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Superconductivity and Abelian chiral anomalies

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Motivated by the geometric character of spin Hall conductance, the topological invariants of generic superconductivity are discussed based on the Bogoliuvov-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 q helicity. Topological origins of the nodal structures of superconducting gaps are also discussed.

I. INTRODUCTION

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 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 in statistical mechanics to the quantum states without any spontaneous symmetry breaking.[7] We also point out an importance of boundary effects for topologically nontrivial systems. Bulk properties are closely related to edge states and localized states near impurities and vortices.[8–12]

Topologically nontrivial structures in superconductors also have a long history. Recently, following a prediction of flux phases for correlated electron systems,[13] spin Hall conductance is defined for superconductors based on the Bogoliuvov-de Gennes (BdG) equation.[14–17] As for singlet states and triplet states besides equal-spin-pairing states, a map to a parameter space which represents the BdG Hamiltonian is considered.[18] In the parameter space, the Dirac monopole exists and the Chern numbers are analyzed.[19]

In this paper, we establish a topological characterization of *general* superconductors based on the BdG equation on lattices. The energy spectrum of the BdG Hamiltonian are fully used to calculate the Chern numbers of the superconductors. As for the unitary superconductors, condensed matter realizations of chiral anomalies for non-Abelian connections are given explicitly. Topological consideration is useful to distinguish superconductivities with the same pairing symmetry. The present analysis also clarifies nodal structures of superconducting gaps with various anisotropic order parameters, which is closely related to the quantum Hall effect in three dimensions.[20,21] Various types of the nodal structures are not accidental but have fundamental topological origins. A possible time-reversal symmettry-breaking and an unconventional gap structure are proposed based on the experiments.[22]

II. BOGOLIUVOV-DE GENNES HAMILTONIAN

Let us start from the following Hamiltonian on lattices with spin-rotation symmetry:

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

where $c_{i\sigma}$ is the electron annihilation operator with spin σ at site i, $t_{ij} = t_{ji}^*$, $V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4} = (V_{ij}^{\sigma_4\sigma_3;\sigma_2\sigma_1})^*$, $V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4} = V_{ji}^{\sigma_2\sigma_1;\sigma_4\sigma_3}$, and μ is a chemical potential. Summations over repeated spin indices σ are implied hereafter.

The mean field Bardeen–Cooper–Schrieffer approximation leads to

$$\mathcal{H} = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij} (\Delta_{ij}^{\sigma_4\sigma_3 *} c_{j\sigma_3} c_{i\sigma_4} + h.c.) - \mu \sum_i c_{i\sigma}^\dagger c_{i\sigma},$$

where the order parameters ($\Delta_{ij}^{\sigma\sigma'} = -\Delta_{ji}^{\sigma'\sigma}$) are given by

$$\Delta_{ij}^{\sigma_1\sigma_2} = V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4} \langle c_{j\sigma_3} c_{i\sigma_4} \rangle.$$

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 $V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4}$. Let us consider the two cases separately:[26,27] (i) singlet states $\mathbf{\Delta}_{ij}=-\tilde{\mathbf{\Delta}}_{ij}=\psi_{ij}i\sigma_y$, $(\psi_{ij}=\psi_{ji})$ and (ii) triplet states $\mathbf{\Delta}_{ij}=\tilde{\mathbf{\Delta}}_{ij}=(\mathbf{d}_{ij}\cdot\boldsymbol{\sigma})i\sigma_y$, $(\mathbf{d}_{ij}=-\mathbf{d}_{ji})$, where $(\mathbf{\Delta}_{ij})^{\sigma\sigma'}=\Delta_{ij}^{\sigma\sigma'}$ is a 2×2 matrix in the spin space and $\sim$ denotes matrix transpose. (See Appendix A for details.) Now assume the translational symmetry, namely, $t_{ij}=t(i-j)$, $\mathbf{\Delta}_{ij}=\mathbf{\Delta}(i-j)$ 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 4×4 matrix $\mathbf{h}_k$ as

$$\mathcal{H}=\sum_k \mathbf{c}_k^\dagger\mathbf{h}_k\mathbf{c}_k,$$

$$h_k=\begin{pmatrix}\epsilon_k\sigma_0 & \mathbf{\Delta}_k \\ \mathbf{\Delta}_k^\dagger & -\epsilon_k\sigma_0\end{pmatrix}$$

where $\mathbf{c}_k^\dagger=(c_\uparrow^\dagger(\mathbf{k}),c_\downarrow^\dagger(\mathbf{k}),c_\uparrow(-\mathbf{k}),c_\downarrow(-\mathbf{k}))$ with $c_\sigma(\mathbf{k})=(1/\sqrt{V})\Sigma_j e^{i\mathbf{k}\cdot\mathbf{r}_j}c_{j\sigma}$, $\varepsilon_k=\Sigma_\ell e^{-i\mathbf{k}\cdot\mathbf{r}_\ell}t(\ell)-\mu$, $\mathbf{\Delta}_k=\Sigma_\ell e^{-i\mathbf{k}\cdot\mathbf{r}_\ell}\mathbf{\Delta}(\ell)$, $\mathbf{\Delta}_{-k}=-\tilde{\mathbf{\Delta}}_k$, and

$$\sigma_0=\begin{pmatrix}1 & 0 \\ 0 & 1\end{pmatrix}.$$

The order parameter is given by

$$\mathbf{\Delta}_k=\psi_k i\sigma_y,\quad \tilde{\mathbf{\Delta}}_k=-\mathbf{\Delta}_k$$

for singlet states and

$$\mathbf{\Delta}_k=(\mathbf{d}_k\cdot\boldsymbol{\sigma})i\sigma_y,\quad \tilde{\mathbf{\Delta}}_k=\mathbf{\Delta}_k$$

for triplet states (ψ_k is even and $\mathbf{d}_k$ is odd in $\mathbf{k}$).[28]

The BdG Hamiltonian has a particle-hole symmetry. If

$$\mathbf{h}_k\begin{pmatrix}\mathbf{u}_k \\ \mathbf{v}_k\end{pmatrix}=E_k\begin{pmatrix}\mathbf{u}_k \\ \mathbf{v}_k\end{pmatrix},$$

then

$$C\begin{pmatrix}\mathbf{u}_k \\ \mathbf{v}_k\end{pmatrix}$$

is also an eigenstate with energy $-E_k$ where $C=\rho_x K$ for singlet states and $C=-i\rho_y K$ for triplet states ($\mathbf{u}_k$ and $\mathbf{v}_k$ are the two-component vectors and K is a complex conjugate operator and the Pauli matrices $\boldsymbol{\rho}$ operate on the two component blocks).[33] Then it is useful to consider

$$\mathbf{h}_k^2=\epsilon_k^2\rho_0+\begin{pmatrix}\mathbf{\Delta}_k\mathbf{\Delta}_k^\dagger & 0 \\ 0 & \mathbf{\Delta}_k^\dagger\mathbf{\Delta}_k\end{pmatrix}.$$

For singlet states, we have

$$\mathbf{\Delta}_k\mathbf{\Delta}_k^\dagger=\mathbf{\Delta}_k^\dagger\mathbf{\Delta}_k=|\psi_k|^2\sigma_0$$

and for triplet states

$$\mathbf{\Delta}_k\mathbf{\Delta}_k^\dagger=|\mathbf{d}_k|^2\sigma_0+\mathbf{q}_k\cdot\boldsymbol{\sigma}$$

with a real vector $\mathbf{q}_k=i\mathbf{d}_k\times\mathbf{d}_k^*$, which we call q helicity († represents Hermite conjugate and ∗ complex conjugate).

III. CHERN NUMBERS FOR UNITARY STATES

Singlet order and triplet order with vanishing q helicity are called unitary since

$$\mathbf{\Delta}_k\mathbf{\Delta}_k^\dagger=\mathbf{\Delta}_k^\dagger\mathbf{\Delta}_k\propto\sigma_0.$$

Nonunitary triplet states $(\mathbf{q}_k\neq0)$ will be discussed later. For unitary states, we define a unitary matrix $\mathbf{\Delta}_k^0$ by

$$\mathbf{\Delta}_k=|\Delta_k|\mathbf{\Delta}_k^0,$$

where $|\Delta_k|=|\psi_k|$ for singlet states and $|\Delta_k|=|\mathbf{d}_k|$ 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.[5,10,11] Instead, one can define non-Abelian vector potentials and fluxes following definitions of generalized non-Abelian connections.[29]

Let us assume that the states are M-fold degenerate ($M=2$ in the present unitary case) as $|\alpha\rangle$, $\alpha=1,\cdots,M$. Then a non-Abelian connection is defined by

$$A_\mu^{\alpha\beta}=\langle\alpha|\partial_\mu|\beta\rangle,\quad \mathcal{A}^{\alpha\beta}=A_\mu^{\alpha\beta}dk_\mu$$

where $\partial_\mu=\partial_{k_\mu}$, $\mu=x,y,z$. (Summation over the repeated indices μ is also assumed.) A unitary transformation of a degenerate state

$$|\alpha\rangle\rightarrow|\bar{\alpha}\rangle=|\alpha\rangle\omega^{\alpha\bar{\alpha}}$$

$$\boldsymbol{\omega}\boldsymbol{\omega}^\dagger=\boldsymbol{\omega}^\dagger\boldsymbol{\omega}=\sigma_0$$

causes "a gauge transformation"

$$\bar{\mathcal{A}}=\boldsymbol{\omega}^\dagger\mathcal{A}\boldsymbol{\omega}+\boldsymbol{\omega}^\dagger d\boldsymbol{\omega}.$$

Then the field strength

$$\mathcal{F}=d\mathcal{A}+\mathcal{A}\wedge\mathcal{A}$$

is gauge covariant since

$$\bar{\mathcal{F}}=\boldsymbol{\omega}^\dagger\mathcal{F}\boldsymbol{\omega}.$$

One may also write it as

$$\mathcal{F}=\frac{1}{2!}\mathbf{F}_{\mu\nu}dk_\mu\wedge dk_\nu,$$

$$\mathbf{F}_{\mu\nu}=\partial_\mu\mathbf{A}_\nu-\partial_\nu\mathbf{A}_\mu+[\mathbf{A}_\mu,\mathbf{A}_\nu].$$

Then "a magnetic field" in the μ direction is

$$B_\mu=\tfrac{1}{2}\epsilon_{\mu\nu\lambda}\mathrm{Tr}\mathbf{F}_{\nu\lambda}.$$

Since $\mathrm{Tr}\,\mathcal{F}$ is unitary invariant, so is B_μ. The total flux passing through the $\nu\lambda$ plane is given by an integral of the magnetic field B_μ over the two-dimensional Brillouin zone $T_{\nu\lambda}^2$ (k_μ is fixed). The first Chern number is[2,28]

$$C_\mu(k_\mu)=\frac{1}{2!}\epsilon_{\mu\nu\lambda}\frac{1}{2\pi i}\int_{T_{\nu\lambda}^2}\mathrm{Tr}\mathcal{F}=\frac{1}{2!}\frac{1}{2\pi i}\int_{T_{\nu\lambda}^2}dk_\nu\wedge dk_\lambda B_\mu.$$

This is the Abelian chiral anomaly discussed in the non-Abelian gauge theories.[2,30] Here we have considered the cu-

bic lattice. Extensions to other lattice structures are straightforward.

IV. DIRAC MONOPOLES IN THE PARAMETER

The BdG equation for the *unitary* states

$$\begin{pmatrix} \epsilon_k \sigma_0 & |\Delta_k| \Delta_k^0 \\ |\Delta_k| (\Delta_k^0)^{-1} & -\epsilon_k \sigma_0 \end{pmatrix} \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix} = E_k \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix}$$

reduces to an equation

$$\begin{pmatrix} \epsilon_k & |\Delta_k| \\ |\Delta_k| & -\epsilon_k \end{pmatrix}_\rho \otimes \sigma_0 \begin{pmatrix} \mathbf{u}_k \\ \Delta_k^0 \mathbf{v}_k \end{pmatrix} = E_k \begin{pmatrix} \mathbf{u}_k \\ \Delta_k^0 \mathbf{v}_k \end{pmatrix}.$$

Thus the energies are given by

$$E_k = \pm R$$

($R = \sqrt{\epsilon_k^2 + |\Delta_k|^2}$) and the states are doubly degenerate. The band with energy $-R$ is the superconducting condensates of pairs. On the other hand, the band with energy $+R$ represents quasiparticle excitations. By a parameterization: $\epsilon_k = R \cos\theta$ and $|\Delta_k| = R \sin\theta$, eigenvectors of condensate ($E_k = -R$) are

$$\begin{pmatrix} \mathbf{u}_k \\ \Delta_k^0 \mathbf{v}_k \end{pmatrix} = |R, \theta\rangle_\rho \otimes |\alpha\rangle_\sigma,$$

where

$$|R, \theta\rangle_\rho = \begin{pmatrix} -\sin\dfrac{\theta}{2} \\ \cos\dfrac{\theta}{2} \end{pmatrix}$$

and $|\alpha\rangle_\sigma$, ($\alpha = 1, 2$) are arbitrary orthonormalized states in the σ space. Now let us take eigenstates of the Δ_k^0 with eigenvalues $e^{-i\phi_\alpha}(\alpha = 1, 2)$

$$\Delta_k^0 |\alpha\rangle_\sigma = e^{-i\phi_\alpha} |\alpha\rangle_\sigma$$

to calculate the Chern numbers.[34] The degenerate orthonormal eigenvetor for the condensate band $E_k = -R$ is given by[18]

$$|\psi_\alpha\rangle = \begin{pmatrix} \mathbf{u}_k \\ \mathbf{v}_k \end{pmatrix}_\alpha = \begin{pmatrix} -\sin\dfrac{\theta}{2} |\alpha\rangle_\sigma \\ e^{i\phi_\alpha}\cos\dfrac{\theta}{2} |\alpha\rangle_\sigma \end{pmatrix}.$$

The connection is given by

$$A_\mu^{\alpha\beta} = \langle \psi_\alpha | \partial_\mu | \psi_\beta \rangle = \langle \mathbf{R}_\alpha | \partial_\mu | \mathbf{R}_\beta \rangle_\rho \langle \alpha | \beta \rangle_\sigma + \langle \mathbf{R}_\alpha | \mathbf{R}_\beta \rangle_\rho \langle \alpha | \partial_\mu | \beta \rangle_\sigma$$

$$= A_\mu^{\alpha\beta}(\rho)\delta_{\alpha\beta} + \langle \mathbf{R}_\alpha | \mathbf{R}_\beta \rangle_\rho A_\mu^{\alpha\beta}(\sigma),$$

where

$$A_\mu^{\alpha\beta}(\rho) = \langle \mathbf{R}_\alpha | \partial_\mu | \mathbf{R}_\beta \rangle_\rho$$

with

$$|\mathbf{R}_\alpha\rangle_\rho = |R, \theta, \phi_\alpha\rangle_\rho = \begin{pmatrix} -\sin\dfrac{\theta}{2} \\ e^{i\phi_\alpha}\cos\dfrac{\theta}{2} \end{pmatrix}.$$

We also have

$$A_\mu^{\alpha\beta}(\sigma) = \langle \alpha | \partial_\mu | \beta \rangle_\sigma = (\mathbf{U}^\dagger \partial_\mu \mathbf{U})_{\alpha\beta}$$

with $\mathbf{U} = (|1\rangle_\sigma, |2\rangle_\sigma)$. Then the total magnetic field in the parameter space is

$$B_\mu = B_\mu(\rho) + B_\mu(\sigma),$$

where $B_\mu(\rho) = \varepsilon_{\mu\nu\lambda}\mathrm{Tr}\partial_\nu \mathbf{A}_\lambda(\rho)$ and $B_\mu(\sigma) = \varepsilon_{\mu\nu\lambda}\mathrm{Tr}\,\partial_\nu \mathbf{A}_\lambda(\sigma)$. Since $B_\mu(\sigma)$ vanishes by the "sum rule" among the filled bands, we have $B_\mu = B_\mu(\rho)$.[35] It implies that the Chern numbers $C_{\alpha,\mu}$ of the condensed band in the μ direction are given by the sum of the Chern numbers of the two vectors $|R_\alpha\rangle_\rho$, ($\alpha = 1, 2$) which are the eigenstates of the 2×2 Hamiltonians

$$\mathbf{h}_k^\alpha = \begin{pmatrix} \epsilon_k & e^{i\phi_\alpha}|\Delta_k| \\ e^{-i\phi_\alpha}|\Delta_k| & -\epsilon_k \end{pmatrix} = \boldsymbol{\sigma} \cdot \mathbf{R}_\alpha,$$

where $R_{\alpha,X} = R\sin\theta\cos\phi_\alpha$, $R_{\alpha,Y} = R\sin\theta\sin\phi_\alpha$, and $R_{\alpha,Z} = R\cos\theta$. Namely they are $C_\mu = \Sigma_\alpha C_{\alpha,\mu}$. Now we have reduced the problem to calculate the Chern numbers of the eigenstates of the 2×2 matrices $\mathbf{h}_k^\alpha$. By mapping from the two-dimensional Brillouin zone to the three-dimensional space, $T_{\nu\lambda}^2 \ni (k_\nu, k_\lambda) \rightarrow \mathbf{R}_\alpha$, we obtain a closed oriented surface $R_\alpha(T_{\nu\lambda}^2)$. The wrapping degree of the map around the origin gives a charge of the Dirac monopole sitting there. This is the Chern number $C_\mu(k_\mu)$.[18,31]

For the present degenerate case, the map from a two-dimensional point to *two* three-dimensional points $T_{\nu\lambda}^2 \ni (k_\nu, k_\lambda) \rightarrow \{\mathbf{R}_{\alpha=1}, \mathbf{R}_{\alpha=2}\}$ defines (fixing k_μ) the surfaces $\{\mathbf{R}_{\alpha=1}(T_{\nu\lambda}^2), \mathbf{R}_{\alpha=2}(T_{\nu\lambda}^2)\}$ which determine the two covering degrees of the maps around the origins, $N_{\alpha;\nu\lambda}(k_\mu)$, ($\alpha = 1, 2$). 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

$$C_\mu(k_\mu) = \frac{1}{2!}\epsilon_{\mu\nu\lambda}N_{\nu\lambda}(k_\mu),$$

$$N_{\nu\lambda}(k_\mu) = \sum_\alpha N_{\alpha;\nu\lambda}(k_\mu).$$

The Chern numbers defined here for the unitary superconductors satisfy $C_{\nu\lambda}(k_\mu) = 4 \times$ integer for the singlet order and $C_{\nu\lambda}(k_\mu) = 2 \times$ integer for the triplet order.[36]

V. NONUNITARY STATES

In these triplet states, there is no degeneracy in solutions of the BdG equation. There are four quasiparticle bands, which are classified by the q helicity as

$$(\boldsymbol{\sigma}\cdot\mathbf{q}_k)\mathbf{u}_\pm = \pm q_k\mathbf{u}_\pm, \quad q_k = |\mathbf{q}_k|,$$

$$\mathbf{h}_k^2\psi_j^\pm = (\epsilon_k^2 + |\mathbf{d}_k|^2 \pm q_k)\psi_j^\pm,$$

$$\psi_1^\pm = \begin{pmatrix} \mathbf{u}_\pm \\ \mathbf{v}_\pm \end{pmatrix}, \quad \psi_2^\pm = \begin{pmatrix} \mathbf{u}_\pm \\ -\mathbf{v}_\pm \end{pmatrix},$$

$$\mathbf{v}_\pm = -i\sigma_y\mathbf{u}_\mp.$$

Then states with helicity $+q_k$ and energy $\pm E_{+q} = \pm\sqrt{\epsilon_k^2 + |\mathbf{d}_k|^2 + q_k}$, are

$$|\pm E_{+q}\rangle = \mathbf{U}_{+q}\boldsymbol{\eta}_{\pm E}^{+q},$$

where

$$\mathbf{U}_{+q} = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_+ & \mathbf{u}_+ \\ \mathbf{v}_+ & -\mathbf{v}_+ \end{pmatrix}$$

and the orthonormal vectors $\boldsymbol{\eta}_{\pm E}^{+q}$ are determined as the eigenvectors of the reduced 2×2 Hamiltonian

$$\widetilde{\mathbf{h}}_{+q} = \mathbf{U}_{+q}^\dagger\mathbf{h}\mathbf{U}_{+q}$$

with energies $\pm E_{+q}$. The Hamiltonian $\widetilde{\mathbf{h}}_{+q}$ is traceless and it can be expressed by as

$$\widetilde{\mathbf{h}}_{+q} = \boldsymbol{\sigma}\cdot\mathbf{R}_{+q}$$

where $\mathbf{R}_{+q}$ is a real vector given by

$$\mathbf{R}_{+q} = (\epsilon, \operatorname{Im} d_{+-}, \operatorname{Re} d_{+-}),$$

$$d_{+-} = \mathbf{u}_+^\dagger(\mathbf{d}_k\cdot\boldsymbol{\sigma})\mathbf{u}_-.$$

As for the helicity $-q_k$ state, one can follow almost the same procedure and obtain the reduced BdG Hamiltonian similarly. (See Appendix II for the details.) Here we can define several topological invariants. As discussed above, the states with $\pm q_k$ helicities and energies $\pm E_{\pm q}$ are nondegenerate,

$$\mathbf{h}_k|\varepsilon_e E_{\varepsilon_q}\rangle = \varepsilon_e E_{\varepsilon_q}|\varepsilon_e E_{\varepsilon_q}\rangle, \quad \mathbf{Q}_k|\varepsilon_e E_{\varepsilon_q}\rangle = \varepsilon_q|\varepsilon_e E_{\varepsilon_q}\rangle,$$

$$\mathbf{Q}_k = \begin{pmatrix} \boldsymbol{\sigma}\cdot\mathbf{q}_k & O \\ O & -\sigma_y\boldsymbol{\sigma}\cdot\mathbf{q}_k\sigma_y \end{pmatrix}, \quad [\mathbf{h}_k, \mathbf{Q}_k] = 0,$$

where

$$E_{\varepsilon_q}(\mathbf{k}) = \sqrt{|\varepsilon_k|^2 + |\mathbf{d}_k|^2 + \varepsilon_q}$$

($\varepsilon_q = \pm q_k$ and $\varepsilon_e = \pm$). Then the standard Chern number $C_\mu^0(k_\mu)$ in the μ direction for a fixed k_μ is obtained by the standard way.[5]

We also have topological invariants in the μ direction $N_\mu^q(k_\mu)$. They are wrapping degrees around the origin of the map $(k_\nu, k_\lambda) \to \mathbf{q}(\mathbf{k}) = \mathbf{q}_k$, which define closed surfaces $\mathbf{q}(T_{\nu\lambda}^2)$ in three dimensions.[18] Further we have other topological invariants $N_\mu^\pm(k_\mu)$, which are also wrapping degrees of the map around the origin, $(k_\nu, k_\lambda) \to \mathbf{R}_{\pm q}(\mathbf{k})$. (The reduced Hamiltonians are $\widetilde{\mathbf{h}}_{\pm q} = \mathbf{R}_{\pm q}\cdot\boldsymbol{\sigma}$ for the q helicity $\pm q_k$.)

VI. GAP NODES OF SUPERCONDUCTORS AS A QUANTUM PHASE TRANSITION

Up to this point, we have had the superconducting gap open in k space. However, the above analysis is also useful for gapless superconductivities. In fact, the nodal structure of the superconducting gap is characterized by the topological description. Formally we have treated a three-dimensional superconductivity as a collection of two-dimensional systems parameterized by, say, k_z. In **R** space, closed surfaces parameterized by (k_x, k_y) are generically away from the monopole at the origin. As k_z is changed, the surfaces move around and they can pass through the monopole. Since the distance between a point on a surface and the monopole gives half of the energy gap $E_g(k_x, k_y; k_z)$, the gap closes at a value of k_z when the monopole is on the surface. Thus the nodal structure of the three-dimensional superconductivity is *point like generically*. When the two-dimensional Chern number jumps as k_z varies, the superconducting gap has to be closed due to a topological stability of the Chern numbers. Also the nonzero Chern number implies that the corresponding two-dimensional system has a nontrivial topological order. Then the superconducting node is considered as the critical point of the quantum phase transition.

To make the discussion clear, let us take an example $\Delta_k = d_z(\sin k_x + i\sin k_y)\sigma_x$, $\epsilon_k = -2t(\cos k_x + \cos k_y + \cos k_z) - \mu$, $(t>0)$.[18] This is an analogue of the Anderson-Brinkman-Morel (ABM) state in ^{3}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 $\mathbf{d}_k \to (0, 0, d_z(k_x + ik_y))$ in the limit of $\mu \to -6t+0$, $\mathbf{k} \to 0$.) Then there are two quantum phase transitions changing the Chern numbers between $-2\rightleftarrows 0$ for $-6t < \mu < -2t$, which correspond to gap nodes at the north and south poles on the Fermi surface, respectively. In Fig. 1, the surface $\mathbf{R}_1(T_{xy}^2)$ for this example is shown with the monopole at the origin.

Other nodal structures are also expected by changing the Chern numbers $-2\rightleftarrows +2$ for $-2t < \mu < 2t$ and $0\rightleftarrows +2$ 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 $d_z \ne 0$. 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 $R_X - R_Z$ plane and one can expect a situation where the monopole moves along the surface when k_z is changed.[31] 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. A detailed discussion on this point will be given elsewhere.[32]
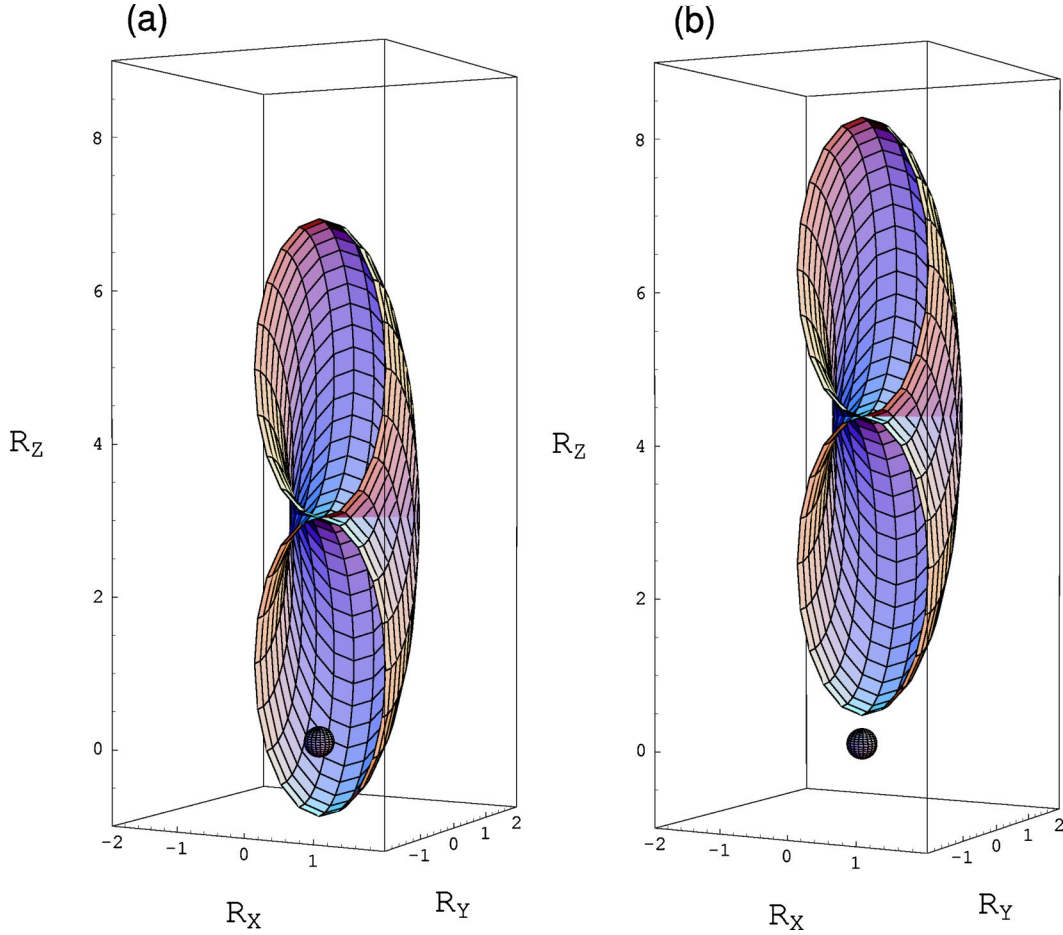
FIG. 1. (Color online) Examples of closed surfaces $R_1(T_{xy}^2)$ which are cut by the R_Y–R_Z plane. The monopole is at the origin, $t=d_z$ $=1$, $\mu=-5$: (a)$k_z=0$ and (b)$k_z=-2\pi/5$.

APPENDIX A: A MEAN FIELD THEORY ON LATTICE

Define a pairing amplitude $x_{ij}^{\sigma\sigma'}$ as

$$x_{ij}^{\sigma\sigma'} = \langle c_{i\sigma}c_{j\sigma'}\rangle = -x_{ji}^{\sigma'\sigma}.$$

The last equation follows from the anticommutation relation between Fermion operators. Then defining an order parameter as

$$\Delta_{ij}^{\sigma_1\sigma_2} = V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4}x_{ji}^{\sigma_3\sigma_4},$$

and inserting $c_{j\sigma_3}c_{i\sigma_4}=x_{ji}^{\sigma_3\sigma_4}+\delta_{ji}^{\sigma_3\sigma_4}$, the mean field Hamiltonian $\mathcal{H}$ is given by

$$H = \mathcal{H} + \mathcal{H}_0 + \mathcal{O}(\delta^2),$$

$$\mathcal{H}_0 = -\sum_{ij} V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4}x_{ji}^{\sigma_2\sigma_1*}x_{ji}^{\sigma_3\sigma_4} = -\sum_{ij}\Delta_{ij}^{\sigma_4\sigma_3*}(x_{ji}^{\sigma_3\sigma_4}),$$

$$\mathcal{H} = \sum_{ij} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma} + \sum_{ij}(\Delta_{ij}^{\sigma_4\sigma_3*}c_{j\sigma_3}c_{i\sigma_4}+\Delta_{ij}^{\sigma_1\sigma_2}c_{i\sigma_1}^{\dagger}c_{j\sigma_2}^{\dagger}),$$

where we note

$$(\Delta_{ij}^{\sigma_4\sigma_3})* = (V_{ij}^{\sigma_4\sigma_3;\sigma_2\sigma_1})*(x_{ji}^{\sigma_2\sigma_1})* = V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4}(x_{ji}^{\sigma_2\sigma_1})*,$$

$$V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4}(x_{ji}^{\sigma_2\sigma_1})*(x_{ji}^{\sigma_3\sigma_4}) = \Delta_{ij}^{\sigma_4\sigma_3*}(x_{ji}^{\sigma_3\sigma_4}) = (x_{ji}^{\sigma_2\sigma_1})*\Delta_{ij}^{\sigma_1\sigma_2}.$$

The self-consistent equation is given by

$$\frac{\partial F}{\partial\Delta_{ij}^{\sigma_4\sigma_3*}} = 0, \quad e^{-\beta F} = \mathrm{Tr}\, e^{-\beta(\mathcal{H}+\mathcal{H}_0)},$$

$$0 = \mathrm{Tr}\, e^{-\beta\mathcal{H}}(c_{j\sigma_3}c_{i\sigma_4} - x_{ji}^{\sigma_3\sigma_4}),$$

$$x_{ji}^{\sigma_3\sigma_4} = \langle c_{j\sigma_3}c_{i\sigma_4}\rangle_{\mathcal{H}},$$

$$\Delta_{ij}^{\sigma_1\sigma_2} = V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4}\langle c_{j\sigma_3}c_{i\sigma_4}\rangle_{\mathcal{H}},$$

where $\mathcal{H}_0$ is a ground state energy.

We require the SU(2) invariance at the mean field level. Since the Hamiltonian is invariant under the transformation, the pairing amplitude is transformed as

$$x_{ij}^{\sigma_1\sigma_2} \rightarrow x_{ij}'^{\sigma_1\sigma_2} = \langle c_{j\sigma_2}' c_{i\sigma_1}' \rangle' = \langle c_{j\sigma_2}' c_{i\sigma_1}' \rangle = U^{\sigma\sigma_1'} U^{\sigma'\sigma_2'} \langle c_{j\sigma_2'} c_{i\sigma_1'} \rangle$$

$$= U^{\sigma_1\sigma_1'} U^{\sigma_2\sigma_2'} x_{ij}^{\sigma_1'\sigma_2'}.$$

Then the order parameter is transformed as

$$\Delta_{ij}^{\sigma_1\sigma_2} = V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4} x_{ji}^{\sigma_3\sigma_4} \rightarrow \Delta_{ij}'^{\sigma_1\sigma_2} = V_{ij}^{\sigma_1\sigma_2;\sigma_3\sigma_4} x_{ji}'^{\sigma_3\sigma_4}$$

$$= U^{\sigma_1\sigma_1'} U^{\sigma_2\sigma_2'} \Delta_{ij}^{\sigma_1'\sigma_2'}.$$

Also the ground state energy is invariant as $\mathcal{H}_0 \rightarrow \mathcal{H}_0' = \mathcal{H}_0$.

As for the infinitesimal transformation

$$U^{\sigma\sigma'} = \left(\cos\frac{\delta\theta}{2} - \hat{n}\cdot\boldsymbol{\sigma}\sin\frac{\delta\theta}{2} \right)_{\sigma\sigma'} = \delta_{\sigma\sigma'} - \delta\theta i\hat{n}\cdot\mathbf{s}_{\sigma\sigma'},$$

$$\mathbf{s} = \frac{1}{2}\boldsymbol{\sigma},$$

we have

$$\delta\Delta_{ij}^{\sigma_1\sigma_2} = \Delta_{ij}'^{\sigma_1\sigma_2} - \Delta_{ij}^{\sigma_1\sigma_2} = \delta\theta i\hat{n}\cdot(\mathbf{s}_{\sigma_1\sigma_1'} + \mathbf{s}_{\sigma_2\sigma_2'})\Delta_{ij}^{\sigma_1'\sigma_2'}.$$

We further require that the order parameters belong to an irreducible representation of the total spin $\mathbf{J} = \mathbf{s}\otimes\boldsymbol{\sigma}_0 + \boldsymbol{\sigma}_0\otimes\mathbf{s}$, which consists of the singlet and the triplet.

As for the singlet, the base is given by

$$|0\rangle_S = \frac{1}{\sqrt{2}}(\Delta_{ij}^{\uparrow\downarrow} - \Delta_{ij}^{\downarrow\uparrow}),$$

$$J_\pm|0\rangle_S = 0,$$

$$J_z|0\rangle_S = 0.$$

In this singlet case, we assume without losing generality

$$\Delta_{ij}^{\sigma\sigma'} = -\Delta_{ij}^{\sigma'\sigma}.$$

As for the triplet case, the bases are given by

$$|+1\rangle_T = \Delta_{ij}^{\uparrow\uparrow},$$

$$|0\rangle_T = \frac{1}{\sqrt{2}}(\Delta_{ij}^{\uparrow\downarrow} + \Delta_{ij}^{\downarrow\uparrow}),$$

$$|-1\rangle_T = \Delta_{ij}^{\downarrow\downarrow},$$

$$J_\pm|m\rangle_T = \sqrt{(1\mp m)(2\pm m)}|m\pm1\rangle_T,$$

$$J_z|m\rangle_T = m|m\rangle_T.$$

As in the singlet case, we can assume without losing generality that

$$\Delta_{ij}^{\sigma\sigma'} = \Delta_{ij}^{\sigma'\sigma}.$$

In the following, we consider the above two cases separately:

$$\text{singlet} \quad \Delta_{ij}^{\sigma\sigma'} = -\Delta_{ij}^{\sigma'\sigma} = \Delta_{ji}^{\sigma\sigma'},$$

$$\text{triplet} \quad \Delta_{ij}^{\sigma\sigma'} = \Delta_{ij}^{\sigma'\sigma} = -\Delta_{ji}^{\sigma\sigma'},$$

which are written in matrix notation as singlet

$$\text{singlet} \quad \boldsymbol{\Delta}_{ij} = -\tilde{\boldsymbol{\Delta}}_{ij} = \begin{pmatrix} & \psi_{ij} \\ -\psi_{ij} & \end{pmatrix} = \psi_{ij} i\sigma_y,$$

$$\psi_{ij} = \psi_{ji} \ (\text{even}),$$

$$\text{triplet} \quad \boldsymbol{\Delta}_{ij} = -\tilde{\boldsymbol{\Delta}}_{ij} = \begin{pmatrix} -d_{ij}^x + id_{ij}^y & d_{ij}^z \\ d_{ij}^z & d_{ij}^x + id_{ij}^y \end{pmatrix} = (\mathbf{d}_{ij}\cdot\boldsymbol{\sigma})i\sigma_y,$$

$$\mathbf{d}_{ij} = -\mathbf{d}_{ji} \ (\text{odd}).$$

Now let us assume a translation symmetry

$$t_{ij} = t(i-j),$$

$$\Delta_{ij}^{\sigma\sigma'} = \Delta^{\sigma\sigma'}(i-j),$$

and define Fermion operators in a momentum representation $c_j = (1/\sqrt{V})\Sigma_k e^{i\mathbf{k}\cdot\mathbf{r}_j} c(\mathbf{k})$. Now we have

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_i,$$

$$\mathcal{H}_t = \sum_k \epsilon(\mathbf{k}) c_\sigma^\dagger(\mathbf{k}) c_\sigma(\mathbf{k}),$$

$$\mathcal{H}_i = \sum_k \Delta^{\sigma\sigma'}(\mathbf{k}) c_\sigma^\dagger(\mathbf{k}) c_{\sigma'}^\dagger(-\mathbf{k}) + \text{h.c.},$$

$$\epsilon(\mathbf{k}) = \sum_\ell e^{i\mathbf{k}\cdot\mathbf{r}_\ell} t(\ell),$$

$$\Delta^{\sigma\sigma'}(\mathbf{k}) = \sum_\ell e^{-i\mathbf{k}\cdot\mathbf{r}_\ell} \Delta^{\sigma\sigma'}(\ell).$$

As for the order parameters, we have

$$\Delta^{\sigma\sigma'}(-\mathbf{k}) = -\Delta^{\sigma'\sigma}(\mathbf{k}),$$

which is a consequence of the Fermion anticommutation relation. It is expressed in matrix form as

$$\boldsymbol{\Delta}(-\mathbf{k}) = -\tilde{\boldsymbol{\Delta}}(\mathbf{k}).$$

Finally we have for the BdG Hamiltonian as

$$\mathcal{H} = \sum_k{}' \mathbf{c}^\dagger(\mathbf{k})\mathbf{h}(\mathbf{k})\mathbf{c}(\mathbf{k}) + \text{const.}$$

$$\mathbf{h}(\mathbf{k}) = \begin{pmatrix} \epsilon(\mathbf{k}) & \boldsymbol{\Delta}(\mathbf{k}) \\ \boldsymbol{\Delta}^\dagger(\mathbf{k}) & -\epsilon(-\mathbf{k}) \end{pmatrix} = \begin{pmatrix} \epsilon(\mathbf{k}) & \boldsymbol{\Delta}(\mathbf{k}) \\ \boldsymbol{\Delta}^\dagger(\mathbf{k}) & -\epsilon(\mathbf{k}) \end{pmatrix}$$

$$\text{if } \epsilon(\mathbf{k}) = \epsilon(-\mathbf{k})$$

$$c(\mathbf{k}) = \begin{pmatrix} c_\uparrow(\mathbf{k}) \\ c_\downarrow(\mathbf{k}) \\ c_\uparrow^\dagger(-\mathbf{k}) \\ c_\downarrow^\dagger(-\mathbf{k}) \end{pmatrix}.$$

The condition $\epsilon(\mathbf{k}) = \epsilon(-\mathbf{k})$ is guaranteed by assuming the hopping elements t_{ij} to be real, that is, the absence of the magnetic field.

As for the order parameter, we assume the two possibilities as an ansatz as

$$\text{singlet } \mathbf{\Delta}(\mathbf{k}) = \begin{pmatrix} & \psi(\mathbf{k}) \\ -\psi(\mathbf{k}) & \end{pmatrix} = \psi(\mathbf{k})i\sigma_y$$

$$\psi(-\mathbf{k}) = \psi(\mathbf{k}) \text{ (even)},$$

$$\tilde{\mathbf{\Delta}}(\mathbf{k}) = -\mathbf{\Delta}(\mathbf{k}),$$

$$\text{triplet } \mathbf{\Delta}(\mathbf{k}) = \begin{pmatrix} -d_x(\mathbf{k}) + id_y(\mathbf{k}) & d_z(\mathbf{k}) \\ d_z(\mathbf{k}) & d_x(\mathbf{k}) + id_y(\mathbf{k}) \end{pmatrix}$$

$$= (\mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma})i\sigma_y$$

$$\mathbf{d}(-\mathbf{k}) = -\mathbf{d}(\mathbf{k}) \text{ (odd)},$$

$$\tilde{\mathbf{\Delta}}(\mathbf{k}) = \mathbf{\Delta}(\mathbf{k}).$$

APPENDIX B: REDUCED HAMILTONIANS FOR NONUNITARY STATES

Let's consider the eigenvalue problem

$$\begin{pmatrix} \boldsymbol{\epsilon} & \mathbf{\Delta} \\ \mathbf{\Delta}^\dagger & -\boldsymbol{\epsilon} \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = E \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}.$$

Due to the particle hole symmetry, it is enough to consider $\mathbf{h}^2$ as

$$\begin{pmatrix} \boldsymbol{\epsilon} & \mathbf{\Delta} \\ \mathbf{\Delta}^\dagger & -\boldsymbol{\epsilon} \end{pmatrix} \begin{pmatrix} \boldsymbol{\epsilon} & \mathbf{\Delta} \\ \mathbf{\Delta}^\dagger & -\boldsymbol{\epsilon} \end{pmatrix} = \begin{pmatrix} \epsilon^2 + \mathbf{\Delta}\mathbf{\Delta}^\dagger & 0 \\ 0 & \epsilon^2 + \mathbf{\Delta}^\dagger\mathbf{\Delta} \end{pmatrix}$$

$$\mathbf{\Delta}\mathbf{\Delta}^\dagger\mathbf{u} = \lambda^2\mathbf{u}$$

$$\mathbf{\Delta}^\dagger\mathbf{\Delta}\mathbf{v} = \lambda^2\mathbf{u},$$

$$E = \pm\sqrt{\epsilon^2 + \lambda^2}, \ (\lambda = \text{real}).$$

For the singlet case, we have

$$\begin{pmatrix} \epsilon & & & \psi \\ & \epsilon & -\psi & \\ & -\psi^* & -\epsilon & \\ \psi^* & & & -\epsilon \end{pmatrix} \begin{pmatrix} u_\uparrow \\ u_\downarrow \\ v_\uparrow \\ v_\downarrow \end{pmatrix} = E \begin{pmatrix} u_\uparrow \\ u_\downarrow \\ v_\uparrow \\ v_\downarrow \end{pmatrix}.$$

It decouples as

$$\begin{pmatrix} \epsilon & \psi \\ \psi^* & -\epsilon \end{pmatrix} \begin{pmatrix} u_\uparrow \\ v_\downarrow \end{pmatrix} = E \begin{pmatrix} u_\uparrow \\ v_\downarrow \end{pmatrix}$$

$$\begin{pmatrix} \epsilon & \psi^* \\ \psi & -\epsilon \end{pmatrix} \begin{pmatrix} v_\downarrow \\ u_\uparrow \end{pmatrix} = -E \begin{pmatrix} v_\downarrow \\ u_\uparrow \end{pmatrix}.$$

This was considered in previous work.[18]

For the triplet case, using $(\boldsymbol{\sigma}\cdot\mathbf{A})(\boldsymbol{\sigma}\cdot\mathbf{B}) = \mathbf{A}\cdot\mathbf{B} + i\boldsymbol{\sigma}(\mathbf{A}\times\mathbf{B})$, we have

$$\mathbf{\Delta}\mathbf{\Delta}^\dagger = i(\mathbf{d}\cdot\boldsymbol{\sigma})\sigma_y(-i)\sigma_y(\mathbf{d}^*\cdot\boldsymbol{\sigma}) = |\mathbf{d}|^2 + i\boldsymbol{\sigma}\cdot(\mathbf{d}\times\mathbf{d}^*).$$

Thus $\mathbf{u}$ is determined by the eigen problem by

$$(\boldsymbol{\sigma}\cdot\mathbf{q})\mathbf{u}_\pm = \pm q\mathbf{u}_\pm, \ (q = |\mathbf{q}|),$$

$$\mathbf{q} = i\mathbf{d}\times\mathbf{d}^*.$$

Then as far as $q \neq 0$ (nonunitary case), we have $\mathbf{u}_\pm$ as

$$\mathbf{\Delta}\mathbf{\Delta}^\dagger\mathbf{u}_\pm = (|\mathbf{d}|^2 + \boldsymbol{\sigma}\cdot\mathbf{q})\mathbf{u}_\pm = (|\mathbf{d}|^2 \pm q)\mathbf{u}_\pm,$$

$$\lambda^2 = |\mathbf{d}|^2 \pm q$$

$$\mathbf{u}_\alpha^\dagger\mathbf{u}_\beta = \delta_{\alpha\beta}.$$

Note that this $\mathbf{q}$ is real ($\mathbf{q}^* = -i\mathbf{d}^*\times\mathbf{d} = i\mathbf{d}\times\mathbf{d}^* = \mathbf{q}$). Thus the quasiparticle energy is given by

$$E = \pm\sqrt{\epsilon^2 + |\mathbf{d}|^2 \pm q}.$$

Since $\mathbf{\Delta}^\dagger\mathbf{\Delta} = \sigma_y(\boldsymbol{\sigma}\cdot\mathbf{d}^*)(\boldsymbol{\sigma}\cdot\mathbf{d})\sigma_y = \sigma_y(|\mathbf{d}|^2 - \boldsymbol{\sigma}\cdot\mathbf{q})\sigma_y$, we have

$$\mathbf{\Delta}^\dagger\mathbf{\Delta}\mathbf{v}_\pm = -i\sigma_y(|\mathbf{d}|^2 - \boldsymbol{\sigma}\cdot\mathbf{q})\mathbf{u}_\mp = -i(|\mathbf{d}|^2 \pm q)\sigma_y\mathbf{u}_\mp$$

$$= (|\mathbf{d}|^2 \pm q)\mathbf{v}_\pm,$$

$$\mathbf{v}_\pm = -i\sigma_y\mathbf{u}_\mp.$$

In summary, we constructed eigenstates of $\mathbf{h}^2$ as

$$\mathbf{h}^2\begin{pmatrix} \mathbf{u}_\pm \\ \mathbf{v}_\pm \end{pmatrix} = (\epsilon^2 + |\mathbf{d}|^2 \pm q)\begin{pmatrix} \mathbf{u}_\pm \\ \mathbf{v}_\pm \end{pmatrix}$$

$$\mathbf{h}^2\begin{pmatrix} \mathbf{u}_\pm \\ -\mathbf{v}_\pm \end{pmatrix} = (\epsilon^2 + |\mathbf{d}|^2 \pm q)\begin{pmatrix} \mathbf{u}_\pm \\ -\mathbf{v}_\pm \end{pmatrix}.$$

Then the energy is given for the helicity $+q$ state as

$$\pm E_{+q} = \pm\sqrt{\epsilon^2 + |\mathbf{d}|^2 + q}.$$

The eigenstate of the full Hamiltonian $\mathbf{h}$ is determined as a linear combination of

$$\frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_+ \\ \pm\mathbf{v}_+ \end{pmatrix}$$

as

$$|\pm E_{+q}\rangle = \alpha_{\pm E}^{+q}\frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_+ \\ \mathbf{v}_+ \end{pmatrix} + \beta_{\pm E}^{+q}\frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_+ \\ -\mathbf{v}_+ \end{pmatrix} = \mathbf{U}_{+q}\begin{pmatrix} \alpha_{\pm E}^{+q} \\ \beta_{\pm E}^{+q} \end{pmatrix}$$

$$\equiv \mathbf{U}_{+q}\boldsymbol{\eta}_{\pm E}^{+q},$$

$$\boldsymbol{\eta}_{\pm E}^{+q} = \begin{pmatrix} \alpha_{\pm E}^{+q} \\ \beta_{\pm E}^{+q} \end{pmatrix},$$

$$(\boldsymbol{\eta}_a^{+q})^\dagger\boldsymbol{\eta}_b^{+q} = \delta_{ab}, \ a,b = \pm E$$

$$\mathbf{U}_{+q} = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_+ & \mathbf{u}_+ \\ \mathbf{v}_+ & -\mathbf{v}_+ \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_+ & \mathbf{u}_+ \\ -i\sigma_y\mathbf{u}_- & i\sigma_y\mathbf{u}_- \end{pmatrix},$$

$$\mathbf{h}|\pm E_{+q}\rangle = \mathbf{h}\mathbf{U}_{+q}\boldsymbol{\eta}_{\pm E}^{+q} = \pm E_{+q}\mathbf{U}_{+q}\boldsymbol{\eta}_{\pm E}^{+q}.$$

That is

$$\mathbf{h}\mathbf{U}_{+q}(\boldsymbol{\eta}_{+E}^{+q},\boldsymbol{\eta}_{-E}^{+q}) = \mathbf{U}_{+q}(\boldsymbol{\eta}_{+E}^{+q},\boldsymbol{\eta}_{-E}^{+q})\begin{pmatrix} E_{+q} & \\ & -E_{+q} \end{pmatrix}.$$

This $\mathbf{U}_{+q}$ is 4×2, which satisfies

$$\mathbf{U}_{+q}^\dagger\mathbf{U}_{+q} = \mathbf{I}_2,$$

$$\mathbf{U}_{+q}\mathbf{U}_{+q}^\dagger = \begin{pmatrix} \mathbf{u}_+\mathbf{u}_+^\dagger & O \\ O & \mathbf{v}_+\mathbf{v}_+^\dagger \end{pmatrix}.$$

The vector $\boldsymbol{\eta}_{\pm E}^{+q}$ is an eigenvector of the 2×2 matrix

$$\widetilde{\mathbf{h}}_{+q} = \mathbf{U}_{+q}^\dagger\mathbf{h}\mathbf{U}_{+q}$$

with energy $\pm E_{+q}$ ($\widetilde{\mathbf{h}}_{+q}\boldsymbol{\eta}_{\pm E}^{+q} = \pm E_{+q}\boldsymbol{\eta}_{\pm E}^{+q}$).

Since $\widetilde{\mathbf{h}}_{+q}$ is traceless as $\mathrm{Tr}\widetilde{\mathbf{h}}_{+q} = \mathrm{Tr}\mathbf{U}_{+q}^\dagger\mathbf{U}_{+q} = \mathrm{Tr}_2\boldsymbol{\epsilon}\mathbf{u}_+\mathbf{u}_+^\dagger - \mathrm{Tr}_2\boldsymbol{\epsilon}\mathbf{v}_+\mathbf{v}_+^\dagger = 0$ and Hermitian, it is expanded by the Pauli matrices with real coefficients as

$$\widetilde{\mathbf{h}}_{+q} = \boldsymbol{\sigma}\cdot\mathbf{R}_{+q},$$

$$\mathbf{R}_{+q} = \tfrac{1}{2}\mathrm{Tr}\,\boldsymbol{\sigma}\widetilde{\mathbf{h}}_{+q},$$

$$E_{+q} = |\mathbf{R}_{+q}| = \sqrt{\epsilon^2 + |\mathbf{d}|^2 + q}.$$

For the helicity $-q$ state, we change $\mathbf{u}_+$, $\boldsymbol{v}_+ \to \mathbf{u}_-$, $\boldsymbol{v}_-$ in $\mathbf{U}_{+q}$ to obtain $\mathbf{U}_{-q}$ as

$$\mathbf{U}_{-q} = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_- & \mathbf{u}_- \\ \mathbf{v}_- & -\mathbf{v}_- \end{pmatrix} = \begin{pmatrix} \mathbf{u}_- & \mathbf{u}_- \\ -i\sigma_y\mathbf{u}_+ & i\sigma_y\mathbf{u}_+ \end{pmatrix},$$

$$\widetilde{\mathbf{h}}_{-q} = \mathbf{U}_{-q}^\dagger\mathbf{h}\mathbf{U}_{-q} = \boldsymbol{\sigma}\cdot\mathbf{R}_{-q},$$

$$\mathbf{R}_{-q} = \frac{1}{2}\mathrm{Tr}\,\boldsymbol{\sigma}\widetilde{\mathbf{h}}_{-q}$$

$$\widetilde{\mathbf{h}}_{-q}\boldsymbol{\eta}_{\pm E}^{-q} = \pm E_{-q}\boldsymbol{\eta}_{\pm E}^{-q},$$

$$E_{-q} = |\mathbf{R}_{-q}| = \sqrt{\epsilon^2 + |\mathbf{d}|^2 - q}.$$

Further let us define

$$\mathbf{U} = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{u}_+ & \mathbf{u}_+ \\ \mathbf{u}_- & -\mathbf{u}_- \end{pmatrix}$$

and rewrite $\mathbf{U}_{\pm q}$ as

$$\mathbf{U}_{+q} = \begin{pmatrix} 1_2 & \\ & -i\sigma_y \end{pmatrix}\mathbf{U}$$

$$\mathbf{U}_{-q} = \begin{pmatrix} 1_2 & \\ & -i\sigma_y \end{pmatrix}\begin{pmatrix} & 1_2 \\ 1_2 & \end{pmatrix}\mathbf{U}\sigma_z.$$

Then we have for $\mathbf{R}_{+q}$, ($\slashed{d} = \boldsymbol{\sigma}\cdot\mathbf{d}$)

$$\mathbf{R}_{+q} = \frac{1}{2}\mathrm{Tr}\,\boldsymbol{\sigma}\mathbf{U}^\dagger\begin{pmatrix} \epsilon & \slashed{d} \\ \slashed{d}^* & -\epsilon \end{pmatrix}\mathbf{U}$$

$$= \frac{1}{2}\mathrm{Tr}\boldsymbol{\sigma}\begin{pmatrix} \mathrm{Re}d_{+-} & \epsilon - i\mathrm{Im}\,d_{+-} \\ \epsilon + i\mathrm{Im}\,d_{+-} & -\mathrm{Re}\,d_{+-} \end{pmatrix} = (\epsilon, \mathrm{Im}\,d_{+-}, \mathrm{Re}\,d_{+-})$$

$$d_{+-} = \mathbf{u}_+^\dagger\slashed{d}\mathbf{u}_- = \mathbf{u}_+^\dagger(\boldsymbol{\sigma}\cdot\mathbf{d})\mathbf{u}_-.$$

As for the negative helicity state, a similar reduced Hamiltonian is obtained by a parallel argument as

$$\mathbf{R}_{-q} = (\epsilon, -\mathrm{Im}\,d_{+-}^*, \mathrm{Re}\,d_{+-}^*),$$

$$d_{+-}^* = \mathbf{u}_+^\dagger\slashed{d}^*\mathbf{u}_- = \mathbf{u}_+^\dagger(\boldsymbol{\sigma}\cdot\mathbf{d}^*)\mathbf{u}_-.$$

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[33] The 4×4 matrices are spanned by $\rho_i \otimes \sigma_j, i, j = 0, \ldots, 3$.

[34] It is a similar procedure to fix phases of states for nondegenerate cases.

[35] $B_\mu(\sigma) = \epsilon_{\mu\nu\lambda} \mathrm{Tr} \partial_\nu (\mathbf{U}^{-1} \partial_\lambda \mathbf{U}) = -\epsilon_{\mu\nu\lambda} \mathrm{Tr}(\mathbf{U}^{-1} \partial_\nu \mathbf{U})(\mathbf{U}^{-1} \partial_\lambda \mathbf{U}) = 0.$ It also completes a general proof of the sum rule for the nondegenerate states, that is, the sum of the Chern numbers for all bands is zero.

[36] For the singlet case, we have $N_{1;\nu\lambda} = N_{2;\nu\lambda}$, since $\phi_1 = \phi_2 + \pi$.[18,31] Further each $N_{2;\nu\lambda}$ is even. For the triplet case, $N_{1;\nu\lambda} \neq N_{2;\nu\lambda}$ generically. However, the sum of them is even since we can show $\phi_1 = +\vartheta + \mathrm{Arg}\ \delta$, $\phi_2 = -\vartheta + \mathrm{Arg}\ \delta + \pi$ with some function ϑ where $\mathbf{d} \cdot \boldsymbol{\sigma}$ is unitary equivalent to $\delta\sigma_z(|\delta| = |\mathbf{d}|)$. We use a base which diagonalizes $\boldsymbol{\Delta}^0_k$. Another base which diagonalizes $\mathbf{d} \cdot \boldsymbol{\sigma}$ is also useful.