Explicit Gauge Fixing for Degenerate Multiplets: A Generic Setup for Topological Orders

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We supply basic tools for the study of the topological order of a multiplet which is an eigenspace of a finite-dimensional normal operator with continuous parameters. We allow intrinsic degeneracies within the multiplet where a well-known standard procedure does not work. As an important example, we give novel expressions for a spin Hall conductance for unitary superconductors with equal spin pairing. Generic topological orders will be treated in this unified manner particularly with nontrivial topological degeneracies.

KEYWORDS: Chern numbers, degeneracy, topological orders

It has been gradually clarified that many physically important phenomena have origins in their topological orders. Some of them include (fractional and integer) quantum Hall effects, Haldane spin chains, solitons in polyacetylenes, anisotropic superconductors and superfluids, chirality order in an itinerant magnetism, spin transport (spintronics) as a realistic application of Thouless pumping, and polarizations in insulators, and the exotic electronic states of graphite. Strong correlations between electrons cause exotic mean field states and effective quasiparticles such as composite fermions which can also be discussed in terms of the topological orders. In many cases, the topological order itself is hidden in bulk systems but exhibits apparent physical consequences at the boundaries of the systems, such as in edge states of the quantum Hall effects, local moments near impurities in the Haldane spin chains, vortices and zero-bias conductance peaks in anisotropic superconductivities and boundary local moments in carbon nanotubes.

In many cases, nontrivial topological orders appear by restricting their physical space in a manner in which a type of gauge structure naturally emerges. To characterize the quantum state of a specific system, one must explicitly determine gauge invariant quantities for the physical states. The (first) Chern number is such a candidate and it has been used for several characterizations of topologically nontrivial states.

In this paper, we present a generic setup for the discussion of the topological order explicitly, particularly focusing on gauge fixing. A standard procedure for fixing gauge was reported by Kohmoto. This is well known today. However, the procedure does not work when degeneracy exists. If degeneracy is accidental, that is, it exists at certain special parameter values, it is negligible. However, in several interesting situations such as in unitary superconductors, degeneracy is due to an intrinsic symmetry, that is, the standard procedure cannot be applied for any values of the parameters (see below). In such cases, the present generic gauge fixing procedure is essentially important, particularly for numerical calculations of Chern numbers. We extend the standard procedure to general situations which allow intrinsic degeneracies of eigenstates. A typical situation where our method is crucial is the calculation of spin Hall conductances for numerically obtained BCS Hamiltonians, where the order parameters are given numerically by minimizing the mean field free energy. Then quasiparticle states are obtained by diagonalizing a Bogoliubov-de Gennes equation. When the order is unitary, it has an intrinsic degeneracy which prevents direct applications of the standard procedure to the calculation of the spin Hall conductance. Also, when a physical ground state has a nontrivial topological order and it lives on a genus Riemann surface, a fundamental topological degeneracy can occur with degeneracies with some integer . A typical situation is the fractional quantum Hall effect with the filling factor . In such a degenerate case, the present extension is indispensable. Further generic expressions in the present paper can be applied to a wide range of physically interesting situations.

Multiplet and Unitary Equivalence: Let us consider taking a normal operator , in an dimensional linear space. This implies that is diagonalizable by a unitary matrix, , as . Note that normal operators include hermite, skew-hermite, unitary and skew-unitary operators. Also, we assume that the operator is labeled by a set of continuous parameters as , where is a -dimensional parameter space. Various physical realizations of the operator are (i) momentum-dependent Hamiltonians in the quantum Hall effect and an anisotropic superconductivity, (ii) parameter-dependent Hamiltonians in the discussion of Thouless pumping and the Berry phase, and (iii) a time evolution operator, . Now construct an -dimensional multiplet (a linear space) with the parameters which we considered...
The document discusses the concept of topological invariants in the context of superconductivity and quantum Hall effects. It explains how certain parameters specify a collection of fluxes passing through the system, which can be described by wave functions in the quantum Hall effects. The document also mentions some examples of concrete topological orders that will be studied. It discusses the gauge freedom and ambiguity in specifying the basis of the multiplet \( W \), which can be clarified by changing the basis. This leads to ambiguity in specifying the basis of the system. The document also introduces the Chern number and how it can be calculated using the integral of the trace log determinant. It explains how the Chern number is found in literature.

A global connection over the full surface \( S \) is not allowed to exist in a system with a nontrivial topological order. Then let us divide the integral region \( S \) into several patches \( S_R \) (for \( R = 0, 1, 2, \ldots \)), where the connection \( A_R \) is locally defined within \( S_R \) as \( A(x) = A_R(x) \). Furthermore, we assume each \( S_R, R = 1, 2, \ldots \), does not share any boundaries with \( \partial S_0 = - \bigcup_{R \geq 1} \partial S_R \). When the connection \( A_R \) is related to \( A_0 \) by the gauge transformation \( \omega_{0R} \), \( A_R = \omega_{0R} A_0 \omega_{0R}^{-1} + \omega_{0R}^{-1} d \omega_{0R} \), the Chern number \( C_S \) is written using the Stokes theorem as \( C_S = \frac{1}{4 \pi} \int_{S_R} \text{Im} \text{Tr} \omega_{0R}^{-1} d \omega_{0R} \).

Explicit Gauge Fixing: Topological invariants are usually given by gauge-dependent quantities. To evaluate the expression, one must fix the gauge. Without fixing it, we cannot have any well-defined derivative. Now let us explicitly fix the gauge for the multiplet. Although the basis \( \Psi \) has a gauge freedom, a projection operator into the multiplet \( \mathbf{P} = \Psi \Psi^\dagger \) is a gauge-invariant. Define a non-normalized basis, \( \Phi_\tilde{\Phi}^\dagger \), from a generic basis, \( \Phi \) (an \( N \times M \) matrix), as \( \Phi_\tilde{\Phi}^\dagger = \mathbf{P} \Phi = \Psi \eta_\Phi \) (\( \eta_\Phi = \Psi \Phi \)). The overlap matrix of the basis \( \Phi_\tilde{\Phi}^\dagger \) is generically semipositive definite. Then, only if the determinant of the matrix \( \Phi_\tilde{\Phi}^\dagger \) is nonzero, we can define a normalized wavefunction, \( \tilde{\Psi}_\Phi = \Psi \Phi_\tilde{\Phi}^\dagger \), where \( \Phi_\tilde{\Phi} \equiv U_\Phi^{ij} \text{diag}(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_M}) U_\Phi \) with \( \Phi_\tilde{\Phi}(\eta_\Phi = \tilde{\Psi}_\Phi \tilde{\Phi}^\dagger \mathbf{U}_\Phi \). This \( \Phi_\tilde{\Phi} \) is hermitean and positive definite. Now we define the connection \( A_\tilde{\Phi} \) with the gauge fixing by \( \tilde{\Phi} \) as \( A_\tilde{\Phi} = \tilde{\Psi}_\Phi \tilde{\Phi}^\dagger d \tilde{\Phi}^\dagger \). This is well defined unless \( \det \Phi_\tilde{\Phi} = 0 \).

Define regions \( S^\Phi_R, R = 1, 2, \ldots \), as (infinitesimally) small neighborhoods of zeros \( x_R^\Phi \) of \( \det \Phi_\tilde{\Phi} \) and \( S_0^\Phi \) as a rest of \( S \) as

\[
S = \bigcup_{R \geq 0} S^\Phi_R, \quad \det \Phi_\tilde{\Phi}(x) \begin{cases} \neq 0 & \forall x \in S^\Phi_R, x \neq x_R^\Phi \in S^\Phi_R, R = 1, 2, \ldots. \\ = 0 & \forall x \in S_0^\Phi \end{cases}
\]

We use this gauge for the region \( S^\Phi_R \) and for the region \( S_0^\Phi \), we use a different gauge by \( \tilde{\Phi} \), with \( \det \Phi_\tilde{\Phi} \neq 0 \) everywhere in \( S_0^\Phi \). The transformation matrix between \( \Phi_\tilde{\Phi} \) and \( \Phi_\tilde{\Phi}^\dagger \) is obtained as \( \omega = \eta_\Phi \eta_\Phi^{-1} \eta_\Phi^\dagger \). Since \( \eta_\Phi \) and \( \eta_\Phi^\dagger \) are strictly positive definite at the boundaries \( \partial S_0^\Phi \), we have \( \text{Im} \text{Tr} \log \omega = - \text{Im} \text{Tr} \log \tilde{\Phi}^\dagger \mathbf{P} \Phi \). Finally, we obtain an expression for the first Chern number with explicit gauge fixing as

\[
C_S = - N^T_S(S) = - \sum_{R \geq 1} \eta^R_\Omega(S^\Phi_R)
\]

where \( N^T_S(S) \) is the total number of signed vertices with the vorticity \( \eta^R_\Omega(S^\Phi_R) \) inside the region \( S_R, R \geq 1 \). Since \( \Omega = \text{Arg det} \eta_\Phi \), all the vertices of \( \Omega(\tilde{\Phi}, \Phi) \) are given by zeros of \( \det \eta_\Phi \), \( (x^\Phi) \) and \( \det \eta_\Phi(x^\Phi) \). The Chern number is obtained by summing up the vorticity only at \( x^\Phi \). This form of Chern number is not found in literature.
Since we assume that the two-dimensional surface $S$ is compact and $\Omega$ is regular except at $x_1^{\phi}, \cdots, x_1^{\phi}$, a union of curves $\{(URS^p_R) \cup (URS^q_R)\}$ is contractible to a point within a region where $\Omega$ is well defined. This implies that $N^T \Omega (I \Psi, \Psi) = N^T I \Omega \Psi, \Psi)$. That is, the vector field $\Omega$ depends on the gauge (choice of $\Phi$) but the total vorticity $N^T \Omega (S)$ is a gauge invariant of the multiplet $W$. None of the vortices has any direct physical meaning. Only the total number of vortices $N^T \Omega (S)$ has a physical significance.

The projection $P$ is essential for carrying out the present gauge fixing procedure. It has also an integral representation, $P = \frac{1}{2\pi i} \oint \Omega T (z)$, where $\Omega T = (I - L)^{-1}$ and the closed curve $\Gamma$ encloses all of the eigenvalues $\epsilon_1, \cdots, \epsilon_N$ inside, but not those $\epsilon_{M+1}, \cdots, \epsilon_N$ on the complex plane. From this form of projection, the stability condition of the generic gap $\phi$ for obtaining a well-defined multiplet is clear. The first Chern number has an apparently gauge-independent form given by $\text{Tr} \mathcal{F} = -\text{Tr} \mathcal{P} \mathcal{F} \mathcal{P}$ as well. Also, the Chern number for the multiplet is expressed as

$$C_S = \frac{1}{2\pi i} \sum_{k \in 1} \int_S dL \{ G_C (\epsilon_k) \} \{ G_C (\epsilon_k) \} dL \psi_k, n,$$

where $G_C = (I - P) \Omega T$. This is equivalent to a Kubo formula in the case of the quantum Hall effect. This formula is particularly important since mathematical objects such as Chern numbers have a direct relation with a physical quantity such as a Hall conductance. Surprisingly, this is observable in a bulk system.

**Sum Rules:** Assume the multiplet $W$ is a direct sum of orthogonal multiplets $W_1$ and $W_2$ as $W = W_1 \oplus W_2$, which is expressed by bases $\Psi_1$ and $\Psi_2$ (orthonormalized in each multiplet) as $\Psi = (\Psi_1, \Psi_2)$, where

$$\Psi_1 = I_{M_1}, \quad \Psi_2 = I_{M_2}, \quad \Psi_1 \Psi_2 = O_{M_1 M_2}, \quad \text{and} \quad \Psi_1 \Psi_2 = O_{M_2 M_1}.$$

The connection is given as $\mathcal{A} = \left( \begin{array}{cc} \Psi_1 & \Psi_2 \\ \Psi_2 & \Psi_1 \end{array} \right) (d \Psi_1, d \Psi_2)$. Thus, a trace of the connection is additive as $\text{Tr} \mathcal{A} = \text{Tr} \mathcal{A}_1 + \text{Tr} \mathcal{A}_2$, where $\mathcal{A}_1 = \Psi_1 d \Psi_1$ and $\mathcal{A}_2 = \Psi_2 d \Psi_2$. From this simple observation in the connection level, a sum rule for Chern numbers is as follows: $C_S(W_1 \oplus W_2) = C_S(W_1) + C_S(W_2)$. The sum rule in the field strength level was previously discussed. A simple consequence of the present sum rule is the total sum rule, that is, the Chern number of the total multiplet $W_T$ always vanishes; $\sum_i C_S(W_i) = C_S(\oplus W_i) = 0$, since $P_{\oplus W_i} = I_N$.

One-Dimensional Example ($\text{dim } W = 1$): When the multiplet is one-dimensional, such as $\Psi = \psi$ and $(P)_{ij} = \psi_i \psi_j^*$, we have $\Phi = P = (P)_{N1} = \psi_i \psi_j \psi_j^* \psi_i$ by taking $\Phi$ and $\Phi'$ as $t \Phi = (1, 0, \cdots, 0)$ and $t \Phi = (0, \cdots, 0, 1)$. Then the Chern number is given as

$$C_S = -\frac{1}{2\pi} \int_{S^0_R} d \text{Im} \log(\psi_1/\psi_N), \quad S^0_R = S \setminus \bigcup_{R \geq 1} S^R_R,$$

where $S^0_R$ includes a single zero of $\det \mathcal{O}_\psi = |\psi_1|^2$. This is a well-known classic expression.

**Multiplet of Several Landau Levels:** When one considers two-dimensional electrons on a lattice with the flux $\phi$ per plaquette, one-particle states are given by $q$ bands when $\phi = p/q$ with the mutually prime $p$ and $q$. Furthermore, the spectrum is given by the famous Hofstadter’s butterfly. When the fermi energy $E_F$ is in the $j$-th energy gap from below, the Hall conductance $\sigma$ is given by the sum of the Chern numbers of the $j$ bands. In this case, take a multiplet from a filled fermi sea ($W = FS$) and construct the basis of the multiplet from the $j$ Bloch states $\psi_j(k)$ below $E_F$ as $\Psi = (\psi_1, \cdots, \psi_j, M = j$, then the Chern number $C_{TFS}$ naturally gives the Hall conductance $\sigma_{xy}$ which is the sum of the Chern numbers of the filled bands.

**Dirac Monopole:** When the dimension of the total Hilbert space $N$ is 2, only the nontrivial multiplet is one-dimensional $M = 1$. Then take an hermite Hamiltonian $H(x) = R(x) \cdot \sigma$ for the normal operator $L$ where $\sigma$’s are Pauli matrices and $R(x)$ is a real three-dimensional vector $(R, \theta, \phi)$ is a polar coordinate of $R$. As an example, consider the multiplet $\Psi_-$ with the energy $-R$ as $\Psi_- = (\sin \theta \hat{x}, e^{i \phi(x)} \cos \theta \hat{y})$. The projection is given as $P_- = \Psi \Psi_- = (\sin^2 \theta \hat{x} - e^{-i \phi(x)} \cos \theta \cos^2 \theta \hat{y} \cos \theta \hat{y} \hat{x})$. Using a gauge by $\Phi$ and $\Phi'$ as $t \Phi = (\cos \xi, e^{i \xi} \hat{x})$ and $t \Phi = (\cos \xi, e^{i \xi} \hat{y})$, we have $\mathcal{O}_\phi = 0$ and $\det \mathcal{O}_\phi = 0$ give $(\theta(x), \phi(x)) = (\xi, \tilde{\xi})$ and $(\xi, \tilde{\xi})$, respectively. This clearly shows that the positions of the vortices defined by the vector field $\Omega = \text{Arg}(-\sin \frac{\pi}{2} \cos \xi + e^{+i(\xi - \tilde{\xi})} \cos \frac{\pi}{2} \sin \frac{\pi}{2})(-\sin \frac{\pi}{2} \cos \xi + e^{-i(\xi - \tilde{\xi})} \cos \frac{\pi}{2} \sin \frac{\pi}{2}) \hat{y}$ is gauge-dependent and do not have any direct physical meaning. One can choose the positions of the vortices as one wishes.

**Unitary Superconductors:** Let us first consider the simplest case, that is, the unit cell includes only one site. Then the Bogoliubov-de Gennes equation for generic superconductivity is given in a momentum space by a $4 \times 4$ secural equation, $H' = E \psi, H'' = \left( \begin{array}{cc} \epsilon_2 & \Delta \\ \Delta^\dagger & -\epsilon_2 \end{array} \right)$. As for the unitary order, the order parameter matrix $\Delta$ is written as $\Delta = \| \Delta \| \Delta$, $\| \Delta \| \geq 0, \| \Delta \| = \| \Delta \| = 1$, where $\Delta_0$ is a $2 \times 2$ unitary matrix. Then the eigenstates (quasiparticle) are doubly degenerate as $\psi_\pm(w) = (-\sin \frac{\pi}{2} w \cos \frac{\pi}{2} \Delta_0, w)$, for example, for the $E = -R$ state where $w$ is a normalized arbitrary two-component vector, $w^* w = 1, R = \sqrt{|\Delta|^2 + \epsilon^2}, \epsilon = R \cos \theta$ and $| \Delta | = R \sin \theta$. Now let us construct a multiplet for the degenerate $E = -R$ quasiparticle bands as $\Psi_- = (\psi_0(w_1), \psi_0(w_2))$, where $w_1$ and $w_2$ form an arbitrary two-dimensional orthonormalized complete set: $w^*_j w_j = \delta_{ij}, w_j w_j + w_j^* w_j = I_2$. Then the projections $P_{-}$ are given in a gauge invariant form as $P_{-} = \left( \begin{array}{cc} I_2 & \Delta_0 \\ -\Delta_0 & I_2 \end{array} \right)$. Now let us fix the gauge by choosing $\Phi = \{ 0_2, I_2 \}$ and $\Phi = \{ I_2, 0_2 \}$. Then we have $\det \mathcal{O}_\phi = \cos \theta \cdot \Omega = \text{Arg} \det \Delta = \text{Arg} \Delta$. Since the overlap determinant $\det \mathcal{O}_\phi = 0$ vanishes at $\theta = \pi$ for the multiplet $W_-$, the Chern number...
ber is given by

$$C_S^- = -\frac{1}{2\pi} \sum_p \oint_p d\arg \det \Delta,$$

where $p$'s are points on the surface $S$ which are specified by $\theta = \pi$, that is, $|\Delta(p)| = 0$ and $\epsilon(p) = R(p) = -E(p)$. This is a novel expression for the generic spin Hall conductance for the unitary superconductors with equal spin pairing. In the previous work, the Chern number was given as the sum of two integers using an eigenvalue equation for the unitary matrix $\Delta_0$. Here, we give a direct expression only using the order parameter matrix $\Delta$. Furthermore, if one parameterizes the unitary $2 \times 2$ matrix $\Delta_0$ as $\Delta_0 = e^{i\theta} e^{i\hat{n} \cdot \vec{p}}$, $|\hat{n}| = 1$, we have

$$C_S^- = -\frac{1}{2} \sum_p \oint_p d\theta.$$

The present method is crucially important and efficient when the order parameter is given by numerically solving a BCS self-consistent equation with a large unit cell. Even in this generic situation, to evaluate the spin Hall conductance, we must determine the (2n - 1)-dimensional spheres $S^n_R$ enclosing $(2n - 2)$-dimensional regions $P^n_R$ which are defined by the zero of $\det \mathcal{O}_n$ in $S^n$. They should also help in the characterization of the topological order in complex situations.

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