
Physics Documentation

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

CLASSICAL MECHANICS:

1.1 Phase space Lagrangian

1.1.1 Regular derivation

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

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

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

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

indicating that $H = p\dot{q} - L$ is conserved in the motion, which is called *Hamiltonian* with physical meaning of energy.

On the other hand, from:

$$\begin{aligned}
 dL(q, \dot{q}) &= \frac{\partial L}{\partial q} dq + \frac{\partial L}{\partial \dot{q}} d\dot{q} \\
 &= \dot{p} dq + p d\dot{q} \\
 &= \dot{p} dq + d(p\dot{q}) - \dot{q} dp \\
 \Rightarrow d(p\dot{q} - L) &= -\dot{p} dq + \dot{q} dp \\
 dH(q, p) &= -\dot{p} dq + \dot{q} dp
 \end{aligned}$$

which means dH is the total differential with respect to q and p . And from:

$$dH = \frac{\partial H}{\partial q} dq + \frac{\partial H}{\partial p} dp$$

we get

$$\dot{p} = -\frac{\partial H}{\partial q} \quad \dot{q} = \frac{\partial H}{\partial p}$$

This is the **Hamilton canonical equations**.

The total derivative with time is:

$$\begin{aligned}
 \frac{dH}{dt} &= \frac{\partial H}{\partial t} + \frac{\partial H}{\partial q} \dot{q} + \frac{\partial H}{\partial p} \dot{p} \\
 &= \frac{\partial H}{\partial t}
 \end{aligned}$$

where Hamilton's equations are used. It also indicates that if H is not depend on time explicitly, we have the conservation of energy.

Note: From Lagrangian to Hamiltonian, we did a *Legendre transformation*, makes the dependence $L(q, \dot{q}, t)$ to $H(q, p, t)$, i.e., L is a function in *configuration space* (q, \dot{q}) , but H is in *phase space* (q, p) .

1.1.2 Dynamic system

Mathematically, a continuous-time dynamical system is defined to be a system of first order differential equations

$$\dot{\mathbf{z}} = \mathbf{f}(\mathbf{z}, t), \quad t \in \mathbb{R}$$

where \mathbf{f} is known as the vector field and \mathbb{R} is the set of real numbers. The space in which \mathbf{z} is defined is called phase space.

Lagrange's equations do not form a dynamical system, because they implicitly contain second-order derivatives, \ddot{q} . However, there is a standard way to obtain a system of first-order equations from a second-order system, which is to double the size of the space of time-dependent variables by treating the generalized velocities u as independent of the generalized coordinates, so that the dynamical system is $\dot{q} = u, \dot{u} = \ddot{q}(q, u, t)$. Then the phase space is of dimension $2n$. This trick is used very frequently in numerical problems, because the standard numerical integrators require the problem to be posed in terms of systems of first-order differential equations.

In the particular case of Lagrangian mechanics, expanding out $\frac{d}{dt} \frac{\partial L}{\partial \dot{q}}$ using the chain rule and moving all but the highest-order time derivatives to the right-hand side,

$$\sum_{j=1}^n \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} \ddot{q}_j = \frac{\partial L}{\partial q_i} - \frac{\partial^2 L}{\partial \dot{q}_i \partial t} - \sum_{j=1}^n \frac{\partial^2 L}{\partial \dot{q}_i \partial q_j} \dot{q}_j$$

The matrix H acting on \ddot{q} , whose elements are given by $H_{i,j} \equiv \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}$, is called the *Hessian matrix*. It is a kind of generalized mass tensor, and for our method to work we require it to be *nonsingular*, so that its inverse, H^{-1} , exists and we can find \ddot{q} . Then our dynamical system becomes:

$$\begin{aligned} \dot{q} &= u, \\ \dot{u} &= H^{-1} \cdot \left[\frac{\partial L}{\partial q} - \frac{\partial L}{\partial \dot{q} \partial t} - \frac{\partial^2 L}{\partial \dot{q} \partial q} \cdot \dot{q} \right] \end{aligned}$$

Momentum instead of velocity

We can achieve our aim of finding 2n first-order differential equations by using many choices of auxiliary variables other than u . These will be more complicated functions of the generalized velocities, but the extra freedom of choice may also bring advantages.

In particular, Hamilton realized that it is very natural to use as the new auxiliary variables the set $p = \{p_i | i = 1, \dots, n\}$ defined by

$$p_i \equiv \frac{\partial}{\partial \dot{q}_i} L(q, \dot{q}, t)$$

where p_i is called the **canonical momentum** conjugate to q_i .

At this moment, we shall assume that the above equation can be solved to give \dot{q} as a function of q and p

$$\dot{q} = u(q, p, t).$$

The Lagrange's equations immediately give us

$$\dot{p} = \frac{\partial L(q, \dot{q}, t)}{\partial q} \Big|_{\dot{q}=u(q,p,t)}$$

The above two equations do indeed form a dynamical system, but so far it looks rather unsatisfactory: now u is defined only implicitly as a function of the phase-space variables q and p , yet the right-hand side of above equation involves a partial derivative in which the q -dependence of u is ignored!

We can fix the latter problem by holding p fixed in partial derivatives with respect to q (because it is an independent phase-space variable) but then subtracting a correction term to cancel the contribution coming from the q -dependence of u . Applying the chain rule, we get

$$\begin{aligned} \dot{p} &= \frac{\partial L(q, u, t)}{\partial q} - \frac{\partial L}{\partial u} \frac{\partial u}{\partial q} \\ &= \frac{\partial L(q, u, t)}{\partial q} - p \frac{\partial u}{\partial q} \\ &= \frac{\partial}{\partial q} [L(q, u, t) - p \cdot u] \\ &= - \frac{\partial H}{\partial q} \end{aligned}$$

where we have already defined the Hamiltonian $H(q, p, t) = p \cdot u?L(q, u, t)$ is a function of (q, p) .

Given the importance of $\partial H/\partial q$ it is natural to investigate whether $\partial H/\partial p$ plays a significant role as well. Differentiating $H(q, p, t) = p \cdot u?L(q, u, t)$ we get

$$\begin{aligned}\frac{\partial H}{\partial p} &= u(q, p, t) - \left[p - \frac{\partial}{\partial u} L(q, u, t) \right] \frac{\partial u}{\partial p} \\ &= \dot{q}\end{aligned}$$

the above two equations are just the **Hamilton's equations** we derived before.

1.1.3 Phase space Lagrangian

The equation $H(q, p, t) \equiv p \cdot \dot{q} - L(q, \dot{q}, t)$ suggest we define $L_{ph}(q, \dot{q}, p, t) \equiv p \cdot \dot{q} - H(q, p, t)$. If $\dot{q} = u(q, p, t)$ were identically satisfied, even on arbitrarily varied phase-space paths, then L_{ph} would simply be L expressed in phase-space coordinates.

However, one can easily construct a counter example to show that this is not the case: consider a variation of the path in which we can vary the direction of its tangent vector, at some point $z \equiv (q, p)$, while keeping this point fixed. Then \dot{q} changes, but u remains the same. Thus L_{ph} and L are the same value only on the subset of paths (which includes the physical paths) for which $p \cdot \dot{q} = p \cdot u(q, p, t)$.

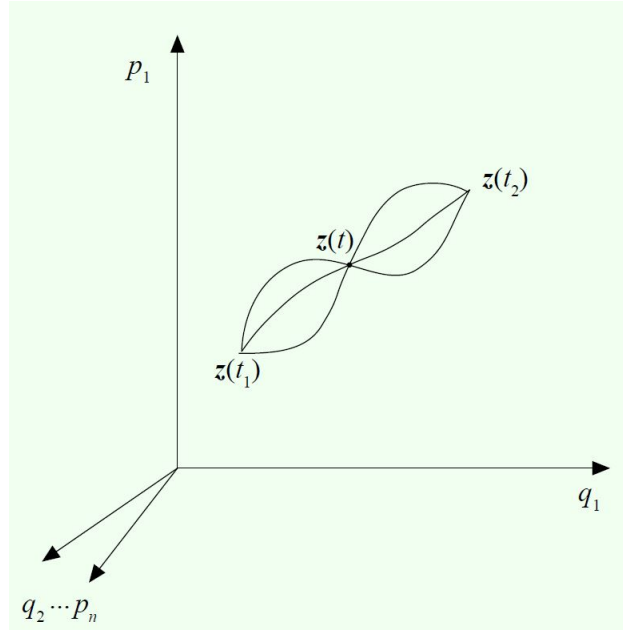


Figure 1.1: **Fig. 1** Phase-space variations of different paths.

Replacing L by L_{ph} in $S = \int L dt$ we define the phase-space action integral

$$S_{ph}[q, p] = \int_{t_1}^{t_2} dt L_{ph}(q, p, \dot{q}, t) = \int_{t_1}^{t_2} dt (p \cdot \dot{q} - H(q, p, t))$$

We know from variational calculus that S_{ph} is stationary under arbitrary variations of the phase-space path (with endpoints fixed), explicitly, we get:

$$\begin{aligned}\delta S_{ph} &= \delta \int_{t_1}^{t_2} dt (p \cdot \dot{q} - H(q, p, t)) \\ &= \int_{t_1}^{t_2} dt \left(\delta p \cdot \dot{q} + p \cdot \delta \dot{q} - \delta p \frac{\partial H(q, p, t)}{\partial p} - \delta q \frac{\partial H(q, p, t)}{\partial q} \right) \\ &= p \delta q \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} dt \left\{ \delta p \cdot \left[\dot{q} - \frac{\partial H(q, p, t)}{\partial p} \right] - \delta q \cdot \left[\dot{p} + \frac{\partial H(q, p, t)}{\partial q} \right] \right\}\end{aligned}$$

which gives us the **Hamilton's equations**:

$$\dot{p} = -\frac{\partial H}{\partial q} \quad \dot{q} = \frac{\partial H}{\partial p}$$

Note: More generally, the phase-space Lagrangian can depend on \dot{p} as well, and makes the Lagrange's equations become:

$$\begin{aligned}\frac{\delta L_{ph}(q, \dot{q}, p, \dot{p})}{\delta q} &= \frac{\partial L_{ph}}{\partial q} - \frac{d}{dt} \frac{\partial L_{ph}}{\partial \dot{q}} = 0 \\ \frac{\delta L_{ph}(q, \dot{q}, p, \dot{p})}{\delta p} &= \frac{\partial L_{ph}}{\partial p} - \frac{d}{dt} \frac{\partial L_{ph}}{\partial \dot{p}} = 0\end{aligned}$$

References

1. L.D. Landau & E.M. Lifshitz, *Mechanics*.
2. Lecture notes by **Bob Dewar** on website [Classical Mechanics](#).

TOPOLOGICAL INSULATOR:

2.1 Lecture notes

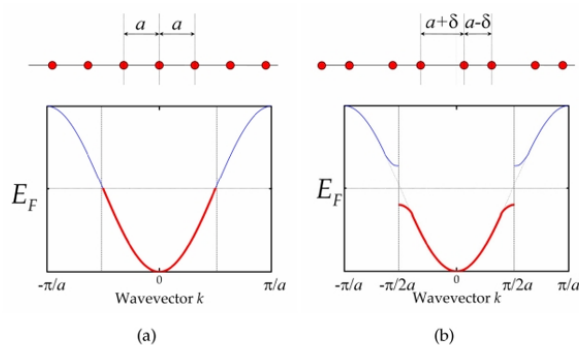
Here is the lecture notes on TI, which is based on the lecture notes given by Janos Asboth, Laszlo Oroszlany, and Andras Palyi, [Here](#) is the resource, and you can also download a copy [here](#).

2.1.1 Lecture 1 : 1-d SSH model

The Su-Schrieffer–Heeger (SSH) model

The simplest non-trivial topology : 1-d lattice.

Peierls instability makes the atoms dimerize.



Polyacetylene Structure:



Tight-binding method-first quantization

Tight-binding method: Single electron total Hamiltonian in atom chain:

$$H = \frac{p^2}{2m} + U(x)$$

with periodical potential: $U(x + na) = U(x)$

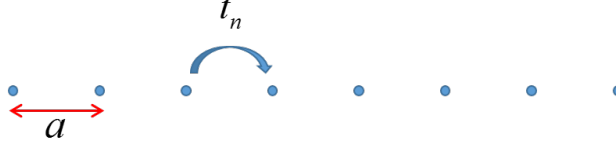


Figure 2.1: 1-d atom chain

Assume single atom potential $V(x)$ with Hamiltonian

$$H_0 = \frac{p^2}{2m} + V(x)$$

and well solved eigen-value and eigen-wave-function:(consider only one state)

$$H_0\phi(x) = E_0\phi(x)$$

Do the combination

$$\psi(x) = \sum_n a_n \phi_n$$

with $\phi_n = \phi(x - x_n)$, $x_n = na$. Define $\Delta U(x) = U(x) - V(x)$, and substitute following equation

$$H\psi = (H_0 + \Delta U)\psi = E\psi$$

we get

$$\sum_n \langle \phi_m | \Delta U(x - x_n) | \phi_n \rangle a_n = (E - E_0)a_m$$

Define: $\langle \phi(x - ma + na) | \Delta U(x) | \phi(x) \rangle = -J(x_m - x_n)$

We get:

$$-\sum_n J(x_m - x_n)a_n = (E - E_0)a_m$$

Because of the Tranformation symmetry of the Hamiltonian, the resulting wavefunction $\psi(x)$ should take Bloch form, which means we should have the solution $a_m = e^{ikx_m}$, then, we get

$$E - E_0 = -\sum_n J(x_n)e^{-ikx_n}$$

Consider only the nearest-hopping interaction, define $J_0 = J(0)$, $J = J(\pm a)$, then we have:

$$\begin{aligned} E - E_0 + J_0 &= -J(e^{ika} + e^{-ika}) \\ &= -2J\cos ka \end{aligned}$$

Second quantization

In the second quantization language, the expectation value of energy becomes a operator, set $\mathcal{H} = \frac{p^2}{2m} + U(x)$, we have

$$H = \langle \psi | \mathcal{H} | \psi \rangle \Rightarrow \hat{H} = \sum_{m,n} \hat{c}_m^\dagger H_{mn} \hat{c}_n$$

with $\psi \rightarrow \hat{\psi} = \sum_n \hat{c}_n \phi_n$, $H_{mn} = \langle \phi | \mathcal{H} | \phi \rangle$ ϕ_n is a orthonormal and complete basis in *Hilbert space*, like plane-waves e^{ikx} or energy eigen-states of H_0 , \mathcal{H} is the energy operator in single particle first quantization picture, which can only act on Hilbert space, while the second quantization energy operator \hat{H} acts on *Fock space*. Here, in tight-binding method, ϕ_n is the wave-function of site n of the energy eigen-state H_0 .

Consider only the nearest interaction, we have:

$$\hat{H} = \sum_{n=1}^M \hat{c}_n^\dagger \hat{c}_{n+1} t_n + h.c.$$

h.c. means hermitian conjugation. Rewrite it in matrix form: $\hat{H} = \sum_{mn} \hat{c}_m \tilde{H}_{mn} c_n$, we have

$$\tilde{H}_{mn} = \begin{pmatrix} 0 & t_1 & 0 & \cdots & t_M^* \\ t_1^* & 0 & t_2 & \cdots & 0 \\ 0 & t_2^* & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_M & 0 & 0 & t_{M-1}^* & 0 \end{pmatrix}$$

In the case when $t = t_n$, \hat{c}_n satisfy the Bloch condition, we can transform it into momentum space, with $\hat{c}_n = \frac{1}{\sqrt{M}} \sum_k \hat{c}_k e^{ikx_n}$,

we can easily get

$$\hat{H} = \sum_k \hat{c}_k^\dagger \hat{c}_k (t e^{ika} + t^* e^{-ika}) = \sum_k \hat{c}_k^\dagger \hat{c}_k E(k)$$

which gives us the dispersion relation:

$$\begin{aligned} E(k) &= t e^{ika} + t^* e^{-ika} \\ &= 2t \cos ka \quad \text{for } t \text{ is real} \end{aligned}$$

On the other hand, keep in mind that we would get $c_n = e^{ik(n-1)a} c_1$, that is

$$\hat{H} = \begin{pmatrix} \hat{c}_1^\dagger & \hat{c}_2^\dagger & \cdots & \hat{c}_M^\dagger \end{pmatrix} \begin{pmatrix} 0 & t & 0 & \cdots & t^* \\ t^* & 0 & t & \cdots & 0 \\ 0 & t^* & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t & 0 & 0 & t^* & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_M \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} c_1^\dagger & c_1^\dagger e^{-ika} & \dots & c_1^\dagger e^{-ik(M-1)a} \end{pmatrix} \begin{pmatrix} 0 & t & 0 & \dots & t^* \\ t^* & 0 & t & \dots & 0 \\ 0 & t^* & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t & 0 & 0 & t^* & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_1 e^{ika} \\ \vdots \\ c_1 e^{ik(M-1)a} \end{pmatrix}$$

$$= \begin{pmatrix} c_1^\dagger & \dots & c_1^\dagger \end{pmatrix} \begin{pmatrix} te^{ika} + t^* e^{-ika} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & te^{ika} + t^* e^{-ika} \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_1 \end{pmatrix}$$

which also gives us $E(k) = te^{ika} + t^* e^{-ika}$.

More generally, t_n can be different from each other, for example, if they are all different up to 4, but have a super-periodicity with $t_5 = t_1$, then there will have 4 sub-bands, in the example we will consider below, we have two t , $t_1 \neq t_2$, and we have two sub-bands.

If each atom have a valance electron, then the above mentioned energy band structure $E(k) = 2t \cos ka$ is not the stable fundamental mode, it will dimerizes to lower the total energy, that means we'll get following coupling case:



with the Hamiltonian:

$$H = \sum_{n=1}^N (v_n c_{n,1}^\dagger c_{n,2} + w_n c_{n,2}^\dagger c_{n+1,1} + h.c.)$$

with $M = 2N$.

Review

In 1-d atom chain, we have got the Hamiltonian in second-quantization frame as:

$$\hat{H} = \sum_{n=1}^M \hat{c}_n^\dagger \hat{c}_{n+1} t_n + h.c.$$

$h.c.$ means hermitian conjugation. Rewrite it in matrix form: $\hat{H} = \sum_{mn} \hat{c}_m H_{mn} \hat{c}_n$, we have

$$\hat{H} = \begin{pmatrix} c_1^\dagger & c_2^\dagger & \dots & c_M^\dagger \end{pmatrix} \begin{pmatrix} 0 & t_1 & 0 & \dots & t_M^* \\ t_1^* & 0 & t_2 & \dots & 0 \\ 0 & t_2^* & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_M & 0 & 0 & t_{M-1}^* & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_M \end{pmatrix}$$

$$\hat{H} = \begin{pmatrix} c_1^\dagger & c_2^\dagger & \cdots & c_M^\dagger \end{pmatrix} \begin{pmatrix} 0 & t_1 & 0 & \cdots & t_M^* \\ t_1^* & 0 & t_2 & \cdots & 0 \\ 0 & t_2^* & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ t_M & 0 & 0 & t_{M-1}^* & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_M \end{pmatrix}$$

t_n can differ from each other.

1. For a open chain with M atoms, we have $t_M = 0$, and this matrix will give us M eigen-values and eigen-functions.
2. Possess translational invariance with $c_{n+1} = c_1 e^{ikna}$, it will be diagonalized with $H(k) = t e^{ika} + t^* e^{-ika}$.
3. Staggered hopping parameters with $t_1 \neq t_2$, but have property $c_{2n+1} = c_1 e^{iknb}$, $c_{2n+2} = c_2 e^{iknb}$. We can block the Hamiltonian up in 2×2 blocks and also pair up c_{2n+1}, c_{2n+2} .

The Hamiltonian:

$$H = \sum_{n=1}^N (v_n c_{n,1}^\dagger c_{n,2} + w_n c_{n,2}^\dagger c_{n+1,1} + h.c.)$$

with $M = 2N$.



For a more beautiful notation, define $\mathbf{c}_n^\dagger = (c_{n,1}^\dagger, c_{n,2}^\dagger) = (c_{2n-1}^\dagger, c_{2n}^\dagger)$, then we have

$$H = \sum_{m,n=1}^N \mathbf{c}_m^\dagger H_{mn} \mathbf{c}_n$$

with

$$\mathbf{c}_n^\dagger H_{nn} \mathbf{c}_n = \begin{pmatrix} c_{n,1}^\dagger & c_{n,2}^\dagger \end{pmatrix} \begin{pmatrix} 0 & v_n \\ v_n^* & 0 \end{pmatrix} \begin{pmatrix} c_{n,1} \\ c_{n,2} \end{pmatrix} = \begin{pmatrix} c_{n,1}^\dagger & c_{n,2}^\dagger \end{pmatrix} U_n \begin{pmatrix} c_{n,1} \\ c_{n,2} \end{pmatrix}$$

and

$$\mathbf{c}_n^\dagger H_{n,n+1} \mathbf{c}_{n+1} = \begin{pmatrix} c_{n,1}^\dagger & c_{n,2}^\dagger \end{pmatrix} \begin{pmatrix} 0 & 0 \\ w_n & 0 \end{pmatrix} \begin{pmatrix} c_{n+1,1} \\ c_{n+1,2} \end{pmatrix} = \begin{pmatrix} c_{n,1}^\dagger & c_{n,2}^\dagger \end{pmatrix} T_n \begin{pmatrix} c_{n+1,1} \\ c_{n+1,2} \end{pmatrix}$$

$$\mathbf{c}_{n+1}^\dagger H_{n+1,n} \mathbf{c}_n = \begin{pmatrix} c_{n+1,1}^\dagger & c_{n+1,2}^\dagger \end{pmatrix} T_n^\dagger \begin{pmatrix} c_{n,1} \\ c_{n,2} \end{pmatrix}$$

when $|m - n| > 1$, we have $H_{mn} = 0$.

For example, for 6 cells (12 sites), we have

$$H = \begin{pmatrix} U_1 & T_1 & 0 & \cdots & T_6^\dagger \\ T_1^\dagger & U_2 & T_2 & \cdots & 0 \\ 0 & T_2^\dagger & U_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T_6 & 0 & 0 & \cdots & U_6 \end{pmatrix}$$

$$H_{mn} = \begin{pmatrix} U_1 & T_1 & 0 & \cdots & T_6^\dagger \\ T_1^\dagger & U_2 & T_2 & \cdots & 0 \\ 0 & T_2^\dagger & U_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T_6 & 0 & 0 & \cdots & U_6 \end{pmatrix}$$

- Open chain: $T_6 = 0$.
- Closed chain with translational symmetry, $T_n = T, U_n = U$, with

$$U = \begin{pmatrix} 0 & v \\ v^* & 0 \end{pmatrix}, T = \begin{pmatrix} 0 & 0 \\ w & 0 \end{pmatrix}$$

Using three Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We get

$$U = \text{Re}(v)\sigma_x - \text{Im}(v)\sigma_y, T = \frac{1}{2}w(\sigma_x - i\sigma_y)$$

Using $\mathbf{c}_n = e^{ik(n-1)b}\mathbf{c}_1$, we have

$$\hat{H} = \begin{pmatrix} \mathbf{c}_1^\dagger & \mathbf{c}_2^\dagger & \cdots & \mathbf{c}_N^\dagger \end{pmatrix} \begin{pmatrix} U & T & 0 & \cdots & T^\dagger \\ T^\dagger & U & T & \cdots & 0 \\ 0 & T^\dagger & U & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T & 0 & 0 & T^\dagger & U \end{pmatrix} \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \\ \vdots \\ \mathbf{c}_N \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} \mathbf{c}_1^\dagger & \mathbf{c}_1^\dagger e^{-ikb} & \cdots & \mathbf{c}_1^\dagger e^{-ik(N-1)b} \end{pmatrix} \begin{pmatrix} U & T & 0 & \cdots & T^\dagger \\ T^\dagger & U & T & \cdots & 0 \\ 0 & T^\dagger & U & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T & 0 & 0 & T^\dagger & U \end{pmatrix} \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_1 e^{ikb} \\ \vdots \\ \mathbf{c}_1 e^{ik(N-1)b} \end{pmatrix}$$

$$= \begin{pmatrix} \mathbf{c}_1^\dagger & \cdots & \mathbf{c}_1^\dagger \end{pmatrix} \begin{pmatrix} U + Te^{ikb} + T^\dagger e^{-ikb} & & \\ & \ddots & \\ & & U + Te^{ikb} + T^\dagger e^{-ikb} \end{pmatrix} \begin{pmatrix} \mathbf{c}_1 \\ \vdots \\ \mathbf{c}_1 \end{pmatrix}$$

which gives us $H = H(k) \oplus H(k) \cdots \oplus H(k) = \oplus_{n=1}^N H(k)$ with

$$H(k) = U + Te^{ikb} + T^\dagger e^{-ikb} = \mathbf{h}(k) \cdot \sigma$$

with

$$\begin{aligned} h_x(k) &= \text{Re}(v) + |w| \cos(kb + \arg(w)) \\ h_y(k) &= -\text{Im}(v) + |w| \sin(kb + \arg(w)) \\ h_z(k) &= 0 \end{aligned}$$

with $w = |w|e^{i\arg(w)}$.

$$H(k) = \mathbf{h}(k) \cdot \sigma$$

with

with eigen-energy

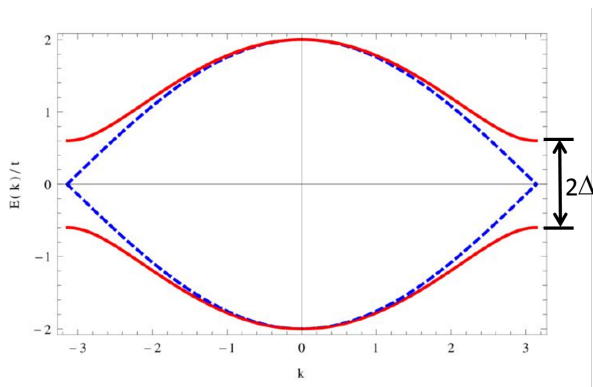
$$E(k) = |(h)(k)| = \pm \sqrt{h_x^2 + h_y^2 + h_z^2} = \pm \sqrt{|v|^2 + |w|^2 + 2|v||w|\cos(kb + \arg(v) + \arg(w))}$$

and eigen-wavefunctions

$$|\pm\rangle = \begin{pmatrix} \pm e^{-i\phi(k)} \\ 1 \end{pmatrix}$$

with $\tan\phi = h_y/h_x$.

For example, set $\arg(v) = \arg(w) = 0$, we have



Can not tell the difference $|v| - |w| = \pm\delta$.

Energy-band description is not completed, it can give us many information, but not the whole, others are hidden in the wave-function. Alternatively, recalling $H(k) = \mathbf{h}(k) \cdot \sigma$, the Hamiltonian should contain the whole information, but we have only used $|h|$, in topological aspect, $\mathbf{h}(k)$ will suffice.

Set $\arg(v) = 0, kb = [0, 2\pi]$, we have two cases

- $|w| < |v|$, **inter < intra**
- $|w| > |v|$, **inter > intra**

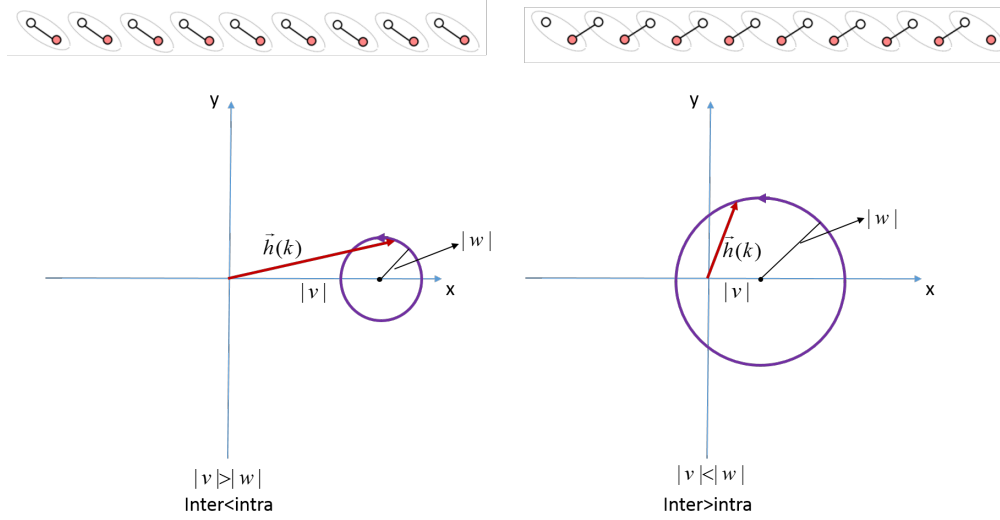


Figure 2.2: two cases

winding number

$H(k) = \mathbf{h}(k) \cdot \sigma$, $\mathbf{h}(k) = 0$ is a degenerate point with $|v| = |w|$, two bands cross, define $h(k) = h_x(k) + ih_y(k)$, we have

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

$$\ln(h) = \ln(|h|)e^{i\arg(h)} = \ln(|h|) + i\arg(h)$$

define

$$\nu = \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk \frac{d}{dk} \ln(h(k))$$

When

- $|w| > |v|, \nu = 1$, **inter > intra**
- $|w| < |v|, \nu = 0$, **inter < intra**

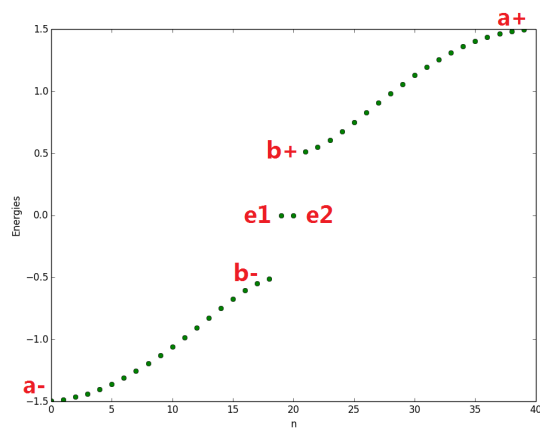
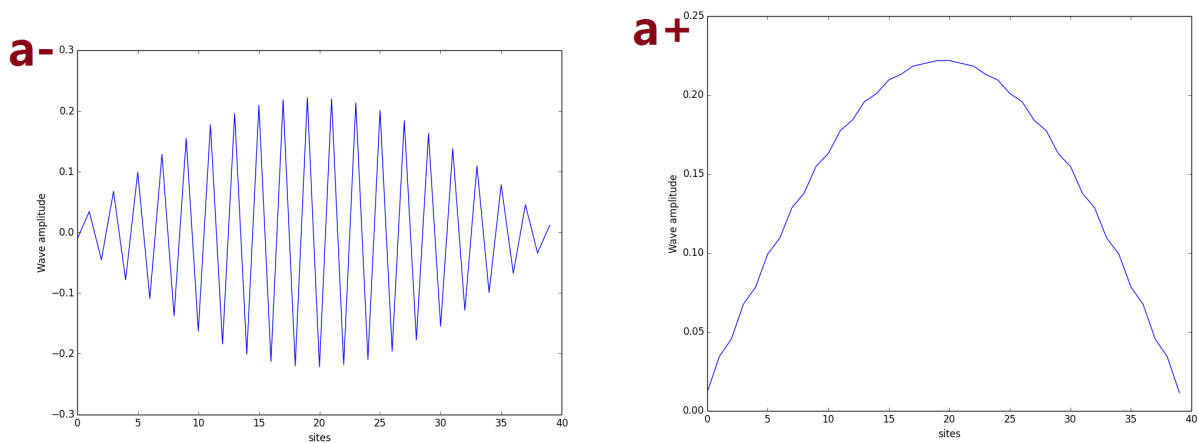
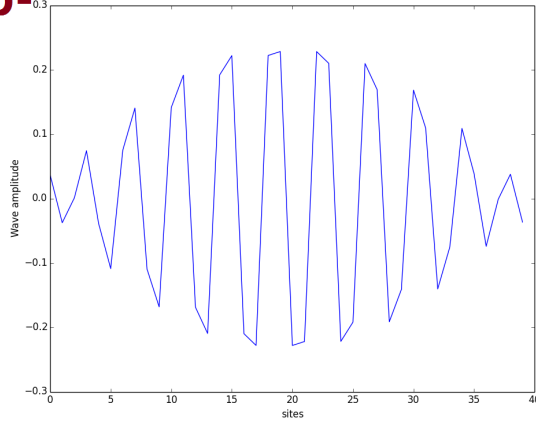


Figure 2.3: eigen-energy

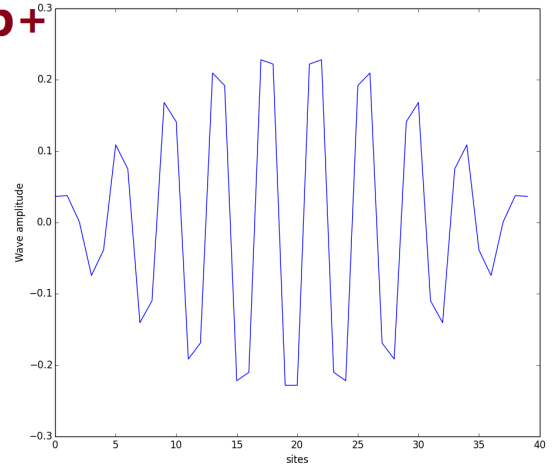
A example, $N = 20$, $M = 2N = 40$, $w = 1$, $v = 0.5$, we get eigen-energys:



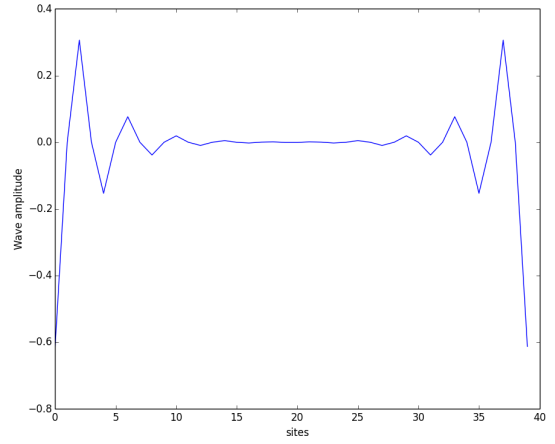
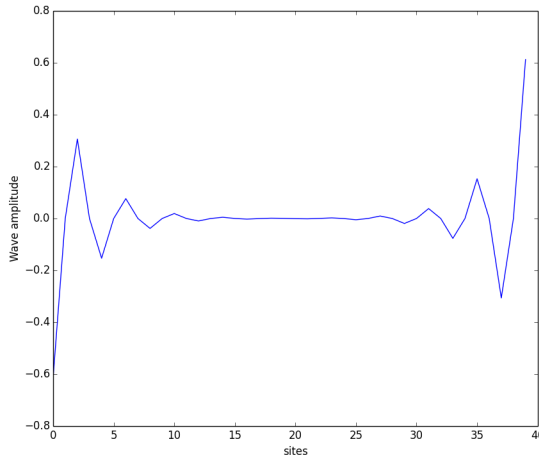
b-



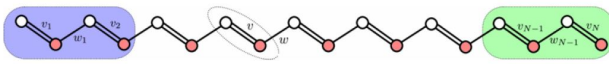
b+



Edge-states:



Chiral symmetry



Recalling the Hamiltonian:

$$H = \sum_{n=1}^N (v_n c_{n,1}^\dagger c_{n,2} + w_n c_{n,2}^\dagger c_{n+1,1} + h.c.)$$

Define projector operators:

$$P_A = \sum_n c_{n,1}^\dagger c_{n,1}, P_B = \sum_n c_{n,2}^\dagger c_{n,2}$$

and the chiral operator $\Sigma_z = P_A - P_B$, The matrix elements of Σ_z vanish, $\langle 0|c_r \Sigma_z c_s^\dagger|0\rangle = 0$ if sites r and s are in different unit cells.

In first-quantization, we have

$$H = \sum_{n=1}^N (v_n |n, 1\rangle \langle n, 2| + w_n |n, 2\rangle \langle n+1, 1| + h.c.)$$

and

$$P_A = \sum_n |n, 1\rangle \langle n, 1|, P_B = \sum_n |n, 2\rangle \langle n, 2|$$

In matrix form, we have

$$\Sigma_z = \sigma_z \oplus \sigma_z \oplus \cdots \oplus \sigma_z = \bigoplus_{n=1}^N \sigma_z$$

Σ_z is *local*, it does not mix site between unit cells, and inherits the algebra from σ_z :

$$\Sigma_z^\dagger \Sigma_z = 1$$

$$\Sigma_z^2 = 1$$

Recalling

$$\begin{pmatrix} U_1 & T_1 & 0 & \cdots & T_N^\dagger \\ T_1^\dagger & U_2 & T_2 & \cdots & 0 \\ 0 & T_2^\dagger & U_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T_N & 0 & 0 & T_{N-1}^\dagger & U_N \end{pmatrix}$$

There are no **onsite terms** in the Hamiltonian, so we have

$$\Sigma_z H \Sigma_z = -H$$

This is the chiral symmetry.

Note: Actually, here, H is defined in momentum space, but Σ_z in real space, we should write $\tilde{H} = U^\dagger H U$ for some unitary matrix U , but the property survives!

Consequences: For eigenstates $|\psi_n\rangle$ of H , we have

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

$$H \Sigma_z |\psi_n\rangle = -\Sigma_z H |\psi_n\rangle = -\Sigma_z E_n |\psi_n\rangle = -E_n \Sigma_z |\psi_n\rangle$$

If

- $E_n \neq 0$, two orthonormal states $|\psi_n\rangle, \Sigma_z|\psi_n\rangle$, which gives

$$\begin{pmatrix} \alpha^* & \beta^* \end{pmatrix} \begin{pmatrix} \alpha \\ -\beta \end{pmatrix} = 0$$

$$\Rightarrow |\alpha|^2 = |\beta|^2$$

- $E_n = 0$, $\Sigma_z|\psi_n\rangle = \pm|\psi_n\rangle$, gives $|\psi_n\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $|\psi_n\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
-

2.2 Berry's Phase

2.2.1 Preliminary

2.2.2 some topics

- fiber bundle
- gauge/parallel transport
- symmetry

2.3 Weyl Semi-metal

2.3.1 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):

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

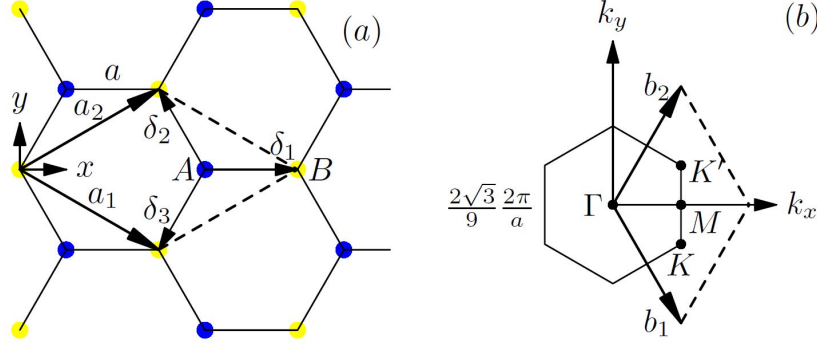


Figure 2.4: **Fig. 1** Crystal Structure of Graphene: \vec{a}_1 and \vec{a}_2 are Bravais crystal vectors for a Graphene unit cell. Each primitive unit cell has two atomic sites, A and B. $\vec{\delta}_i$ specifies B-s' position around A site. (b) Brillouin Zone for Graphene \vec{b}_1 and \vec{b}_2 are 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 ϕ changes 2π , 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 $\psi(\vec{k})$ 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 ϕ 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 ϕ (Fig. 2(c)) winds one round too.

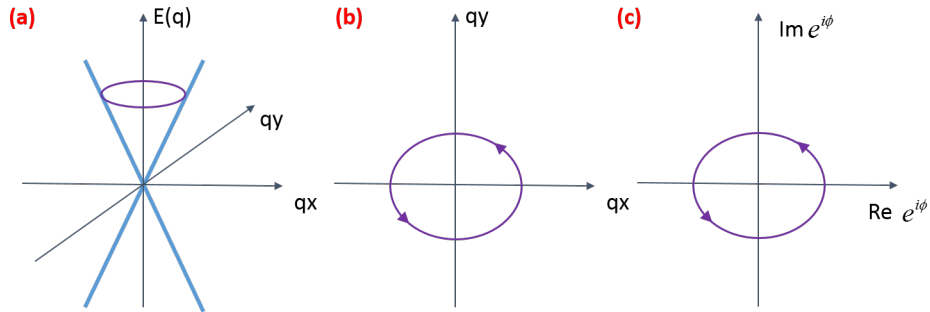


Figure 2.5: **Fig. 2** Dirac cone and the winding of \vec{q} and ϕ

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

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 get:

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

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*.

2.3.2 Three dimension: Weyl semi-metal and Chern number

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

$$H(\vec{k}) = [-2t_x(\cos k_x - \cos k_0) + m(2 - \cos k_y - \cos k_z)]\sigma_x + 2t_y \sin k_y \sigma_y + 2t_z \sin k_z \sigma_z$$

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 $v_x = 2t_x \sin k_0, v_y = 2t_y, v_z = 2t_z$. 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 $C = 1$.

2.3.3 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:

$$H_{k_x}(k_y, k_z) = \vec{h}(\vec{k}) \cdot \sigma = [-2t_x(\cos k_x - \cos k_0) + m(2 - \cos k_y - \cos k_z)]\sigma_x + 2t_y \sin k_y \sigma_y + 2t_z \sin k_z \sigma_z$$

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

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:

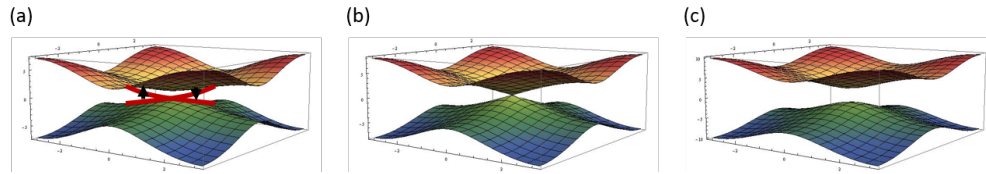


Figure 2.6: **Fig. 3** Typical energy band dispersion with (a) $k_x = 0$, (b) $k_x = k_0 = 1$, (c) $k_x = 2$.

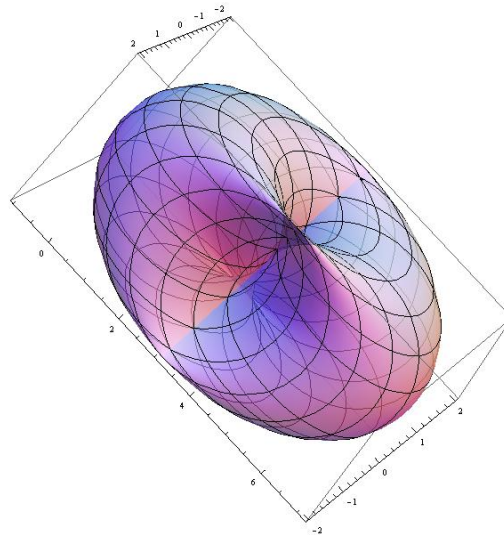


Figure 2.7: **Fig. 4** Typical torus of $\vec{h}(k_y, k_z)$ with $k_x = 0$.

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 $C = 0$ (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:

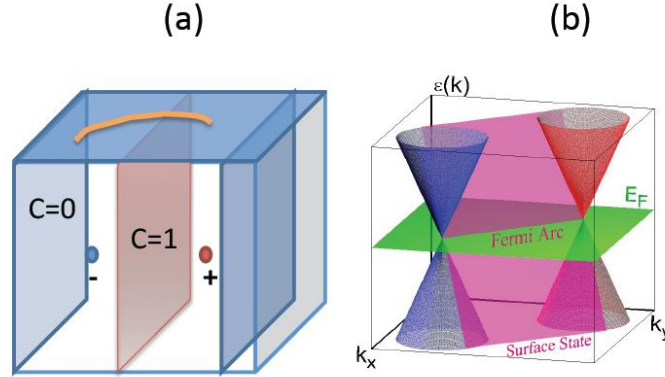


Figure 2.8: **Fig. 5** Fermi arc.

Alternatively, we can look at the Bulk-boundary corresponding another way. The Weyl points behave like “magnetic” monopoles in momentum space whose charge is given by the chirality; they are actually a source of “Berry flux” rather than magnetic flux.

Consider a curve in the surface Brillouin zone encircling the projection of the bulk Weyl point, which is traversed counterclockwise as we vary the parameter $\lambda : 0 \rightarrow 2\pi$; $\mathbf{k}_\lambda = [k_x(\lambda), k_y(\lambda)]$ [see Fig. 6(a)]. We show that the energy λ of a surface state at momentum \mathbf{k}_λ crosses $E = 0$ at some value of λ . Consider $H(\lambda, k_z) = H(\mathbf{k}_\lambda, k_z)$, which can be interpreted as the gapped Hamiltonian of a two-dimensional system (with λ and k_z as the two momenta). The two periodic parameters λ, k_z define the surface of a torus in momentum space. The Chern number of this two-dimensional band structure is given by the Berry curvature integration: $\frac{1}{2\pi} \int \mathcal{F} dk_z d\lambda$, which, by the Stokes theorem, simply corresponds to the net monopole density enclosed within the torus. This is obtained by summing the chiralities of the enclosed Weyl nodes. Consider the case when the net chirality is unity, corresponding to a single enclosed Dirac node. Then, the two-dimensional subsystem is a quantum Hall insulator with unit Chern number. When the system is given a boundary at $z = 0$, we expect a chiral edge state for this subsystem [see Fig. 6(b)]. Hence, this surface state crosses zero energy somewhere on the surface Brillouin zone \mathbf{k}_{λ_0} . Such a state can be obtained for every curve enclosing the Weyl point. Thus, at zero energy, there is a Fermi line in the surface Brillouin zone, that terminates at the Weyl point momenta [see Fig. 6(c)]. An arc beginning on a Weyl point of chirality c has to terminate on a Weyl point of the opposite chirality. Clearly, the net chirality of the Weyl points within the (λ, k_z) torus was a key input in determining the number of these states. If Weyl points of opposite chirality line up along the k_z direction, then there is a cancellation and no surface states are expected.

References:

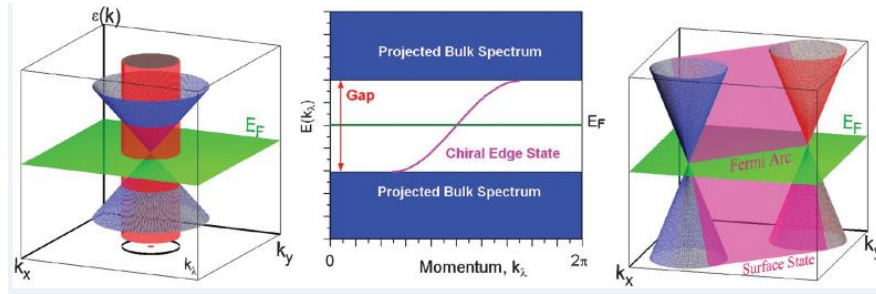


Figure 2.9: **Fig. 6** Illustration of surface states arising from bulk Weyl points.

1. (a) Wan, A.M. Turner, A. Vishwanath, and S.Y. Savrasov, Physical Review B **83**, 205101 (2011).
24. A.M. Turner, A. Vishwanath, and C.O. Head, Topological Insulators **6**, 293 (2013).
25. (a) Haldane, Physical Review Letters **93**, 206602 (2004).

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 many-body 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) ε_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 $t \rightarrow -\infty$, 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

SOME TOPICS WANT TO EXPLORE

- Green's Function
- Dirac, Majorana, Weyl fermions

SOMETHING ABOUT PYTHON

5.1 Python 学习

1. 数组初始化

初始化一维数组

```
p1=[1]*100
```

初始化二维数组 100*10

```
p2=[[1] * 100 for i in xrange(10)]
```

#Below does not work!

```
p2=[[1] * 100]*10
```

#Or we can use:

```
p2=[[None for col in range(100)] for row in range(10)]
```

初始化三维数组 2*3*4

```
p3=[[[1] * 2 for i in xrange(3)] for j in xrange(4)]
```

#Or

```
p3=[[[1 for i in xrange(2)] for j in xrange(3)] for k in xrange(4)]
```

#Or

```
p3=[]
```

```
for i in range(2):
```

```
    p3.append([])
```

```
    for j in range(3):
```

```
        p3[i].append([])
```

```
        for k in range(4):
```

```
            p3[i][j].append(0)
```

1. python 中的内积 dot 是没有复共轭的, vdot 有, 而 matlab dot(a,b) 是对 a 取复共轭的。

