# physics Documentation

***Release 0.1***

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Contents

Welcome! This is the place for me to write some notes on physics. Contents will be added indefinitely.

CHAPTER 1

# Classical Mechanics:

## 1.1 Phase space Lagrangian

The climax part of classical mechanics lies in **the Lagrangian and Hamiltonian form**. It starts with the extremal principle, the real motion of a mechanical system is the one makes the variation of *the action* $S$ vanish, i.e.,

$$\delta S = \delta \int L(q, \dot{q}, t) dt = 0$$

When the Lagrangian is not depend on time explicitly, we get

$$\delta L = \frac{\partial L}{\partial q}\delta q + \frac{\partial L}{\partial \dot{q}}\delta \dot{q} = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\delta q\right) + \left[\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\right]\delta q$$

which gives us *the Lagrangian equation*:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}$$

Define the *canonical momentum* $p = \frac{\partial L}{\partial \dot{q}}$, we have

$$\dot{p} = \frac{\partial L}{\partial q}$$

We can easily prove that energy is an *integral of motion* (which is a conserved quantity in motion) based on the homogeneity of time. When the Lagrangian does not depend on time explicitly, we found that its total derivative is

$$\begin{aligned}\frac{dL}{dt} =& \frac{\partial L}{\partial q}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} \\ =& \frac{d}{dt}\left(p\dot{q}\right)\end{aligned}$$

We have used Lagrangian equation in the above derivation,and we have now

$$\frac{d}{dt}\left(p\dot{q} - L\right) = 0$$

indicating that is conserved in the motion, which is called *Hamiltonian* with physical meaning of energy.

CHAPTER 2

# Topological Insulator:

## 2.1 Berry's Phase

### 2.1.1 Preliminary

### 2.1.2 some topics

- fiber bundle
- graphene(trival Weyl semi-metal)
- gauge/parallel transport
- symmetry

## 2.2 Weyl Semi-metal

### 2.2.1 Graphene

In the tight-binding approximation, when only nearest neighborhood couplings are considered, the Hamiltonian of Graphene can be written as:

$$\hat{H}(\vec{k}) = -t \begin{pmatrix} 0 & h(\vec{k}) \\ h^*(\vec{k}) & 0 \end{pmatrix}$$

where $h(\vec{k}) = \sum_{\vec{\delta}_i} e^{i\vec{k}\cdot\vec{\delta}_i} = |h(\vec{k})|e^{i\phi(\vec{k})}$, $\vec{\delta}_i$ are three position vectors shown in the following diagram.

Then the Hamiltonian is:

$$\hat{H}(\vec{k}) = -t|h(\vec{k})| \begin{pmatrix} 0 & e^{i\phi(\vec{k})} \\ e^{-i\phi(\vec{k})} & 0 \end{pmatrix}$$

with the eigen-value: $E(\vec{k}) = -t|h(\vec{k})|$ and eigen-function (only show one of the two):

$$u(\vec{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi(\vec{k})/2} \\ e^{-i\phi(\vec{k})/2} \end{pmatrix} e^{i\psi(\vec{k})}$$

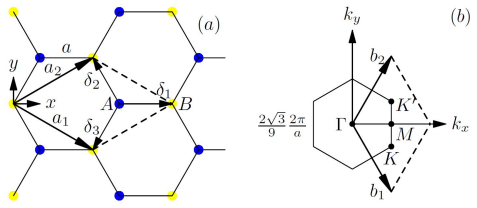


Figure 2.1: **Fig. 1** Crystal Structure of Graphene: $\vec{a}_1$ and $\vec{a}_2$ are Bravais crystal vectors for a Graphene unit cell. Each primitive unit cell has two atomic sties, A and B. $\vec{\delta}_i$ specifies B-s' position around A site. (b) Brillouin Zone for Graphene $\vec{b}_1$ and $\vec{b}_2$ are reciprocal vector basis for intrinsic Graphene. Its corners are known as K and K' points.

We should notice that the $1/2$ factor is quite important here, when $\phi$ changes $2\pi$, the wave-function does not return to its original value, but with a minus sign. If instead, we want the wave-function to be single valued, the function :math:‘psi(vec{k})‘should change accordingly.

At the vicinity of Dirac point (K or K', here we expand the things near K), we have:

$$\begin{aligned}\hat{H}(\vec{K}+\vec{q}) =& \alpha \begin{pmatrix} 0 & q_x + iq_y \\ q_x - iq_y & 0 \end{pmatrix} = \alpha(q_x\sigma_x - q_y\sigma_y) \\ =& \alpha|q| \begin{pmatrix} 0 & e^{i\phi(\vec{q})} \\ e^{-i\phi(\vec{q})} & 0 \end{pmatrix}\end{aligned}$$

We can see that the general $\phi$ turn out to be the angle of $\vec{q}$ with the x axis. Then, wind a circle around the Dirac point K at some energy in the band structure shown below (Fig. 2(a)), the corresponding $\phi$ (Fig. 2(c))winds one round too.

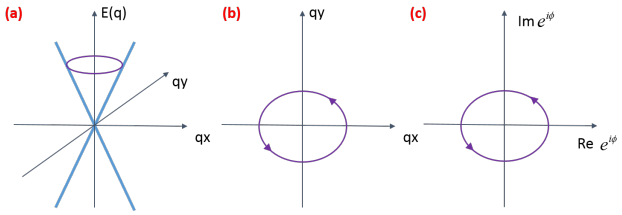


Figure 2.2: **Fig. 2** Dirac cone and the winding of $\vec{q}$ and $\phi$

So, if $\vec{q}$ circles around the Dirac point one turn, $\phi$ changes from 0 to $2\pi$, in order to keep the basic wave-function $u(\vec{q})$ single-valued, $\psi$ **must** changes $\pi$.

More explicitly, we calculate the vector potential in momentum space with:

$$\vec{A}(\vec{k}) = i\langle u^\dagger | \nabla_{\vec{k}u(\vec{k})\rangle = -\nabla\psi(\vec{k})}$$

Then we got:

$$\gamma = \oint \vec{A}\cdot d\vec{k} = -\psi(\phi = 2\pi) + \psi(\phi(0)) = -\pi$$

We got the Berry's phase $\gamma = \pm\pi$. It is this non-trivial phase of the equal-frequency surface that makes us call it **Weyl semi-metal**, and the *Dirac points* called *Weyl nodes*.

### 2.2.2 Three dimension: Weyl semi-metal and Chern number

In three dimension, things can goes the same way. Using a simple model with Hamiltonian:

$$H(\vec{k}) = \left[-2t_x\left(cosk_x - cosk_0\right) + m\left(2 - cosk_y - cosk_z\right)\right]\sigma_x + 2t_y sink_y\sigma_y + 2t_z sink_z\sigma_z$$

It has two Weyl nodes: $\vec{K} = \pm(k_0, 0, 0)$, which means if we treat $k_x$ as a variable, only when $k_x = \pm k_0$, the corresponding energy band $E_{k_x}(k_y, k_z)$ is crossing at the point $k_y, k_z = (0, 0)$.

Also, at the Weyl node (say $k_x = k_0$), we have:

$$H(\vec{K} + \vec{q}) = v_x q_x \sigma_x + v_y q_y \sigma_y + v_z q_z \sigma_z$$

with $v_x = 2t_x sink_0, v_y = 2t_y, v_z = 2t_z$. Without loss of generality, we can set $v_x = v_y = v_z$ (the only effect is the shape changing from sphere to ellipsoid, which has no effect on the topology), then we get:

$$H(\vec{K} + \vec{q}) = v\vec{q} \cdot \vec{\sigma}$$

with eigen-value: $E(\vec{k}) = v|\vec{q}|$ and eigen-function (only show one of the two):

$$u(\vec{k}) = \begin{pmatrix} sin\frac{\theta}{2} \\ -cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} e^{i\chi}$$

It is easy to find that this wave-function will give us a magnetic field with a monopole at $\vec{K}$, which will give us non-trivial equal-frequency surface Chern number $C = 1$.

### 2.2.3 Bulk-boundary corresponding

In order to see things clearer, also, to see the connection of Weyl semi-metal with Topological insulator, we treat $k_x$ as a variable, the Hamiltonian is:

$$H_{k_x}(k_y, k_z) = \vec{h}(\vec{k}) \cdot \sigma = \left[-2t_x\left(cosk_x - cosk_0\right) + m\left(2 - cosk_y - cosk_z\right)\right]\sigma_x + 2t_y sink_y \sigma_y + 2t_z sink_z \sigma_z$$

For example, we set $t_x = t_y = t_z = 1, m = 2, k_0 = 1$, three typical energy band dispersion shown below:

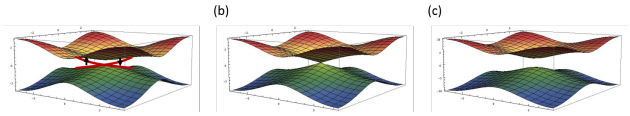


Figure 2.3: **Fig. 3** Typical energy band dispersion with (a) $k_x = 0$, (b) $k_x = k_0 = 1$, (c) $k_x = 2$.

To see if the system with $k_x \neq k_0$ is a topological insulator or not, we can plot the diagram of $\vec{h}(k_y, k_z)$, and see how many times the resulting torus incorporates the origin point. Typical shape of the torus shows below:

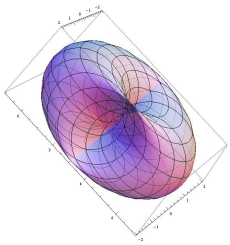

Figure 2.4: **Fig. 4** Typical torus of $\vec{h}(k_y, k_z)$ with $k_x = 0$.

We found that at the region $k_x = [-k_0, k_0]$, the origin point is in the torus once with Chern number $C = 1$, outside of that, we got $C = 1$ (Noticing we have $k_x = [-\pi, \pi]$) . This is why we plot the edge state in Fig. 4(a), but not in Fig. 4(c). In the non-trivial case, for any energy inside the gap, we get a edge state, so different $k_x$ will give us a edge-state line, which is called *Fermi-arc*, especially, when we look at the case of Fermi surface with energy $E = 0$, the Fermi-arc stretch from one Weyl node to another, like the picture shown below:

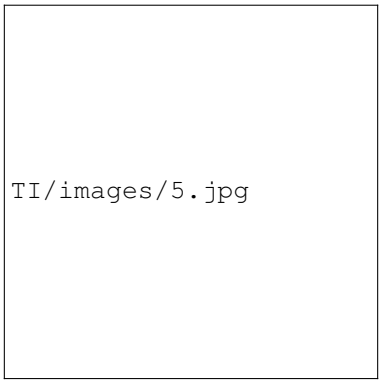


Figure 2.5: **Fig. 5** Fermi arc.

CHAPTER 3

# Condensed Matter Physics:

## 3.1 Linear response theory

### 3.1.1 Kubo formula

Many times, the world shows us as a **black box**, we can only get limited knowledge about it and the rest are filled with our *theories*, in this way, theories can always changing and are never completed. we always use a probe to probe a system and check its response to this probe, and naturally, we expect when the perturbation of the probe is ignorable to the system, the response should be linear to the probe, which is called **linear response theory**. The most important result of linear response theory is consummated by *Kubo formula*, we are now going to derive it.

#### Zero temperature

Let $\hat{H}_0$ be the full manybody Hamiltonian for some isolated system that we are interested in, and assume the existence of a set of eigenkets $\{|n\rangle\}$ that diagonalize $\hat{H}_0$ with associated eigenvalues (energies) $\varepsilon_n$.

In addition to $\hat{H}_0$, we now turn on an external probe potential $\hat{V}(t)$, such that the total Hamiltonian $\hat{H}(t)$ satisfies:

$$\hat{H}(t) = \hat{H}_0 + e^{\eta t}\hat{V}(t)$$

**Note:** The additional factor $e^{\eta t}$ means we switch on the external potential adiabatically from $t \to -\infty$, we'll see later that it is this factor gives us the way to detour the *singular points*, it is an *analytical continuation* which is a reflection of *causality*.

The Schrödinger equation of the system now reads:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = (\hat{H}_0 + e^{\eta t}\hat{V}(t))|\psi(t)\rangle$$

**Warning:** us the way to detour the singular points, it is an analytical continuation which is a reflection of causality.

**Important:** us the way to detour the singular points, it is an analytical continuation which is a reflection of causality.

**Hint:** us the way to detour the singular points, it is an analytical continuation which is a reflection of causality.

## 3.2 Fermi's Golden rule

CHAPTER 4

# Some topics want to explore

- Phase-space Lagrangian

CHAPTER 5

# Indices and tables

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