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Plateau transitions in the pairing model: Topology and selection rule

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Based on the two-dimensional lattice fermion model, we discuss transitions between different pairing states. Each phase is labeled by an integer which is a topological number and characterized by vortices of the Bloch wave function. The transitions between phases with different integers obey a selection rule. Even without a magnetic field, edge states necessarily exist in the superconductor if the topological number is nonzero. They reflect the topological character of the bulk. Transitions driven by randomness are also discussed numerically.

Quantum phase transitions between different superconducting states have attracted much interest recently. In Refs. 1 and 2, for example, its possible realization in a high-$T_c$ superconductor was proposed, which is accompanied by the time-reversal symmetry breaking. Further, there is a recent observation that it has some similarity to the plateau transition in the integer quantum Hall effect (IQHE).3–6 One of the claims is that each phase is labeled by an integer (analog of the Hall conductance in the IQHE) and there can be transitions between phases with different integers.

In this paper, based on the lattice fermion model, we investigate the problem. The integer for each phase is defined by a topological invariant of the U(1) fiber bundle (the Chern number).3,7,8 The U(1) fiber bundle is a geometrical object which is composed of the Brillouin zone (torus) and the Bloch wave functions (fiber). Due to its topological stability, a singularity in the U(1) fiber bundle necessarily occurs with the change of the Chern number. The singularity is identified with the energy-gap closing9–14 The Chern number is closely related to zero points (vortices) of the Bloch wave function. Focusing on the motion of the vortices near the singularity, we give a general proof of a selection rule of the transitions. Due to the intrinsic symmetry of the system, the selection rule differs from that of the IQHE.15 We also investigate the properties of the edge states and how they reflect the topological character of the bulk. The transition due to the change of randomness strength is a typical example of the disorder-driven transition numerically.

The Hamiltonian is

$$\mathcal{H} = \sum_{l,m} c_l^\dagger \mathbf{H}_{lm} c_m = \sum_{l,m} c_l^\dagger \begin{pmatrix} t_{lm} & \Delta_{lm} \\ \Delta_{ml}^* & -t_{ml} \end{pmatrix} c_m,$$

(1)

where $c_l^\dagger = (c_n^\dagger, c_{-n}^\dagger)$, $c_n = (c_n^1, c_n^2)$, and $n = (n_x,n_y) \in \mathbb{Z}^2$.

This is an extension of the lattice fermion model discussed in connection with the plateau transition in the IQHE.11–14 Here we comment on the relation between this Hamiltonian and the superconductivity. Under the unitary transformation $c_n \rightarrow d_n$, $c_{-n} \rightarrow d_{-n}$ (for $\forall n$), the Hamiltonian (1) is equivalent to

$$\mathcal{H} = \sum_{l,m} [d_l^\dagger t_{lm} d_m + d_l^\dagger t_{ml} d_m + d_l^\dagger \Delta_{lm} d_m + d_{-m}^\dagger \Delta_{ml}^* d_m].$$

This is the pairing model for the singlet superconductivity. In the context of superconductivity, the pair potential $\Delta_{lm}$ should be determined by a self-consistent equation. Although the effect is interesting itself, it is beyond the scope of this paper. Further, the conditions $t_{lm} = t_{ml}$ and $\Delta_{lm} = \Delta_{ml}^*$ are imposed and they correspond to the Hermiticity and the SU(2) symmetry, respectively. The SU(2) symmetry leads to the condition

$$- (\sigma_y H_{lm} \sigma_y)^* = H_{lm}.$$

(2)

Due to the SU(2) symmetry, we can restrict ourselves to the sector $\Sigma_m d_l^\dagger \sigma^y d_m = 0$ without loss of generality. This is equivalent to the half-filled condition for the Hamiltonian (1), which we impose in the following arguments.

Now let us define a topological invariant (the Chern number) for our model. It is a key concept in the following arguments. Put the system on a torus, which is $L_x \times L_y$ and periodic in both $x$ and $y$ directions. Define the Fourier transformation by $c_n = 1/\sqrt{L_x L_y} \sum_k e^{i k \cdot n} c(k)$ where $k = (k_x,k_y)$ is on the Brillouin zone $(-\pi,\pi) \times (-\pi,\pi)$. Assuming $H_{lm}$ to be invariant under translations, we obtain $\mathcal{H} = \sum_k c(k)^\dagger \mathbf{H}(k) c(k)$ where $\mathbf{H}(k) = \Sigma_{l,m} e^{-i k \cdot l} \sigma^y \Delta_{lm}^*$. The $\mathbf{H}(k)$ has two eigenvectors and eigenvalues. They correspond to the Bloch wave functions and the energy bands, respectively. To satisfy the half-filled condition, the lower band is occupied for the ground state. We denote the Bloch wave function for the lower band by $(a(k),b(k))$. Then the topological invariant [the Chern number of the U(1) fiber bundle] is defined as

$$C = \frac{1}{2\pi i} \int dk \cdot \hat{z} \cdot (\nabla_k \times \mathbf{A}),$$

(3)

where $\mathbf{A} = (a^*(k) b^*(k)) \nabla_k \hat{z} (a(k),b(k))$ and $\hat{z} = (0,0,1)$.3,7,8 The integration $\int dk$ is over the Brillouin zone which can be identified with a torus. For simplicity, we assumed $H_{lm}$ to be

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invariant under translations. However, a generalization to a multiband system (including a random system) is possible. It is crucial for the following arguments to rewrite the above formula in terms of a zero point of the Bloch wave function (vortex) and the winding number (charge). To be explicit, let us perform the gauge fixing of the Bloch wave function for the lower-energy band. We note that the Chern number itself does not depend on the gauge fixing. To define the gauge, we use the rule \(a(k) = 1\) and introduce a notation \(b(k) = b'(k)e^{-iik} [b'(k) \in R]\). An ambiguity in the gauge fixing occurs when \(a(k) = 0\). Around the zero point (vortex) in the Brillouin zone, it is necessary to change the way of the gauge fixing—for example, as \(b(k) = 1\). Then the Chern number (3) is rewritten as

\[
C = \sum_i C_i, \quad C_i = \frac{1}{2\pi} \int_{\partial R_i} d\kappa \nabla \xi(k),
\]

where the summation is taken over all vortices of \(a(k)\) and \(R_i\) is a region surrounding the \(i\)th vortex which does not contain other zeros of either \(a(k)\) or \(b(k)\). Here \(C_i\) is an integer and we call it the charge of the \(i\)th vortex.

Let us discuss the \(d_{2\ldots 2} + id_{xy}\) model on a torus as an example. The model is defined by \(t_{n+e_x, e_y} = t_{e_x, e_y} = t\), \(\Delta_n + e_x, e_y = -\Delta_n + e_x, e_y = \Delta_{2\ldots 2} - \gamma^2\), and \(\Delta_n - e_x, e_y = -\Delta_n + e_x, e_y = i\Delta_{xy}\) for \(\forall n\) \([e_x = (1,0), e_y = (0,1), t > 0, \Delta_{2\ldots 2}, \Delta_{xy} \in R]\) and the other matrix elements are zero. Then

\[
H(k) = \begin{pmatrix}
A(k) & B(k) \\
B^*(k) & -A(k)
\end{pmatrix},
\]

where \(A(k) = 2t(\cos k_x + \cos k_y)\) and \(B(k) = 2\Delta_{2\ldots 2}(\cos k_x - \cos k_y) + 2i\Delta_{xy}(\cos(k_x + k_y) - \cos(k_x - k_y))\). The energy spectrum is given by \(E = \pm \sqrt{A(k)^2 + |B(k)|^2}\). When \(\Delta_{xy} = 0\), the upper band and the lower band touch at points \((\pm \pi/2, \pm \pi/2)\) in the Brillouin zone. The low-lying excitations around the gap-closing points are described by massless Dirac fermions. By turning on a finite \(\Delta_{xy}\), the mass generation occurs in the Dirac fermions. The vortex position is given by \(a(k) = 0\) and it is \((k_x, k_y) = (0, 0)\). Using \(B(k) = B'(k)e^{i\Delta_{xy}}[B'(k) \in R]\), the charge of the vortex is \(1/2\pi \int_{(0,0)} d\kappa \nabla \xi(k) = 2 \text{sgn}(\Delta_{xy}/\Delta_{2\ldots 2})\). Since there is no other vortex, the Chern number \(C\) is given by

\[
C = 2 \text{sgn}(\Delta_{xy}/\Delta_{2\ldots 2}).
\]

Here we note that, as in the case of the IQHE on a lattice, the Chern number can take various integer values in general cases—e.g., a multiband system and a model with a different \(T\)-broken pairing symmetry. Even in these cases, there are universal features in this problem. They are, for example, the existence of edge states without a magnetic field and a selection rule as discussed below.

As in the IQHE,\(^{17-19}\) the edge states play a crucial role in the problem.\(^{20-23}\) The edge states reflect the bulk properties and it is possible to detect the topological character of the bulk through the edge states. We also note that the existence of the edge states even without a magnetic field can justify the network model in Ref. 4. In order to discuss the edge states, put the system on a cylinder which is \(L_x \times L_y\) and periodic only in \(y\) direction. Further we impose an open boundary condition in the \(x\) direction. Define the Fourier transformation by \(c_n = 1/\sqrt{L_x} \sum_k e^{ik_n} c_n(k_x)\) where \(k_x\) is on \((-\pi, \pi)\). Then \(H = \sum_k c^*_l(k_x) H_{lm}(k_x)c_m(k_x)\) where \(H_{lm}\) is assumed to be invariant under translations in the \(y\) direction and \(H_{l m_{q}}(k_x) = \sum_{l_{q}-m_{q}} e^{-ik_{x}(l_{q}-m_{q})} H_{lm}\). The relation (2) can be rewritten as \(-\langle \sigma_x H_{lm_{q}}(k_x) \sigma_y \rangle = H_{lm_{q}}(k_x)\). Define an eigenvector \(u\) by \(\sum_{m_{q}} H_{lm_{q}}(k_x)u_{m_{q}} = Eu_{l}\). Now we show that there are two basic operations \(\mathcal{P}\) and \(\mathcal{Q}\) on the vector. They are defined by \((\mathcal{P}u)_{n_{x}} = \langle \sigma_x \rangle u_{n_{x}}\) and \((\mathcal{Q}u)_{n_{x}} = u_{n_{x}+1}\). Then \(\sum_{m_{q}} H_{lm_{q}}(k_x)\langle \mathcal{P}u \rangle_{m_{q}} = \langle -E \rangle (\mathcal{P}u)_{l}\). Further, when there is a reflection symmetry, we can obtain another relation \(\sum_{m_{q}} H_{lm_{q}}(k_x)\langle \mathcal{Q}u \rangle_{m_{q}} = E (\mathcal{Q}u)_{l}\). Based on the symmetry, we shall discuss basic properties of the edge states. Consider a case when \(u\) is an eigenstate which is localized spatially on the left (or right) boundary, i.e., a left (or right)-hand edge state. Then, from the above argument, \(\mathcal{P}u, \mathcal{Q}u, \mathcal{P} \mathcal{Q}u\) are classified into two left-hand edge states and two right-hand edge states. Now, as in the argument of the IQHE,\(^{24}\) let us introduce a fictitious flux through the cylinder and change it from 0 to flux quanta \(\Phi/e\). Due to the symmetry, the number of edge states which move from one boundary to the other is necessarily even. We shall consider the \(d_{2\ldots 2} + id_{xy}\) model on a cylinder as an example. In Fig. 1, the energy spectrum is shown. It is confirmed that the energy spectra of the edge states appear in pairs and the number of the edge states which move from one boundary to the other as the fictitious flux is added is even and coincides with the Chern number. In other words, the edge states directly reflect the topological character of the bulk. Therefore, even without a magnetic field, the edge states necessarily exist in the superconductor if the Chern number is nonzero.

As discussed above, each phase in our model is labeled by the Chern number. The vortices move as the Hamiltonian is perturbed. The Chern number, however, does not change in general. Due to the topological stability, the change of the Chern number is necessarily accompanied by a singularity in the U(1) fiber bundle. The singularity is identified with the energy-gap closing. Focusing on the singularity, we can prove a selection rule from a general point of view (see also Refs. 10–14). The selection rule is closely related to the
SU(2) symmetry in our model. Let us introduce a parameter \( g \) in the Hamiltonian. Assume that, when \( g = g_0 \), the energy gap closes at several zero-energy points in the Brillouin zone. Next focus on the region near one of the gap-closing points \((k_x^0, k_y^0)\), i.e., 
\[\mathbf{p} = (k_x^0 - k_z^0, k_y^0 - k_x^0, g - g_0) \sim \mathbf{0}.\]
Then the leading part of the Hamiltonian is, generally, given by

\[H_0(p) = v_0 p + (\sigma_x, \sigma_y, \sigma_z) v p. \tag{6}\]

where \( v_0 \) is a \( 1 \times 3 \) vector, \( \sigma_{(x,y,z)} \) is a \( 2 \times 2 \) Pauli matrix, and \( v \) is a \( 3 \times 3 \) matrix. Now let us introduce the standard form, which is convenient for the following arguments.\(^{11}\)

Choosing a unitary transformation \( U \) appropriately, one can obtain 
\[\hat{U}H_0(p)\hat{U}^{-1} = v_0 p + (\sigma_x, \sigma_y, \sigma_z) D \mathbf{T} p\]
where \( D \) is \( \text{diag}(1,1,\text{sgn}(\det v)) \) and \( \mathbf{T} \) is an upper triangle matrix with positive diagonal elements. Let us perform \( Tp \rightarrow p \) [the parity-conserving affine transformation on \((k_x, k_y)\) and the rescaling on \( g \)] and the redefinition \( v_0 \mathbf{T}^{-1} \rightarrow v_0 \). Finally the standard form is obtained as

\[H_1(p) = v_0 p + \sigma_x p_x + \sigma_y p_y + \sigma_z p_z, \tag{7}\]

This is equivalent to the Hamiltonian \( \mathcal{H}(k) \) where \( A(k) = p_x, \text{sgn}(\det v) \) and \( B(k) = p_y, -ip_z \). Performing the same analysis, one can find that a vortex moves from one band to the other at the gap closing, and the conclusion is that the change of the Chern number is practically determined by \( \text{sgn}(\det v) \) and \( v \). To summarize, the linearized Hamiltonian near the dual gap-closing point \( (-k_x^0, -k_y^0) \) which exists due to the symmetry. Here the relation derived from Eq. (2) plays a crucial role and it is given by 
\[H(-k) = - \left( \sigma_x H(k) \sigma_y \right)^*.\]

Therefore
\[H(-k_x^0 - p_x, -k_y^0 - p_y, g) = - (\sigma_x H(k_x^0 + p_x, k_y^0 + p_y, g) \sigma_y)^* - v_0 p + (\sigma_x, \sigma_y, \sigma_z) v p. \tag{8}\]

where \( w = v \text{diag}(-1, -1, 1) \). It gives \( \text{sgn}(\det v) = \text{sgn}(\det w) \). Therefore the change of the Chern number due to gap closings always occurs in pair with the same sign and the total change is \( \Delta C = \pm 2 \) generally. This is the selection rule. On the other hand, in the absence of the relation (2) [or SU(2) symmetry], the above argument does not hold and it leads to the rule \( \Delta C = \pm 1 \). Now we note the results in Ref. 4 where the network model with the same symmetry as our model was investigated. Although their model is different from the lattice fermion model considered here, their selection rule still applies: this suggests the universality. Assuming that the system belongs to a phase with a vanishing Chern number by tuning parameters in the Hamiltonian, the selection rule implies that the Chern number is always even, which supports the result based on the edge states.

Finally, we comment on the disorder-driven transition based on the random \( d_{x^2-y^2} + id_{xy} \) model. It is defined by 
\[t_{ij} = t_{ij}^0 + \delta t_{ij} \quad \text{and} \quad \Delta_{ij} = \Delta_{ij}^0 + \delta \Delta_{ij}, \]
where \( \delta t_{ij} \) and \( \delta \Delta_{ij} \) denote the randomness. Here the hermiticity and the SU(2) symmetry are imposed on \( t_{ij} \) and \( \Delta_{ij} \), respectively. It has an intimate connection with the random Dirac fermion problem.\(^{21-26}\) It is to be noted that the SU(2) symmetry is kept even in the presence of randomness and the model is interesting as the Anderson localization problem.\(^{16}\) As discussed above, the Chern number is \( \pm 2 \) in the absence of randomness. On the other hand, in the presence of sufficiently strong randomness, it is expected that all the vortices disappear through the pair annihilation of vortices with opposite charges and the Chern number vanishes.\(^{13,14}\) By the numerical diagonalization, we treated the disorder-driven transition for the \( \delta t_{ij} = \delta t_{ij} f_i \) and \( \delta \Delta_{ij} = \delta \Delta_{ij} g_j \) where the \( f_i \)'s and \( g_j \)'s are uniform random numbers chosen from \([-W/2, W/2]\). The model was also studied extensively in Ref. 27. In Fig. 2, the density of states is shown in the case \( \Delta_{ij}^0 \neq 0 \). It can be seen that the two energy bands come closer and finally touch, as the randomness strength is increased. The transition \( C = \pm 2 \sim 0 \) with the gap closing is a natural consequence from the selection rule. The exploration of the global phase diagram and the field-theoretical description are left as future problems.

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