Research Note; The Flat Band in Kagome Lattice

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ABSTRACT

This note reports the energy bands of Kagomi Lattices, well known as a lattice with basket-liked structure. We use tight-binding method and notice the existence of flat band which implies the full degeneration of wave vectors and infinity effective mass of electrons. Further, we calculate the Berry phase of this system. Previous works have been done by Liu, Liu, and Wu [3]

KEYWORDS: Kagome Lattice, Tight-Binding Model, Band Structure, Berry Phase

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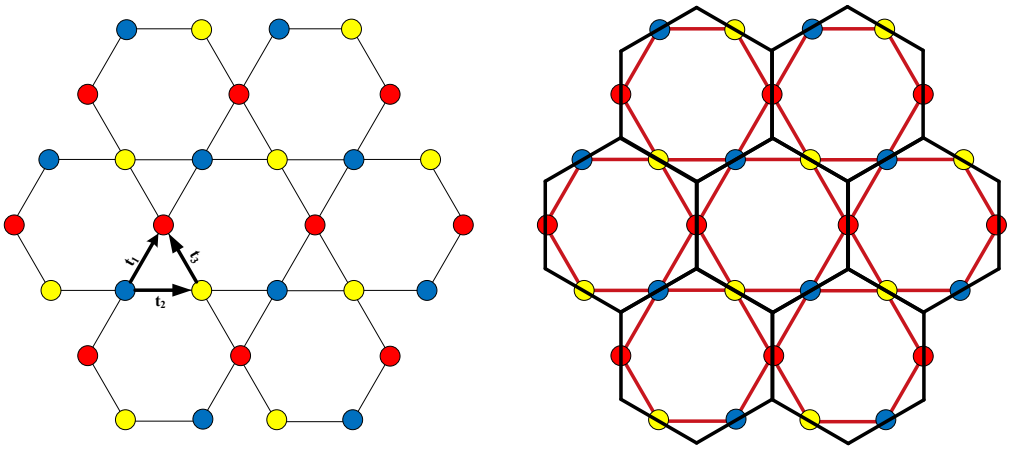
1. Kagome Lattice

1.1. Introduction

Figure1(a)shows the structure of Kagome Lattice



(a) Sturcture of Kagome Lattice (b) Line Graph

Figure 1: Sturcture of Kagome Lattice

We use colours to represent inequivalent sites in kagome lattice whose Bravais lattice is hexagonal. This interesting structure looks like a traditional Japanese basket as called.
Here introduces a graph conception. The line graph of origin graph $G(V, E)$ is defined by $L(V_L, E_L)$ which has these properties:

1. V_L is the E in G
2. V_{Li} and V_{Lj} are connected if E_i and E_j are incident

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. Figure1(b) shows this relation. Due to some theories of graph[4], 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 introduce the kagome lattice.

1.2. Energy Bands

For simplify, we consider carbon based kagome lattice. The cell vectors of kagome lattice are

$$\begin{cases} t_1 = \frac{a}{2}\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \\ t_2 = \frac{a}{2}(1, 0) \\ t_3 = \frac{a}{2}\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \end{cases} \tag{1.1}$$

We set blue is 1, yellow is 2 and red is 3.

$$M_{ij} = E_i \delta ij + \sum_{\mathbf{t_I}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t_I}} \int \phi_i(\mathbf{r}) V(\mathbf{r} - \mathbf{t_I}) \phi_j(\mathbf{r} - \mathbf{t_I}) dr \tag{1.2}$$

where $\mathbf{t_I}$ is the nearest atom vector. Since the high symmetry, we can use a t to represent the integration.
So, we have(here we set the $E_i = 0$ for simplify):

$$\begin{cases} M_{11} = 0 \\ M_{22} = 0 \\ M_{33} = 0 \\ M_{12} = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t_1}} + \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{t_1}} = 2\cos(\frac{k_x a}{2}) \\ M_{13} = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t_2}} + \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{t_2}} = 2\cos(\frac{k_x a}{4} + \frac{\sqrt{3}k_y a}{4}) \\ M_{23} = \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t_3}} + \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{t_3}} = 2\cos(-\frac{k_x a}{4} + \frac{\sqrt{3}k_y a}{4}) \end{cases} \tag{1.3}$$

Now we calculate the eigenvalue of equation(1.3), that is

$$\det \begin{Vmatrix} 0 & 2\cos(\frac{k_x a}{2}) & 2\cos(\frac{k_x a}{4} + \frac{\sqrt{3}k_y a}{4}) \\ 2\cos(\frac{k_x a}{2}) & 0 & 2\cos(-\frac{k_x a}{4} + \frac{\sqrt{3}k_y a}{4}) - E(k) \\ 2\cos(\frac{k_x a}{4} + \frac{\sqrt{3}k_y a}{4}) & 2\cos(-\frac{k_x a}{4} + \frac{\sqrt{3}k_y a}{4}) & 0 \end{Vmatrix} = 0 \tag{1.4}$$

The analysis solutions is:

$$\begin{cases} E_1 = -2 \\ E_{2/3} = 1 \pm \sqrt{3 + 2\cos(k_x) + 4\cos\left(\frac{k_x}{2}\right)\cos\left(\frac{\sqrt{3}k_y}{2}\right)} \end{cases} \tag{1.5}$$

The solutions plotted by MATLAB is shown in Figure 2

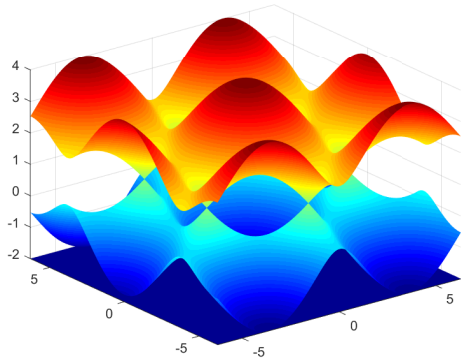


Figure 2: Energy Bands of Kagome Lattice

The dark blue plane represent the flat band in kagome lattice. The effective mass of this bands takes $\frac{1}{m^*} = \frac{1}{\hbar}\frac{\partial^2 E}{\partial k^2}$, implies that infinity mass and extremely localized wave function

2. Berry Phase

The Berry Phase describe the phase change by a systum moving along a circuit on a adiabatic surface.

2.1. Hellmann-Feynman Theorem

Consider a Hamiltonian which depends on parameter(s) indicated by $\mathbf{R}$. The $\mathbf{R}$ can be wave-vector $\mathbf{k}$, configuration of atoms R. We assume that the electron can adapt to the change of Hamiltonian quickly thus:

$$H(\mathbf{R})\,|\phi_n(r;\mathbf{R})\rangle = E_n(\mathbf{R})\,|\phi_n(r;\mathbf{R})\rangle \tag{2.1}$$

and the orthonormality relations shows:

$$\langle\phi_n(r;\mathbf{R})\,|\,H(\mathbf{R})\,|\,\phi_m(r;\mathbf{R})\rangle = E_n\delta_{mn} \tag{2.2}$$

$$\langle\phi_n(r;\mathbf{R})\,|\,\phi_m(r;\mathbf{R})\rangle = \delta_{mn} \tag{2.3}$$

The derivation of equation (2.2) and equation (2.3) gives

$$\left\langle \phi_n(r;\mathbf{R}) \left| \frac{\partial H(\mathbf{R})}{\partial \mathbf{R}_i} \right| \phi_n(r;\mathbf{R}) \right\rangle = \frac{\partial E_n(\mathbf{R})}{\partial \mathbf{R}_i} \tag{2.4}$$

$$\left\langle \phi_m(r;\mathbf{R}) \left| \frac{\partial H(\mathbf{R})}{\partial \mathbf{R}_i} \right| \phi_n(r;\mathbf{R}) \right\rangle = [E_n(\mathbf{R}) - E_m(\mathbf{R})] \left\langle \phi_m(r;\mathbf{R}) \left| \frac{\partial}{\partial \mathbf{R}_i} \phi_n(r;\mathbf{R}) \right. \right\rangle \tag{2.5}$$

$$\left\langle \phi_n(r;\mathbf{R}) \left| \frac{\partial}{\partial \mathbf{R}_i} \phi_n(r;\mathbf{R}) \right. \right\rangle = pure\ imaginary\ part \tag{2.6}$$

2.2. Berry Phase and Berry Curvature

Consider a closed circuit C drawn in parameter space, at every point $\mathbf{R}$ there is a state vector and continuous to the parameter. It's hard to think and describe mathematically without conception of fiber bundle. But we can roughly imagine a 3-D vector field on a curve, and roughly use the simple vector analysis.
I skip all the derivation and collect them in Appendix. Define $d\varphi$ as

$$\mathrm{e}^{id\varphi} \equiv \frac{\langle \phi_n(r;\mathbf{R}+d\mathbf{R}) \,|\, \phi_n(r;\mathbf{R}) \rangle}{|\langle \phi_n(r;\mathbf{R}+d\mathbf{R}) \,|\, \phi_n(r;\mathbf{R}) \rangle|} \tag{2.7}$$

It's ill define since the $d\varphi$ is various under the gauge transformation, however,

$$\gamma(C) = \oint d\varphi = i \oint \langle \phi_n(r;\mathbf{R}) \,|\, \nabla_{\mathbf{R}} \phi_n(r;\mathbf{R}) \rangle \cdot d\mathbf{R} \tag{2.8}$$

is well defined(easy to check). Notice that we apply Taylor series in Equation (2.7). This γ is called Berry Phase.
The Berry phase can be interpreted as a phase acquired by the wave-function as the parameters appearing in the Hamiltonian are changing slowly in time. Consider the time dependent Schrödinger equation.[1][2]

$$i\hbar \frac{\partial}{\partial t} \Phi(t) = H(\mathbf{R}(t)) \Phi(t) \tag{2.9}$$

Thus, $\Phi(t) = e^{i\gamma(t)} e^{-i/\hbar \int E(t)dt} \phi(t)$ is the solution of Equation (2.9).

2.3. Berry Phase in Kagome Lattice

For the Flat Bands, the eigenvector of Equation(1.3) is
$\left(\sin(-\frac{k_x}{4} + \frac{\sqrt{3}k_y}{4}), -\sin(\frac{k_x}{4} + \frac{\sqrt{3}k_y}{4}), \sin(\frac{k_x}{2}) \right)$
, implies the real-valued wave-function. That's to say, the Berry phase and Berry curvature is vanished. Further, since the Hamiltonian is a real symmetric matrix, every eigenvector is real-valued and the Berry phase is vanished.

3. Further Works

In next two weeks, I prepare to read some papers and handle the nontrivial Berry phase like gapped graphene-liked materials, and Berry magnetic monopole.

References

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Appendix A. Formula

(1.3) to (1.4):

set $\frac{k_x a^{'}}{2} = a$, $\frac{k_x a^{'}}{4} + \frac{\sqrt{3} k_y a^{'}}{4} = b$, $-\frac{k_x a^{'}}{4} + \frac{\sqrt{3} k_y a^{'}}{4} = c$, and $a + c = b$

$$\det \begin{Vmatrix} -E(k) & 2\cos(a) & 2\cos(b) \\ 2\cos(a) & -E(k) & 2\cos(c) \\ 2\cos(b) & 2\cos(c) & -E(k) \end{Vmatrix} = 0 \tag{Appendix A.1}$$

$$E(k)(4\cos^2 a + 4\cos^2 b + 4\cos^2 c) + 16\cos a \cos b \cos c - E^3(k) = 0 \tag{Appendix A.2}$$

using the fact that $2\cos a \cos b \cos c = \cos^2 a + \cos^2 b + \cos^2 c - 1$

$$(E(k) + 2)(4\cos^2 a + 4\cos^2 b + 4\cos^2 c) = E^3(k) + 8 \tag{Appendix A.3}$$

$$(E(k) + 2)(4\cos^2 a + 4\cos^2 b + 4\cos^2 c - 3 - (E(k) - 1)^2) = 0 \tag{Appendix A.4}$$

(2.8):

using the Taylor series and notice that the norm is two-ordered infinity small.

$$1 + id\varphi = 1 - \langle \phi_n(r; \mathbf{R}) \,|\, \nabla_{\mathbf{R}} \phi_n(r; \mathbf{R}) \rangle \cdot d\mathbf{R} \tag{Appendix A.5}$$

$$d\varphi = i \langle \phi_n(r; \mathbf{R}) \,|\, \nabla_{\mathbf{R}} \phi_n(r; \mathbf{R}) \rangle \cdot d\mathbf{R} \tag{Appendix A.6}$$

(**??**)

$$H\Phi(t) = e^{i\gamma(t)} e^{-i/\hbar \int E(t) dt} E(t) \phi(t) \tag{Appendix A.7}$$

$$i\hbar \frac{\partial}{\partial t} \Phi(t) = (1/\hbar \gamma^{'}(t) + E(t) - i/\hbar \frac{\partial}{\partial t}) \phi(t) e^{i\gamma(t)} e^{-i/\hbar \int E(t) dt} \tag{Appendix A.8}$$

Compare (Appendix A.7) and (Appendix A.8)

$$\gamma^{'}(t) = i\phi^*(t) \frac{\partial}{\partial t} \phi(t) \tag{Appendix A.9}$$

, which is Berry Phase.