KIAS-SNU 2019 Winter School Problem Set

Topology of One-dimensional Insulator

We want to study the topology in one-dimensional insulators, namely Su-Schrieffer-Heeger chain. The system contains two atomic sites, A and B. See the Fig. 1 below.

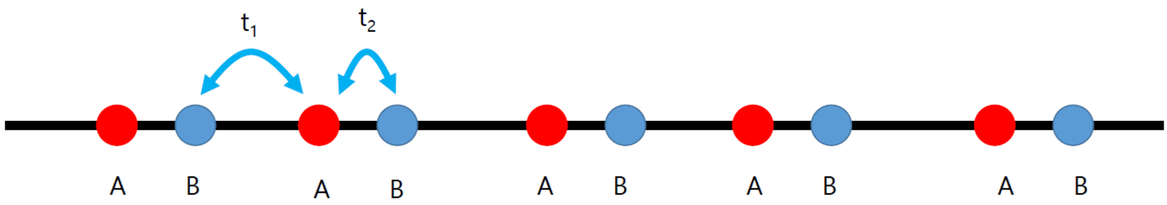

Figure 1 Su-Schrieffer-Heeger chain.

The simplest Hamiltonian of the system describes the hopping of the electrons around the sites.

$$\mathrm{H}_0 = \sum_x -t_1|x,B\rangle\langle x+1,A| - t_2|x,A\rangle\langle x,B| + H.C.$$

Here, t_1 may be different from t_2. The system is in the periodic boundary condition and the length L$\in \mathrm{Z}^+$: $|1,\mathrm{A/B}\rangle = |\mathrm{L}+1,\mathrm{A/B}\rangle$.

1. Energy and ground state:

a) Find the single-electron energy spectrum by performing the Fourier transformation on the site x.

b) When the Fermi level is at zero, i.e., $\mathrm{E_f} = 0$, show that the system is an insulator as far as $\mathrm{t}_1 \neq t_2$.

2. Topology of insulating ground state:

In this problem, we will see that the two insulators, one with $\mathrm{t}_1 > t_2$ and the other with $\mathrm{t}_2 > t_1$, are topologically different.

a) For $\mathrm{t}_1 > t_2$, find the energy eigenstate $|\mathrm{k}\rangle$ of the single-particle spectrum with the momentum k, which is filled at the zero temperature.

b) For $t_2 > t_1$, find the energy eigenstate $|k\rangle$ of the single-particle spectrum with the momentum k, which is filled at the zero temperature.

c) Calculate the Berry's connection:

$$A(k) = \ -i\ \langle k|\partial_k|k\rangle$$

for the above two cases.

d) Calculate the "winding number" of the Berry's connection:

$$P = \frac{1}{2\pi}\oint A(k)dk$$

for the two cases. Show that the quantity P changes only at $t_1 = t_2$ where the system becomes a metal.

3. Physical Meaning of P:

The physical meaning of P above is in fact the uniform polarization density of the one-dimensional insulator. **In this problem, we want to test this numerically, so use mathematica or matlab.**

Remember that the uniform polarization P manifests itself when the system is truncated to the open boundary condition.

$$Q_{boundary} = P \cdot \hat{n}$$

where $\hat{n}$ is the unit vector normal to the boundary. In this model, $\hat{n}$ is $\pm\hat{x}$ and the polarization is along x-direction, so the boundary charge $Q_{boundary} = \pm\frac{1}{2}$.

We will explicitly calculate the boundary charge for the chain with the finite length =4 and open boundary condition. See Fig 2. The model is described by $H = H_0 + V$.

$$H_0 = \sum_{x=1,2,3,4} (-t_1|x,B\rangle\langle x+1,A| - t_2|x,A\rangle\langle x,B| + H.C.)$$

Here there are no sites of label x=5, or x=0, and so we drop out the terms involving those sites.

We also include infinitesimal term:

$$V = \sum_{x=1,2,3,4} -\mu[|x,B\rangle\langle x,B| - |x,A\rangle\langle x,A|]$$

Here we take $\mu = 10^{-2}$, which is significantly smaller than $|t_1|, |t_2|$.

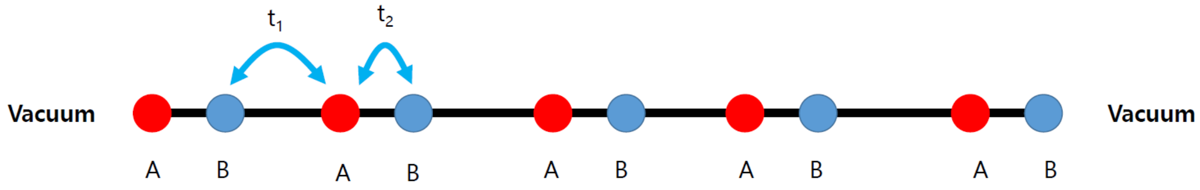

Figure 2. Su-Schrieffer-Heeger chain with the open boundary condition.

a) Write down the matrix form of the Hamiltonian explicitly. Numerically diagonalize the spectrum and find the eigenstate. (You don't need to show the states explicitly.)

b) Compute the charge localized at the boundary. This is done by computing

$$Q_{\text{numerical}} = \sum_{x=1,2} \sum_{E<0} |\Psi_E(x,A)|^2 + |\Psi_E(x,B)|^2 \quad \text{mod } 1$$

Calculate $Q_{\text{numerical}}$ for $t_1 \neq t_2$ and show that it agrees with **d) in problem 2**.