

Prof. Yang Qi on topological classification of free fermion models

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1 Antiunitary symmetry of free fermions

Consider the following second quantized Hamiltonian:

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

where operators with $\hat{}$ 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

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

and

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

So the Hamiltonian transforms as

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

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

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

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

$$THT^{-1} = H^*. \quad (6)$$

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

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

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

$$\mathcal{C} c_i \mathcal{C}^{-1} = c_i^{\dagger}, \quad \mathcal{C} c_i^{\dagger} \mathcal{C}^{-1} = c_i, \quad (8)$$

then we have

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

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 $|\mathbf{i}\rangle$ to $\langle \mathbf{i}|$. 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

$$c_{\mathbf{k}}^{\dagger} \xrightarrow{\mathcal{C}} c_{-\mathbf{k}} \quad (10)$$

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

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

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 $\mathcal{H} \rightarrow \mathcal{H}^*$ should be *antiunitary* to keep naturalness.

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

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

and the second quantized Hamiltonian under (11) transforms as

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

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

$$H = -C H^* C^{-1}. \quad (13)$$

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,

$$\mathcal{S} = \mathcal{T} \mathcal{C} \quad (14)$$

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

$$S H S^{-1} = -H. \quad (15)$$

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

$$T H(\mathbf{k}) T^{-1} = H(-\mathbf{k})^*. \quad (16)$$

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

$$C H(-\mathbf{k})^* C^{-1} = -H(\mathbf{k}). \quad (17)$$

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

$$S H(\mathbf{k}) S^{-1} = -H(\mathbf{k}). \quad (18)$$

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:

$$H = \sum_{\mathbf{k}, \alpha} \xi_{\mathbf{k}} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha} - V \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}, \alpha, \beta} c_{\mathbf{k}'-\mathbf{q}, \alpha}^\dagger c_{\mathbf{k}+\mathbf{q}, \beta}^\dagger c_{\mathbf{k}\beta} c_{\mathbf{k}'\alpha}, \quad (19)$$

can be turned into

$$H = \sum_{\mathbf{k}, \alpha} \xi_{\mathbf{k}} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha} + \sum_{\mathbf{k}} (\Delta c_{-\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}\uparrow}^\dagger + \Delta^* c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}), \quad (20)$$

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 quasiparticles 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

$$H = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta \\ -\Delta^* & -\xi_{\mathbf{k}} \end{pmatrix} \Psi_{\mathbf{k}}, \quad \Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{-\mathbf{k},\downarrow}^\dagger \end{pmatrix}. \quad (21)$$

This Hamiltonian has a particle-hole symmetry. Because $\xi_{\mathbf{k}} = \xi_{-\mathbf{k}}$, we have

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}} & -\Delta \\ -\Delta^* & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = - \begin{pmatrix} \xi_{-\mathbf{k}} & -\Delta \\ -\Delta^* & -\xi_{-\mathbf{k}} \end{pmatrix}^*. \quad (22)$$

But the particle-hole symmetry is actually *redundant*. BdG Hamiltonians without this symmetry aren't qualified theories of superconductors. 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 $\Psi_{\mathbf{k}}$ should be $2d$ dimensional to include all possible terms. (In the BCS case there are two kind of fermions and Ψ is 2-dimensional, but we can always introduce $c_{\mathbf{k}\downarrow}$ and $c_{-\mathbf{k},\uparrow}^\dagger$ components and assign zero matrix elements for them, and the resulting first-quantized Hamiltonian still has a particle-hole symmetry.) 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 must be a particle-hole symmetry to make sure the spectrum of the first quantized Hamiltonian reflects this fact.

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. Sometimes it's just a redundancy: the C matrix acting on a state gives exactly the state itself. Consider, for example, the following simplest case:

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} = \frac{1}{2} \sum_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k}}^\dagger & c_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \xi_{\mathbf{k}} & \\ & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}} \\ c_{\mathbf{k}}^\dagger \end{pmatrix} + \text{const}, \quad (23)$$

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)

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

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

3 The 10-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 these symmetries are present,

- Class A: no time reversal symmetry, no particle-hole symmetry, no chiral symmetry. An insulator with charge conservation. Example: Chern-insulators, IQHE.
- Class AIII: no time reversal symmetry, no particle-hole symmetry, but there is a chiral symmetry. Example: SSH model.
- Class D: no time reversal, but there is a particle-hole symmetry. This is a superconductor. It actually may not have any physical symmetry other than the fermion parity symmetry. Example: 1D Kitaev chain, 2D $p + i$ superconductor.
- Class DIII: $T = -1$,