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SSH Model-2

聂嘉会

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1 Bulk boundary correspondence

Now, let's consider a little more complex lattice geometry based on SSH model, as shown below,

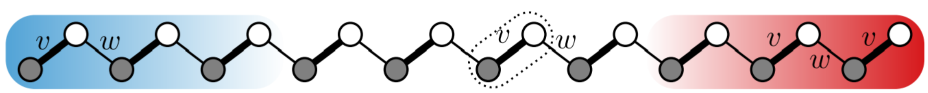


Fig. 1. SSH model-2

where the blue sector, white sector and red sector are three sectors with equal length of $\frac{L}{3}$ but different interaction parameters. If we write the formal SSH Hamiltonian as

$$\mathcal{H} = \sum_i v c_{A,i}^\dagger c_{B,i} + w c_{A,i+1}^\dagger c_{B,i} + \text{h.c.}, \tag{1}$$

then the parameters set in each sector are chosen as

$$\begin{cases} v = 1, w = 0, \text{ blue/head sector: trivial insulator} \\ v = \cos(\alpha i + \phi), w = \sin(\alpha i + \phi), \text{ white/middle sector: transition zone} \\ v = 0, w = 1, \text{ red/tail sector: topological insulator} \end{cases}. \tag{2}$$

Here, parameters α, ϕ are chosen such that the v, w are connected smoothly. We could first identify their general forms. Assuming there are N unit cells in total, and m cells in blue and red section respectively, so $N-2m$ cells are in the middle sector. We number the first cell as 0 for numerical convenience, then we should set the mth cell's parameters belong to the blue sector and the $(N-m-1)$th cell's parameters belong to the red sector. Thus we get

$$\cos(\alpha m + \phi) = 1, \ \cos(\alpha(N-m-1) + \phi) = 0 \tag{3}$$

and this gives us

$$\begin{cases} \alpha = \frac{\pi}{2(N-2m-1)} \\ \phi = -\frac{m\pi}{2(N-2m-1)} \end{cases}. \tag{4}$$

Note that if $N-2m-1=0$, which means there is only one unit cell in the transition zone, then we may set it as a gap-closing transition point for $v = w = \frac{1}{2}$. The Hamiltonian is built by three blocks, each one characterizes the dynamic on each of the three sectors.

This lattice geometry implies that we connect a topological insulator with a trivial insulator with a smooth transition zone, and inside this zone there must be a gap-closing point, which is exactly the edge state. Numerical simulation shows that this edge state is robust, since it only corresponds with the right topological insulator's nontrivial bulk with a nonzero topological invariant inside it.

The code is as follow.

```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import math
import cmath
import seaborn

N=27 #number of unit cells
m=9 #length of head or tail

cm = plt.cm.get_cmap('Oranges') #get colorbar

#build the OBC Hamiltonian
hamiltonian = np.zeros((2*N,2*N))

for i in range(0,2*m,2):
    hamiltonian[i,i+1] = 1
    hamiltonian[i+1,i] = 1
for i in range(1,2*m,2):
    hamiltonian[i,i+1] = 0
    hamiltonian[i+1,i] = 0
for i in range(2*m,2*(N-m)+1,2):
    if N-2*m-1 == 0:
        hamiltonian[i,i+1] = 1/2
        hamiltonian[i+1,i] = 1/2
    else:
        hamiltonian[i,i+1] = math.cos(((math.pi)/(2*(N-2*m-1)))*(i/2)-(m*math.pi)/(2*(N-2*m-1)))
        hamiltonian[i+1,i] = math.cos(((math.pi)/(2*(N-2*m-1)))*(i/2)-(m*math.pi)/(2*(N-2*m-1)))
for i in range(2*m+1,2*(N-m)+1,2):
    if N-2*m-1 == 0:
        hamiltonian[i,i+1] = 1/2
        hamiltonian[i+1,i] = 1/2
    else:
        hamiltonian[i,i+1] = math.sin(((math.pi)/(2*(N-2*m-1)))*((i-1)/2)-(m*math.pi)/(2*(N-2*m-1)))
        hamiltonian[i+1,i] = math.sin(((math.pi)/(2*(N-2*m-1)))*((i-1)/2)-(m*math.pi)/(2*(N-2*m-1)))
for i in range(2*(N-m),2*N,2):
    hamiltonian[i,i+1] = 0
```

```python
    hamiltonian[i+1,i] = 0
for i in range(2*(N-m)+1,2*N-1,2):
    hamiltonian[i,i+1] = 1
    hamiltonian[i+1,i] = 1

#solve the eigen-problem
eigenvalue, eigenvector = np.linalg.eig(hamiltonian)
#divide the eigenvalues from three sectors
eigen1 = eigenvalue[:2*m]
eigen2 = eigenvalue[2*m:2*(N-m)]
eigen3 = eigenvalue[2*(N-m):2*N]
eigen1.sort()
eigen2.sort()
eigen3.sort()

#number the eigenvalues
k1 = np.arange(0,2*m)
k2 = np.arange(2*m,2*(N-m))
k3 = np.arange(2*(N-m),2*N)
k = np.arange(0,2*N)
z = eigen2

#plot the spectrum
plt.scatter(k1,eigen1,c="b",marker = "o",s=30,alpha=1,norm=1)
plt.scatter(k2,eigen2,c=z, marker = "o",s=30,alpha=1)
plt.scatter(k3,eigen3,c="r",marker = "o",s=30,alpha=1,norm=1)
plt.colorbar()
plt.xlabel("eigenstate", fontdict={'size': 16})
plt.ylabel("energy", fontdict={'size':16})
plt.title("OBC-"+str(N)+"cells-"+str(m)+"flat", fontdict={'size': 20})
plt.savefig('OBC-'+str(N)+"-"+str(m)+'.jpg', dpi=300)
plt.show()
```

Let us first simulate the case of $m = \frac{N}{3}$. The spectrum in real space is shown in Fig. 2.

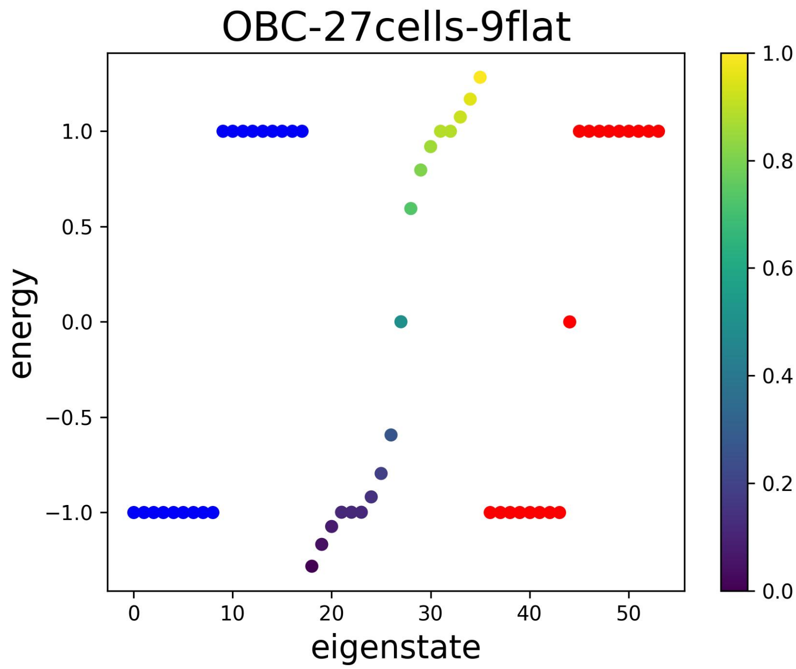
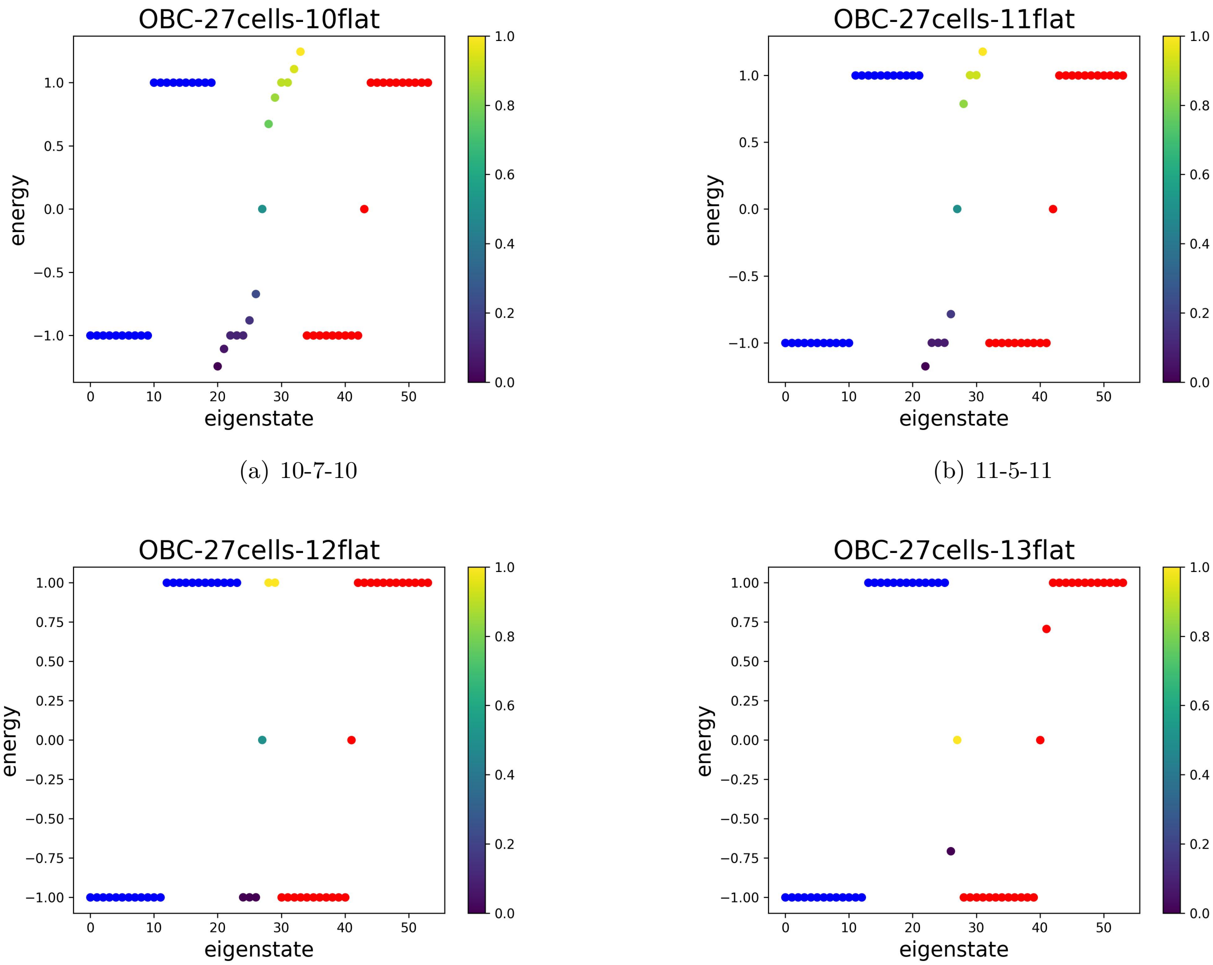


Fig. 2. The spectrum of 27 cells chain of 9-9-9 lattice geometry. The blue band denotes the trivial insulator sector, the red band denotes the topological insulator sector, and the gradient color band denotes the middle transition sector.

From the spectrum above, we can find that there are two edge states. One is in the middle transition sector, and one is in the topological sector. This is what we have expected: in the smooth transition from left trivial bulk to right topological bulk, there must exists an edge state; the other is located at the right end of the chain.

Now, we may shrink the size of the middle region as a continue process, and see how the spectrum flow. The following simulations are as follows.



(a) 10-7-10

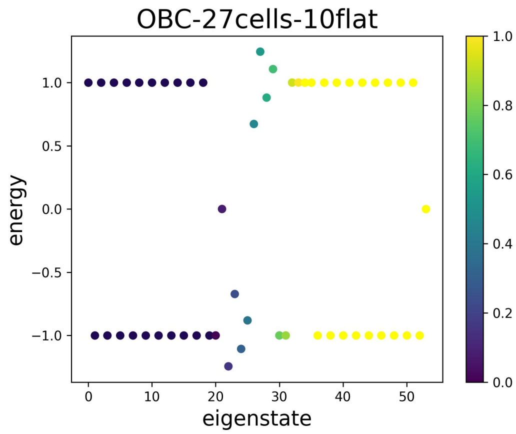
(b) 11-5-11

(c) 12-3-12

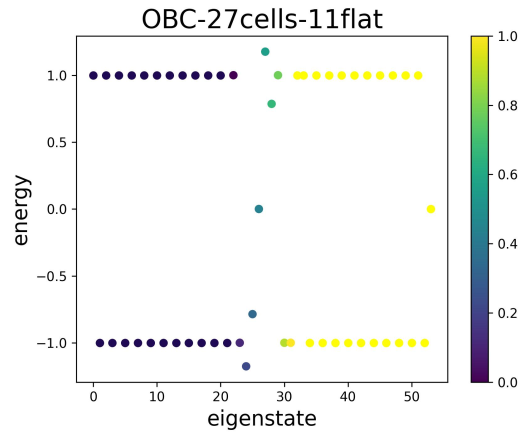
(d) 13-1-13

Fig. 3. The evolution of spectrum sorted by energy

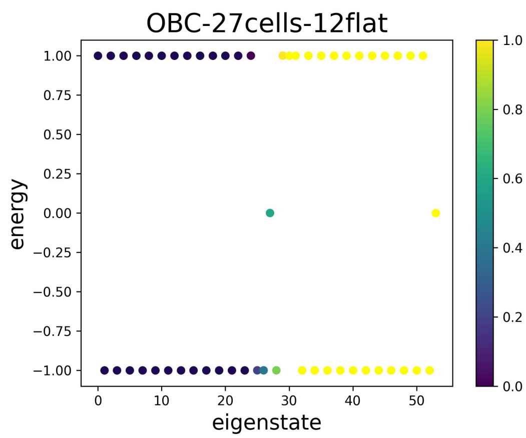
It may be more helpful and clearer if we plot the eigenstates of each sector by their locations instead of their eigenvalues, then we get



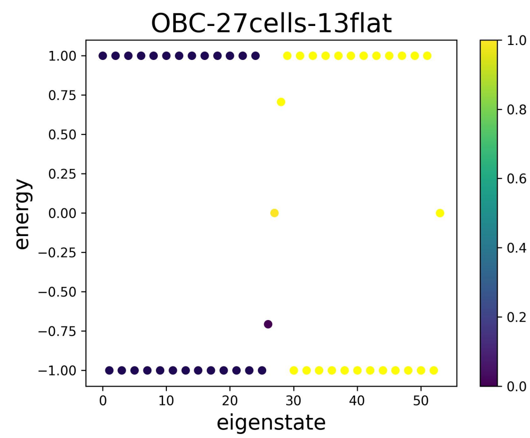
(a) 10-7-10



(b) 11-5-11



(c) 12-3-12



(d) 13-1-13

Fig. 4. The evolution of spectrum sorted by locations

We find that while we are shrinking the middle transition sector, its contribution to the spectrum has a steady point, which is exactly the edge state. Such edge state is robust under the shrink operation. Thus we can see it is due to the fact that the change of the topology in this model from right to left requires a band gap-closing existing.

Finally, if we go to the limit of vanishing the middle region, we rediscover a combination of Fig. 4 and Fig. 5 in Notes-1:

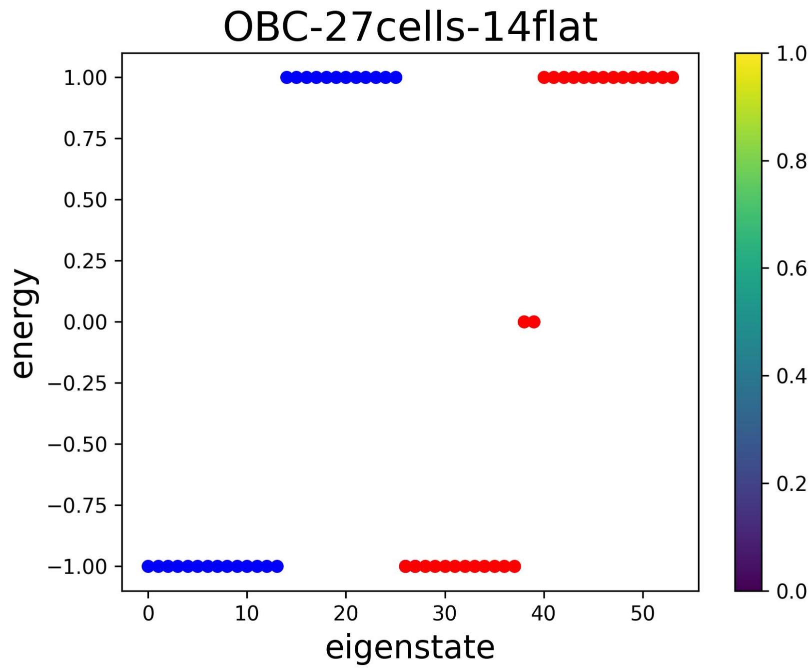


Fig. 5. 13-0-14

2 Chiral symmetry

The more fundamental reason why such edge state is topologically robust with the strong correspondence of bulk and edge is the symmetry class that a certain model is in. In SSH model, it is the chiral symmetry that protects the edge state. In Notes-1 we have found the chiral transformation operator $\Gamma = P_A - P_B$, and under such transformation the Hamiltonian changes as follow:

$$\Gamma\mathcal{H}\Gamma = -\mathcal{H}. \tag{5}$$

Physically, the existence of chiral symmetry is due to the fact that there is no onsite dynamic. In the chiral basis, the chiral operator is diagonalized and is represented as σ_z. Then the chiral symmetry $\sigma_z\mathcal{H}\sigma_z = -\mathcal{H}$ implies that the 2-band Hamiltonian contains only σ_x term and σ_y term due to the antisymmetry of Pauli operators. This constrains the normalized Hamiltonian vector on the equator of the Bloch sphere, so that the closed curve mapped from periodic BZ cannot deform continually (homotopically) on the sphere. Thus, the only two shape classes are the loop fully around the equator (enclose the origin) or bending along a half equator (disclose the origin). The former is topological while the latter is trivial. The loop in one class cannot deform continually to the other unless the band gap is closed so that the normalized Hamiltonian vector goes to a singularity. Because of this, in our model there must be an edge state protect by the chiral symmetry.

We can try to add onsite dynamics to our Hamiltonian numerically, and see what will happen. We just need to add block-diagonal matrices of $t\sigma_z$ for each cell. The modified part of the code is as follow.

```
… …
t = 1 #add external potential to break chiral symmetry
… …
for i in range(2*m,2*(N-m),2):
    hamiltonian[i,i] = t
for i in range(2*m+1,2*(N-m),2):
    hamiltonian[i,i] = -t
… …
```

Do the same simulation for $N = 27, m = 9$,

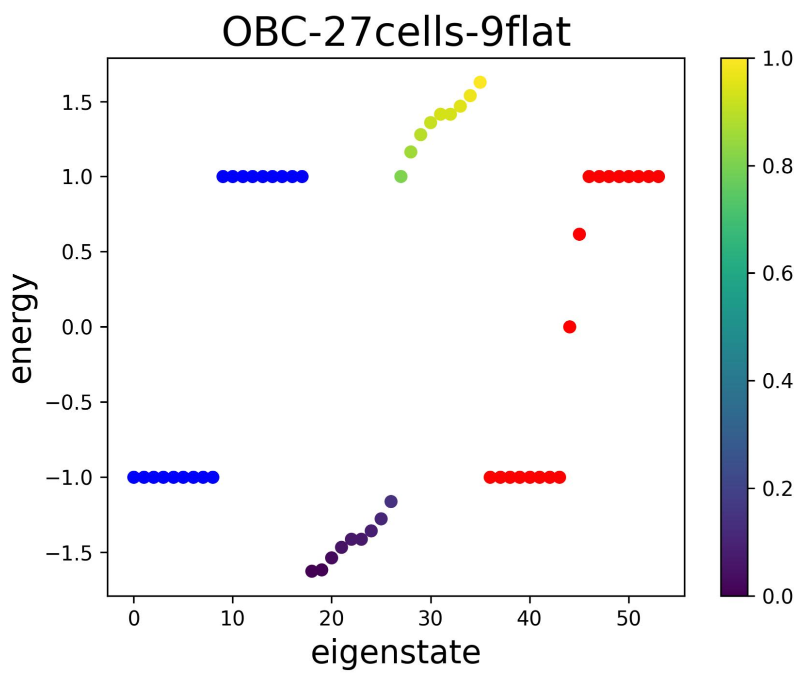


Fig. 6. 9-9-9 lattice geometry with chiral symmetry broken in middle region

We find that the edge state in middle region has vanished, and while the middle region shrinking, two kinds of insulators connect smoothly for now the Hamiltonian vector can move along the upper or lower part of the Bloch sphere to deform from trivial loop to topological loop.

In general, winding number is well-defined in topological quantum material in the presence of chiral symmetry in odd dimension. Bloch Hamiltonians belong to this class have the form of

$$\mathcal{H}(\mathbf{k}, \mathbf{r}) = \begin{pmatrix} 0 & D(\mathbf{k}, \mathbf{r}) \\ D^{\dagger}(\mathbf{k}, \mathbf{r}) & 0 \end{pmatrix}, \tag{6}$$

if we eliminate the occupied Fermi sea by redefining Hamiltonian matrix to Q matrix, then the off-diagonal part q induces a map from the base manifold $\mathrm{BZ}^d \times \mathcal{M}^D$ to $\mathrm{U}(N)$, where we can get the fundamental group $\pi_{d+D}(\mathrm{U}(N))$ which is nontrivial when $d + D$ is odd. And such maps are characterized by the winding number:

$$\nu_{2n+1}[q] = \int_{\mathrm{BZ}^d\times\mathcal{M}^D} \frac{(-1)^n n!}{(2n+1)!}\left(\frac{i}{2\pi}\right)^{n+1} \mathrm{Tr}\left[(q^{-1}dq)^{2n+1}\right]. \tag{7}$$

Physically, such winding number is related to the crystal polarization inside the material. By fixing one band, we can show that it is the average of position operator.

References

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[4] Notes: physics and manipulation of 2 by 2 Hermitian matrices. Biao Huang

[5] Classification of topological quantum matter with symmetries. Ching-Kai Chiu, Jeffrey C.Y. Teo, Andreas P. Schnyder, and Shinsei Ryu. Rev. Mod. Phys. 88, 035005