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SSH Model-1

聂嘉会

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1 Hamiltonian

SSH model refers to a one dimension lattice staggered by two different atoms. The dimerized structure forms two sublattices which we may label as A and B. The unit cell of this lattice model is shown below:

图 1: SSH model

SSH model is renowned as the simplest one-dimensional topological insulator model. This model is loaded a tight-binding Hamiltonian written in the second quantized form in real space:

$$\mathcal{H} = \sum_{i\in\mathbb{Z}} (t+\delta t) c^{\dagger}_{A,i} c_{B,i} + (t-\delta t) c^{\dagger}_{A,i+1} c_{B,i} + \text{h.c.}, \tag{1}$$

where $t \in \mathbb{R}$ describes the hopping amplitudes between $(t-\delta t)$ or in $(t+\delta t)$ the unit cells. The first term denotes electron hopping from B atom to A atom in one unit cell, and the second term denotes the case between two adjacent cells, while the Hermite conjugate just denotes the reverse process. This Hamiltonian owns a chiral symmetry for there is no hopping in sublattices:

$$\Gamma\mathcal{H}\Gamma = -\mathcal{H},\ \Gamma = \sum_i |i,A\rangle\langle i,A| - \sum_i |i,B\rangle\langle i,B|\,. \tag{2}$$

This can be shown by noticing that the Hamiltonian only contain terms like $|i,A\rangle\langle i',B|$ or the Hermite conjugate. This chiral symmetry results in three things:

- The Hamiltonian has no z component in Pauli space;
- The energy spectrum is symmetry;
- From the first point there may exist a well-defined winding number for Hamiltonian in Pauli space.

Here, the index i is put formally, and we can apply two different boundary conditions to specify it: the periodic boundary condition and the open boundary condition. Assuming there are N cells in total, then the former refers to that N cells form a closed circle: $c_{N+1} = c_1$; while the latter refers to just a chain with two open boundaries, so summation over hoppings between cells is just up to the $N-1$ term. The

periodic boundary condition only reveals the bulk information, but the open boundary condition gives us the edge information.

Applying periodic boundary condition, the Hamiltonian can be written as:

$$\mathcal{H} = \sum_{i=1}^{N} (t+\delta t) c_{A,i}^{\dagger} c_{B,i} + (t-\delta t) c_{A,i+1}^{\dagger} c_{B,i} + \text{h.c.}, \tag{3}$$

by the discrete spatial translation symmetry, we can transform it into momentum space by using Fourier transformation on the creation and annihilation operators for A and B:

$$\begin{aligned} c_{A,j} &= \frac{1}{\sqrt{N}} \sum_{k} e^{ikj} a_k, \\ c_{B,j} &= \frac{1}{\sqrt{N}} \sum_{k} e^{ikj} b_k, \end{aligned} \tag{4}$$

where $k \in [-\pi, \pi]$ is the first BZ. Thus the Hamiltonian is transformed as

$$\begin{aligned} \mathcal{H} &= \sum_{j=1}^{N} (t+\delta t) \Big[\frac{1}{\sqrt{N}} \sum_{k} e^{-ikj} a_k^{\dagger} \Big] \Big[\frac{1}{\sqrt{N}} \sum_{k'} e^{ik'j} b_{k'} \Big] + (t-\delta t) \Big[\frac{1}{\sqrt{N}} \sum_{k} e^{-ik(j+1)} a_k^{\dagger} \Big] \Big[\frac{1}{\sqrt{N}} \sum_{k'} e^{ik'j} b_{k'} \Big] + \text{h.c.} \\ &= \sum_{k} (t+\delta t) a_k^{\dagger} b_k + (t-\delta t) e^{-ik} a_k^{\dagger} b_k + \text{h.c.} \\ &= \sum_{k} \left(a_k^{\dagger}, b_k^{\dagger} \right) \begin{pmatrix} 0 & (t+\delta t) + (t-\delta t) e^{-ik} \\ (t+\delta t) + (t-\delta t) e^{ik} & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \\ &=: \sum_{k} \psi_k^{\dagger} \boldsymbol{h}(t,k) \cdot \boldsymbol{\sigma} \psi_k, \end{aligned} \tag{5}$$

where $\boldsymbol{h}(t,k) = ((t+\delta t) + (t-\delta t)\cos k, (t-\delta t)\sin k, 0)$ can be seen as a Hamiltonian vector operator in Pauli space, and $\psi_k = \begin{pmatrix} a_k \\ b_k \end{pmatrix}$ is an annihilation spinor operator.

2 Spectrum

Since we have written the Hamiltonian in a 2×2 matrix form, the spectrum can be obtained by diagonalizing $\boldsymbol{h}(t,k) \cdot \boldsymbol{\sigma}$. This is a classical 2-band Hamiltonian, we then get the dispersion relationships:

$$E(k) = \pm \sqrt{\boldsymbol{h} \cdot \boldsymbol{h}} = \pm \sqrt{(t+\delta t)^2 + (t-\delta t)^2 + 2(t+\delta t)(t-\delta t)\cos k}. \tag{6}$$

Define the shperical angles in Pauli space, we find that the Hamiltonian lays on the $\sigma_x - \sigma_y$ plane because of chiral symmetry:

$$\begin{aligned} \theta_k &= \arccos \frac{h_z}{|h|} = \frac{\pi}{2}, \\ e^{i\phi_k} &= \frac{h_x + i h_y}{|h_x + i h_y|} = \frac{(t+\delta t) + (t-\delta t) e^{ik}}{\sqrt{(t+\delta t)^2 + (t-\delta t)^2 + 2(t+\delta t)(t-\delta t)\cos k}}. \end{aligned} \tag{7}$$

Under Northern gauge, the eigenstates are

$$
\begin{aligned}
|+\rangle &= \begin{pmatrix} \cos\frac{\theta_k}{2} e^{-i\phi_k} \\ \sin\frac{\theta_k}{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi_k} \\ 1 \end{pmatrix}, \\
|-\rangle &= \begin{pmatrix} \sin\frac{\theta_k}{2} e^{-i\phi_k} \\ -\cos\frac{\theta_k}{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\phi_k} \\ -1 \end{pmatrix}.
\end{aligned} \tag{8}
$$

For the spectrum, when we adjust the parameter δt, it begins to flow. We notice that when $\delta t = 0$, the energy gap closes. In other articles, if we use v, w instead of $t + \delta t, t - \delta t$, the critical point is $v/w = 1$. The physical meaning is clear: when we reduces δt from positive to negative, the dominant mechanism shifts from inner cell hopping to adjacent cell hopping, and the shift point is $\delta t = 0$.

3 Winding number

The flow of energy spectrum shows that system has a phase transition point. We define the phases of SSH model as:

$$
\begin{cases} \text{topological trivial phase} : \delta t > 0; \\ \text{topological nontrivial phase} : \delta t < 0. \end{cases} \tag{9}
$$

The word "topological" is related to the fact that there exists a bulk invariant in thet case $\delta t < 0$, and such invariant is topological invariant in k-space. First, let us calculate the Berry phase of the system, where the basic derivation can be found in Bernevig's book. In short, Berry phase characterizes the nontrivial topological effect of a quantum system. It is known that for the 2-band Hamiltonian, the Berry phase on the negative band is:

$$
\begin{aligned}
\gamma &= -\mathrm{Im} \int_{-\pi}^{\pi} dk \, \langle - | \nabla_k | - \rangle \\
&= -\mathrm{Im} \int_{-\pi}^{\pi} dk \frac{1}{2} e^{i\phi_k} \nabla_k (e^{-i\phi_k}) \\
&= \frac{1}{2} \int_{-\pi}^{\pi} dk \frac{(t+\delta t)(t-\delta t)\cos k + (t-\delta t)^2}{(t+\delta t)^2 + (t-\delta t)^2 + 2(t+\delta t)(t-\delta t)\cos k} \\
&= \frac{1}{2} \pi [\mathrm{sgn}(t+\delta t) - \mathrm{sgn}(\delta t)].
\end{aligned} \tag{10}
$$

This calculation is shown below, when we use the Hamiltonian to do the equivalent calculation. We find that the Berry phase depends on the sign of the parameter δt. If $\delta t > 0$, the Berry phase is zero, thus the phase is topological trivial——there is no topological excitation (or monopole) in the manifold of system in k-space. However if $\delta t < 0$, the Berry phase is π, and the phases is topological nontrivial——for the manifold of system in k-space has enclosed a monopole. The topological invariant is just $\nu = \frac{1}{\pi}\gamma$.

Here I have to clarify the term "monopole" and "manifold of system" I have used. The base space is the one-dimensional k-space or the first BZ, and the "manifold of system" is a circle (actually a two-dimensional family of circles but here we fix the parameter t, and due to the periodicity, in general it

should be a directed closed loop) as the deformation of the energy band given by the map:

$$f : [-\pi, \pi] \to \mathbb{R}^2, \begin{cases} h_x = (t + \delta t) + (t - \delta t)\cos k \\ h_y = (t - \delta t)\sin k \end{cases}, \tag{11}$$

which is a circle $(h_x - (t + \delta t))^2 + h_y^2 = (t - \delta t)^2$. "Monopole" refers to a topology charge creates Berry flux located in a system's degenerate point that often created by setting all the parameters to zero. Here it is located in the point $(h_x = 0, h_y = 0)$. When we adjust δt from positive value to negative value, the circle begins to flow along the negative direction of h_x axis towards the origin and becomes bigger. When the system reach the critical point, say $\delta t = 0$, the circle just touches the origin (monopole). Before that, according to Gauss' theorem, the net flux goes through the manifold is zero; after, the monopole is inside the circle, so the net flux goes through the manifold is nonzero, which, by integrating over the surface, gives us a nonzero Berry phase.

The topological invariant thus relates to the number of the monopole. However, we need to remind ourselves that the map f may contribute additional degrees. If f is a degenerate map, which in this case doubles the winding times of the circle——that is, in fact there are two circles enclose the monopole, then we need to double the number we previously get. In our case, the degree of f is just 1. So the true topological invariant is the winding number——the times of the circle winding the origin.

In the parameter space, we have several ways to adjust the ground state manifold adiabatically to enter the topological nontrivial phase. In this figure copied from arXiv:1509.02295, we can see that there are basically three ways: (a) shifting the center of the circle (reducing the intercell hopping amplitude), (b) enlarging the radius of the circle (enhancing the betweencell hopping amplitude), and (c) lifting the circle in z dimension (introducing a sublattice chemical potential to break the chiral symmetry temporarily).

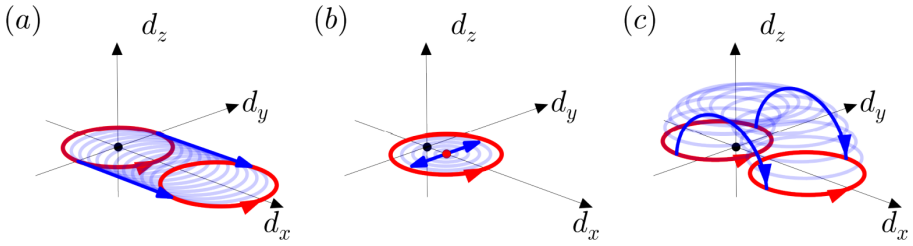

图 2: ways to moving ground state manifold

The winding number can also be calculated by Hamiltonian in a more complex-analytic way. Complexifying the Hamiltonian into $h = h_x - ih_y = (t + \delta t) + (t - \delta t)e^{-ik}$. Then it is obvious that the winding number

is the integrate invariant in the complex plane:

$$\begin{aligned}\nu &= \frac{1}{2\pi i}\int_{\mathrm{BZ}}\frac{dh}{h}\\ &= \frac{1}{2\pi i}\int_{-\pi}^{\pi}dk\frac{\partial}{\partial_k}\ln h\\ &= \frac{1}{2\pi i}\ln((t+\delta t)+(t-\delta t)e^{-ik})\Big|_{-\pi}^{\pi}\\ &= \frac{1}{2}[\mathrm{sgn}(t+\delta t)-\mathrm{sgn}(\delta t)].\quad (\text{when } \delta t<0,\ \text{we need to shift the brunch by } e^{\pm i\pi} \text{ respectively})\end{aligned} \tag{12}$$

The result is equivalent with the way by using eigenstate to calculate the Berry phase.

4 Numericial simulation

From above we calculate the bulk properties of SSH model by applying the periodic boundary condition to the Hamiltonian. If we use the open boundary condition, we should notice that there exist two disconnected isolate edge modes.

The Hamiltonian with open boundary condition is as follow:

$$\mathcal{H} = \sum_{i=1}^{N}(t+\delta t)c_{A,i}^{\dagger}c_{B,i} + \sum_{i=1}^{N-1}(t-\delta t)c_{A,i+1}^{\dagger}c_{B,i} + \mathrm{h.c.}, \tag{13}$$

here we notice that the discrete translation symmetry for the overall chain is broken. However we could first get to know the fully dimerized limits of it. If we fully close the betweencell hoppings by setting

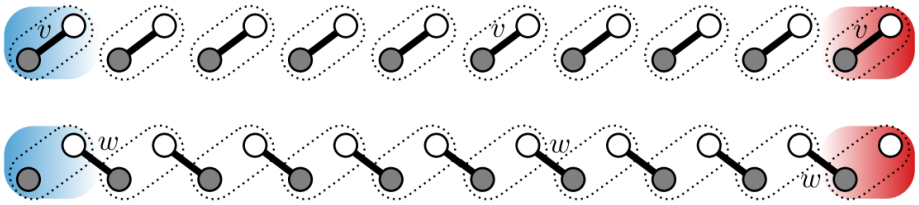

图 3: two fully dimerized limits

$t+\delta t = 1, t-\delta t = 0$, the model becomes trivial for now the Hamiltonian can be written like $\mathcal{H} = \sum_{i=1}^{N}|i,A\rangle\langle i,B| + |i,B\rangle\langle i,A|$, then the eigenstates are obvious:

$$\mathcal{H}(|i,A\rangle \pm |i,B\rangle) = \pm(|i,A\rangle \pm |i,B\rangle). \tag{14}$$

There is no special edge modes, and it is related to a topological trivial bulk.

If we fully close the innercell hoppings by setting $t+\delta t = 0, t-\delta t = 1$, the model is topologically nontrivial, for now the Hamiltonian can be written like $\mathcal{H} = \sum_{i=1}^{N-1}|i+1,A\rangle\langle i,B| + |i,B\rangle\langle i+1,A|$, and eigenstates are:

$$\mathcal{H}(|i,B\rangle \pm |i+1,A\rangle) = \pm(|i,B\rangle \pm |i+1,A\rangle). \tag{15}$$

However, there also exists a single zero energy mode in both edges:

$$\mathcal{H}|1,A\rangle = \mathcal{H}|N,B\rangle = 0. \tag{16}$$

And we know at this time the bulk is in the topological phase, has winding number 1.

We now do a numericial simulation to see the energy spectrum under open boundary condition. (Sorry for my poor coding ability, the code is self-learned online).

The code is as follows.

```
import numpy as np
import matplotlib.pyplot as plt
import cmath

v=1 #intercell hopping
w=0.2 #betweencell hopping
N=8 #number of unit cells

#build the OBC Hamiltonian
hamiltonian = np.zeros((2*N,2*N))
for i in range(0,2*N,2):
    hamiltonian[i,i+1] = v
    hamiltonian[i+1,i] = v
for i in range(1,2*N-1,2):
    hamiltonian[i,i+1] = w
    hamiltonian[i+1,i] = w

#solve the eigen-problem
eigenvalue, eigenvector = np.linalg.eig(hamiltonian)
eigenvalue.sort()

k = np.arange(0,2*N)

#draw the spectrum
plt.scatter(k, eigenvalue)
plt.xlabel("eigenstate", fontdict={'size': 16})
plt.ylabel("energy", fontdict={'size':16})
plt.title("PBC", fontdict={'size': 20})
plt.show()
```

Plot $t+\delta t = 0.2, t-\delta t = 1, N = 8$ case and $t+\delta t = 1, t-\delta t = 0.2, N = 8$ case, here we get an trivial insulator (latter) and a topological insulator (former), we find:

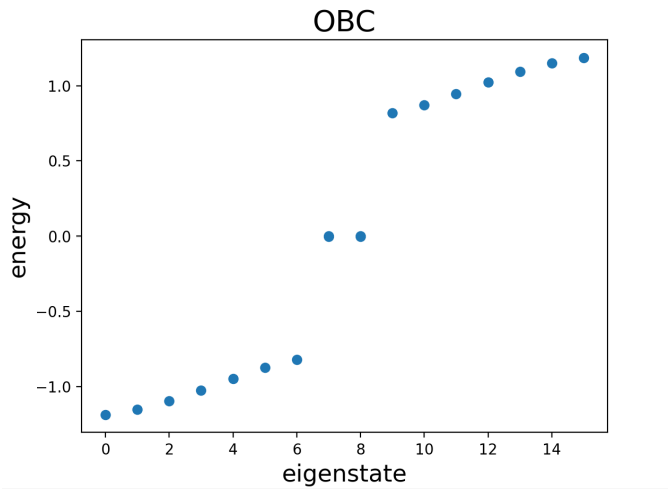

图 4: $t+\delta t=0.2, t-\delta t=1, N=8$

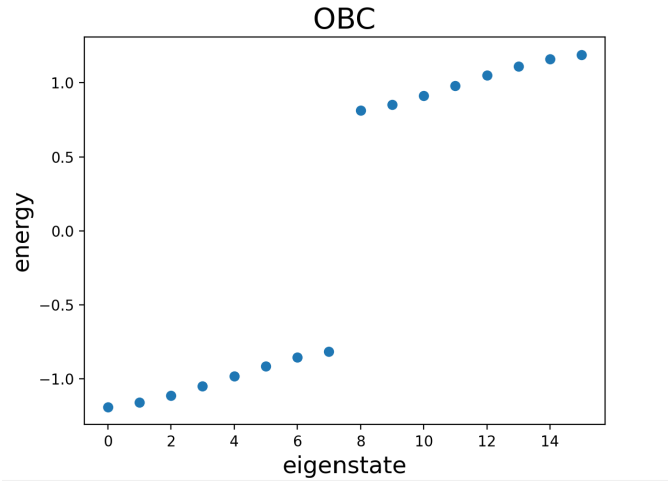

图 5: $t+\delta t=1, t-\delta t=0.2, N=8$

We can see there are two zero energy edge modes for $\delta t<0$ phase, however they vanish in $\delta t>0$ phase.

As a contrast, we can plot the spectrum for the periodic boundary condition. Here, we just need to add a hopping term between the first cell and the last cell. The added part is as follows:

```
……
hamiltonian[0,2*N-1] = w
hamiltonian[2*N-1,0] = w
……
```

Plot $t+\delta t=0.2, t-\delta t=1, N=8$ case and $t+\delta t=1, t-\delta t=0.2, N=8$ case, we find:

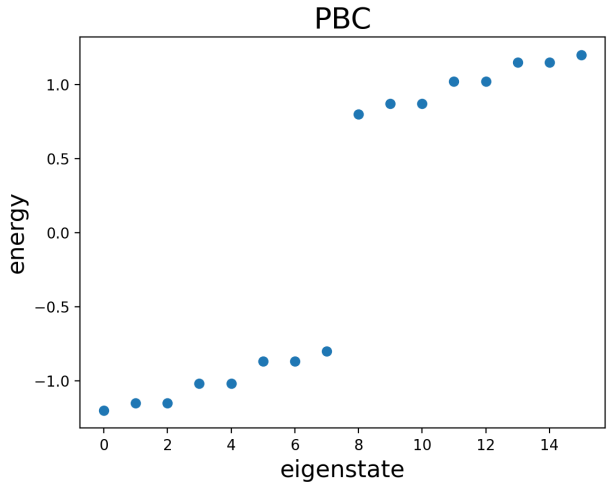

图 6: $t + \delta t = 0.2, t - \delta t = 1, N = 8$

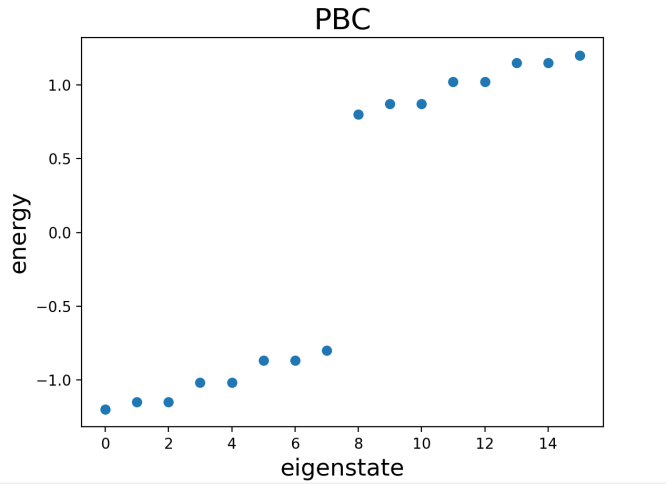

图 7: $t + \delta t = 1, t - \delta t = 0.2, N = 8$

There are no zero energy edge modes.

5 Questions

- 卷绕数的一般定义是什么？按照这里的几何图像，它描述沿着 BZ，基态流形在参数空间绕原点的次数。如果是高维的情况是否就变成了 “覆盖”，比如SU(2) 到SO(3)，有卷绕数 2？是否存在流形不连通的情况？那个时候该怎么定义卷绕数。

- arXiv:1509.02295 里作者说了 bulk-boundary correspondence，在这里确实体现为在 OBC 下 bulk 里非平庸的拓扑数导致有边界态存在。不过这里作者又说什么 domain wall，比如一条链的两侧的那一个原子或一对原子也算做边界态？这里我不是很清楚他在说什么。

- 开放边界条件和周期边界条件对系统本质的影响是什么？我理解的是后者只能够给出 bulk 内部的性质，而开边界可以给出边缘态的信息，不过这二者应该在热力学极限下没有区别？以及我之前见到的全是周期边界条件，这样才能够做傅里叶变换解能谱，开放边界条件一般怎么精确解？
- 那篇文章里，作者通过手征对称性就预知了系统可能存在非零卷绕数，一般手征对称性存在的类似系统，除了能谱对称，哈密顿矢量可以构成一个闭合回路，还有什么直接的信息？
- 导致系统进入拓扑相的本质是什么？
- 这个模型的简化版本之前上高量课听姜老师讲过，加上对 Berry phase 有些了解，看了下网上一些文章理论框架大致清楚了。不过计算机模拟部分花了半天时间，因为之前只上过一门计算机导论课，平时基本上没自己编过程序，寒假刚好安装了 Python 准备学学。这里现学了下怎么构造矩阵算特征值。。。计算部分平时需要学到什么程度？还是边做边学？

References

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