Topological quantum phase transitions in superconductivity on lattices

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Topological quantum phase transitions in superconductivity are discussed on two-dimensional lattices. The main focus is on the Chern number for superconducting states. Each superconductivity is characterized by the Chern number, and the quantum phase transition is associated with topological changes of the quasiparticle Bloch function in the Brillouin zone. For the superconducting case, the Chern number has several equivalent but different topological expressions given by vortices, the Dirac monopole, and strings. We demonstrate quantum phase transitions by these topological quantities both for singlet and triplet cases.

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The quantum phase transition is a drastic change of a ground state when physical parameters of a system are varied. This is a phase transition at zero temperature with quantum fluctuation, which raises many interesting physical questions. Recently substantial number of works have focused on the topic reflecting its importance. Typical examples include the Mott transition in strongly correlated systems and the Hall plateau transition in the quantized Hall effect.[1–4] The latter is special in the sense that the ground state is characterized by a quantized quantity (quantized Hall conductance σ_{xy}). As is known today, its quantization originates from a topological character of the Hall conductance.[5–8] Then the transition is governed by topological objects such as the Chern numbers; vortices, and edges states.[6–9] Each phase is characterized by the different topological quantum number although the symmetry of the state is not necessarily different. It is quite different from usual phase transitions and is characteristic to the topological quantum phase transition.[10] There have been several features for this type of the phase transition. Some of them are a special form of a selection rule, and the possible stability of the phase, which puts special importance on the topological transitions and discriminates from other quantum phase transitions.[4,10]

Recently, there have been trials to extend the concept of this topological phase transition to unconventional singlet superconductivity.[11–14] In the discussions, mapping the system into the standard quantum Hall system is essential. Here the ''spin'' Hall conductance plays a main role, which is given by the Chern numbers. A nontrivial example of such states is given by time-reversal symmetry breaking superconductivity.[12–16] Leaving its reality apart, the topological phase transition in superconductivity raises important theoretical questions how the topological character restricts transition types. In this paper, we take the generalized Bogoliuvov-de Gennes (B-dG) Hamiltonian for superconductivity to discuss the topological quantum phase transition and demonstrate the topological character using several topological expressions.

Search for spin triplet superconductivity has also long history but several important materials have been found recently, which raised intense reinvestigations of triplet superconductivity. One of the interesting aspects of the triplet state is its rich structure of the order parameters, which allows the existence of nontrivial topological structures. On this point, the topological characters of the chiral p-wave superconductivity is investigated by several groups.[13,14,17,18] In this paper, we treat this spin triplet case on a two-dimensional lattice based on the same strategy as the spin singlet case. Then we can characterize the triplet state by the Chern number and several topological expressions as well.[19]

Comparing to the usual Quantum Hall effect with many Landau bands, there are only two quasiparticle bands of quasiparticles (and quasiholes) in the superconductivity. This special but simple situation allows us to use the interesting Berry's parameterization. Then the gauge fixing to calculate the explicit Chern number also produces an interesting topological expression. Using this gauge fixing, we establish a relation between several different topological expressions.

The Chern number. To demonstrate the topological transition in superconductivity, we investigate systems described by the following B-dG Hamiltonian for superconducting quasiparticles

$$H=\sum_{ij}\ (t_{ij}^{\sigma}c_{i\sigma}^{\dagger}c_{j\sigma}+\Delta_{ij}c_{i\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}+\Delta_{ij}^{*}c_{j\downarrow}c_{i\uparrow})-\mu\sum_{i\sigma}\ c_{i\sigma}^{\dagger}c_{i\sigma}.$$

In this paper, we assume the system is translationally invariant as $t_{ij}^{\sigma}=t^{\sigma}(i-j)$ and $\Delta_{ij}=\Delta(i-j)$. Then the Hamiltonian is written as

$$H=\sum_{k}\ \boldsymbol{c}^{\dagger}(\boldsymbol{k})\boldsymbol{h}(\boldsymbol{k})\boldsymbol{c}(\boldsymbol{k}),\quad \boldsymbol{h}(\boldsymbol{k})=\begin{pmatrix}\epsilon^{\uparrow}(\boldsymbol{k}) & \Delta(\boldsymbol{k})\\ \Delta^{*}(\boldsymbol{k}) & -\epsilon^{\downarrow}(-\boldsymbol{k})\end{pmatrix},$$

where $\boldsymbol{c}^{\dagger}(\boldsymbol{k})=[c_{\uparrow}^{\dagger}(\boldsymbol{k}),c_{\downarrow}(\boldsymbol{k})]$, $\epsilon^{\sigma}(\boldsymbol{k})=\Sigma_j e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_j}t^{\sigma}(j)-\mu$ and $\Delta(\boldsymbol{k})=\Sigma_j e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_j}\Delta(j)$. We further require $t_{ij}^{\uparrow}=t_{ji}^{\downarrow}$. Then we have $\epsilon^{\uparrow}(\boldsymbol{k})=\epsilon^{\downarrow}(-\boldsymbol{k})\equiv\epsilon(\boldsymbol{k})$. Generically various realizations of order parameters are determined by the self-consistent equation. Here let us assume a form of the order parameters to discuss topological quantum phase transitions.

The ''spin'' Hall conductance of the superconducting state on a lattice is given by the generalized Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) formula as $\sigma=-(e^2/h)C$, where $C\equiv(1/2\pi i)\int_{T^2}d\boldsymbol{S}_k\cdot\mathrm{rot}_k\boldsymbol{A}_k$, $\boldsymbol{A}_k=\langle\boldsymbol{k}|\boldsymbol{\nabla}_k\boldsymbol{k}\rangle$.[6–8,11–13,20] The Chern number C, is given by a total vorticity of the quasiparticle Bloch function $|\boldsymbol{k}\rangle$ for the *negative-energy* quasiparticle, $\boldsymbol{h}(\boldsymbol{k})|\boldsymbol{k}\rangle=-E(\boldsymbol{k})|\boldsymbol{k}\rangle$, $E(\boldsymbol{k})=\sqrt{\epsilon(\boldsymbol{k})^2+|\Delta(\boldsymbol{k})|^2}$ since the quantum-mechanical average is taken over the grand canonical ensemble. The integration is over the Brillouin zone, which is topologically a torus T^2, and $d\boldsymbol{S}=(dk_x,0,0)\times(0,dk_y,0)=(0,0,dk_xdk_y)$ is an infinitesimal area. The Chern number has an apparent topological expression that is written as a winding number of a relative phase of the Bloch function[7,8]

$$C=-N_{winding}\equiv-\sum_l \frac{1}{2\pi}\oint_{\partial R_l} d\boldsymbol{k}\cdot\boldsymbol{\nabla}\,\mathrm{Im}\,\ln\frac{|\boldsymbol{k}\rangle_1}{|\boldsymbol{k}\rangle_2}.$$

The summation is over the poles of $|\boldsymbol{k}\rangle_1/|\boldsymbol{k}\rangle_2$ (zeros of the the second component of the Bloch function $|\boldsymbol{k}\rangle_2$) in the Brillouin zone (R_l is a small area around each pole).[7,8]

By the Berry's parametrization,[21] the Hamiltonian $\boldsymbol{h}(\boldsymbol{k})$ can be written as

$$\boldsymbol{h}(\boldsymbol{k})=\boldsymbol{R}(\boldsymbol{k})\cdot\boldsymbol{\sigma},$$

where $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ are the Pauli matrices and $\boldsymbol{R}=(R_x,R_y,R_z)=[\mathrm{Re}\,\Delta(\boldsymbol{k}),-\mathrm{Im}\,\Delta(\boldsymbol{k}),\epsilon(\boldsymbol{k})]$. Then the expression for the Chern number is rewritten by these coordinates in $\boldsymbol{R}$ space as

$$C=\frac{1}{2\pi i}\int_{R(T^2)} d\boldsymbol{S}_R\cdot\mathrm{rot}_R\boldsymbol{A}_R,$$

where $\boldsymbol{A}_R=\langle\boldsymbol{R}|\boldsymbol{\nabla}_R\boldsymbol{R}\rangle$ and $|\boldsymbol{k}\rangle=|\boldsymbol{R}(\boldsymbol{k})\rangle$. In a particular gauge (a phase convention of the vector), it is written as $|\boldsymbol{R}\rangle=\binom{-\sin\theta/2}{e^{i\phi}\cos\theta/2}$, where (R,θ,ϕ) is a polar coordinate of $\boldsymbol{R}$. The integral region $R(T^2)$ is a closed surface in three-dimensional parameter space mapped from the Brillouin zone T^2. As is well known, the corresponding vector potential defines a magnetic monopole at the origin in the three-dimensional space as $\mathrm{div}\,\mathrm{rot}\,\boldsymbol{A}_R=-2\pi i\,\delta_R(\boldsymbol{R})$.[21–23] Therefore, by the Gauss' theorem, we have another expression for the Chern number as

$$C=-\int_{R(T^2)} dV\,\delta_R(\boldsymbol{R})=-N[R(T^2),O]=-N_{covering},$$

where $N_{covering}=N[R(T^2),O]$ is a degree of covering by the closed surface $R(T^2)$ around the origin O. This is another topological expression characterizing the negative-energy band.

Now let us calculate the winding number $N_{winding}$ by this gauge. In the present gauge, $\boldsymbol{\nabla}_k\,\mathrm{Im}\,\ln|\boldsymbol{k}\rangle_1/|\boldsymbol{k}\rangle_2=-\boldsymbol{\nabla}_k\phi$ and we have $N_{winding}=(1/2\pi)\Sigma_{P_-}\oint_{R(\partial R_l)}d\boldsymbol{R}\cdot\boldsymbol{\nabla}_R\phi$. Since the zeros of the second component of the Bloch function are defined by $\cos\theta/2=0$, we rewrite the above equation as

$$C=-N_{winding}=-\sum_{P_-} I[R(T^2),z_-],$$

where z_- is a negative z axes in the $\boldsymbol{R}$ space (the Dirac string) and P_-'s are intersection points of the closed surface $R(T^2)$ and the Dirac string z_-. The integer $I[R(T^2),z_-]$ is an intersection number that gives the multiplicity of the local covering at P_-'s. It is a positive integer when the Dirac string z_- is parallel to the normal vector of the surface $(\widehat{\partial\boldsymbol{R}/\partial k_x})\times(\widehat{\partial\boldsymbol{R}/\partial k_y})$ and a negative integer when it is antiparallel. $N_{winding}$ is apparently integral and zero if the origin is outside the surface. It is one of the advantages of the present expression.

Now we have established a relation for the two topological integers as

$$N_{covering}=N_{winding},$$

$$N[R(T^2),O]=\sum_{P_-} I[R(T^2),z_-].$$

This relation is physically apparent but it confirms the consistency of the discussion.

Demonstration. As is discussed above, the Chern number is a topological quantity and is stable against small perturbation. Each superconducting state is characterized by an integer and the topological quantum transition is associated with topological change of geometrical objects, one of which is the relative phases of the Bloch functions of the quasiparticles and the others are the closed surface $R(T^2)$ and the Dirac string z_-. The topological transition of the superconductivity is clearly observed by investigating these topological objects.

Now let us take following two examples of the order parameters to demonstrate the topological transition.

$$\text{Case I:}\quad \text{singlet},\quad \Delta_{ij}=\Delta_{ji},$$

$$\Delta_{i,i}=\Delta_0,\quad \Delta_{i,i+\hat{x}}=-\Delta_{i,i+\hat{y}}=\Delta_{x^2-y^2},$$

$$\Delta_{i,i+\hat{x}+\hat{y}}=-\Delta_{i+\hat{x},i+\hat{y}}=i\Delta_{xy},$$

$$\text{Case II:}\quad \text{triplet},\quad \Delta_{ij}=-\Delta_{ji},$$

$$\Delta_{i,i+\hat{x}}=-i\Delta_{i,i+\hat{y}}=\Delta_x,$$

where $\Delta_{x^2-y^2}$ and Δ_{xy} are real. The hopping $t_{ij}^{\sigma}=t$, is also real and only nonzero on the nearest-neighbor links. We have $\epsilon(\boldsymbol{k})=-2t(\cos k_x+\cos k_y)-\mu$, for the both cases, and $\Delta(\boldsymbol{k})=\Delta_0+2\Delta_{x^2-y^2}(\cos k_x-\cos k_y)+2i\Delta_{xy}[\cos(k_x+k_y)-\cos(k_x-k_y)]$ for the singlet case (Case I) and $\Delta(\boldsymbol{k})=2i\Delta_x(\sin k_x+i\sin k_y)$ for the triplet case (Case II).

In Fig. 1, the relative phase of the Bloch function, $\mathrm{Arg}(|\boldsymbol{k}\rangle_1/|\boldsymbol{k}\rangle_2)$, for the singlet case is shown. For small Δ_0, one can see the charge two vortices at the pole of $|\boldsymbol{k}_1\rangle/|\boldsymbol{k}_2\rangle$ (circle) split into two independent ones and contribute to the nontrivial Chern numbers. Note that only the poles (circles) of $|\boldsymbol{k}\rangle_1/|\boldsymbol{k}\rangle_2$ contribute to the Chern numbers although the zeros (squares) also give vortices. When Δ_0 is sufficiently large, they finally annihilate in pairs with negative vortices defined by the zeros of $|\boldsymbol{k}\rangle_1/|\boldsymbol{k}\rangle_2$ (squares). Another topological objects, the closed surface $R(T^2)$ and the Dirac string z_- is shown for the singlet case in Fig. 2. One can see the covering degree of mapping $T^2\rightarrow R(T^2)$ is two if Δ_0 is sufficiently small. The intersection number of the closed surface $R(T^2)$ and the Dirac string z_- is also two, which can be easily checked for this example. In general, the order parameter may have more complicated momentum dependence, and calculating the covering degree of mapping is not trivial at all. Therefore, the intersection number $I[R(T^2),z_-]$ helps

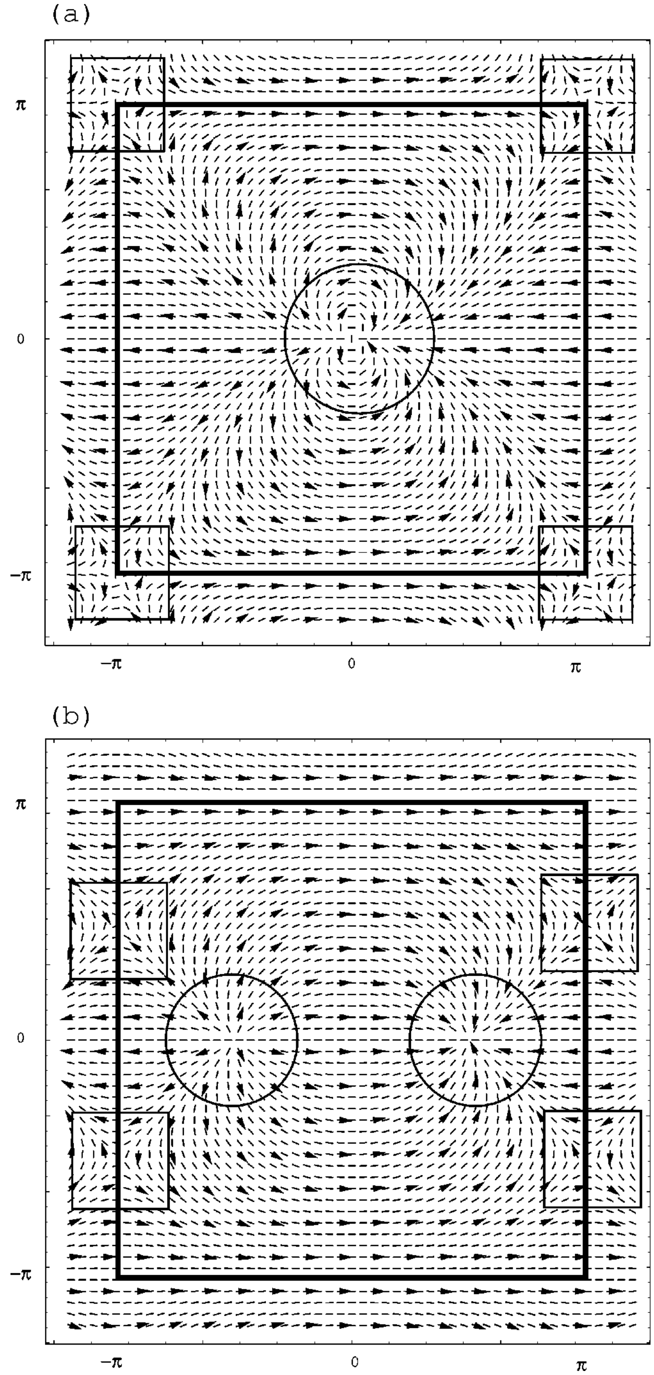

FIG. 1. Relative phases, $\mathrm{Arg}(|\boldsymbol{k}\rangle_1/|\boldsymbol{k}\rangle_2)=\mathrm{Im}\ln|\boldsymbol{k}\rangle_1/|\boldsymbol{k}\rangle_2$ of the quasiparticle Bloch function in the Brillouin zone (solid square). The circles and the squares include the poles and the zeros of $|\boldsymbol{k}\rangle_1/|\boldsymbol{k}\rangle_2$, respectively. Note that only the circles (poles) contribute to the total Chern number. The spin singlet case with (a) $\Delta_0=0$, $\Delta_{x^2-y^2}=t$, $\Delta_{xy}=0.5t$, $\mu=0$ (the vorticity of the pole at the origin is $+2$), (b) $\Delta_0=2t$, $\Delta_{x^2-y^2}=t$, $\Delta_{xy}=0.5t$, $\mu=0$ (there are two vorticity $+1$ vortices at the poles).

us to determine the Chern number concretely. It is also easy to see that the Chern number vanishes if $|\Delta_0|$ or $|\mu|$ is sufficiently large since the surface $R(T^2)$ does not include the origin. In this singlet case, the origin O, is doubly covered since $\boldsymbol{R}(\boldsymbol{k})=\boldsymbol{R}(-\boldsymbol{k})[\Delta(\boldsymbol{k})=\Delta(-\boldsymbol{k})]$. It implies the selection

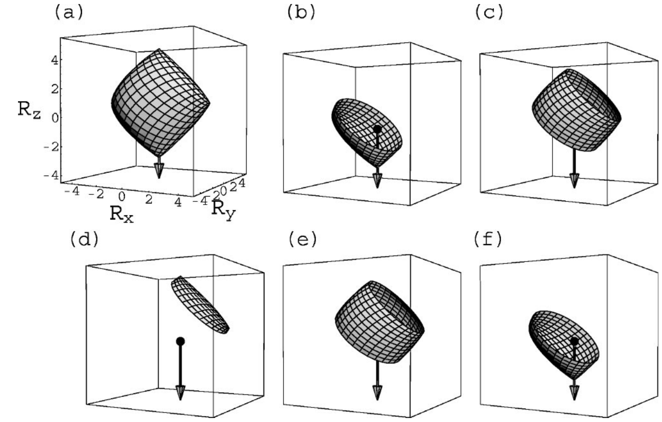

FIG. 2. Mapped Brillouin zone $R(T^2)$ by the Berry's parametrization. The monopole at the origin O and the Dirac string z_- are also shown. The spin singlet case with $\Delta_0=0$, $\Delta_{x^2-y^2}=t$, $\Delta_{xy}=t$, $\mu=-t$; (a) is the total surface $R(T^2)$, $k_x\in[0,2\pi]$, $k_y\in[0,2\pi]$, and (b)–(f) are parts of the surface to show how it covers the origin. They are drawn for $k_x\in[0,2\pi]$ and (b): $k_y\in[0,2\pi/5]$, (c): $k_y\in[2\pi/5,4\pi/5]$, (d): $k_y\in[4\pi/5,6\pi/5]$, (e): $k_y\in[6\pi/5,8\pi/5]$, (f): $k_y\in[8\pi/5,2\pi]$. The monopole O is doubly covered by surface $R(T^2)$.

rule $\Delta C=\pm 2$.[12] Another interesting case is given by the $\Delta_{xy}=0$. In this case, the energy gap collapses and the gapless Dirac dispersion prevent from determining the Chern number without ambiguity (if $|\mu|$ is small). This situation is evident by the present discussion since the surface $R(T^2)$ is collapsed into a diamond shaped two-dimensional region $\boldsymbol{R}=\lambda_1\boldsymbol{v}_1+\lambda_2\boldsymbol{v}_2-(0,0,\mu)$, $\lambda_{1,2}\in[-1,1]$, $\boldsymbol{v}_1=(\Delta_{x^2-y^2},0,-2t)$ and $\boldsymbol{v}_2=(-\Delta_{x^2-y^2},0,2t)$. When the origin O is on this region, the Chern number is ill defined and the dispersion is gapless. This condition is clearly given by $|\mu|\leqslant 2t$. Otherwise, there is an energy gap and the Chern number is zero.

The triplet case, the case II, gives a little tricky situation. As shown in Fig. 3, the covering degree of mapping around the origin is $+1$ or -1 depending on the parameter detail. The surface $R(T^2)$ is self-intersecting and a local coordinate $[\boldsymbol{e}_x(\boldsymbol{R}),\boldsymbol{e}_y(\boldsymbol{R}),\boldsymbol{n}(\boldsymbol{R})]$ on the surface has a different chirality depending on the position of the surface where $\boldsymbol{e}_\alpha(\boldsymbol{R})=\widehat{\partial\boldsymbol{R}/\partial k_\alpha}$, $(\alpha=x,y)$ are tangent vectors and $\boldsymbol{n}(\boldsymbol{R})$ is a normal vector of the surface at $\boldsymbol{R}$. In other words, inside and outside of the surface are exchanged on intersecting lines. Of course, the surface $R(T^2)$ itself is orientable always. At the

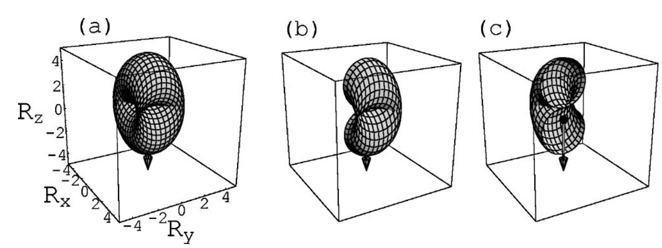

FIG. 3. Same as Fig. 2 for the spin triplet case with $\Delta_0=0$, $\Delta_x=-t$, $\mu=-t$; (a) is the total surface $R(T^2)$, $k_x\in[0,2\pi]$, $k_y\in[0,2\pi]$; (b) and (c) are drawn for $k_x\in[0,2\pi]$ and (b): $k_y\in[0,\pi]$, (c): $k_y\in[\pi,2\pi]$.

transition, the selection rule for the triplet case is $\Delta C = \pm 1$ generically. However, the transition in which the origin O passes through this intersecting point, say, changing the chemical potential μ, the Chern number can change its sign as $C: \pm 1 \to \mp 1$, $(\Delta C = \pm 2)$.

In conclusion, we have demonstrated the topological quantum phase transition in superconductivity on lattices by using several topological expressions for the Chern number. They are the winding number of the relative phase of the quasiparticle Bloch function $N_{winding}$ and the covering degree $N_{covering}$ of mapping $T^2 \to R(T^2)$ around the Dirac monopole at origin. The winding number also has another expression given by the intersection number $I[R(T^2), z_-]$ of the closed surface $R(T^2)$ and the Dirac string z_-.

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