Motivated by the geometric character of spin Hall conductance, the topological invariants of generic superconductivity are discussed based on the Bogoliubov-de Gennes equation on lattices. They are given by the Chern numbers of degenerate condensate bands for unitary order, which are realizations of Abelian chiral anomalies for non-Abelian connections. The three types of Chern numbers for the \( x, y \) and \( z \)-directions are given by covering degrees of some doubled surfaces around the Dirac monopoles. For nonunitary states, several topological invariants are defined by analyzing the so-called \( g \)-helicity. Topological origins of the nodal structures of superconducting gaps are also discussed.

The importance of quantum-mechanical phases in condensed matter physics has been recognized and emphasized for recent several decades. The fundamental character of a vector potential is evident in the Aharonov-Bohm effect where the \( U(1) \) gauge structure is essential and a magnetic field in itself plays only a secondary role \[1\]. Topological structures in quantum gauge field theories have also been studied and extensive knowledge has been accumulated \[2\]. Quantum mechanics itself supplies a fundamental gauge structure \[3\]. It is known as geometrical phases in many different contexts, where gauge structures emerge by restricting physical spaces. The quantum Hall effect is one of the key phenomena to establish the importance of geometrical phases \[4\]. The topological character of the Hall conductance was first realized by the Chern number expression, where the Bloch functions define “vector potentials” in the magnetic Brillouin zone accompanied with a novel gauge structure \[5\]. Further the ground state of the fractional quantum Hall effect is a complex many-body state where another kind of gauge structure emerges \[6\]. These quantum states with nontrivial geometrical phases are characterized by topological orders which extend an idea of order parameters, which is closely related to the quantum Hall effect in three-dimensions \[16\], \[17\]. Various types of the nodal structures are not accidental but have fundamental topological origins. A possible time-reversal symmetry-breaking and an unconventional gap structure are proposed based on the experiments \[32\].

**Bogoliubov-de Gennes hamiltonian.** Let us start from the following hamiltonian on lattices with spin-rotation symmetry:

\[
H = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij} V_{ij}^{\sigma_1 \sigma_2 ; \sigma_3 \sigma_4} c_{i\sigma_1}^\dagger c_{j\sigma_2} c_{j\sigma_3} c_{i\sigma_4} - \mu \sum_i c_{i\sigma}^\dagger c_{i\sigma}
\]

where \( c_{i\sigma} \) is the electron annihilation operator with spin \( \sigma \) at site \( i \), \( t_{ij} = t_{ji} \), \( V_{ij}^{\sigma_1 \sigma_2 ; \sigma_3 \sigma_4} = (V_{ij}^{\sigma_2 \sigma_1 ; \sigma_3 \sigma_4})^* \), \( V_{ij}^{\sigma_1 \sigma_2 ; \sigma_3 ; \sigma_4} = V_{ji}^{\sigma_2 \sigma_1 ; \sigma_3 ; \sigma_4} \) and \( \mu \) is a chemical potential. Summations over repeated spin indices \( \sigma \) are implied hereafter. The mean field BCS approximation leads to:

\[
\mathcal{H} = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij} (\Delta_{ij}^{\sigma_1 \sigma_2} c_{j\sigma_2} c_{i\sigma_1} + \text{h.c.}) - \mu \sum_i c_{i\sigma}^\dagger c_{i\sigma},
\]

where the order parameters \( \Delta_{ij}^{\sigma_1 \sigma_2} = -\Delta_{ji}^{\sigma_2 \sigma_1} \) are given by \( \Delta_{ij}^{\sigma_1 \sigma_2} = V_{ij}^{\sigma_2 \sigma_1 ; \sigma_3 \sigma_4} (c_{j\sigma_2} c_{i\sigma_1}) \). The usual mean field theory leads to the gap equation of which a solution gives an order parameter. Here we do not follow this.
procedure but a priori assume order parameters which may be realized for some interactions $V_{\sigma\sigma'}\sigma\sigma'$. Let us consider the two cases separately. (i) singlet states $\Delta_{ij} = -\Delta_{ji} = \psi_{ij}i\sigma y_1$, $\psi_{ij} = \psi_{ji})$ and (ii) triplet states $\Delta_{ij} = \Delta_{k\ell} = (d_{ij} \cdot \sigma)i\sigma y_1$, $d_{ij} = -d_{ji}$, where $(\Delta_{ij})^{\sigma\rho} = \Delta_{ji}^{\rho\sigma}$ is a $2 \times 2$ matrix in the spin space and $\sigma$ denotes matrix transpose. Now assume the translational symmetry, namely, $t_{ij} = t(i-j)$, $\Delta_{ij} = \Delta(i-j)$ and also the absence of a magnetic field, that is, $t(i-j)$ to be real. Then, except a constant, the BdG Hamiltonian is given by a $4 \times 4$ matrix $h_k$ as

$$\mathcal{H} = \sum_k c_k^\dagger h_k c_k,$$

where $c_k = (c_k^\dagger (k), c_k^\dagger (-k), c_k(-k), c_k(-k))$ with $c_k(k) = 1/\sqrt{V} \sum \delta^{ij}\delta^{r\ell} c_{ijr\ell}$, $c_k = \sum \epsilon^{ij}\epsilon^{r\ell} c_{ijr\ell} t(\ell) - \mu$, $\Delta_k = \sum \epsilon^{ij}\epsilon^{r\ell} \Delta(\ell), \Delta_{-k} = -\Delta_k$, $\sigma_0 = (1 0 0 1)$, and $V$ is a volume of the system. The order parameter is given by $\Delta_k = \psi_{ij}i\sigma y_1$, $\Delta_k = \Delta_k$ for singlet states and $\Delta_k = (d_{ij} \cdot \sigma)i\sigma y_1$, $\Delta_k = \Delta_k$ for triplet states ($\psi_k$ is even and $d_k$ odd in $k$).

The BdG Hamiltonian has a particle-hole symmetry. If $h_k(u_k \upsilon_k)$, then $C(u_k \upsilon_k)$ is also an eigenstate with energy $-E_k$ where $C = \rho y K$ for singlet states and $C = -\rho y K$ for triplet states ($u_k$ and $\upsilon_k$ are the two-component vectors and $K$ is a complex conjugate operator and the Pauli matrices $\rho$ operate on the two component blocks.) Then it is useful to consider $h_k^2 = c_k^2 \rho_0 + \left(\Delta_k \Delta_k^\dagger \right)_k$. For singlet states, we have $\Delta_k \Delta_k^\dagger = \Delta_k \Delta_k^\dagger = |\psi_k|^2 \sigma_0$ and for triplet states, $\Delta_k \Delta_k^\dagger = |d_k|^2 \sigma_0 - q_k \cdot \sigma$, with a real vector $q_k = d_k \times d_k$, which we call $q$-helicity ($\dagger$ represents hermitian conjugate and * complex conjugate).

**Chern numbers for unitary states.** Singlet order and triplet order with vanishing $q$-helicity are called unitary since $\Delta_k \Delta_k^\dagger = \Delta_k \Delta_k^\dagger \propto \sigma_0$. Nonunitary triplet states $(q_k \neq 0)$ will be discussed later. For unitary states, we define a unitary matrix $\Delta_k^\dagger$ by $\Delta_k = |\Delta_k| \Delta_k^\dagger$, $(|\Delta_k| = |\psi_k|$ for singlet states and $|\Delta_k| = |d_k|$ for triplet states, respectively). Since the spectra are doubly degenerate as will be shown later, fixing phases of the states is not enough to determine Chern numbers by the standard procedure. Instead, one can define non-Abelian vector potentials and fluxes following definitions of generalized non-Abelian connections.

Let us assume that the states are $M$-fold degenerate $(M = 2$ in the present unitary case) as $|\alpha\rangle$, $\alpha = 1, \ldots, M$. Then a non-Abelian connection is defined by $A_{\mu}^{\alpha\beta} = (\alpha | \partial_\mu | \beta\rangle$, $A_{\mu}^{\alpha\beta} = A_{\mu}^{\alpha\beta} d_{\mu} \rho$ and $\partial_\mu = \partial_{\mu_x} + \partial_{\mu_y} + i \epsilon_{\mu_y\mu_z}$. A unitary transformation of a degenerate state $|\alpha\rangle \rightarrow |\bar{\alpha}\rangle = |\alpha\rangle e^{i\omega_{\alpha\beta}}$ ($\omega$: unitary) causes “a gauge transformation” $\bar{\omega} = \omega^\dagger \omega + \omega^\dagger i\omega$. Then the field strength $F = dA + A \wedge A$ is gauge covariant since $\bar{F} = \omega^\dagger F \omega$. One may write $F = \frac{1}{2} F_{\mu\nu} d_{\mu\nu} \wedge d_{\nu\mu}$, $F_{\mu\nu} = \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu} + [A_{\mu}, A_{\nu}]$, $(A_{\mu})^{\alpha\beta} = A_{\mu}^{\alpha\beta}$. Then “a magnetic field” in the $\mu$-direction is $B_\mu = \frac{1}{2} \epsilon_{\mu\lambda\sigma} \text{Tr} F_{\nu\lambda}$. Since $\mathcal{F}$ is unitary invariant, so is $B_\mu$. The total flux passing through the $\nu\lambda$-plane is given by an integral of the magnetic field $B_\mu$ over the two-dimensional Brillouin zone, $T_{\nu\lambda}^2$, ($k_\mu$ is fixed). The first Chern number is $C_{\mu\alpha} = \frac{1}{2\pi} \int_{T_{\nu\lambda}^2} (\Delta_k)^{\alpha\beta} (\bar{\omega})_{\alpha\beta}$. This is the Abelian chiral anomaly discussed in the non-Abelian gauge theories. Here we have considered the cubic lattice. Extensions to other lattice structures is straightforward.

**Dirac monopole in the parameter space.** The BdG equation for the unitary states $(\epsilon_k \sigma_0 - |\Delta_k|) |u_k\rangle = E_k |u_k\rangle$ reduces to

$$(\epsilon_k - \epsilon_0 |\Delta_k|) |u_k\rangle = E_k |u_k\rangle.$$
band in the \( \mu \)-direction, is given by the sum of the Chern numbers of the two vectors \( |R_{\alpha}\rangle \) \((\alpha = 1, 2)\) which are the eigenstates of the 2 \( \times \) 2 hamiltonians

\[
h_k^\alpha = \left( \begin{array}{c|c} 
\epsilon_k & e^{i\theta_{\alpha}} |\Delta_k| \\
\hline
-\epsilon_k & 0 
\end{array} \right) = \sigma \cdot R_\alpha,
\]

where \( R_{\alpha,X} = R \sin \theta \cos \phi_\alpha, \quad R_{\alpha,Y} = R \sin \theta \sin \phi_\alpha \) and \( R_{\alpha,Z} = R \cos \theta \). Namely they are \( C_\mu = \sum_\alpha C_{\alpha,\mu} \). Now we have reduced the problem to calculate the Chern numbers of the eigenstates of the 2 \( \times \) 2 matrices, \( h_k^\alpha \). By mapping from the two-dimensional Brillouin zone to the three-dimensional space, \( T_{\mu \lambda}^2 \ni (k_x, k_y) \rightarrow R_{\alpha} \), we obtain a closed oriented surface \( R_{\alpha}(T_{\mu \lambda}^2) \). The wrapping degree of the map around the origin gives a charge of the Dirac monopole sitting there. This is the Chern number \( C_\mu(k_\mu) \) \([17, 22]\).

For the present degenerate case, the map from a two-dimensional point to two three-dimensional points \( T_{\mu \lambda}^2 \ni (k_x, k_y) \rightarrow \{R_{\alpha=1}, R_{\alpha=2}\} \) defines (fixing \( k_\mu \)) the surfaces \( \{R_{\alpha=1}(T_{\mu \lambda}^2), R_{\alpha=2}(T_{\mu \lambda}^2)\} \) which determine the two covering degrees of the maps around the origins, \( N_{\alpha,\mu}(k_\mu) \), \((\alpha = 1, 2)\). They give the Chern numbers \( C_{\alpha,\mu} \) respectively. Since only the condensed states are filled for the superconducting ground state, the Chern numbers of the unitary states are given by

\[
C_\mu(k_\mu) = \frac{1}{2\pi} \epsilon_{\nu \lambda} N_{\nu \lambda}(k_\mu), \quad N_{\nu \lambda}(k_\mu) = \sum_\alpha N_{\alpha,\nu \lambda}(k_\mu).
\]

The Chern numbers defined here for the unitary superconductors satisfy \( C_{\mu}(k_\mu) = 4 \) for the singlet order and \( C_{\mu}(k_\mu) = 2 \) for the triplet order. \([39]\)

**Nonunitary states.** In these triplet states, there are no degeneracies in solutions of the BdG equation. There are four quasiparticle bands, which are classified by the \( q \)-helicity as

\[
(\sigma \cdot q_\mu) u_+ = \pm q_k u_+, \quad q_k = |q_\mu|,
\]

\[
h_k^\mu \psi_+^\pm = \left( \begin{array}{c|c}
\epsilon_k & e^{i\theta_\mu} |\Delta_k| \\
\hline
-\epsilon_k & 0 
\end{array} \right) \psi_+^\pm = \pm q_k \psi_+^\pm,
\]

\[
\psi_+^\pm = \left( \begin{array}{c}
u_+ \\
-\nu_-
\end{array} \right), \quad \psi_-^\pm = \left( \begin{array}{c}
u_- \\
-\nu_+
\end{array} \right), \quad v_\pm = -i\sigma_y u_\pm.
\]

Then states with helicity \( \pm q_k \) and energy \( \pm E_{+q} = \pm \sqrt{\epsilon_k^2 + |d_k|^2 + q_k} \), are \( |\pm E_{+q}\rangle = U_+ \eta_{+q}^\pm \), where \( U_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} u_+ & u_+ \ 
 v_+ & -v_+
 \end{pmatrix} \) and the orthonormal vectors \( \eta_{+q}^\pm \) are determined as the eigenvectors of the reduced 2 \( \times \) 2 hamiltonian \( h_{+q} = U_+^\dagger h U_+ \) with energies \( \pm E_{+q} \). The hamiltonian \( h_{+q} \) is traceless and it can be expressed by the Pauli matrices, \( h_{+q} = \sigma \cdot R_{+q} \) where \( R_{+q} = (\epsilon, \Im d_{+q}, -\Re d_{+q}) \) is a real vector and \( d_{+q} = u_+^\dagger (d_k \cdot \sigma) u_- \). As for the helicity \( -q_k \) state, one can follow almost the same procedure and obtain the reduced BdG hamiltonian similarly. Here we can define several topological invariants. As discussed above, the states with \( \pm q_k \)-helicities and energies \( \pm E_{\pm q} \) are non-degenerate,

\[
h_k |\epsilon_{E_{\pm q}}\rangle = \epsilon_{E_{\pm q}} |\epsilon_{E_{\pm q}}\rangle, \quad Q_k |\epsilon_{E_{\pm q}}\rangle = \epsilon q_{|\epsilon_{E_{\pm q}}\rangle},
\]

\[
Q_k = \left( \begin{array}{c}
\sigma \cdot q_k & 0 \\
0 & -\sigma \cdot q_k
\end{array} \right), \quad [h_k, Q_k] = 0,
\]

where \( E_{\pm q}(k) = \sqrt{|\epsilon_k|^2 + |d_k|^2 + q_k}, \quad (\epsilon_k = \pm q_k \text{ and } \epsilon_q = \pm) \). Then the standard Chern number \( C^\mu_\mu(k_\mu) \) in the \( \mu \)-direction for a fixed \( k_\mu \) is obtained by the standard way \([13]\).

Also we have topological invariants in the \( \mu \)-direction \( N^\mu_\mu(k_\mu) \). They are wrapping degrees around the origin of the map \( (k_x, k_y) \rightarrow q(k) = q_k \), which define closed surfaces \( q(T_{\mu \lambda}^2) \) in three-dimensions \([13]\). Further we have other topological invariants \( N^\mu_\mu(k_\mu) \), which are also wrapping degrees of the map around the origin, \((k_x, k_y) \rightarrow R_{\pm q}(k) \). (The reduced hamiltonians are \( h_{\pm q} = R_{\pm q} \cdot \sigma \) for the \( q \)-helicity \( \pm q_k \).

Up to this point, topological arguments have been applied to gapful cases. However, the nodal structure of the gap function is, in fact, characterized by the topological description. Formally we have treated a three-dimensional superconductivity as a collection of two-dimensional systems parametrized by, say, \( k_z \). In \( R \)-space, closed surfaces parametrized by \((k_x, k_y) \) are generally away from the monopole at the origin. As \( k_z \) is varied, the surfaces move around and they can pass through the monopole. Since the distance between a point on a surface and the monopole gives a half of the energy gap \( E_q(k_x, k_y; k_z) \), the gap closes at the value of \( k_z \) when the monopole is on the surface. Thus the nodal structure of the superconductivity is point-like generically if the time-reversal symmetry is broken. When the Chern number jumps as \( k_z \) varies, the superconducting gap has to be closed due to topological stability of Chern numbers. Also a non-zero Chern number implies that the corresponding two-dimensional system has a non-trivial topological order. The superconducting node is considered as the critical point of the quantum phase transition between two states with different topological orders.

To make the discussion clear, let us take an example \( \Delta_k = d_0^t \begin{pmatrix} \sin k_x + i \sin k_y \sigma_x \end{pmatrix} \epsilon_{k} = -2t \cos k_x + \cos k_y \cos k_z - \mu, \quad (t > 0) \) \([17]\). This is an analogue of the Anderson-Brinkman-Morel(ABM) state in \( 3^\text{He} \) superfluid. For a fixed value of \( k_z \), the surface is reduced to that of the chiral \( p \)-wave order parameter with a modified chemical potential, \( \mu - 2t \cos k_z \). (we can recover the ABM state, \( d_k \rightarrow (0, 0, d_0^t(k_z + ik_y)) \) in the limit of \( \mu \rightarrow -6t + 0, k \rightarrow 0 \)) There are two quantum phase transitions which are accompanied by jumps of the Chern number between \(-2 \) and \(+2 \) for \(-6t < \mu < 2t \). These correspond to the gap nodes at the north and south poles on the Fermi surface. In Fig. 1, surfaces \( R_{\pm}(T_{\mu \lambda}^2) \) are shown with the monopole at the origin. The Chern number jumps between \(+2 \) and \(+2 \) for \(-2t < \mu < 2t \) and \(+2 \) for \(2t < \mu < 6t \).
For line nodes, we need additional constraints to keep the monopole on the closed surfaces when \( k_z \) is varied. To make a discussion simple, we take singlet order or triplet order with \( d_x = d_y = 0 \) and \( d_z \neq 0 \). Further let us require that the order parameters are real, namely we have a time-reversal symmetry. Then the closed surfaces in the \( R \)-space collapse into a board like region on the \( R_x - R_y \) plane and one can expect a situation where the monopole moves along the surface when \( k_z \) is varied.

Thus a line node appears in the superconducting gap. As shown in this example, the nodal structure of the superconductivity has a fundamental relation to topological order. The detailed discussion on this point will be given elsewhere.\[26\]

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[31] A nontrivial gauge structure in superfluid \(^3\)He was discussed from a different point of view by [23, 24].
[32] Possible point nodes in superconductivities of the filled-sketterudite PrOs\(_2\)Sb\(_12\) associate with a breaking of a time-reversal symmetry are discussed in [25, 26].
[33] The sum is over a half of the Brillouin zone to avoid double counting.
[34] The 4 \( \times \) 4 matrices are spanned by \( \rho_1 \otimes \sigma_j, i, j = 0, \cdots, 3 \).
[35] Summation over the repeated indices \( \mu \) is assumed.
[36] \( T_{2 \lambda} = \{ (k_x, k_y) \mid k_x, k_y \in [0, 2\pi) \} \) and \( k_\mu \) runs over \([0, \pi]\) to avoid double counting.
[37] It is a similar procedure to fix phases of states for non-degenerate cases [5].
[38] \( R_\mu (\sigma) = \sum_{\nu \lambda} \epsilon_{\mu \nu \lambda} \text{Tr} d_\nu (U^{-1} \partial_\nu U) = -\epsilon_{\mu \nu \lambda} \text{Tr} (U^{-1} \partial_\nu U (U^{-1} \partial_\nu U)) = 0 \). It also completes a general proof of the sum rule for the non degenerate states, that is, the sum of the Chern numbers for all bands is zero.
[39] For the singlet case, we have \( N_{1, \mu \lambda} = N_{2, \mu \lambda} \) since \( \phi_1 = \phi_2 + \pi \). Further each \( N_{2, \mu \lambda} \) is even [17, 22]. For the triplet case, \( N_{1, \mu \lambda} \neq N_{2, \mu \lambda} \) generically. However, the some of them is even since we can show \( \phi_1 = +\theta + \text{Arg} \delta \), \( \phi_2 = -\theta + \text{Arg} \delta + \pi \) with some function \( \theta \) where \( d \cdot \sigma \) is unitary equivalent to \( \delta \sigma_3 \). We use a base which diagonalizes \( \Delta_\mu \). Another base which diagonalizes \( d \cdot \sigma \) is also useful. We thank A. Vishwanath for the communication on this point.

FIG. 1: Examples of closed surfaces \( R_1 (T_{xy}) \) which are cut by the \( R_y - R_z \)-plane. The monopole is at the origin. \( t = d_z = 1, \mu = -5 \): (a) \( k_x = 0 \), (b) \( k_x = -2\pi/5 \).