Majorana edge modes at topological insulator-superconductor-ferromagnet junctions in three dimensions

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Abstract. Recently the condition for the existence of gapless modes in arbitrary topological defects is proposed [Jeffrey C. Y. Teo and C. L. Kane, Phys. Rev. B 82, 115120 (2010)]. It is suggested that the existence of gapless modes follows from topologically nontrivial Hamiltonian which varies with adiabatic material-parameters characterizing the defects. We show that such adiabatic approach fails in cases of the existence of Majorana edge modes at topological insulator-superconductor-ferromagnet junctions. It is pointed out that quantum corrections beyond adiabatic quasiclassical approximation are required for the evaluation of second Chern number associated with the line junction.

1. Introduction
Certain classes of three-dimensional (3D) topological insulator-superconductor-ferromagnet junction possess chiral Majorana edge fermions at line defects [1]. Recently the general condition for the existence of gapless modes in arbitrary topological defects such as the topological insulator-superconductor-junctions is proposed [2]. It is suggested that the existence of gapless modes follows from topologically nontrivial Hamiltonian which varies with adiabatic material parameters characterizing the defects. In the case of line defects, the existence of chiral edge modes on the line defects follows from the topologically nontrivial ground state characterized by the second Chern number. We examine the second Chern number in 3D topological insulator-superconductor-ferromagnet junction systems, and show that such adiabatic approach fails in this case.

2. Effective two dimensional model
We briefly review the emergence scenario of chiral Majorana edge fermions in 3D topological insulator-superconductor-ferromagnet junction. The effective model of the 3D topological insulators considered by [3] is

\[ H = v |k| \sigma \cdot k + (m + \epsilon k^2) \mu_3 - \mu. \]  

Here \( \sigma = (\sigma_1, \sigma_2, \sigma_3) \) and \( \mu = (\mu_1, \mu_2, \mu_3) \) are the Pauli matrices representing spin, and orbital degrees of freedom, respectively, and \( \mu \) is a chemical potential. In the case where \( \epsilon > 0 \), the region with \( m > 0 \) describes a trivial insulator, while \( m < 0 \) describes a topological insulator.
We consider surface geometry in which \( z > 0 \) is vacuum and \( z < 0 \) is a topological insulator. The wave function of helical Dirac fermions localized in the surface is

\[
\Phi^{(0)}_{\chi, k_x, k_y}(x, y, z) = u_i \sinh \left( \frac{v_z}{2e} \sqrt{1 + \frac{4e}{v^2} \left( m + \epsilon \left( k_x^2 + k_y^2 \right) \right)} \right) e^{\frac{v_x}{e} i (k_x x + k_y y)},
\]

up to a normalization factor. Here \( u_i (i = 1, 2) \) is the spinor for the helical Dirac fermions, and we take \( u_1 = i (\frac{1}{\sqrt{2}}, 0, -\frac{1}{\sqrt{2}}, 0) \), \( u_2 = i (0, -\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}) \) in the basis of spin and orbital degrees of freedom, \( (|\mu_3 = 1, \sigma_3 = 1; \mu_3 = 1, \sigma_3 = -1; \mu_3 = -1, \sigma_3 = 1; |\mu_3 = -1, \sigma_3 = -1) \). The condition \( m + \epsilon (k_x^2 + k_y^2) < 0 \) corresponds to the localized wave function. The low-energy effective Hamiltonian \( H_{\text{HD}} \) describing helical Dirac fermions is derived by projecting Hamiltonian (1) onto the Hilbert space spanned by \( U = (\Phi^{(0)}_{1, k_x, k_y}, \Phi^{(0)}_{2, k_x, k_y}) \),

\[
H_{\text{HD}} = U^\dagger H U = v k_x \tilde{\sigma}_1 + v k_y \tilde{\sigma}_2 - \mu.
\]

Here the Pauli matrices \( \tilde{\sigma} = (\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_3) \) are defined for the space spanned by \( u_1, u_2 \).

Next we introduce an uniform ferromagnetic perturbation \( H_B = \mathbf{h} \cdot \mathbf{\sigma} \), which induces the mass gap in the helical Dirac fermions because of breaking time-reversal symmetry. The effective perturbed Hamiltonian is also given by the projection, \( H_B \mapsto U^\dagger H_B U = h_x \tilde{\sigma}_3 \). Hence the effective two dimensional surface BdG Hamiltonian describing the 3D topological insulator-superconductor-ferromagnet junction is

\[
H = \tau_3 (v k_x \tilde{\sigma}_1 + v k_y \tilde{\sigma}_2 - \mu) + h_x \tilde{\sigma}_3 + |\Delta| \tau_1.
\]

Here \( \tau = (\tau_1, \tau_2, \tau_3) \) are the Pauli matrices for the particle-hole space. We assume the s-wave gap symmetry for superconductivity, and the phase of gap function is fixed. The first Chern number \( \text{Ch}_1 := \frac{i}{\pi} \int_{T^2} \text{tr} \mathcal{F} \) of this systems is given by \( \text{Ch}_1 = -\text{sgn}(h) \Theta(h^2 - |\Delta|^2 - \mu^2) \). \( \mathcal{F} \) is Berry curvature. A proof is as follows: \( \det H = \left( v^2 k^2 + h^2 - |\Delta|^2 - \mu^2 \right)^2 + 4v^2 k^2 |\Delta|^2 \), then the gap closes when \( h^2 = |\Delta|^2 + \mu^2 \) is satisfied. The first Chern number changes only when the parameters cross this point. So there are three different topological phases: (1) \( h^2 > |\Delta|^2 + \mu^2, h > 0 \), (2) \( h^2 > |\Delta|^2 + \mu^2, h < 0 \), (3) \( h^2 < |\Delta|^2 + \mu^2 \). To calculate the first Chern number, it is sufficient to consider only the case of \( \mu = 0 \). When \( \mu = 0 \), \( [H, \tau_1 \tilde{\sigma}_3] = 0 \), thus the system is decoupled as

\[
V = \frac{1}{\sqrt{2}} \begin{pmatrix}
\frac{1}{\delta_3} & -1 \\
\delta_3 & \frac{1}{\delta_3}
\end{pmatrix},
\]

where

\[
V^\dagger HV = \begin{pmatrix}
v k_x \tilde{\sigma}_1 + v k_y \tilde{\sigma}_2 + (h + |\Delta|) \tilde{\sigma}_3 & 0 \\
0 & v k_x \tilde{\sigma}_1 + v k_y \tilde{\sigma}_2 + (h - |\Delta|) \tilde{\sigma}_3
\end{pmatrix}.
\]

The first Chern number is the sum of the two sectors, \( \text{Ch}_1 = -\frac{1}{2} \text{sgn}(h + |\Delta|) - \frac{1}{2} \text{sgn}(h - |\Delta|) \), and in the case of \( \mu \neq 0 \), \( \text{Ch}_1 = -\text{sgn}(h) \Theta(h^2 - |\Delta|^2 - \mu^2) \). \( \Theta(x) \) is a step function. Thus, the domain wall chiral Majorana fermion occurs at the line defects when \( h^2 - |\Delta|^2 - \mu^2 > 0 \). The sign of \( h \) decides chirality. It is noted that this condition is similar to that for realization of the chiral Majorana mode in Rashba s-wave superconductors [4].

The above result has an implication for the recently discovered superconductor Cu_xB_2Se_3 [5, 6]. The ARPES experiments for this system revealed that the surface helical Dirac fermion in the normal state has the chemical potential \( \mu \sim 0.1 \text{eV} \). Thus, in this material, it is difficult to realize the chiral Majorana edge fermion since the Zeeman energy of the order \( \sim 0.1 \text{eV} \) is unrealistic. On the other hand, the zero energy Majorana bound state appears in the mixed state of this system, provided that the total vorticity inside the system is odd [7].
3. Second Chern number in three-dimensions

Next, we examine the existence of chiral Majorana edge fermion in 3D topological insulator-superconductor-ferromagnet junction by use of method of ref.[2]. We will see that this approach fails to reproduce the results obtained in the section 2. The second Chern number is defined by the ground state of the adiabatic Hamiltonian $H(k, s)$ where $s(r) \in S^1$ is the adiabatically space-dependent material-parameters which change along contours surrounding the defects. The Hamiltonian describing 3D topological insulator-superconductor-ferromagnet junction systems is

$$H = \tau_3 (v \mu_1 \sigma \cdot k + m s(r) [s(r)] - \mu [s(r)]) + h [s(r)] \sigma_3 + |\Delta| [s(r)] |\tau_1. \tag{7}$$

For simplicity, we put $\epsilon = 0$, so the helical Dirac fermion on the surface of topological insulator is a domain wall type. We set the line defect geometry in which the material parameter $m [s(r)]$ changes slowly from $m < 0$ in the region $z < 0$, to $m > 0$ in the region $z > 0$, and also the parameter $h^2 - |\Delta|^2 - \mu^2 < 0$ changes from a negative value in the region $y < 0$, to positive value in the region $y > 0$. The second Chern number is defined by $\text{Ch}_2 = -\frac{1}{8\pi^2} \int_{T^3 \times S^1} \text{tr} [\mathcal{F} \wedge \mathcal{F}].$ $F = F(k, s)$ is a Berry curvature given by the ground state wave function of the adiabatic Hamiltonian $H(k, s)$. It is noted that in the calculation of the second Chern number the variables $k$ and $r$ of $H(k, s(r))$ are treated as independent parameters. Thus, this calculation is based on quasiclassical approximation. In the following, we show that this quasiclassical approach for the second Chern number fails for topological insulator-superconductor-ferromagnet junction.

Within the quasiclassical approximation, the gap closing condition is given by

$$\det H = \left( v^2 k^2 + m^2 + |\Delta|^2 + \mu^2 - h^2 \right)^2 - 4\mu^2 \left( v^2 k^2 + m^2 \right) + 4v^2 (k_x^2 + k_y^2) h^2 = 0. \tag{8}$$

The second Chern number is well defined only when the energy spectrum is fully gapped. But, at the large fermion region $(h^2 - |\Delta|^2 - \mu^2 > 0)$ in the surface of the topological insulator $(m = 0)$, $\min_k (\det H) = -4\mu^2 \left( h^2 - |\Delta|^2 \right) \leq 0$, so there exists the gap closing points in the Brillouin zone. This means that in the 3D topological insulator-superconductor-ferromagnet junction the second Chern number is not well-defined for the adiabatic Hamiltonian $H(k, s(r))$.

Contrastively, as pointed out in ref [2], in 3D topological insulator-superconductor-antiferromagnet junction, $H = \tau_3 (v \mu_1 \sigma \cdot k + m \mu_3) + h_{af} \mu_2 + |\Delta| \tau_1$, the nontrivial second Chern number (for simplicity, we set $\mu = 0$) is well-defined. The gap closing condition is $\det H = \left( v^2 k^2 + m^2 + |\Delta|^2 - h_{af}^2 \right)^2 + 4h_{af}^2 (v^2 k^2 + m^2) = 0$, which determine the gap closing points in the parameter region $\{(m, |\Delta|, h_{af}) \mid m = 0, h_{af} = \pm |\Delta| \}$. The gap closing points constitute the line defects in 3-dimensional parameter space $(m, |\Delta|, h_{af})$. The adiabatic parameter can wind around these line, and thus, it is possible that the second Chern number is nontrivial. Hence, in the case of antiferromagnetic junction, the adiabatic quasiclassical approach is sufficient to determine the existence of of gapless modes.

4. Conclusions

In the 3D topological insulator-superconductor-ferromagnet junction systems, the Teo-Kane’s adiabatic approach for the calculation of the second Chern number doesn’t work since the bulk energy gap of three dimensional Hamiltonian is closed at certain adiabatic parameters. Such problem is general in Teo-Kane’s adiabatic approach. In some cases, quantum corrections beyond the quasiclassical approximation is required for a well-defined topological number. In fact, for 3D topological insulator-superconductor-ferromagnet junction, it is possible to cure this point by including the first order quantum corrections which give rise to effective “antiferromagnetic field” breaking explicitly both time-reversal symmetry and inversion symmetry.
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