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Topological Classification and Stability of Fermi Surfaces

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In the framework of the Cartan classification of Hamiltonians, a kind of topological classification of Fermi surfaces is established in terms of topological charges. The topological charge of a Fermi surface depends on its codimension and the class to which its Hamiltonian belongs. It is revealed that six types of topological charges exist, and they form two groups with respect to the chiral symmetry, with each group consisting of one original charge and two descendants. It is these nontrivial topological charges which lead to the robust topological protection of the corresponding Fermi surfaces against perturbations that preserve discrete symmetries.

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For a Fermi gas at zero temperature, a Fermi surface (FS) naturally arises as the boundary separating the occupied and empty states in (ω, k) space. As is known, when weak interactions or perturbations and disorders are introduced, some FSs still survive though the occupation of states may be shifted dramatically, while some others are easily gapped. Such a kind of FS stability originates from its topological property of the Green’s function or the Feynman propagator for fermionic particles, G(ω, k) = (iω − H)⁻¹, which was first pointed out by Volovik in Ref. [1]. Generally speaking, an FS is robust against weak interactions or perturbations and disorders, if it has a nontrivial topological charge that provides the protection; otherwise, it is vulnerable and easy to be gapped. The most general case is that a Hamiltonian is not subject to any symmetry, where the topological charge is formulated by the homotopy group π[GL(N, C)]. This general case was addressed in Refs. [1,2] and analyzed in the framework of the K theory [3]. Notably, real physical systems have normally certain symmetries, making it necessary and significant to develop a corresponding theory for symmetry-preserving cases.

It is known that the symmetry of a quantum system can always have either a unitary representation or an antiunitary one in the corresponding Hilbert space. The unitary symmetries, such as rotation, translation, and parity symmetries, are easy to be broken by weak interactions or perturbations and disorders, while the antiunitary symmetries, such as the time-reversal symmetry (TRS) and charge conjugate or particle-hole symmetry (PHS), can usually be preserved. Thus we are motivated to develop a unified theory to classify the FSs of systems with the two so-called reality symmetries, namely, TRS and PHS, which seems to be fundamentally important. In this Letter, by taking into account the two reality symmetries and introducing six types of topological charges, a new kind of complete classification of all FSs is obtained, explicitly illustrated in Table II. Moreover, an intrinsic relationship between the symmetry class index and the codimension number is established, which provides us a unique way for realizing any type of FS with a high codimension.

Let us first introduce how to classify all sets of Hamiltonian involving the above-mentioned two reality symmetries, as done in the random matrix theory [4,5]. It turns out that the chiral symmetry (CS) has to be introduced for a complete set of classification. If a unitary symmetry represented by K can anticommute with the Hamiltonian H, i.e., {K, H} = 0, it corresponds to the CS. In fact, the combined symmetry of TRS and PHS is a kind of chiral symmetry. On the other hand, two chiral symmetries can be combined to commute with H, which makes H diagonal. Thus it is sufficient to consider only one chiral symmetry. Based on these considerations [6–8], a kind of complete classification of all sets of Hamiltonian can be obtained with respect to the three symmetries. As is known, the TRS and PHS are both antiunitary and can be expressed in a unified form:

\[ H(k) = \epsilon_c C H^T(-k) C^{-1} \]

where \( \epsilon_c \) = +1(-1) denotes TRS (PHS) and \( \eta_c = \pm 1 \). As a result, each reality symmetry may take three possible types (even, odd, and absent), and thus there are nine classes. In addition, considering that the chiral symmetry may be preserved or not when both reality symmetries are absent, we can have ten classes, as summarized in Table I, which is the famous Cartan classification of Hamiltonians in the random matrix theory [4,5], which may be easily understood in the present framework [6–9].

For a system with spatial dimension d, the FS is a compact submanifold of dimension \( d - p \) if the (ω, k) space is compact. We may define the codimension of the FS as p. Topological charges can be defined on a chosen \( p \)-dimensional submanifold in the (ω, k) space enclosing the FS in its transverse dimension. The two reality symmetries are essentially different from the CS, which lies in that each of the reality symmetries relates a k point to the \( -k \) point in k space, while the CS acts on every k.
This difference leads to the requirement that a chosen submanifold in \((\omega, k)\) space has to be centrosymmetric around the origin in order to preserve either of the reality symmetries.

Generally, the topological property of an FS depends on its codimension and symmetry \([10]\). After the detailed analysis, we are able to classify all classes in an appropriate form illustrated in Table II, which is one of main results of this work. In each case, as seen in Table II, a kind of topological charge is designated to the FS. Topological charges \(0, Z, Z_2^{(1,2)},\) and \(2Z\) correspond, respectively, to \(0,\) an integer, an integer of mod \(2,\) and an even integer. As illustrated in the table, the ten classes can be divided into real and complex cases according to whether or not they have either of the reality symmetries. On the other hand, they can also be put into the chiral and nonchiral cases depending on whether or not they have the CS. Actually, from this kind of classification, we can find that there are six types of topological charges, which form two groups in terms of the CS, with each group consisting of an original one \((Z)\) and the two descendants \((Z_2^{(1)}, Z_2^{(2)})\) \([11]\). In the chiral or nonchiral real case, all of the four types of FSs can be realized for any given number of codimension. It is also clear that the complex and real cases have different periodicities: One is of a twofold periodicity, while the other is of an eightfold one. Obviously, for the complex case, we can introduce a matrix element \(C(p, i)\) to denote the topological charges listed in Table II, where \(i = \text{odd (even)}\) number corresponds to the class A (AIII) and \(p\) is the number of the codimension. In this way, \(C(p, i)\) satisfies the relation \(C(p, i) = C(p + n, i + n)\) with \(n\) an integer and \(i \mod 2\). For the real case, we can also introduce another matrix element \(R(p, i)\), where \(i = 1, \ldots, 8\) denote the classes AI, BDI, D, DIII, AII, CLI, C, and CI, respectively. Intriguingly, we can also find

\[
R(p, i) = R(p + n, i + n)
\]

with \(i \mod 8\), which establishes an intrinsic relationship between the symmetry class index and the codimension number. More significantly, based on this relationship, we are able to realize any type of FS with a high codimension by reducing its codimension to an experimentally accessible one with the same CS, i.e., \(p = 1, 2, 3\). Actually, the above relation and the twofold periodicity as well as the eightfold one originated from the Bott periodicity of \(GL(N, C)\). In particular, the present eightfold periodicity is induced by the two reality symmetries enforcing on the twofold Bott periodicity and, thus, is different from the eightfold Bott periodicity for \(O(N)\) and \(Sp(N)\) \([12]\).

Let us look at the most general case, i.e., the class A, in the absence of any symmetry. The basic idea to classify FSs in terms of the topology may be learned from this case, which was already discussed in Ref. \([3]\). We here follow it for a pedagogical purpose. The Green’s function can be written as

\[
G(\omega, k) = \frac{1}{i\omega - H(k)},
\]

which is regarded as an \(N\)-dimensional matrix. FSs are defined to be connected to the zero energy. Formulating topological charges in terms of the Green’s function has an advantage when handling interacting systems, which is addressed in Refs. \([3, 13, 14]\). Generally, the FS consists of branches of compact manifolds in \(k\) space. For a specific branch with dimension \(d - p,\) a \(p\)-dimensional sphere \(S^p\) can always be picked up from \((\omega, k)\) space to enclose this branch in its transverse dimension. \(G^{-1}(\omega, k)\) is nonsingular for each \((\omega, k)\) restricted on the \(S^p\); in other words, it is a member of \(GL(N, C)\). Then \(G^{-1}(\omega, k)\) restricted on the \(S^p\) can be regarded as a mapping from \(S^p\) to \(GL(N, C)\). As all these mappings can be classified by the homotopy group \(\pi_p[GL(N, C)]\), \(G^{-1}(\omega, k)\) on the \(S^p\) is in a certain homotopy class. In the so-called stable regime, \(N > p/2\), \(\pi_p[GL(N, C)]\) satisfies the Bott periodicity \([12]\):

\[
\pi_p[GL(N, C)] \simeq \mathbb{Z}/p \simeq \mathbb{Z}/p\mathbb{Z}.
\]
Since physical systems are always in the stable regime, only the mappings on $S^p$ for FSs with the odd codimension $p = 2n + 1$ can be in a nontrivial homotopy class, while ones for the even codimension $p$ are always trivial. In other words, FSs with the even codimension $p$ are always trivial and vulnerable against weak perturbations, while ones with odd codimension can be classified by $\pi_p(GL(N, \mathbb{C})) \cong \mathbb{Z}$, and its stability is topologically protected against any weak perturbations for the nontrivial one. We emphasize that, since the class A is not subject to any symmetry, the perturbation can be quite arbitrary. In addition, the concrete shape of the $S^p$ is irrelevant in principle, and the only requirement is that it is an orientable compact submanifold in $(\omega, \mathbf{k})$ space with dimension $p$, which is distinctly different from the cases of reality symmetries. The homotopy number of a mapping for an FS is named as the topological charge of the FS, which can be calculated from the following formula:

$$N_p = C_p \int_{S^p} \text{tr}(GdG^{-1})^p$$

with

$$C_p = -\frac{n!}{(2n + 1)! (2\pi i)^{n+1}}.$$  

The $\mathbb{Z}$ type of FSs in class A is thus obtained. Once an FS has nontrivially this topological charge, it can survive under any weak perturbations in the absence of any symmetry [15]. But the topologically trivial FSs can be gapped due to the perturbations. Both cases can be seen in $^3\text{He}$ [1], where two Fermi points in $^3\text{He}$-A phase are topologically protected with charge $\pm 2$ individually, while the Fermi line in the planar phase cannot be topologically charged because its codimension is even. The FS of another simple model Hamiltonian $\mathcal{H} = g(\mathbf{k}) \cdot \mathbf{\sigma}$ belongs also to this topological class [16], where $\sigma_i$ are Pauli matrices.

We now turn to consider the case when the system has a chiral symmetry denoted by $\mathcal{K}$, i.e.,

$$\{ \mathcal{H}, \mathcal{K} \} = 0.$$  

Systems with this symmetry have a crucial property: For any eigenstate $|\alpha\rangle$ of $H$ with the energy $E_\alpha$, $K|\alpha\rangle$ is also an eigenstate of $H$ but with the energy $-E_\alpha$. The Hamiltonian associated with this symmetry can always be diagonalized in $\mathbf{k}$ space on the basis that diagonalizes $\mathcal{K}$ and thus can be written as

$$h(\mathbf{k}) = \begin{pmatrix} 0 & u(\mathbf{k}) \\ u^\dagger(\mathbf{k}) & 0 \end{pmatrix}.$$  

On the $S^p$ that is chosen to enclose an FS of dimension $d = p$, $h(\mathbf{k})$ also takes this form, which makes the topological charge defined in Eq. (4) always vanishing. However, $u(\mathbf{k})$ can be regarded as a mapping from $S^{p-1}$ (set $\omega = 0$) to $GL(N/2, \mathbb{C})$, which may be in a nontrivial homotopy class of $\pi_{p-1}(GL(N/2, \mathbb{C}))$. In this sense, there exist nontrivial FSs for the even number of codimension, i.e., $p = 2n$. The homotopy number may be calculated as

$$\nu_p = C_{p-1} \int_{S^{p-1}} \text{tr}(u(\mathbf{k})d(u^{-1}(\mathbf{k}))^{p-1}.$$  

As the homotopic number is real, it can also be calculated by $u^\dagger(\mathbf{k})$. Thus the homotopic number can also be expressed by the Green’s function:

$$\nu_p = \frac{C_{p-1}}{2} \int_{S^{p-1}} \text{tr}(\mathcal{K}(GdG^{-1})^{p-1}|_{\omega = 0}).$$

The homotopic number is referred to as the chiral topological charge of the FS.

For this $\mathbb{Z}$-type topological charge in class AIII, if it is nontrivial, the FS is stable against any perturbations that do not break the CS. However, the topological protection is not as stable as that induced by Eq. (4), because the FS is gapped if ever the CS is broken. For instance, the honeycomb lattice model has two Dirac cones with the low-energy effective Hamiltonian $\mathcal{H}_a = k_x^2 + k_y^2$, respectively, with $\sigma_3$ representing the chiral symmetry that is the sublattice symmetry here [17]. The two Dirac cones have $\nu_2 = \pm 1$, respectively, [16], and thus they are topologically stable as far as this chiral symmetry is preserved. More remarkably, according to our present theory, it is noted that the stability of FSs in this model was recently verified in an ultracold atom experiment [18]. In addition, it was also seen clearly from this experiment that if the sublattice symmetry is broken, a gap may be opened in the whole Brillouin zone. It is noted that this type of topological charge was also seen in a superconducting system [19]. Another interesting model Hamiltonian $\mathcal{H} = (k_x^2 - k_y^2)\sigma_1 \pm 2k_xk_y\sigma_2$ also gives out this type of topological charge $\nu_2 = \pm 2$ [16].

When TRS and PHS are considered, many $\mathbb{Z}$-type topological charges vanish. As for the first descendant (i.e., $\mathbb{Z}_2$) of a $\mathbb{Z}$ type in a nonchiral real case, e.g., the case of codimension 2 that is labeled one row above that of codimension 3 ($\mathbb{Z}$-type) in class AII in Table II, the Green’s function restricted on the chosen $S^p$ can be classified by a $\mathbb{Z}_2$-type topological charge. The key idea is that $G(\omega, \mathbf{k})|_{S^p}$ can be continuously extended to $\tilde{G}(\omega, \mathbf{k}; u)$ on the $(p + 1)$-dimensional disk by introducing an auxiliary parameter $u$ (ranging from 0 to 1) with the two requirements: (i) $\tilde{G}(\omega, \mathbf{k}; 0)|_{S^p} = G(\omega, \mathbf{k})|_{S^p}$ and (ii) $\tilde{G}(\omega, \mathbf{k}; 1)|_{S^p}$ is a diagonal matrix, such that $\tilde{G}_{\alpha\alpha} = (i\omega - \Delta)^{-1}$ for empty bands and $\tilde{G}_{\beta\beta} = (i\omega + \Delta)^{-1}$ for occupied bands, where $\Delta$ is a positive constant [13,20]. The validity of the extension is based on the fact that $G(\omega, \mathbf{k})$ restricted on $S^p$ is always trivial in the homotopic sense in this case. This topological charge in terms of Green’s function is formulated as
with
\[ C_p' = -\frac{2(p/2)!}{p!(2\pi i)^{(p/2)+1}}, \]
where \(\sim\) has been dropped for brevity. The topological charge is defined in a similar way to the Wess-Zumino-Witten term in quantum field theory [21], and the \(\mathbb{Z}_2\) character comes from the fact that two different extensions differ to an even integer, as demonstrated in Ref. [13]. As a concrete illustration, we here exemplify this \(\mathbb{Z}_2\)-type topological charge by a model Hamiltonian defined in two spatial dimensions: \(\mathcal{H}(\mathbf{k}) = k_x \sigma_1 + k_y \sigma_2 + (k_x + k_y)\sigma_3\), which has only a TRS with \(C = i\sigma_2\) and \(\eta = -1\) according to Eq. (6) and thus belongs to class AII in Table I and corresponds to the case of \(R(2,5)\) in Table II. The corresponding FS at the origin in the \((\omega, \mathbf{k})\) space is found to have a nontrivial topological charge \(N_p^{(1)} = 1\) from Eq. (6) [16].

For the second descendant with the codimension \(p\) (i.e., \(\mathbb{Z}_2^{(2)}\)), e.g., the case of codimension 3 with two rows above that of codimension 5 in class C in Table II, a \(\mathbb{Z}_2\)-type topological charge can also be defined on the chosen \(S^p\). To define the \(\mathbb{Z}_2\)-type topological charge, the \(G(\omega, \mathbf{k})\) is smoothly extended to a two-dimensional torus \(T^2\) parameterized by the two auxiliary parameters \(u\) and \(v\) (both ranging from \(-1\) to \(1\)) with the three requirements: (i) \(\tilde{G}(\omega, \mathbf{k}; 0,0)|_{S^p} = G(\omega, \mathbf{k})|_{S^p}\), (ii) \(\tilde{G}(\omega, \mathbf{k}; u, v)|_{S^p} = e^{i\mathbf{k} \cdot \mathbf{r}} G(\omega, -\mathbf{k}; -u, -v)|_{S^p} C^{-1}\), referring to Eq. (1), and (iii) \(\tilde{G}(\omega, \mathbf{k}; 1, 1)|_{S^p}\) corresponds to a trivial system, such as \(\tilde{G}_{aa} = (i\omega - \Delta)^{-1}\) for empty bands and \(\tilde{G}_{\beta\beta} = (i\omega + \Delta)^{-1}\) for occupied bands. The corresponding topological charge is defined as [13,20]
\[ N_p^{(2)} = C_{p+2} \int_{S^p \times T^2} \text{tr} (GdG^{-1})^{p+2} \mod 2, \]
where \(\sim\) has been dropped and the \(C_{p+2}\) is defined in Eq. (4). As a topological charge of FSs, its physical meaning is analogous to that of Eq. (6).

Similar to the nonchiral case, a \(\mathbb{Z}\) chiral topological charge is associated with two descendants: a son and a grandson. The \(\mathbb{Z}_2\)-type topological charge of the son originated from the chiral topological charge defined in Eq. (5) in the same spirit of that Eq. (6) originated from Eq. (4), which is given by
\[ N_p^{(1)} = C_p' \int_{S^{p-1}} \int_0^1 du \text{tr}(\mathcal{K}(GdG^{-1})^{p-1} G\partial_\omega G^{-1}|_{\omega=0}) \mod 2, \]
where \(\mathcal{K}\) is the matrix to represent the chiral symmetry, \(S^{p-1}\) is the chosen \(S^p\) restricted on \(\omega = 0\), and \(G\) is extended by an auxiliary parameter ranging from 0 to 1 with the same requirements for introducing Eq. (6). The \(\mathbb{Z}_2\) topological charge for the grandson can also be defined in the same spirit of writing out Eq. (7). We extend the \(G(\omega, \mathbf{k})|_{S^p}\) to a two-dimensional torus \(T^2\) parameterized by two auxiliary parameters \(u\) and \(v\) (both ranging from \(-1\) to \(1\)) with the four requirements: The first three requirements are the same as those of the nonchiral counterpart in Eq. (7), while the fourth one is that the chiral symmetry is preserved on \(T^2\), which also permits that either of the reality symmetries is applicable in the second requirement. The \(\mathbb{Z}_2\) topological charge is written as
\[ \nu_p^{(2)} = C_{p+1} \frac{2}{2} \int_{S^{p-1} \times T^2} \text{tr}(\mathcal{K}(GdG^{-1})^{p+1}|_{\omega=0}) \mod 2, \]
where \(C_{p+1}\) is defined in Eq. (4).

The physical meanings of topological charges for the eight classes with TRS and/or PHS are elaborated as follows. The FS(s) with a certain codimension is always distributed centro symmetrically, since either TRS or PHS relates \(\mathbf{k}\) to \(-\mathbf{k}\). Thus there exist two possibilities: (i) The FS with codimension \(p\) resides at the origin in \((\omega, \mathbf{k})\) space; (ii) the FS(s) is centro symmetric outside of the origin. For the first case, we can choose an \(S^p\) in \((\omega, \mathbf{k})\) space to enclose the FS and use the corresponding formula to calculate the topological charge. If the topological charge is nontrivial, the FS is stable against perturbations provided the corresponding symmetries are preserved. For the second case, the FS(s) is usually spherically distributed, so two \(S^p\)s can be chosen to sandwich the FS(s) in its transverse dimension. The difference of the topological charges calculated from the two \(S^p\)s is the topological charge of the FS(s). If it is nontrivial, the FS(s) is topologically stable when the corresponding symmetries are preserved.

Before concluding this Letter, we wish to emphasize that the topological charges of FSs addressed here are closely connected to topological insulators or superconductors [22], and therefore this work may provide a new and deep insight for studying them.

In conclusion, FSs in all of the ten symmetry classes have been classified appropriately in terms of topological charges. It has been revealed that when an FS is associated with a nontrivial topological charge, this FS is topologically protected by the corresponding symmetry.

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Noting that the Fermi surface may consist of several disconnected parts, each having different topological characteristics, for simplicity and without loss of generality, we here focus only on one branch.

\[ Z \] and \( 2Z \) are regarded to be the same type of topological charge given by Eq. (4) [Eq. (5)] in the chiral (nonchiral) real case, while \( Z_2^{(1)} \) and \( Z_2^{(2)} \) are different types.


Noting that for the square lattice Hubbard model at half filling with a very large \( U \) (no continuum approximation could be used), a seemingly perturbative effect of adding one electron or hole will significantly shift the ground state of the system, such that it is effectively nonperturbative and thus may not be taken care of from the present topological analysis.


