Prof. Yang Qi on topological classification of gapped free fermion models

Jinyuan Wu

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Gapped systems satisfy the adiabatic theorem, so with small perturbation on the Hamiltonian, we can transform the nth eigenstate of one Hamiltonian into the nth eigenstate of another Hamiltonian, and then go back, so in this sense, these states are *equivalent*. This gives a natural criterion of Hamiltonian classification, each equivalence class of which can be said as a homotopy equivalence class, and in this sense, we achieve a *topological classification* of the Hamiltonians.

For free fermions, perturbation of the Hamiltonian is just perturbation of the band structure, so topological classification of Hamiltonians reduces to topological classification of band structures: two band structures that can be connected by a smooth deformation which doesn't cross the Fermi surface (or otherwise when a band crosses the Fermi surface, the system becomes a metal and is gapless).

In the following lectures we discuss topological classification of gapped free fermions. These systems include insulators and the electron-like excitations in superconductors (as well as other systems with certain kind of electron condensation).

It's possible that a topological equivalence class involves several separate subclasses, each of which has a different symmetry group, and a smooth transformation from one class into another inevitably breaks or adds some symmetry. In this case, the subclasses are said to be *symmetry protected* – as long as the symmetry is present, we are sure that perturbation on the Hamiltonian won't get the system out of its subclass.

1 Antiunitary symmetry of free fermions

Consider the following second quantized Hamiltonian:

$$\hat{H} = \sum_{\alpha,\beta} c_\alpha^\dagger H_{\alpha\beta} c_\beta, \tag{1}$$

where operators with ˆ are second quantized operators. In this section, we consider how antiunitary symmetries acts on (1). The action of a unitary group element can be written as

$$g \cdot |\alpha\rangle = |\beta\rangle \, \varphi(g)_{\beta\alpha}, \quad g \cdot \langle\alpha| = \varphi(g)^\dagger_{\alpha\beta} \, \langle\beta| \, , \tag{2}$$

and

$$g \cdot c_\alpha^\dagger = g c_\alpha^\dagger g^{-1} = c_\beta^\dagger \varphi(g)_{\beta\alpha}, \quad g \cdot c_\alpha = g c_\alpha g^{-1} = \varphi(g)^\dagger_{\alpha\beta} c_\beta. \tag{3}$$

So the Hamiltonian transforms as

$$g \cdot \hat{H} = c_{\alpha'}^\dagger \varphi(g)_{\alpha'\alpha} H_{\alpha\beta} \varphi(g)^\dagger_{\beta\beta'} c_{\beta'}. \tag{4}$$

Of course, this is just in the form of basis transition. If the Hamiltonian has the symmetry of g, we have

$$H_{\alpha'\beta'} = \varphi(g)_{\alpha'\alpha} H_{\alpha\beta} \varphi(g)^\dagger_{\beta\beta'}. \tag{5}$$

Suppose $\{|\alpha\rangle\}$ is real with regard of the time reversal operation $\mathcal{T} = T\mathcal{K}$. In this case, the time reversal symmetry doesn't act on the basis, but $\mathcal{K}$ acts on $H_{\alpha\beta}$ and adds a star, so if the system has time reversal symmetry, we have

$$THT^{-1} = H^*. \tag{6}$$

Note that here H is the *first quantized* Hamiltonian, i.e. the coefficient matrix in (1). The operation T is also the *unitary* transformation associated to $\mathcal{K}$, instead of the full *second quantized*

$\mathcal{T}$. We work with first quantization because it's easier: we don't need to actually work with complex conjugate of creation and annihilation operators.

Now we move to the "real" particle-hole symmetry in an insulator. Consider

$$\hat{H} = -\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} (t_{\boldsymbol{ij}} c_{\boldsymbol{i}}^\dagger c_{\boldsymbol{j}} + \text{h.c.}). \tag{7}$$

We use $\mathcal{C}$ to denote the particle-hole transformation from c to $c^\dagger$, i.e.

$$\mathcal{C} c_{\boldsymbol{i}} \mathcal{C}^{-1} = c_{\boldsymbol{i}}^\dagger, \quad \mathcal{C} c_{\boldsymbol{i}}^\dagger \mathcal{C}^{-1} = c_{\boldsymbol{i}}, \tag{8}$$

then we have

$$\mathcal{C}\hat{H}\mathcal{C}^{-1} = -\sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} (t_{\boldsymbol{ij}} c_{\boldsymbol{i}} c_{\boldsymbol{j}}^\dagger + \text{h.c.}) = \sum_{\langle \boldsymbol{i},\boldsymbol{j}\rangle} (t_{\boldsymbol{ji}}^* c_{\boldsymbol{j}}^\dagger c_{\boldsymbol{i}} + \text{h.c.}) = -\hat{H}^* = -\hat{H}^\top. \tag{9}$$

We know the spectrum of the tight-binding model is a cosine curve, so the minus sign comes as is expected, meaning flipping the spectrum with the Fermi surface as a mirror, while the transpose operation comes from flipping $|\boldsymbol{i}\rangle$ to $\langle \boldsymbol{i}|$. Here we need to keep in mind a strange property of particle-hole transformation. $\mathcal{C}$ should be *unitary* in the second quantization formalism, because we want

$$c_{\boldsymbol{k}}^\dagger \xrightarrow{\mathcal{C}} c_{-\boldsymbol{k}} \tag{10}$$

to keep momentum conservation, and if $\mathcal{C}$ is unitary, it doesn't act on a complex factor, so we have

$$\mathcal{C} \cdot c_{\boldsymbol{k}}^\dagger = \mathcal{C} \cdot \frac{1}{\sqrt{N}} \sum_{\boldsymbol{i}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_{\boldsymbol{i}}} c_{\boldsymbol{i}}^\dagger = \sum_{\boldsymbol{i}} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_{\boldsymbol{i}}} c_{\boldsymbol{i}} = c_{-\boldsymbol{k}},$$

which is exactly what we want. However, the first quantization version of $\mathcal{C}$ maps a single-electron wave function in the single electron Hilbert space to the *dual* space, and a map $\mathcal{H} \to \mathcal{H}^*$ should be *antiunitary* to keep naturalness.

The action of $\mathcal{C}$ on an arbitrary basis is

$$\mathcal{C} c_\alpha \mathcal{C}^{-1} = c_\beta^\dagger C_{\beta\alpha}, \quad \mathcal{C} c_\alpha^\dagger \mathcal{C}^{-1} = C_{\alpha\beta}^{-1} c_\beta, \tag{11}$$

and the second quantized Hamiltonian under (11) transforms as

$$\begin{aligned} \mathcal{C}\hat{H}\mathcal{C}^{-1} &= \mathcal{C} c_\alpha^\dagger \mathcal{C}^{-1} H_{\alpha\beta} \mathcal{C} c_\beta \mathcal{C}^{-1} = C_{\alpha\alpha'}^{-1} c_{\alpha'} \underbrace{H_{\alpha\beta}}_{H_{\beta\alpha}^*} c_{\beta'}^\dagger C_{\beta'\beta} \\ &= -c_{\beta'}^\dagger C_{\beta'\beta} H_{\beta\alpha}^* C_{\alpha\alpha'}^{-1} c_{\alpha'} = -c_{\beta'}^\dagger (C H^* C^{-1})_{\beta'\alpha'} c_{\alpha'}. \end{aligned} \tag{12}$$

So the particle-hole symmetry condition for the first quantized Hamiltonian is

$$H = -C H^* C^{-1}. \tag{13}$$

Despite their weirdness, $\mathcal{T}$ and $\mathcal{C}$ can be fully demonstrated by constraints on the coefficient matrix H (i.e. first quantized Hamiltonian) in (1). Classification of free fermion systems is therefore classification of these matrices.

$\mathcal{T}$ and $\mathcal{C}$ have non-trivial multiplication relation: since $\mathcal{T}$ is antiunitary in both first and second quantization formulation, and $\mathcal{C}$ is unitary in second quantization but antiunitary in first quantization,

$$\mathcal{S} = \mathcal{T}\mathcal{C} \tag{14}$$

is unitary in first quantization but antiunitary in second quantization. We call it **chiral symmetry** to keep consistent with the definition in particle physics. The condition that a second quantized Hamiltonian has chiral symmetry can be verified similar to (6) and (13), and we have

$$S H S^{-1} = -H. \tag{15}$$

In the momentum representation, $\mathcal{C}$ is bond to change the momentum in the $\boldsymbol{k} \to -\boldsymbol{k}$ way, because of momentum conservation. The rest of labels (band index, spin, etc.) are mixed together with a finite dimensional matrix. So suppose $H(\boldsymbol{k})$ is the block in H with momentum $\boldsymbol{k}$, and we have

$$TH(\boldsymbol{k})T^{-1} = H(-\boldsymbol{k})^*. \tag{16}$$

where C is the block in the C matrix in (6) that mixes labels other than $\boldsymbol{k}$. Similarly from (13), we have

$$CH(-\boldsymbol{k})^* C^{-1} = -H(\boldsymbol{k}). \tag{17}$$

The chiral symmetry doesn't change the momentum, since it's the multiplication of $\mathcal{T}$ and $\mathcal{C}$, so from (15) we have

$$SH(\boldsymbol{k})S^{-1} = -H(\boldsymbol{k}). \tag{18}$$

Now in a model with multiple bands, it's possible that there are several different particle-hole symmetry: it may be possible that band A's particles are equivalent to *both* band B and band C's holes. But in this case, band B and band C must coincide and there is a symmetry switching B and C, so in the end we only need to define one particle-hole symmetry as the generator: the rest of the particle-hole symmetries can be automatically generated using composition.

2 Particle-hole symmetry in superconductors

The following BCS model of superconductivity:

$$\hat{H} = \sum_{\boldsymbol{k},\alpha} \xi_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\alpha} c_{\boldsymbol{k}\alpha} - V \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\alpha,\beta} c^\dagger_{\boldsymbol{k}'-\boldsymbol{q},\alpha} c^\dagger_{\boldsymbol{k}+\boldsymbol{q},\beta} c_{\boldsymbol{k}\beta} c_{\boldsymbol{k}'\alpha}, \tag{19}$$

can be turned into

$$\hat{H} = \sum_{\boldsymbol{k},\alpha} \xi_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\alpha} c_{\boldsymbol{k}\alpha} + \sum_{\boldsymbol{k}} (\Delta c^\dagger_{-\boldsymbol{k}\downarrow} c^\dagger_{\boldsymbol{k}\uparrow} + \Delta^* c_{\boldsymbol{k}\uparrow} c_{-\boldsymbol{k}\downarrow}), \tag{20}$$

where Δ is the BCS order parameter. (20) is called the **BdG Hamiltonian**, which describes the spectrum of (electron-like) quasiparticles in a BCS superconductor. Note that the order parameter in (20) has quantum fluctuation, but what we are discussing here is the *topological band behavior* of fermions, so ignoring the fluctuation of Δ makes sense. It's possible that the fluctuation of Δ destroys the ordinary BCS order, but it's not the case in 3D. Note also that our current approach – ignoring the fluctuation of Δ, i.e. ignoring the many-body effect introduced by electron interaction – is a non-interaction limit of the general theory of topological classification with interaction.

In 1D and 2D, Mermin–Wagner theorem means the effective theory about fermionic quasi-particles of (19) is not (20), because $U(1)$ symmetry – a continuous symmetry – can't be broken here. But we can always use a 3D bulk state to "induce" a low-dimensional superconducting phase, which has electron pairing anyway and can be described by (20), though this time (20) has nothing to do with BCS mechanism. So henceforth we will work with a free-fermionic model like (20) and ignore what induces superconductivity pairing.

In such a Hamiltonian, the existence of a pairing channel means we have terms like $c_\alpha c_\beta$, and therefore the Hamiltonian can't be recast into (1) from which we can extract the first quantized Hamiltonian H. The solution is a classical procedure in BCS theory: (20) can be rephrased into

$$\hat{H} = \sum_{\boldsymbol{k}} \Psi^\dagger_{\boldsymbol{k}} \begin{pmatrix} \xi_{\boldsymbol{k}} & -\Delta \\ -\Delta^* & -\xi_{\boldsymbol{k}} \end{pmatrix} \Psi_{\boldsymbol{k}}, \quad \Psi_{\boldsymbol{k}} = \begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k},\downarrow} \end{pmatrix}. \tag{21}$$

Often, we call this form of Hamiltonian as the **BdG Hamiltonian** rather than (20).

BdG Hamiltonians often have *redundant* particle-hole symmetry. The point here is that suppose there are d kind of fermions (i.e. possible values of labels other than the momentum), then the existence of $c_\alpha c_\beta$ terms means $\Psi_{\boldsymbol{k}}$ should be $2d$ dimensional to include all possible terms. So the resulting H matrix is $2d \times 2d$ dimensional, the same as the first quantized Hamiltonian of $2d$ kind of fermions, but it describes d kind of fermions anyway. Since d kinds of fermions are actually just holes for the rest d kinds of fermions, there is possibly a particle-hole symmetry to make sure the spectrum of the first quantized Hamiltonian reflects this fact. Consider, for example, the following simplest case:

$$\hat{H} = \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} c_{\boldsymbol{k}}^\dagger c = \frac{1}{2} \sum_{\boldsymbol{k}} \begin{pmatrix} c_{\boldsymbol{k}}^\dagger & c_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} \xi_{\boldsymbol{k}} & \\ & -\xi_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k}} \\ c_{\boldsymbol{k}}^\dagger \end{pmatrix} + \text{const}, \tag{22}$$

the first quantized Hamiltonian of which obviously has a particle-hole symmetry, which is based on the simple fact that (here the complex conjugate operation only applies to the elements of a matrix)

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k}} \\ c_{\boldsymbol{k}}^\dagger \end{pmatrix}^\dagger = \begin{pmatrix} c_{\boldsymbol{k}} \\ c_{\boldsymbol{k}}^\dagger \end{pmatrix}.$$

The BCS BdG Hamiltonian (20) also has a particle-hole symmetry. Because $\xi_{\boldsymbol{k}} = \xi_{-\boldsymbol{k}}$, we have

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \xi_{\boldsymbol{k}} & -\Delta \\ -\Delta^* & -\xi_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = - \begin{pmatrix} \xi_{-\boldsymbol{k}} & -\Delta \\ -\Delta^* & -\xi_{-\boldsymbol{k}} \end{pmatrix}^*. \tag{23}$$

In the BCS case there are two kind of fermions and Ψ is 2-dimensional, so the particle-hole symmetry is not a byproduct of double counting of degrees of freedom. Sometimes the particle-hole symmetry comes from existing symmetries of the Hamiltonian. In the BCS case, it's easy to find that it's just the spin flipping symmetry.

The particle-hole symmetry is not always here. For example, the following superconductor Hamiltonian with the spin rotational symmetry on the z direction:

$$\hat{H} = \sum_{\boldsymbol{k}} \begin{pmatrix} c_{\boldsymbol{k}\uparrow}^\dagger & c_{\boldsymbol{k}\downarrow} \end{pmatrix} \begin{pmatrix} \epsilon_{\boldsymbol{k}\uparrow} & \Delta \\ \Delta & -\epsilon_{-\boldsymbol{k}\downarrow} \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c_{\boldsymbol{k}\downarrow}^\dagger \end{pmatrix}. \tag{24}$$

Its first quantized Hamiltonian don't have any $\mathcal{T}, \mathcal{C}$ or $\mathcal{S}$ symmetry and therefore can't be distinguished from, say, the first quantized Hamiltonian of IQHE.

A superconductor has *more* symmetry than a similar insulator because its first quantized Hamiltonian has a particle-hole symmetry, while it has *fewer* actual symmetry than a similar insulator because it breaks the $U(1)$ symmetry.

3 The ten-fold way

So there are several possibility of these three weird symmetries. $\mathcal{T}$ and $\mathcal{C}$ symmetries may simply not exist, which we denote as $T = 0$ or $C = 0$. When $\mathcal{T}$ is present, for fermions we have $\mathcal{T}^2 = -1$ (fermion parity) and for bosons $\mathcal{T}^2 = 1$. It's also possible to redefine $\mathcal{T}$ in a fermionic system so that $\mathcal{T}'^2 = 1$ (see discussion around (**??**) in the last lecture). We denote the $\mathcal{T}^2 = 1$ case as $T = 1$, and the $\mathcal{T}^2 = -1$ case $T = -1$. For both fermionic and bosonic systems it can be verified that $\mathcal{C}^2 = 1$ (for multiple band systems, it may be the case that several bands A, B, C, etc. overlap and $\mathcal{C}$ turn A into B, B into C, etc., and in this case $\mathcal{C}^2 = 1$ still works for the specific definition of $\mathcal{C}$ which only exchange ban labels in pairs), but for certain types of $SU(2)$ superconductors, it's useful to define $\mathcal{C}$ such that $\mathcal{C}^2 = -1$. So for $\mathcal{C}$ we also have $C = 0, \pm 1$. If both $\mathcal{C}$ and $\mathcal{T}$ are present, $\mathcal{S}$ is bond to be a symmetry, while if only one of them is present, $\mathcal{S}$ can't be a symmetry. This leaves us a final choice for systems where $T = 0, C = 0$ and $\mathcal{S}$ may be present or absent. So in the end, the symmetry of a free fermionic or bosonic system concerning $\mathcal{C}$, $\mathcal{T}$ and $\mathcal{S}$ has $3 \times 3 - 1 + 2 = 10$ possibilities, called **the ten-fold way**. Here we list the notation for these symmetry classes and some examples [1].

- Class A: $T = 0,\ C = 0,\ S = 0$. Without the particle-hole symmetry, typically this is an insulator, and therefore charge conservation holds. Example: Chern-insulators, IQHE. But a superconductor like (24) can also be a realization of this symmetry class.
- Class AIII: $T = 0,\ C = 0,\ S = 1$. Again, typically an insulator, while superconductors are also possible. Example: SSH model.
- Class D: $T = 0,\ C = 1,\ S = 0$. This class is typically realized as a superconductor, which actually may not have any physical symmetry other than the fermion parity symmetry. Example: 1D Kitaev chain, 2D $(p + ip)$ superconductor. Of course, this class can also be implemented by an insulator with a real particle-hole symmetry.

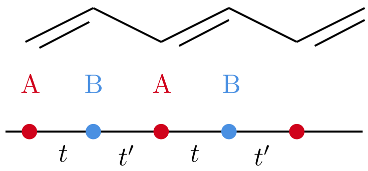

Figure 1: The lattice of the SSH model

- Class DIII: $T=-1, C=1, S=1$. Usual superconductors belong to this class, in which $\mathcal{T}^2$ is the fermion parity symmetry. 1D topological superconductors are in this class.
- Class AII: $T=-1, C=0, S=0$. Topological insulators in the ordinary sense are in this class.
- Class CII: $T=-1, C=-1, S=1$. This is a strange symmetry class. $C=-1$ means the symmetry class can be realized by a $SU(2)$ superconductor, but typically in this case we define $T=1$. Another way to think of this symmetry class is to realize it as an insulator with charge-hole symmetry.
- Class C: $T=0, C=-1, S=0$. This can be realized by a $SU(2)$ superconductor.
- Class CI: $T=1, C=-1, S=0$. This can also be realized by a $SU(2)$ superconductor with time reversal symmetry, in which we redefine $\mathcal{T}$ by attaching an i factor to it so that $T=1$.
- Class AI: $T=1, C=0, S=0$. A spinless insulator can realize this symmetry class. For electronic systems without spin-orbital coupling, by considering states with the following form
$$\frac{1}{\sqrt{2}}(|\boldsymbol{k},\uparrow\rangle+|\boldsymbol{k},\downarrow\rangle)$$
we can construct a "spinless" subspace.
- Class BDI: $T=1, C=1, S=0$. A typical realization is a spinless superconductor, like a p-wave superconductor in which the pairing order parameter Δ is real.

4 The SSH model

4.1 The Hamiltonian, topological phases and the winding number

Band structures in class A and class AIII may be classified by their Chern numbers. It can be proved that the possible Chern classes of class A and class AIII gapped free fermion are

The **SSH model** is first a tight-binding model on a polyacetyene chain. From the lattice structure Figure 1 on page 5, we can write down the second quantized Hamiltonian

$$\begin{aligned}\hat{H} &= -t\sum_i (a_i^\dagger b_i + \text{h.c.}) - t'\sum_i (b_i^\dagger a_{i+1} + \text{h.c.}) \\ &= \sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} 0 & -t-t'\mathrm{e}^{-\mathrm{i}k} \\ -t-t'\mathrm{e}^{\mathrm{i}k} & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix}.\end{aligned} \tag{25}$$

The first quantized Hamiltonian is

$$H(k) = \begin{pmatrix} 0 & -t-t'\mathrm{e}^{-\mathrm{i}k} \\ -t-t'\mathrm{e}^{\mathrm{i}k} & 0 \end{pmatrix} =: \begin{pmatrix} 0 & D(k) \\ D^*(k) & 0 \end{pmatrix}. \tag{26}$$

Now we check the chiral symmetry. Consider the following definition:

$$\mathcal{S}: a_i \mapsto a_i^\dagger, \quad b_i \mapsto -b_i^\dagger, \quad \mathrm{i} \mapsto -\mathrm{i}. \tag{27}$$

This is a typical definition of chiral operation, which involves both flipping c and $c^\dagger$ ($\mathcal{C}$) and the complex conjugate ($\mathcal{T}$). Under this transformation,

$$a_k = \sum_i a_i \mathrm{e}^{-\mathrm{i}kr_i} \mapsto \sum_i a_i^\dagger \mathrm{e}^{\mathrm{i}kr_i} = a_k^\dagger, \tag{28}$$

$$b_k = \sum_i b_i \mathrm{e}^{-\mathrm{i}kr_i} \mapsto -\sum_i b_i^\dagger \mathrm{e}^{\mathrm{i}kr_i} = -b_k^\dagger, \tag{29}$$

so the first quantization transformation is

$$S = \tau^z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}, \tag{30}$$

and we find

$$SH(k)S^{-1} = -H(k), \tag{31}$$

so indeed the SSH model has a chiral symmetry.

All information of a SSH band structure is stored in $D(k)$ in (26). We see $D(k)$ is a circle on the complex plane, and it can't go over the origin (which means the gap is closed). It's easy to check that when $t = t'$, the gap is closed. This is the critical point which separate the $t > t'$ topological phase and the $t < t'$ topological phase.

We consider the *flattened* Hamiltonian, in which the energy of occupied eigenstate is assigned as -1, and the energy of unoccupied states is assigned as 1. This means $H^2 = 1$, and all bands of this Hamiltonian is flatten. We usually denote it as Q to distinct it from the real Hamiltonian H. For the SSH model, it's

$$Q(k) = \begin{pmatrix} 0 & g(k) \\ g^*(k) & 0 \end{pmatrix}, \quad g(k) = \frac{D(k)}{|D(k)|} =: \mathrm{e}^{\mathrm{i}\theta(k)}, \tag{32}$$

and we have

$$Q(k)^2 = \begin{pmatrix} g(k)g^*(k) & \\ & g(k)g^*(k) \end{pmatrix} = 1. \tag{33}$$

So now a winding number can be defined for θ, which can also be calculated by

$$W = \mathrm{i} \int \frac{\mathrm{d}k}{2\pi} g^*(k) \partial_k g(k), \tag{34}$$

because

$$W = \mathrm{i} \int \frac{\mathrm{d}k}{2\pi} g^*(k) \partial_k g(k) = \mathrm{i} \int \frac{\mathrm{d}k}{2\pi} \mathrm{i} \partial_k \theta = -\int_0^{2\pi} \mathrm{d}\theta = -\theta(k)|_{k=0}^{2\pi}. \tag{35}$$

Note that $\theta(k)$ can be multivalued, as long as $g(2\pi) = g(0)$, which means

$$\theta(2\pi) - \theta(0) = 2\pi n, \quad n \in \mathbb{Z},$$

so we find $W \in \mathbb{Z}$.

Here a possible paradox occurs: we can decide the topological property of Q (and hence H) by calculating the winding number, while the shape of bands of Q and a trivial flat band model created by highly localized Wannier functions are the same. So what's the information loss after we diagonalize the Hamiltonian? Actually the topological information is stored in the *basis* after diagonalization.

4.2 Polarization

Now we turn to a concept first developed in *ab initio* calculation: the microscopic definition of charge polarization. Now we use n (instead of i) to denote the site index and α the sublattice label (and hence the band index). We have

$$\boldsymbol{P} = \langle n\alpha | \boldsymbol{r} | n\alpha \rangle, \quad P_x = \langle n\alpha | x | n\alpha \rangle. \tag{36}$$

Now we are going to show that P_x is actually given by the Berry phase on the x direction.

A Bloch state is in the form of

$$\psi_{k\alpha}(x) = \mathrm{e}^{\mathrm{i}kx} u_{n\alpha}(x), \tag{37}$$

which in the bra-ket notation is

$$|\psi_{k\alpha}\rangle = \mathrm{e}^{\mathrm{i}k\hat{x}} |u_{kn}\rangle . \tag{38}$$

The Wannier function is

$$|n\alpha\rangle = \frac{1}{\sqrt{N}} \sum_k \mathrm{e}^{\mathrm{i}k(\hat{x}-x_n)} |u_{kn}\rangle \tag{39}$$

When the polarization is uniform enough, we have

$$\begin{aligned} P_x &= \sum_{\alpha<0} \langle n=0,\alpha|\hat{x}|n=0,\alpha\rangle = \frac{1}{N} \sum_{k,k',\alpha<0} \langle u_{k'\alpha}|\mathrm{e}^{-\mathrm{i}k'\hat{x}} \hat{x} \mathrm{e}^{\mathrm{i}k\hat{x}}|u_{k\alpha}\rangle \\ &= \frac{\mathrm{i}}{N} \sum_{k,\alpha<0} \langle u_{k\alpha}|\frac{\partial}{\partial k}|u_{k\alpha}\rangle = \sum_{\alpha<0} \int \frac{\mathrm{d}k}{2\pi} \mathrm{i} \langle u_{k\alpha}|\frac{\partial}{\partial k}|u_{k\alpha}\rangle . \end{aligned} \tag{40}$$

This is just the integral

$$P_x = \int \frac{\mathrm{d}k}{2\pi} A_x \tag{41}$$

of the Berry phase

$$A_x = \mathrm{i} \sum_{\alpha<0} \langle u_{k\alpha}|\frac{\partial}{\partial k}|u_{k\alpha}\rangle . \tag{42}$$

The polarization P_x is only well defined mod 1, because we can do a gauge transformation

$$|u_{k\alpha}\rangle \to \mathrm{e}^{\mathrm{i}\theta(k)} |u_{k\alpha}\rangle , \tag{43}$$

and

$$P_x \to P_x + \frac{\theta(2\pi) - \theta(0)}{2\pi}. \tag{44}$$

Now we will find the chiral symmetry in class AIII requires

$$P_x = 0,\ \frac{1}{2} \bmod 1 \tag{45}$$

for the SSH model. The eigenstate of $Q(k)$ can be found as

$$Q \begin{pmatrix} u_k \\ \pm q^*(k) u_k \end{pmatrix} = \begin{pmatrix} \pm q(k) q^*(k) u_k \\ q^*(k) u_k \end{pmatrix} = \pm \begin{pmatrix} u_k \\ \pm q^*(k) u_k \end{pmatrix}. \tag{46}$$

Note that by selecting these states as the basis, we have already chosen a *gauge* for A_x. Since $(u_k, -q^*(k)u_k)$ is the occupied state, we have

$$\begin{aligned} A_x(k) &= \mathrm{i} \begin{pmatrix} u_k^* & -q(k) u_k^* \end{pmatrix} \frac{\partial}{\partial k} \begin{pmatrix} u_k \\ -q^*(k) u_k \end{pmatrix} \\ &= \frac{\mathrm{i}}{2} \operatorname{tr}(q(k) \partial_k q^*(k)) \end{aligned} \tag{47}$$

We find that though Q is as flat as a trivial flat band model constructed by localized Wannier functions, by extracting information from the *basis*, we are able to recover the topological classification obtained previously by the winding number.

5 Class A insulators when $d = 2$

Now we consider the $d = 2$ class A insulators. Examples of this class include IQHE and Chern insulators. The

References

[1] Shinsei Ryu, Andreas P Schnyder, Akira Furusaki, and Andreas W W Ludwig. Topological insulators and superconductors: tenfold way and dimensional hierarchy. *New Journal of Physics*, 12(6):065010, jun 2010.