Inversion symmetry in the extended BHZ model

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We first review the standard BdG setting for symmetries, and how inversion symmetry appears here, and how to transition to a chiral basis.

We then discuss how the BHZ model fits into this framework.

I. STANDARD BDG FOR TIME-REVERSAL SYMMETRIC SUPERCONDUCTORS (DIII)

A superconductor in the mean-field approximation can be described by a single-particle Bogoliubov-de Gennes (BdG) Hamiltonian $\mathcal{H}$. This has the form,

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}. \tag{1}$$

Here h and Δ are possibly quite large matrices. Using $\tau_{x,y,z}$ to denote Pauli matrices acting on the blocks here, this has particle-hole symmetry by construction,

$$\mathcal{P} = \tau_x K; \qquad \tau_x K \mathcal{H} K \tau_x = -\mathcal{H}, \tag{2}$$

with K representing complex conjugation in position basis.

We are interested in superconductors with time-reversal symmetry (that squares to -1). Time-reversal is usually represented by

$$\mathcal{T} = \sigma_y K, \tag{3}$$

where $\sigma_{x,y,z}$ act on spin (or in general some internal degree of freedom). This should act on the BdG Hamiltonian block by block, i.e., we need

$$[\sigma_y, \tau_x] = 0, \tag{4}$$

which holds if we have a tensor product structure.

If we have both particle-hole and time-reversal symmetries, their product, chiral symmetry, is also a symmetry of the system. This is represented in the standard basis used above by

$$\hat{\Gamma} = \tau_x \sigma_y = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}. \tag{5}$$

Although this looks like a 4×4 matrix, there could be any number of internal states, and so each number in the matrix above can correspond to a unit matrix.

A. Chiral basis

We are interested in transforming the Hamiltonian to the chiral basis, where chiral symmetry is represented by

$$\tilde{\Gamma} = \tau_z. \tag{6}$$

To achieve this transformation, we diagonalize $\hat{\Gamma}$.

$$\hat{\Gamma} = |||\setminus \equiv = \mathcal{O}\tau_z\mathcal{O}^\dagger; \tag{7}$$

$$\mathcal{O} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & -i & 0 & i \\ i & 0 & -i & 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ \sigma_y & -\sigma_y. \end{pmatrix} \tag{8}$$

The transformation works by conjugating with $\mathcal{O}$ above, which gives for the particle-hole and time-reversal symmetries,

$$\tau_x K \to \frac{1}{2} \begin{pmatrix} 1 & \sigma_y \\ 1 & -\sigma_y \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} K \begin{pmatrix} 1 & 1 \\ \sigma_y & -\sigma_y \end{pmatrix}$$
$$= \frac{1}{2} \begin{pmatrix} 1 & \sigma_y \\ 1 & -\sigma_y \end{pmatrix} \begin{pmatrix} -\sigma_y & \sigma_y \\ 1 & 1 \end{pmatrix} K = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix} K = i\tau_y\sigma_y K, \tag{9}$$

where we can drop the factor i at the end for simplicity. Similarly, for time reversal,

$$\sigma_y K \to \tau_x \sigma_y K. \tag{10}$$

In the chiral basis, the BdG Hamiltonian is block off-diagonal.

$$\mathcal{H} = \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix}. \tag{11}$$

The particle-hole symmetry acts on D by:

$$D \to -\sigma_y D^T \sigma_y, \tag{12}$$

as can be checked by calculation. For the bulk momentum-space Hamiltonian, the requirement of particle-hole symmetry, $\mathcal{H} = -\mathcal{P}\mathcal{H}\mathcal{P}^{-1}$ thus translates to

$$D(k) = \sigma_y D(-k)^T \sigma_y. \tag{13}$$

As a consequence, in this basis,

$$\det D(k) = \det D(-k). \tag{14}$$

A consequence of the above is that winding number of $\det D(k)$ around some momentum point k_0 is the same as around its time-reversed partner, $-k_0$. Thus topologically protected Weyl nodes come in pairs, where members of a pair have equal charges. Because the net sum of all charges in the Brillouin zone has to be 0, Weyl nodes should come in groups of 4. This was Benjamin Beri's statement.

B. Inversion symmetry

Inversion is an operation that acts in real space by inversion through a center. In momentum space this changes $k \leftrightarrow -k$, but it can also change the internal states by some unitary $\hat{J}$.

We expect inversion to not affect the particle/hole degree of freedom. Not sure about spin, probably should not affect spin either. So it should act elementwise in the chiral basis as well. Thus inversion symmetry gives

$$D(k) = \hat{J} D(-k) \hat{J}^\dagger. \tag{15}$$

This requires

$$\det D(k) = \det D(-k), \tag{16}$$

which is the same requirement as that due to particle-hole symmetry, Eq. (14).

II. OUR CASE, IN SPECIAL BASIS

We are investigating the BHZ model, where we interpret the Hamiltonian as a BdG Hamiltonian. Here the bulk momentum-space Hamiltonian reads,

$$H(k) = \begin{pmatrix} A(k) & B(k) & 0 & -C \\ B(k)^* & -A(k) & C & 0 \\ 0 & C & A(k) & -B(k)^* \\ -C & 0 & -B(k) & A(k), \end{pmatrix} \tag{17}$$

with

$$A(k) = u + v_x \cos k_x + \cos k_y; \tag{18}$$
$$B(k) = v_x \sin k_x - i \sin k_y, \tag{19}$$

and with $()^*$ denoting elementwise complex conjugation (without changing sign of momentum). This is just two layers of QWZ model, with time-reversal symmetry built into the model. The coupling between the layers is such that time reversal symmetry, represented by

$$\mathcal{T} = \tau_y K, \tag{20}$$

is respected. We happen to also have particle-hole symmetry, with

$$\mathcal{T} = \sigma_x K. \tag{21}$$

We can rewrite the coupled BHZ model to the "standard basis" above, and find

$$\mathcal{H}(k) = \begin{pmatrix} A(k) & 0 & B(k) & -C \\ 0 & A(k) & - & -B(k)^* \\ B(k)^* & C & -A(k) & 0 \\ -C & -B(k) & 0 & -A(k), \end{pmatrix} \tag{22}$$

Seen as a BdG Hamiltonian, this is somewhat peculiar. The Hamiltonian $h(k)$ is just a nn hopping on a square lattice, spin independent. The superconducting order parameter is momentum dependent, but in a somewhat weird way.

A. Our inversion symmetry

The BHZ model, without the coupling, has an inversion symmetry that commutes with time reversal. It is represented by

$$\hat{J} = \hat{\sigma}_z. \tag{23}$$

When interpreting the σ matrices as particle-hole operators, all we do is replace $\sigma \leftrightarrow \tau$, the inversion becomes peculiar, it is $\hat{J} = \tau_z$. In the language of the BdG Hamiltonian, it requires

$$h(k) = h(-k); \qquad \Delta(k) = -\Delta(-k). \tag{24}$$

The coupling via C breaks inversion symmetry.

In the chiral basis, this inversion symmetry of ours is transformed to:

$$\hat{J} \to \tau_x. \tag{25}$$

Therefore, this inversion symmetry requires

$$D(k) = D^\dagger(-k), \tag{26}$$

which entails

$$\det D(k) = \det D(-k)^*. \tag{27}$$

Together with particle-hole symmetry, Eq. (14), this amounts to

$$\det D(k) \in \mathbb{R}. \tag{28}$$

Thus our inversion symmetry excludes the presence of topologically protected Weyl nodes, because it prevents $\det D(k)$ from having a phase that could wind.

III. QUESTIONS

Our inversion is pretty specific. What property does it have that prevents protected Weyl nodes?