Fermi-Surface Formula for Topological Invariants in Superconductors

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The BdG Hamiltonian is

$$H_{\boldsymbol{k}} = \begin{pmatrix} h_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta_{\boldsymbol{k}}^\dagger & -h_{-\boldsymbol{k}}^T \end{pmatrix}, \quad \Delta_{\boldsymbol{k}}^T = -\Delta_{-\boldsymbol{k}}. \tag{1}$$

This is equivalent to imposing the following PHS:

$$C H_{\boldsymbol{k}} C^{-1} = -H_{-\boldsymbol{k}}, \quad C = \tau_x K. \tag{2}$$

1 1D, class DIII

We further impose TRS. More generally, let us consider cases where the matrix for TRS depends on k, for instance when an effective TRS exists only on a certain symmetry line:

$$T_k H_k T_k^{-1} = H_{-k}, \quad T_k = \begin{pmatrix} u_{T,k} & \\ & u_{T,-k}^* \end{pmatrix} K, \quad u_{T,-k} u_{T,k}^* = -1. \tag{3}$$

This is equivalent to

$$u_{T,k} h_k^* u_{T,k}^\dagger = h_{-k}, \quad u_{T,k} \Delta_k^* u_{T,-k}^T = \Delta_{-k} = -\Delta_k^T. \tag{4}$$

The chiral symmetry is

$$\Gamma_k = i T_{-k} C = \begin{pmatrix} & i u_{T,-k} \\ i u_{T,k}^* & \end{pmatrix}, \quad \Gamma_k^2 = 1, \tag{5}$$

$$\Gamma_k H_k = -H_k \Gamma_k. \tag{6}$$

Introduce bases with $\Gamma_k = \pm$:

$$\mathcal{U}_{\pm,k} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} \\ \pm i u_{T,k}^* \end{pmatrix}. \tag{7}$$

The bases $\mathcal{U}_{\pm,k}$ generally depend on k. Let q_k be the off-diagonal $(2,1)$ component of H_k in the basis $(\mathcal{U}_{+,k}, \mathcal{U}_{-,k})$. Explicitly,

$$q_k = \mathcal{U}_{-,k}^\dagger H_k \mathcal{U}_{+,k} = h_k + i \Delta_k u_{T,k}^*. \tag{8}$$

In addition to $h_k^\dagger = h_k$, we have

$$(\Delta_k u_{T,k}^*)^\dagger = u_{T,k}^T \Delta_k^\dagger = u_{T,-k} \Delta_{-k}^* = \Delta_k u_{T,k}^*, \tag{9}$$

so $\Delta_k u_{T,k}^*$ is also Hermitian. Thus the expression for q_k is a decomposition into real and imaginary parts. Furthermore,

$$q_k^T = (q_k^\dagger)^* = (h_k - i \Delta_k u_{T,k}^*)^* = h_k^* + i \Delta_k^* u_{T,k} \tag{10}$$

$$= u_{T,k}^\dagger h_{-k} u_{T,k} + i (u_{T,k}^\dagger \Delta_{-k} u_{T,-k}^*) u_{T,k} = u_{T,k}^\dagger (h_{-k} + i \Delta_{-k} u_{T,-k}^*) u_{T,k} = u_{T,k}^\dagger q_{-k} u_{T,k}. \tag{11}$$

Therefore

$$(q_k u_{T,k})^T = -q_{-k} u_{T,k}. \tag{12}$$

At symmetric points $-k \equiv k$, the Pfaffian is therefore defined:

$$\mathrm{Pf}\,[q_k u_{T,k}], \quad k = 0, \pi. \tag{13}$$

Introduce the quantity

$$z[H_k] = \frac{\mathrm{Pf}\,[q_0 u_{T,0}]}{\mathrm{Pf}\,[q_\pi u_{T,\pi}]} \exp \frac{1}{2} \int_0^\pi d \log \det q_k \in \{\pm 1\}. \tag{14}$$

The quantity $z[H_k]$ is quantized to some $\mathbb{Z}_2$ value determined by the matrices $u_{T,k}$:

$$z[H_k]^2 = \frac{\det[q_0 u_{T,0}]}{\det[q_\pi u_{T,\pi}]} \exp \int_0^\pi d \log \det q_k \in \{\pm 1\} = \frac{\det[u_{T,0}]}{\det[u_{T,\pi}]} \in U(1). \tag{15}$$

The matrices $u_{T,k}$ do not depend on the Hamiltonian; they are determined only by the atomic insulator on which the Hamiltonian is defined. To define a topological invariant that is quantized to ± 1 and gives 1 for a trivial Hamiltonian, it is enough to take the ratio with $z[H_k^{\mathrm{triv}}]$ for a trivial Hamiltonian. Define the $\mathbb{Z}_2$ invariant as

$$(-1)^{\nu[H_k]} := \frac{z[H_k]}{z[H_k^{\mathrm{triv}}]} \in \pm 1. \tag{16}$$

Note that in the expressions for $z[H_k]$ and $z[H_k^{\mathrm{triv}}]$, one must use the common bases $\mathcal{U}_{\pm,k}$. As a trivial Hamiltonian H_k^{triv}, one can consider the vacuum with no fermions occupied. Concretely, taking the limit where the chemical potential goes to $\mu \to -\infty$, we may choose

$$h_k \equiv 1, \quad \Delta_k \equiv 0. \tag{17}$$

Then

$$q_k \equiv 1, \tag{18}$$

and hence

$$z[H_k^{\mathrm{triv}}] = \frac{\mathrm{Pf}\,[u_{T,0}]}{\mathrm{Pf}\,[u_{T,\pi}]}. \tag{19}$$

Therefore the $\mathbb{Z}_2$ invariant is given by

$$(-1)^{\nu[H_k]} = \frac{\mathrm{Pf}\,[q_0 u_{T,0}]/\mathrm{Pf}\,[u_{T,0}]}{\mathrm{Pf}\,[q_\pi u_{T,\pi}]/\mathrm{Pf}\,[u_{T,\pi}]} \exp \frac{1}{2} \int_0^\pi d \log \det q_k \in \{\pm 1\}. \tag{20}$$

1.1 Fermi-surface formula

The topological number of a superconductor is determined only near the Fermi surfaces. We compute $z[H_k]$ under the assumptions

(i) there is no Fermi surface at $k = 0, \pi$;

(ii) Δ_k takes a small finite value only near the Fermi surfaces;

(iii) there is no degeneracy on the Fermi surfaces.

If we consider only time-reversal symmetry, degeneracies on the Fermi surfaces can be removed continuously within assumptions (i) and (ii). If other symmetries, for example inversion symmetry, are present, assumption (iii) may fail. Cases where degeneracy is unavoidable must be considered separately.

By the assumptions above, the phase of $\det q_k$ changes only near the Fermi surfaces, where $\det h_k = 0$. Label the Fermi surfaces by n, and write a state on the Fermi surface as $|nk\rangle$. Let $\varepsilon_{nk} = \langle nk|h_k|nk\rangle$. Near the Fermi surface n, q_k is approximated as

$$h_k + i\Delta_k u^*_{T,k} \sim \left(\partial_k \varepsilon_{nk_{nF}}(k - k_{nF}) + i\delta_{nk_{nF}}\right)|nk\rangle\langle nk| + \sum_{m\neq n} \varepsilon_{mk}|mk\rangle\langle mk|. \quad (21)$$

Here we have set

$$\delta_{nk_{nF}} = \langle nk|\Delta_k u^*_{T,k}|nk\rangle|_{k=k_{nF}} \in \mathbb{R}\backslash\{0\}. \quad (22)$$

The term $\sum_{m\neq n}$ denotes the contribution from bands other than the Fermi-surface band. The contribution from the vicinity of the Fermi surface n to the integral $\int d\log\det q_k$ is

$$\int_{k_{nF}-\delta k}^{k_{nF}+\delta k}\int d\log\det q_k = |\log|q_k||\big|_{k_{nF}-\delta k}^{k_{nF}+\delta k} - \pi i \mathrm{sgn}(\partial_k \varepsilon_{nk_{nF}})\mathrm{sgn}(\delta_{nk_{nF}}). \quad (23)$$

Adding the contributions from all Fermi surfaces gives

$$\int_0^\pi d\log\det q_k = \log|\det q_\pi| - \log|\det q_0| - \pi i \sum_{\varepsilon_{nk}=0} \mathrm{sgn}(\partial_k\varepsilon_{nk})\mathrm{sgn}(\delta_{nk}). \quad (24)$$

Therefore

$$\exp\frac{1}{2}\int_0^\pi d\log\det q_k = \frac{\sqrt{|\det q_\pi|}}{\sqrt{|\det q_0|}}\exp -\frac{\pi i}{2}\sum_{\varepsilon_{nk}=0}\mathrm{sgn}(\partial_k\varepsilon_{nk})\mathrm{sgn}(\delta_{nk}). \quad (25)$$

For a sign $\sigma \in \pm 1$,

$$e^{\frac{\pi i}{2}\sigma} = i \times \sigma. \quad (26)$$

Thus

$$\begin{aligned}\exp -\frac{\pi i}{2}\sum_{\varepsilon_{nk}=0}\mathrm{sgn}(\partial_k\varepsilon_{nk})\mathrm{sgn}(\delta_{nk}) &= \prod_{\varepsilon_{nk}=0} -i\mathrm{sgn}(\partial_k\varepsilon_{nk})\mathrm{sgn}(\delta_{nk}) && (27)\\ &= \prod_{\varepsilon_{nk}=0} -i\mathrm{sgn}(\partial_k\varepsilon_{nk})\prod_{\varepsilon_{nk}=0}\mathrm{sgn}(\delta_{nk}) && (28)\\ &= (-i)^{\sum_{\varepsilon_{nk}=0}\mathrm{sgn}(\partial_k\varepsilon_{nk})}\prod_{\varepsilon_{nk}=0}\mathrm{sgn}(\delta_{nk}). && (29)\end{aligned}$$

Under the assumption that there are no Fermi surfaces at $k = 0, \pi$, the numbers N_0, N_π of occupied bands at $k = 0, \pi$ are invariant. The first factor is determined by the numbers of occupied bands N_0, N_π at $k = 0, \pi$:

$$\sum_{\varepsilon_{nk}=0}\mathrm{sgn}(\partial_k\varepsilon_{nk}) = N_0 - N_\pi. \quad (30)$$

Note that by TRS, N_0, N_π are nonnegative even integers. At this stage the $\mathbb{Z}_2$ invariant is

$$(-1)^{\nu[H_k]} = \frac{\mathrm{Pf}\,[q_0 u_{T,0}]/\mathrm{Pf}\,[u_{T,0}]}{\mathrm{Pf}\,[q_\pi u_{T,\pi}]/\mathrm{Pf}\,[u_{T,\pi}]} \times \frac{\sqrt{|\det q_\pi|}}{\sqrt{|\det q_0|}} \times (-1)^{\frac{N_0-N_\pi}{2}} \times \prod_{\varepsilon_{nk}=0}\mathrm{sgn}(\delta_{nk}). \quad (31)$$

We compute the signs of the Pfaffians $\mathrm{Pf}\,[q_0 u_{T,0}]$ and $\mathrm{sgn}\,\mathrm{Pf}\,[q_\pi u_{T,\pi}]$. Set $k = 0, \pi$ and suppress k. By assumptions (i) and (ii), we may replace Δ_k by $\Delta_k \sim 0$ at $k = 0, \pi$.

$$\mathrm{Pf}\,[qu_T] = \mathrm{Pf}\,[hu_T]. \quad (32)$$

Introduce a basis that diagonalizes h. Taking Kramers pairs as $|\chi_{\mathrm{I}}\rangle, |\chi_{\mathrm{II}}\rangle$, choose a basis $U = (|\chi_{\mathrm{I}}\rangle, |\chi_{\mathrm{II}}\rangle, \dots)$ satisfying

$$u_T |\chi_{\mathrm{I}}\rangle^* = |\chi_{\mathrm{II}}\rangle, \quad u_T |\chi_{\mathrm{II}}\rangle^* = -|\chi_{\mathrm{I}}\rangle. \tag{33}$$

If $N \in 2\mathbb{Z}$ is the number of occupied states, then

$$hU = U\Lambda \otimes 1_2, \quad \Lambda = \begin{pmatrix} \epsilon_1 & & \\ & \ddots & \\ & & \epsilon_n \end{pmatrix}, \tag{34}$$

$$u_T U^* = U 1_n \otimes (-i\sigma_y). \tag{35}$$

Here $2n \in 2\mathbb{Z}$ is the total number of bands, and $\epsilon_j \neq 0$ are the energy eigenvalues with Kramers degeneracy. Then

$$\begin{aligned} \mathrm{Pf}\,[hu_T] &= \mathrm{Pf}\,\left[U(\Lambda \otimes 1_2)U^\dagger u_T\right] && (36)\\ &= \mathrm{Pf}\,\left[U(\Lambda \otimes 1_2)(-u_T U^*)^T\right] && (37)\\ &= \mathrm{Pf}\,\left[U(\Lambda \otimes 1_2)(-U 1_n \otimes (-i\sigma_y))^T\right] && (38)\\ &= \mathrm{Pf}\,\left[U(\Lambda \otimes 1_2)(1_n \otimes (-i\sigma_y))U^T\right] && (39)\\ &= \mathrm{Pf}\,\left[U(\Lambda \otimes (-i\sigma_y))U^T\right] && (40)\\ &= \det U \mathrm{Pf}\,[\Lambda \otimes (-i\sigma_y)] && (41)\\ &= \det U \prod_{j=1}^{n} (-\epsilon_j). && (42) \end{aligned}$$

Furthermore,

$$\mathrm{Pf}\, u_T = \mathrm{Pf}\,[U 1_n \otimes (-i\sigma_y) U^T] = \det U (-1)^n, \tag{43}$$

and

$$\sqrt{|\det q|} = \sqrt{|\det h|} = \prod_{j=1}^{n} |\epsilon_j|. \tag{44}$$

Thus we finally obtain

$$\frac{\mathrm{Pf}\,[qu_T]}{\mathrm{Pf}\,[u_T]\sqrt{|\det q|}} = \prod_{j=1}^{n} \mathrm{sgn}\,\epsilon_j = (-1)^{N/2}. \tag{45}$$

Here N is the number of occupied states.

Combining the above, we obtain the Fermi-surface formula for the $\mathbb{Z}_2$ invariant [1]:

$$(-1)^{\nu[H_k]} = \prod_{\varepsilon_{nk}=0} \mathrm{sgn}(\delta_{nk}). \tag{46}$$

The final expression can be extended to the case of degenerate bands. If the labels within a degenerate band are $a = 1, \dots, I_n$, then

$$(-1)^\nu = \prod_{\epsilon_{nk}=0} \mathrm{sgn}\ \det(\langle nak|\Delta_k u_{T,k}^*|nbk\rangle)_{a,b=1,\dots,I_n}. \tag{47}$$

1.2 Example

Assume spin-1/2 and orbital degrees of freedom as internal degrees of freedom, and take

$$u_T = -i\sigma_y, \quad \Delta_k = (\psi_k + \boldsymbol{d}_k \cdot \boldsymbol{\sigma})(i\sigma_y). \tag{48}$$

Then $\Delta_k u_T^* = \psi_k + \boldsymbol{d}_k \cdot \boldsymbol{\sigma}$. Since $\Delta_k u_T^*$ is Hermitian, ψ_k and $\boldsymbol{d}_k$ are Hermitian matrices. The product of the signs of the eigenvalues of $\psi_k + \boldsymbol{d}_k \cdot \boldsymbol{\sigma}$ in the Fermi-surface states $|nak\rangle$ contributes to the $\mathbb{Z}_2$ invariant.

In the simpler situation where there is no orbital degree of freedom and the band is degenerate in spin space, the contribution of a Fermi surface to the $\mathbb{Z}_2$ invariant is

$$\mathrm{sgn}\ \det(\psi_k + \boldsymbol{d}_k \cdot \boldsymbol{\sigma}) = \mathrm{sgn}\,(\psi_k^2 - \boldsymbol{d}_k^2). \tag{49}$$

1.3 DIII plus even mirror symmetry

In addition to TRS, consider the case where there is an additional unitary symmetry that does not change the wave vector:

$$m_k h_k m_k^\dagger = h_k, \quad m_k \Delta_k m_{-k}^T = \Delta_k, \quad m_k^2 = -1, \tag{50}$$

$$u_{T,k} m_k^* = m_{-k} u_{T,k}. \tag{51}$$

The symmetry for the BdG Hamiltonian is

$$M_k = \begin{pmatrix} m_k & \\ & m_{-k}^* \end{pmatrix}. \tag{52}$$

From the relations

$$M_k^2 = -1, \quad T_k M_k = M_{-k} T_k, \quad C M_k = M_{-k} C, \tag{53}$$

the effective AZ class is AIII$_T$. Winding numbers $W_{\pm i}$ can be defined in the $M_k = \pm i$ sectors, and depending on the definition of chirality, they obey a relation $W_i = \pm W_{-i}$. Let us define the winding number in the $M_k = i$ sector.

As in the previous section, introduce the matrix q_k:

$$q_k = h_k + i\Delta_k u_{T,k}^*. \tag{54}$$

Then

$$m_k q_k m_k^\dagger = m_k h_k m_k^\dagger + i m_k \Delta_k m_{-k}^T m_{-k}^* u_{T,k}^* m_k^\dagger = h_k + i\Delta_k u_{T,k}^* = q_k, \tag{55}$$

so q_k decomposes into the $m_k = \pm i$ sectors. Introduce periodic bases $\mathcal{B}_{\pm,k}, \mathcal{B}_{\pm,2\pi} = \mathcal{B}_{\pm,0}$ with $m_k = \pm i$, and write

$$q_{\pm,k} = h_{\pm,k} + i\tilde{\Delta}_{\pm,k}, \tag{56}$$

$$h_{\pm,k} = \mathcal{B}_{\pm,k}^\dagger h_k \mathcal{B}_{\pm,k}, \quad \tilde{\Delta}_{\pm,k} = \mathcal{B}_{\pm,k}^\dagger \Delta_k u_{T,k}^* \mathcal{B}_{\pm,k}. \tag{57}$$

Define the winding numbers by

$$W_{\pm i} = \frac{1}{2\pi i} \oint d \log \det q_{\pm,k}. \tag{58}$$

The Fermi-surface formula is

$$W_{\pm i} = -\frac{1}{2} \sum_{\varepsilon_{nk}^\pm = 0} \mathrm{sgn}(\partial_k \varepsilon_{nk}^\pm) \mathrm{sgn}(\delta_{nk}^\pm). \tag{59}$$

Here

$$\varepsilon_{nk}^\pm = \langle nk | h_{\pm,k} | nk \rangle, \quad \delta_{nk}^\pm = \langle nk | \tilde{\Delta}_{\pm,k} | nk \rangle. \tag{60}$$

For the expression of $W_{\pm i}$, in the present case there is also a symmetry $k \mapsto -k$, so we would like to define a topological invariant on the independent region $k \in [0, \pi]$. Using $u_{T,k} m_k^* = m_{-k} u_{T,k}$, we may set

$$\mathcal{B}_{-,k} = u_{T,-k} \mathcal{B}_{+,-k}^*. \tag{61}$$

Then

$$q_{-,k} = \mathcal{B}_{-,k}^\dagger (h_k + i\Delta_k u_{T,k}^*) \mathcal{B}_{-,k} \tag{62}$$

$$= \mathcal{B}_{+,-k}^T u_{T,-k}^\dagger (h_k + i\Delta_k u_{T,k}^*) u_{T,-k} \mathcal{B}_{+,-k}^* \tag{63}$$

$$= \mathcal{B}_{+,-k}^T (h_{-k}^* - i\Delta_{-k}^* u_{T,k}^T) \mathcal{B}_{+,-k}^* \tag{64}$$

$$= q_{+,-k}^*. \tag{65}$$

From this, one checks that $W_i = W_{-i}$. To define the invariant on the independent integration region $k \in [0, \pi]$, note the relations at TRIM,

$$q_{-,0} = q^*_{+,0}, \quad q_{-,\pi} = q^*_{+,\pi}. \tag{66}$$

Then the following is a well-defined winding number:

$$W_m = \frac{1}{2\pi i}\left(\int_0^\pi d\log\det q_{+,k} + \int_\pi^0 d\log\det q^*_{-,k}\right) \in \mathbb{Z}. \tag{67}$$

Rewriting it,

$$W_m = \frac{1}{2\pi i}\int_0^\pi (d\log\det q_{+,k} + d\log\det q_{-,k}) \in \mathbb{Z}. \tag{68}$$

To obtain a gauge-independent expression that does not depend on the choice of $\mathcal{B}_{\pm,k}$, define

$$W_m[H_k] := \int_0^\pi d\log\det q_k \in \mathbb{R}, \tag{69}$$

and subtract the contribution of the trivial Hamiltonian:

$$W_m[H_k] - W_m[H_k^{\text{triv}}] \in \mathbb{Z}. \tag{70}$$

The Fermi-surface formula is

$$W_m[H_k] - W_m[H_k^{\text{triv}}] = -\frac{1}{2}\sum_{\varepsilon_{nk}=0, k\in(0,\pi)} \text{sgn}(\partial_k\varepsilon_{nk})\text{sgn}(\delta_{nk}). \tag{71}$$

References

[1] Xiao-Liang Qi, Taylor L. Hughes, and Shou-Cheng Zhang, *Topological invariants for the Fermi surface of a time-reversal-invariant superconductor*, Phys. Rev. B **81**, 134508, published 5 April 2010.