Lattice model of three-dimensional topological singlet superconductor with time-reversal symmetry

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We study topological phases of time-reversal invariant singlet superconductors in three spatial dimensions. In these particle-hole symmetric systems the topological phases are characterized by an even-numbered winding number ν. At a two-dimensional (2D) surface the topological properties of this quantum state manifest themselves through the presence of ν flavors of gapless Dirac fermion surface states, which are robust against localization from random impurities. We construct a tight-binding model on the diamond lattice that realizes a topologically nontrivial phase, in which the winding number takes the value ν = ±2. Disorder corresponds to a (non-localizing) random SU(2) gauge potential for the surface Dirac fermions, leading to a power-law density of states ρ(ε) ∼ ε1/7.

The bulk effective field theory is proposed to be the (3+1) dimensional SU(2) Yang-Mills theory with a theta-term at θ = π.

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and momentum $k$ on sublattice $A$ and $B$ of the diamond lattice, respectively, and

$$
\mathcal{H}(k) = \begin{pmatrix}
\Theta_k & \Phi_k & \Delta_k & 0 \\
\Phi_k^* & -\Theta_k & 0 & \Delta_k \\
\Delta_k^* & 0 & -\Theta_k & \Phi_{-k}^* \\
0 & \Delta_{-k}^* & -\Phi_{-k} & \Theta_k
\end{pmatrix}.
$$

(1)

Here, the nearest neighbor hopping term is given by $\Phi_k = \sum_{i=1}^4 t_i e^{ik \cdot s_i}$, the next nearest neighbor hopping term is $\Theta_k = \sum_{i,j, l} t'_{ij} e^{ik \cdot (s_i - s_l)} + \mu_s$, and the pairing potential is $\Delta_k = \sum_{i,j, l} \Delta_{ij} e^{ik \cdot (s_i - s_l)}$, where $s_{i=1,\ldots,4}$ denotes the four first neighbor bond vectors. The nearest and second nearest neighbor hopping amplitudes are parametrized by the vector $t_l$ and the symmetric matrix $t'_{ij}$, respectively. Similarly, the symmetric matrix $\Delta_{ij}$ denotes the singlet BCS pairing order parameter, whereas $\mu_s$ is the staggered chemical potential.

From Eq. (1), the energy eigenvalues $E^\pm_k = \pm \sqrt{|\Phi_k|^2 + |\Theta_k|^2 + |\Delta_k|^2}$ are readily obtained, exhibiting a two-fold degeneracy for each $k$. The symmetry operation that realizes particle-hole symmetry (PHS) for a singlet pairing BdG Hamiltonian is given by

$$
r_y \mathcal{H}^T(-k)r_y = -\mathcal{H}(k),
$$

(2a)

where $r_y$ is the second Pauli matrix acting on the particle-hole space. Hamiltonian (1) automatically satisfies symmetry property (2a), as can be checked easily. If furthermore time-reversal symmetry (TRS) is present, $\mathcal{H}(k)$ obeys

$$
\mathcal{H}^*(-k) = \mathcal{H}(k),
$$

(2b)

which is the case, if the pairing amplitudes $\Delta_{ij}$ are all purely real. The discrete symmetry constraints (2a) and (2b) define the CI symmetry class in the Altland-Zirnbauer classification [10, 11]. It is important to note, that an arbitrary Hamiltonian belonging to symmetry class CI can be brought into block off-diagonal form. This is achieved by means of a unitary transformation which rotates the $r_y$ matrices such that $(r_x, r_y, r_z) \rightarrow (r_x, -r_z, r_y)$. Under this rotation $\mathcal{H}(k)$, Eq. (1), transforms into

$$
\mathcal{H}(k) \rightarrow \begin{pmatrix} 0 & D(k) \\ D^T(k) & 0 \end{pmatrix},
$$

(3a)

where the upper right block is given by

$$
D(k) = \begin{pmatrix}
\Delta_k - i\Theta_k & -i\Phi_k \\
i\Phi_k^* & \Delta_k + i\Theta_k
\end{pmatrix},
$$

(3b)

which satisfies $D^T(-k) = D(k)$, since $\Delta_{-k} = \Delta_k$ and $\Phi_{-k}^* = \Phi_k$.

In order to define a topological invariant for the CI topological insulator, we need to introduce, following Ref. [6], the projection operator $Q(k)$

$$
Q(k) = \begin{pmatrix} 0 & q(k) \\ q^T(k) & 0 \end{pmatrix}, \quad q(k) = \frac{-D(k)}{E^+(k)},
$$

(4)

where, as a consequence of TRI and PHS, $q^T(-k) = q(k)$. The block off-diagonal form of $\mathcal{H}(k)$, and hence of $Q(k)$, is essential to uncover the topological structure of the space of all possible quantum ground states in class CI. It allows us to introduce a topological invariant that classifies maps from the Brillouin zone (BZ) into the space of the projection operators $Q(k)$. This invariant is a winding number defined in Ref. [6] through

$$
\nu[g] = \int \frac{d^3k}{24 \pi^2} \epsilon^{\mu\nu\rho} \text{tr} \left[ (q^{-1} \partial_\mu q)(q^{-1} \partial_\nu q)(q^{-1} \partial_\rho q) \right],
$$

(5)

where the integral is over the 3D BZ [11]. Due to the class CI constraint, $q^T(-k) = q(k)$, $\nu$ can take on only even integer values. (In the absence of any constraint, i.e., for symmetry class AIII [6], the winding number can be an arbitrary integer.) The winding number changes only when the quantum system undergoes a quantum phase transition, which is accompanied by the closing of the bulk gap.

We now turn to a more detailed specification of our lattice model. When $t_l = t$ for all $l = 1, \ldots, 4$

$$
\Phi_k = 2t \left[ e^{i\frac{\pi}{3}} \cos \frac{k_x + k_y}{4} - e^{i\frac{\pi}{6}} \cos \frac{k_x - k_y}{4} \right].
$$

(6)

The pairing potential we consider is “$d_{3z^2-r^2}$”-like, where the pairing amplitude on bonds within the $x-y$ plane differs in sign form the out-of-plane pairing amplitudes [see Fig. 1(a)]

$$
\Delta_k = 4\Delta \left[ \cos \frac{k_x}{2} \cos \frac{k_y}{2} - \cos \frac{k_y}{2} \cos \frac{k_z}{2} - \cos \frac{k_z}{2} \cos \frac{k_x}{2} \right].
$$

(7)

For definitiveness we will take $t$ and $\Delta$ positive throughout the paper. The BCS dispersion given by $\Phi_k$ and $\Delta_k$ has four point nodes (Dirac points), at which the bands are four-fold degenerate

$$
K_{1,\pm} = 2\pi \left( \pm 1/3, 1, 0 \right), \quad K_{2,\pm} = 2\pi \left( 1, \pm 1/3, 0 \right).
$$

Note that PHS and TRI relate $K_{a,+}$ to $K_{a,-}$ ($a = 1, 2$), as $K_{a,-}$ is identified to $-K_{a,+}$ via a translation by reciprocal lattice vectors. The degeneracy at the point nodes can be lifted by a finite staggered sublattice potential or by second neighbor hopping amplitudes, which are parametrized by the symmetric matrix $t'_{ij}$. In order to open up a bulk gap, we choose $t'_{13} = -t'_{14} = +t'_{24} = -t'_{23} \equiv t' \neq 0$, while $t'_{12} = t'_{34} = 0$, in which case the second neighbor hopping term simplifies to [see Fig. 1(a)]

$$
\Theta_k = 4t' \cos \frac{k_z}{2} \left( \cos \frac{k_y}{2} - \cos \frac{k_z}{2} \right) + \mu_s,
$$

(8)

where we have also included a staggered chemical potential.

The BdG Hamiltonian (1) has four energy bands, two of which are occupied. With the choice for the hopping
parameters and gap amplitudes given by Eqs. (6-8) the spectrum has a bulk energy gap, except when \( \pm 6t' = \mu_s \), i.e., when the system undergoes a quantum phase transition between different topological phases. The winding number \( \nu \), Eq. (8), for this model can be computed numerically, by discretizing the integral over the BZ. The numerical evaluation of \( \nu \) as a function of \( \mu_s \) and \( t' \) is shown in Fig. 2(b), where we set \( t = 4 \), and \( \Delta = 2 \). With increasing number of grid points in the BZ the integral converges rapidly to an even integer value. In this way we obtain the phase diagram shown in Fig. 2(a), which contains four distinct gapped phases. The nontrivial phases (\( \nu = \pm 2 \)) occur if \( |\mu_s| > |6t'| \). Inclusion of finite (but small) second neighbor terms \( t_{12}' \) and \( t_{34}' \) shifts the phase boundaries, but does not change the topology of the phase diagram.

When \( \mu_s \) and \( t' \) are small compared to \( t \) [see Fig. 2(a)], an effective low-energy continuum description can be derived by expanding Hamiltonian (3) around the four nodal points \( K_{1,2,\pm} \). Rescaling momenta as \( t k_z/2 \to k_z \), \( t \sqrt{3} k_y/2 \to k_y \), and \( 2t' \sqrt{3} \Delta k_x \to k_x \), and performing a unitary transformation, we find that the low-energy expansion around the node \( K_{1,\pm} \) of the off-diagonal block in Eq. (3a) is given by

\[
D(\vec{q}) = \beta i \sigma_y \left[ \vec{q} \cdot \alpha - i(\mu_s + 6t') \gamma^5 \right], \tag{9}
\]

where \( \vec{q} = (q_x, -q_y, -q_z) \) denotes the deviation of the momentum from \( K_{1,\pm} \). Eq. (4) is identical to the class CI Dirac Hamiltonian for the nodes \( K_{2,\pm} \) is related by symmetry to the result for the nodes \( K_{1,\pm} \) by simultaneously interchanging \( k_x \) with \( k_y \) and replacing the mass term \( \mu_s + 6t' \) with \( \mu_s - 6t' \),

\[
D(\vec{q}) = \beta i \sigma_y \left[ \vec{q} \cdot \alpha - i(\mu_s - 6t') \gamma^5 \right], \tag{11}
\]

where \( \vec{q} = (q_y, -q_x, -q_z) \). Similarly, the winding number within the continuum description for the nodes \( K_{2,\pm} \) is

\[
\nu_2 = -\frac{1}{2} \frac{(\mu_s - 6t')}{|\mu_s - 6t'|} \times 2. \tag{12}
\]

Interestingly, the winding number obtained from the continuum description, \( \nu = \nu_1 + \nu_2 \), reproduces the phase diagram of the lattice model correctly.

A physical consequence of the non-zero winding number \( \nu \) is the appearance of zero-energy surface Andreev bound states with Dirac dispersion. To study these surface states we solve model (4) in a slab geometry, and compute the energy bands for a slab parallel to the (111) surface, both in the trivial and nontrivial phases. As shown in Fig. 3 where we set \( t = 4 \) and \( \Delta = 2 \), there are, in addition to the bulk states, surface Dirac states which cross the band gap. When the bulk topological invariant is \( \nu = 2 \) [Fig. 3(c)] there are two surface Dirac states, whereas there is no such state when the bulk topological invariant is \( \nu = 0 \) [Fig. 3(d)]. Hence, the total number of Dirac states/cones \( N_f = 2 \) is consistent with the bulk characteristics \( \nu = 2 \). \( N_f = 2 \) is the minimal number of Dirac cones required by class CI symmetries. Note,
however, that in any two-dimensional lattice model satisfying the CI symmetries, the possible number of Dirac cones is an integer multiple of \(2N_f\) because of a no-go theorem analogous to the fermion doubling theorem of Ref. [12]. Here, the fermion doubling is avoided since the two-dimensional system is realized as a boundary of a 3D bulk.

The surface Dirac fermion modes cannot be gapped by any deformation of the Hamiltonian respecting time-reversal and particle-hole symmetry. Indeed, this is so because any perturbation respecting the class CI symmetries takes the form of an SU(2) gauge field, which perturbs the surface Dirac fermions in the following way

\[
\mathcal{H} = (k_x + a_x \cdot \sigma) \tau_x + (k_y + a_y \cdot \sigma) \tau_y,
\]

where \(a_{\mu=x,y} = 1,2,3 \in \mathbb{R}\). The gapless nature of this four-component Dirac fermion is stable against arbitrary values of the six real parameters \(a^\mu\), i.e., the non-Abelian gauge potential shifts the location of the Dirac node, but does not lead to a gap. With the inclusion of randomness, small relative to the bulk energy gap, the surface Dirac fermion mode realizes the random SU(2) gauge potential model discussed in Ref. [13]. The random SU(2) gauge potential, known not to be able to localize the potential model discussed in Ref. [13], is applicable to a wide range of systems. There are various ways how the topologically protected surface states in such compounds could be detected experimentally. First of all, because of spin rotation symmetry, the surface conductivity for the spin current is a well-defined quantity, which is unchanged by symmetry preserving perturbations, including disorder. Secondly, the density of states of the surface states can be probed via tunneling experiments. Finally, we argue that by breaking TRS locally at the surface, while keeping the spin-rotation symmetry intact, one can realize the so-called ‘spin quantum Hall effect’ (SQHE) in symmetry class C (unrelated to the ‘quantum spin Hall insulators’ mentioned earlier) at the surface of the CI topological superconductor. This can be seen as follows. Broken TRS (without breaking SU(2) symmetry) allows for the appearance of four additional perturbing potentials in Eq. (13), describing the surface modes. One can check that only one of these additional potentials gives rise to a gap, and hence to a (2D) non-zero Chern integer \(n = \pm 1\); this is one half of the allowed value of the Chern number in any 2D system exhibiting the SQHE [14]. This situation is completely analogous to the half-integer surface QHE of the 3D \(\mathbb{Z}_2\) topological insulator [14, 15, 16].

In the 3D \(\mathbb{Z}_2\) topological insulator, this topological magneto-electric effect can be described by the effective field theory whose action is given by \((3+1)\) QED supplemented with \(\theta = \pi\) term [16, 17]. Since spin is a good quantum number in a singlet superconductor, it is possible to describe its spin transport in terms of an external SU(2) gauge field. Indeed, the effective field theory of the SQHE in TRS-breaking 2D singlet superconductors is known to be the SU(2) Chern-Simons theory at an integer level [17]. Then, following the same reasoning as in the case of the 3D \(\mathbb{Z}_2\) topological insulators, we propose that the effective field theory describing class CI topological superconductor is the \((3+1)\)D SU(2) Yang-Mills theory argumented with the theta term

\[
\mathcal{L} = \frac{\theta}{32\pi^2} \epsilon_{\mu\nu\kappa\lambda} \text{tr} (F_{\mu\nu} F_{\kappa\lambda}),
\]

where \(F_{\mu\nu}\) is the SU(2) field strength and \(\theta = \pi\).

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