Electronic and Topological Properties In Graphene and Kagome Lattices

Final report on Class PH353

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Outline

- Introduction
- Band Structure
- Berry Curvature and Chern Number
- Conclusion

Section 1

Review of Proposal

- (Basic) Learn some basis ideas and theory of solid-state physics and then deduce the band structure of graphene by tight-binding model.
- (Initial Applications) Deduce the band structure in Kagome lattice if time allows.
- (Advanced Applications) Research on Berry curvature and Chern number

WORK TO DO	Begin	Finish
Reading Text Book	Sep. 23rd/Sep. 23rd	Nov. 4th/Oct. 28th
Graphene	TBD/Oct. 28th	Nov. 4th/Nov. 4th
Kagome Lattices	Nov. 19th/Nov. 4th	Nov. 25th/Nov. 18th
Preparation	Nov. 25th/Nov. 15th	Exam Weeks/Dec. 2nd
Berry Curvature	Winter/Nov. 15th	TBD /Dec. 16nd

Introduction

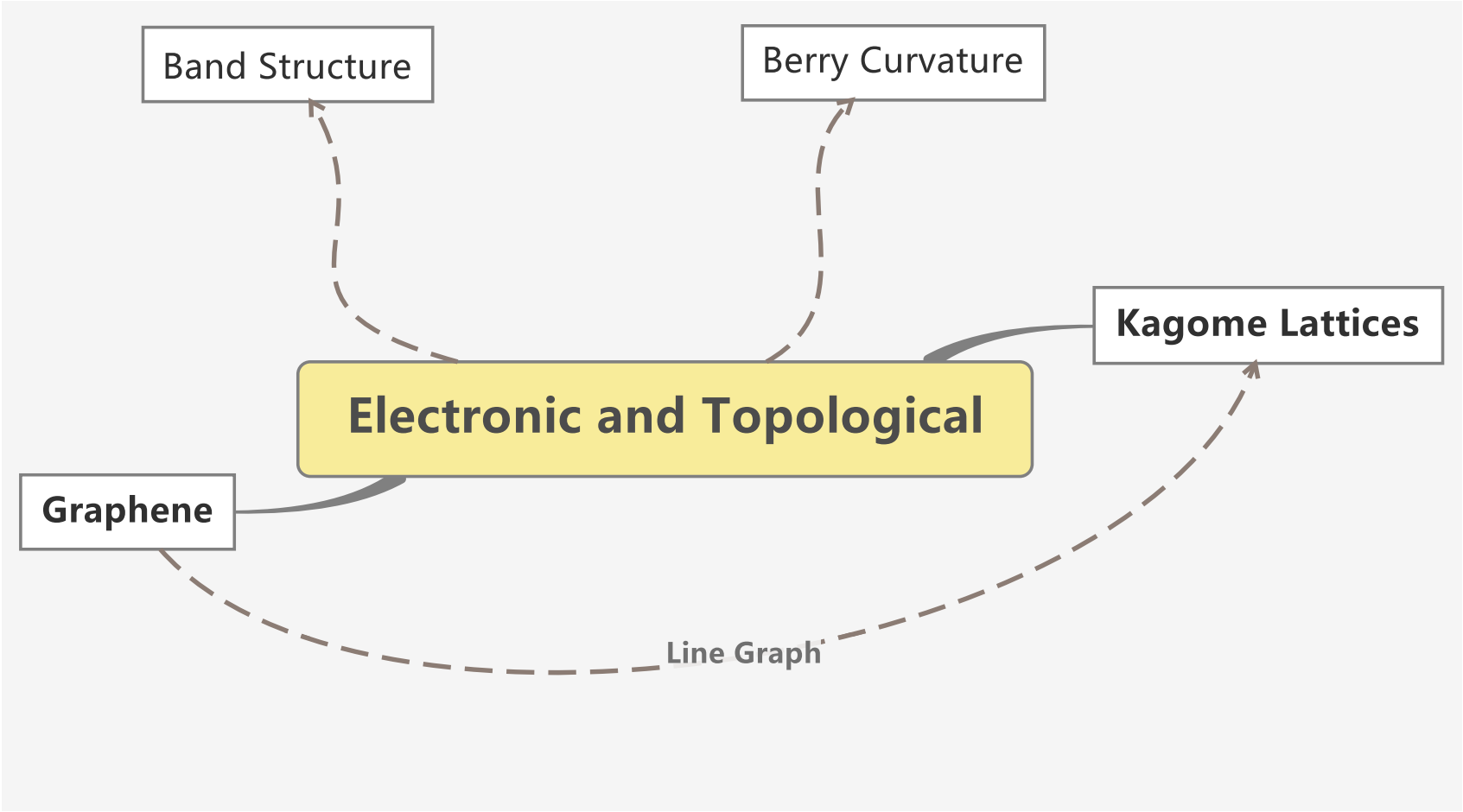


Figure: Mind map

Structure of Two Lattices

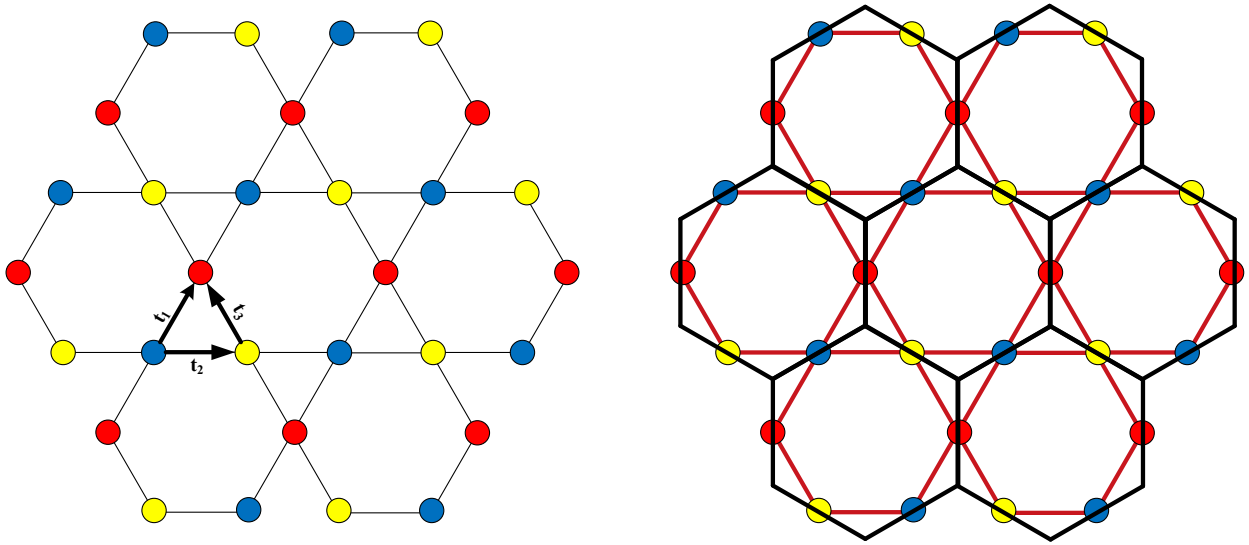


Figure: Structure of Kagome Lattices and Line Graph relation

Line Graph

Given a graph $G = (V_1, E_1)$, its line graph $L(G) = (V_2, E_2)$

- $V_2 = E$
- two vertices of L(G) are adjacent iff their corresponding edges are incident in G.

Section 2

Tight-Binding Model

The main assumption of TBM(LCAO) is that crystal states is linear combinations of atomic orbitals. By some further meticulous semi-empirical approach, one takes that:

Formula

The energy are obtained from

$$||H_{ij} - E\delta_{ij}|| = 0 \tag{1}$$

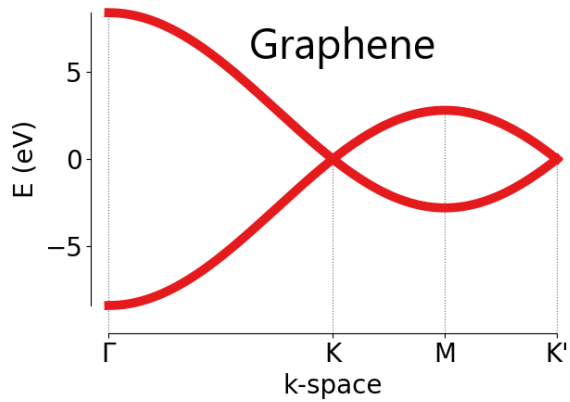
$$H_{ij} = E_i\delta_{ij} + \sum_{\mathbf{t_I}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{t_I}} \int \phi_i^*(\mathbf{r}) V_a(\mathbf{r}-\mathbf{t_I}) \phi_j(\mathbf{r}-\mathbf{t_I}) \tag{2}$$

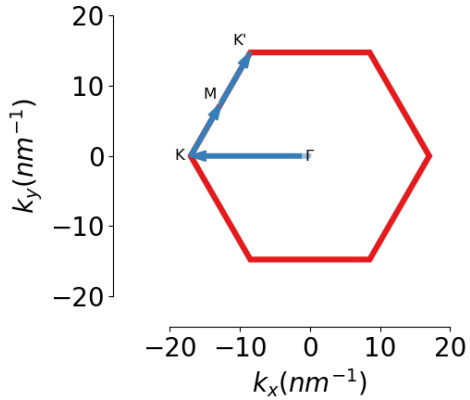
E_i: atomic energy
$\mathbf{t_I}$: first neighbors
ϕ_i: atomic orbitals
$V_a(r)$: atomic-liked potential

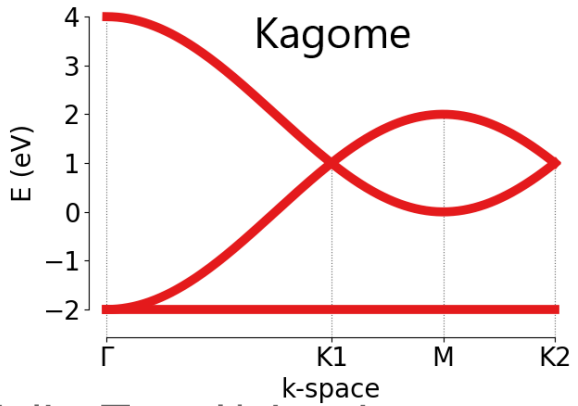
Band Structure in Graphene and Kagome Lattices

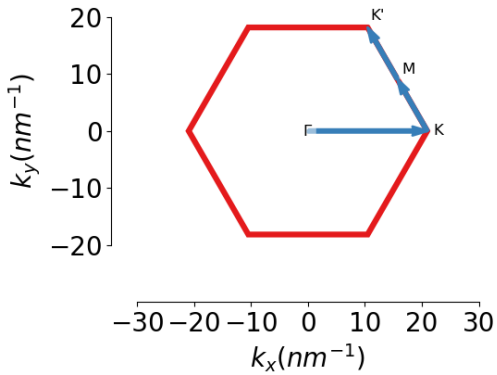
$$E_{\mathrm{gra}} = \pm t\sqrt{1 + 4\cos^2\frac{k_x a}{2} + 4\cos\frac{k_x a}{2}\cos\frac{\sqrt{3}k_y a}{2}}$$

$$E_{\mathrm{kago}} = t(1 \pm \sqrt{1 + 4\cos^2\frac{k_x a}{2} + 4\cos\frac{k_x a}{2}\cos\frac{\sqrt{3}k_y a}{2}})/-2t$$









Discussion

- The upper bands are similar but Kagome have a flat bands$\rightarrow$ **infinite mass**
- Upper bands are degenerate at $K^{'}, K$ and the energy is linear dependent of length of momentum($E = v_F \hbar |k|$) $\rightarrow$ **massless**

The effective mass

The effective mass is defined by

$$\frac{1}{m^*} = \frac{1}{\hbar} \frac{\partial^2 E}{\partial k^2} \tag{3}$$

Section 3

Definition of Berry Phase

The Berry Curvature is defined by the geometric Berry phase which was introduced by Berry in 1984.[**?**]
The Berry Phase was defined by

$$\begin{aligned}\gamma_n(C) &:= i \oint \langle \phi_n(r;\mathbf{R}) \,|\, \nabla_{\mathbf{R}} \phi_n(r;\mathbf{R}) \rangle \cdot d\mathbf{R} \\ &:= \oint A_n(\mathbf{R}) d\mathbf{R}\end{aligned} \tag{4}$$

The Physical means of Berry phase is related to adiabatic evolution;

Physical Meaning

Consider the time dependent Schrödinger equation.

$$i\hbar\frac{\partial}{\partial t}\Phi(t) = H(\mathbf{R}(t))\Phi(t) \tag{5}$$

The evolution of eigenstate can be deduced from TD-Schrödinger equation,

$$\Phi(t) = e^{i\gamma(t)}e^{-i/\hbar\int E(t)dt}\phi(t)$$

($\phi(t)$ is the eigenstate $H(R)\phi(t) = E(R)\phi(t)$)
Besides normal mechanical phase, there is an additional geometric phase change during adiabatic evolution.
topological properties!

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Gauge Transform and Berry Curvature

We now that wave functions can have an arbitrarily phase.
$\phi^{'} = \mathrm{e}^{i\alpha(R)}\phi$

$$A_n^{'}(R) = \left\langle \phi_n^{'}(r;\mathbf{R}) \middle| \nabla_{\mathbf{R}} \phi_n^{'}(r;\mathbf{R}) \right\rangle = A_n(R) - \nabla_{\mathbf{R}}\alpha(R) \tag{6}$$

Roughly apply Stock's law.(whether A is continuous?)

$$B_n(\mathbf{R}) \coloneqq \nabla_{\mathbf{R}} \times A_n(\mathbf{R}) \tag{7}$$

We have:

$$B_n(\mathbf{R}) \coloneqq -\Im \sum_{m(\neq n)} \langle \nabla_{\mathbf{R}} \phi_n \,|\, \phi_m \rangle \times \langle \phi_m \,|\, \nabla_{\mathbf{R}} \phi_n \rangle \tag{8}$$

Berry Curvature in Graphene and Kagome Lattices

Naturally, we use k as parameters. Here we modify the Hamiltonian with a small energy gap to avoid the ill define. (BN lattices)

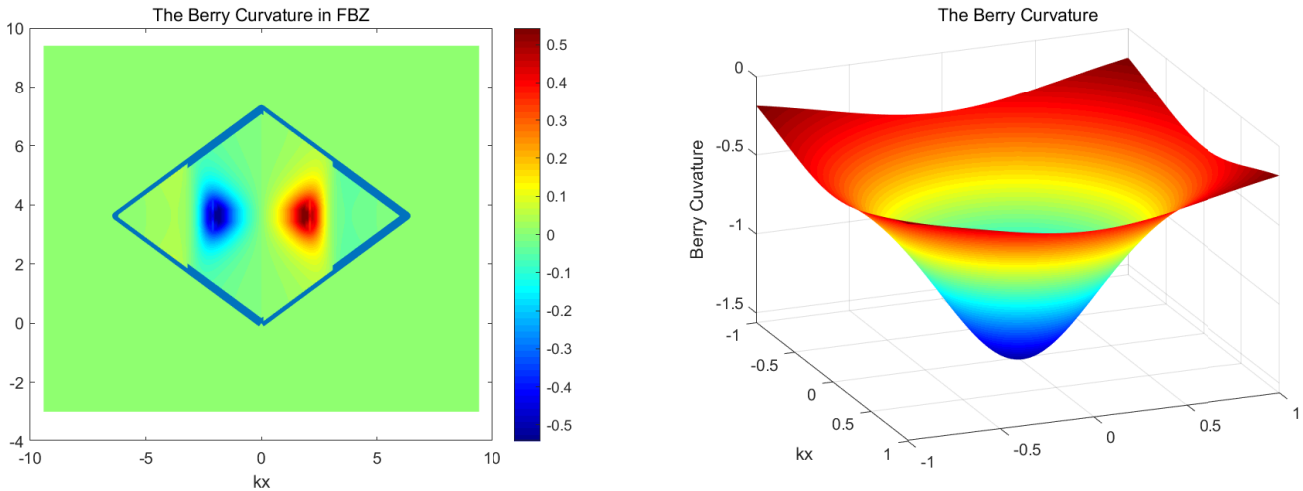

Figure: Graphene

The Berry Curvature in Kagome Lattices vanish everywhere.

Discussion

Time Reversal Symmetry: $B(k) = -B(-k)$
Spatial Inversion Symmetry: $B(k) = -B(k)$
Small energy gap break the spatial inversion symmetry in Graphene but not in Kagome. So Berry Curvature vanishes in kagome lattices.

Chern Number

We naturally extend Gauss-Bonet Theorem into Chern-Gauss-Bonet Theorem:

$$\begin{cases} \iint KdS = 2\pi\chi \text{ (GB-Theorem)} \\ \iint BdS = 2\pi c \text{ (CGB-Theorem)} \end{cases} \tag{9}$$

The χ is Euler characteristic number and c is Chern number. Chern Number is an topological invariable which measure whether there is an obstruction to choosing a perfect gauge to make Berry connection continuity.

Section 4

Conclusion

The band structure of Graphene and Kagome reflect to different types of carriers.
TRS$\rightarrow$0 Chern number$\rightarrow$ trivial topological properties
Further works
Break TRS$\rightarrow$ magnetic field $\rightarrow$ QHE

Thank you!