mathbf{R}}H\,|\,\phi_m(r;\mathbf{R})\rangle}{(E_m - E_n)^2} \\ \times &\langle\phi_m(r;\mathbf{R})\,|\,\nabla_{\mathbf{R}}H\,|\,\phi_n(r;\mathbf{R})\rangle \end{aligned} \quad (5.3)$$

The Berry curvature reflect the topological properties in material called holonomy. When a system go through an adiabatic path, its phase may change. The difference can be gauged by Berry curvature just like how curved the surface were can be measured by Gauss curvature K. We naturally extend Gauss-Bonet Theorem into Chern-Gauss-Bonet Theorem:

$$\begin{cases} \iint KdS = 2\pi\chi \text{ (GB-Theorem)} \\ \iint BdS = 2\pi c \text{ (CGB-Theorem)} \end{cases} \quad (5.4)$$

The χ is Euler characteristic number and c is Chern number.

We calculate the Berry curvature in Graphene and Kagome lattice and reflected their topological and symmetrical properties.[5]

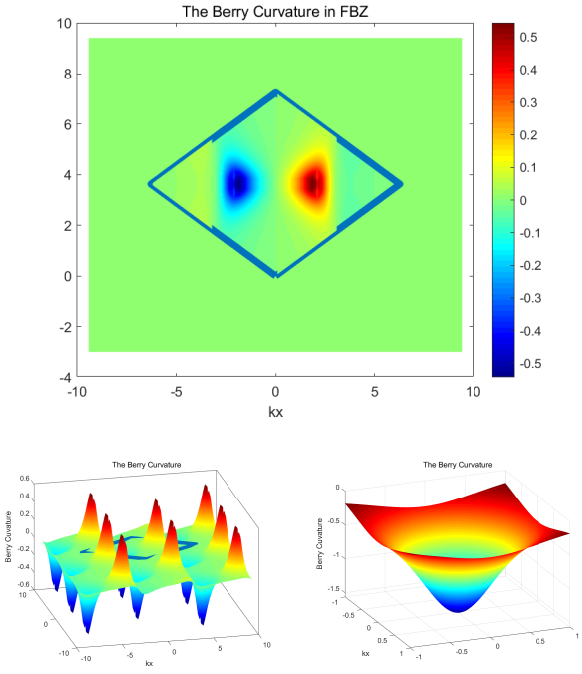

Figure 3: We apply a small gap to graphene to remove the singularity near the degeneracy **Top**: The Berry curvature in the FBZ. **Bottom Left**: The Berry curvature in the large scale certainly repeat the properties in FBZ **Bottom Right**: The Berry curvature near the Dirac Point (Has remove the singularity)

The Berry curvature is vanish everywhere in Kagome Lattice. And Chern Number is vanish in Berry curvature which reflect the symmetric in these two lattice. Time reversal symmetry and inversion symmetry

From Schrödinger Equation

$$(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{k},\mathbf{r}))\Psi(\mathbf{k},\mathbf{r}) = i\hbar\frac{\partial\Psi(\mathbf{k},\mathbf{r})}{\partial t} \quad (5.5)$$

if we apply time reversal operator

$$\begin{aligned}(-\frac{\hbar^2}{2m}\nabla^2 + V(-\mathbf{k},\mathbf{r}))\Psi(-\mathbf{k},\mathbf{r}) &= -i\hbar\frac{\partial\Psi(-\mathbf{k},\mathbf{r})}{\partial t}\\ (-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{k},\mathbf{r}))\Psi(-\mathbf{k},\mathbf{r}) &= -i\hbar\frac{\partial\Psi(-\mathbf{k},\mathbf{r})}{\partial t} \quad \text{TRS}\\ (-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{k},\mathbf{r}))\Psi^*(-\mathbf{k},\mathbf{r}) &= i\hbar\frac{\partial\Psi^*(-\mathbf{k},\mathbf{r})}{\partial t}\end{aligned} \quad (5.6)$$

So TRS leads to $\Psi^*(-\mathbf{k},\mathbf{r}) = \Psi(\mathbf{k},\mathbf{r})$

if we apply inversion operator

$$\begin{aligned}(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{k},-\mathbf{r}))\Psi(\mathbf{k},-\mathbf{r}) &= i\hbar\frac{\partial\Psi(\mathbf{k},-\mathbf{r})}{\partial t}\\ (-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{k},\mathbf{r}))\Psi(\mathbf{k},-\mathbf{r}) &= i\hbar\frac{\partial\Psi(\mathbf{k},-\mathbf{r})}{\partial t} \quad \text{IS}\end{aligned} \quad (5.7)$$

So TRS leads to $\Psi(-\mathbf{k},\mathbf{r}) = \Psi(\mathbf{k},\mathbf{r})$

For Berry curvature, If system is protected by TRS: $B_n(-\mathbf{k}) = -B_n(\mathbf{k})$, or IS:$B_n(-\mathbf{k}) = B_n(\mathbf{k})$. To make it is possible that two properties hold simultaneously, $B(\mathbf{k}) = 0$ is required.[4] Kagome Lattice do.

6 Conclusion

The band structure and kagome lattices looks quite similar but the properties are completely different.The lowest energy ban in kagome lattice is flat which reflects the extremely localized wave function. The Berry curvature in kagome lattices vanish everywhere due to the protection of TRS and IS. Under the TRS, the Chern's number in Graphene also vanish.

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