Prof. Yang Qi on topological classification of free fermion models

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1 Antiunitary symmetry of second quantized Hamiltonian of free fermions

Consider the following second quantized Hamiltonian:

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

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

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

So the Hamiltonian transforms as

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

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

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

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

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

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

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

then we have

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

The minus sign, physically, means 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

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

to keep momentum conservation, and if $\mathcal{C}$ is unitary, we have

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

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 state is

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

$$\mathcal{C} H \mathcal{C}^{-1} = -C H^* C^{-1}. \tag{12}$$

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.

2 Particle-hole symmetry in superconductors

Particle-hole symmetry is another antiunitary symmetry that may concern us for fermionic systems. Consider, for example, the following BCS model of superconductivity:

$$H = \sum_{\boldsymbol{k},\alpha} \xi_{\boldsymbol{k}} c_{\boldsymbol{k}\alpha}^\dagger c_{\boldsymbol{k}\alpha} - V \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},\alpha,\beta} c_{\boldsymbol{k}'-\boldsymbol{q},\alpha}^\dagger c_{\boldsymbol{k}+\boldsymbol{q},\beta}^\dagger c_{\boldsymbol{k}\beta} c_{\boldsymbol{k}'\alpha}, \tag{13}$$

which turns into

$$H = \sum_{\boldsymbol{k},\alpha} \xi_{\boldsymbol{k}} c_{\boldsymbol{k}\alpha}^\dagger c_{\boldsymbol{k}\alpha} + \sum_{\boldsymbol{k}} (\Delta c_{-\boldsymbol{k}\downarrow}^\dagger c_{\boldsymbol{k}\uparrow}^\dagger + \Delta^* c_{\boldsymbol{k}\uparrow} c_{-\boldsymbol{k}\downarrow}), \tag{14}$$

where Δ is the BCS order parameter. (14) is called the **BdG Hamiltonian**, which describes the spectrum of (electron-like) quasiparticles in a BCS superconductor. Note that the order parameter in (14) 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 (13) is not (14), 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 (14), though this time (14) has nothing to do with BCS mechanism. So henceforth we will work with the free-fermionic model (14) and ignore what induces superconductivity pairing.

Now we repeat the classical procedure in BCS theory: (14) can be rephrased into

$$H = \sum_{\boldsymbol{k}} \Psi_{\boldsymbol{k}}^\dagger \begin{pmatrix} \xi_{\boldsymbol{k}} & -\Delta \\ -\Delta^* & -\xi_{\boldsymbol{k}} \end{pmatrix} \Psi_{\boldsymbol{k}}, \quad \Psi_{\boldsymbol{k}} = \tag{15}$$

The particle-hole symmetry is actually a *redundancy*: BdG Hamiltonians without this symmetry aren't qualified theories of superconductors. 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

- 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 $p + \mathrm{i}$ superconductor.
- Class DIII: $T = -1$,