Three-dimensional topological phase on the diamond lattice

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An interacting bosonic model of Kitaev type is proposed on the three-dimensional diamond lattice. Similarly to the two-dimensional Kitaev model on the honeycomb lattice, which exhibits both Abelian and non-Abelian phases, the model has two ("weak" and "strong" pairing) phases. In the weak pairing phase, the auxiliary Majorana hopping problem is in a topological superconducting phase characterized by a nonzero winding number introduced by Schnyder *et al.* [Phys. Rev. B **78**, 195125 (2008)] for the ensemble of Hamiltonians with both particle-hole and time-reversal symmetries. The topological character of the weak pairing phase is protected by a discrete symmetry.

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I. INTRODUCTION

The recent discovery of $\mathbb{Z}_2$ topological insulators, a band insulator with particular topological characters of Bloch wave functions, came as a surprise.[1–9] On the one hand, $\mathbb{Z}_2$ topological insulators are close relatives to more familiar integer quantum Hall (IQH) states.[10,11] Similar to an IQH state in the bulk, they are characterized by a topological invariant ($\mathbb{Z}_2$ invariant). Similar to an IQH state with boundaries, they support stable gapless boundary states that are robust against perturbations. On the other hand, unlike the IQH states, time-reversal symmetry (TRS) is a prerequisite to the existence of $\mathbb{Z}_2$ topological insulators. In fact, as soon as the TRS of a $\mathbb{Z}_2$ topological insulator is broken, it becomes possible to deform in a continuous manner a band insulator with a trivial $\mathbb{Z}_2$ topological number into one with a nontrivial $\mathbb{Z}_2$ number.

Time-reversal symmetry for spin-1/2 particles is not the only discrete symmetry for which a topological distinction of quantum ground states arises. A systematic and exhaustive classification of topological band insulators and mean-field superconductors has been proposed in Ref. 14 by relying on the discrete symmetries of relevance to the theory of random matrices.[12,13] In three spatial dimensions, it was shown that, besides the $\mathbb{Z}_2$ topological insulator in the symplectic symmetry class, there are precisely four more symmetry classes in which topological insulators and/or superconductors are possible.[15,16] For three out of the five symmetry classes of random matrix theory, we introduced a topological invariant ν (winding number), which distinguishes several different topological insulators/superconductors, just like the Chern integer distinguishes different IQH states in two dimensions.[10,11]

While the classification given in Ref. 14 is for noninteracting fermionic systems, strong correlations among electrons (or spins) might spontaneously give rise to these topological phases by forming a nontrivial band structure for some, possibly emergent, fermionic excitations (e.g., spinons).[17] It is the purpose of this paper to demonstrate how topological insulators (superconductors) emerge as a result of strong correlations. We will show that it is possible to design an interacting bosonic model with emergent Majorana fermion excitations, the ground state of which is a topological insulator (superconductor) with nonvanishing winding number, $\nu \neq 0$.

Our model is a natural generalization of the spin-1/2 model on the honeycomb lattice introduced by Kitaev[18] to the three-dimensional diamond lattice with four-dimensional Hilbert space per site. The Kitaev model on the honeycomb lattice has two types of phases: the so-called Abelian and non-Abelian phases. The Abelian phase is equivalent to the toric code model[19] and an exactly solvable model proposed by Wen,[20] which in turn is described by a $\mathbb{Z}_2$ gauge theory. On the other hand, the non-Abelian phase is in the universality class of the Moore-Read Pfaffian state. Each phase corresponds to the weak and strong pairing phases of two-dimensional spinless chiral p-wave superconductor, respectively,[21] the latter of which is an example of a topological superconductor in symmetry class D of Altland-Zirnbauer classification in two dimensions.[12–14]

Similarly to the Kitaev model on the honeycomb lattice, the ground state of our model can be obtained from a Majorana fermionic ground state (with a suitable projection procedure). Our model has two phases, which we also call strong and weak pairing phases. In particular, in the weak pairing phase, the ground state is given by a topological superconducting state in symmetry class DIII of Altland-Zirnbauer classification, and in the universality class of a three-dimensional analog of the Moore-Read Pfaffian state discussed in Ref. 14. The B phase of ^{3}He is also in this universality class.[14,22,23] The topological character of the ground state is protected by a discrete symmetry transformation, which is a combination of time-reversal and a fourfold discrete rotation, the latter of which forms a subgroup of a continuous U(1) symmetry of our model. Spin-1/2 models of Kitaev type on the diamond lattice and on other three-dimensional lattices have been constructed.[24–26] For these models, however, there is no phase analogous to the non-Abelian phase in the original Kitaev model, and the ground states discussed there have a vanishing winding number. Extensions of the spin-1/2 Kitaev model to models with four-dimensional Hilbert space per site have been studied in Refs. 20 and 27–30.

II. LOCAL HILBERT SPACE AND DISCRETE SYMMETRIES

We start by describing the local Hilbert space of our model, defined as it is at each site of some lattice. Consider the four-dimensional Hilbert space spanned by the orthonormal basis

$$|\sigma\tau\rangle, \quad \sigma=\pm 1, \quad \tau=\pm 1. \tag{1}$$

This space can be viewed, if we wish, as describing the four-dimensional Hilbert space of a spin-3/2 degree of freedom, or as a direct product of two spin-1/2 Hilbert spaces. In the latter case, one can view these two spin-1/2 degrees of freedom as, say, originating from spin and orbital. We will denote two sets of Pauli matrices, $\sigma^\mu=\sigma^0,\sigma^x,\sigma^y,\sigma^z$, and $\tau^\mu=\tau^0,\tau^x,\tau^y,\tau^z$ ($\mu=0,1,2,3$), each acting on σ and τ indices, with σ^0 and τ^0 being 2×2 unit matrices.

We shall represent the Hamiltonian in terms of two sets of Dirac matrices $\alpha^{\mu=0,1,2,3}$ (Dirac representation),

$$\alpha^a=\sigma^a\otimes\tau^x, \quad \alpha^0=\sigma^0\otimes\tau^z=\beta=\gamma^0, \tag{2}$$

and $\zeta^{\mu=0,1,2,3}$ (chiral representation),

$$\zeta^a=-\sigma^a\otimes\tau^z, \quad \zeta^0=\sigma^0\otimes\tau^x=\gamma_5, \tag{3}$$

where $a=1,2,3$. The two sets $\{\alpha^\mu\}$ and $\{\zeta^\mu\}$ are related to each other by $\zeta^\mu=i\alpha^\mu i\gamma^5\gamma^0=i\alpha^\mu(\sigma^0\otimes\tau^y)$, and satisfy the Dirac algebra,

$$\{\alpha^\mu,\alpha^\nu\}=\{\zeta^\mu,\zeta^\nu\}=2\delta^{\mu\nu}, \quad \mu,\nu=0,\ldots,3. \tag{4}$$

Discrete symmetries

In the following, we will consider three antiunitary discrete symmetry operations, T, T', and Θ. They are characterized by

$$T^2=+1, \quad \Theta^2=-1, \quad T'^4=-1. \tag{5}$$

In the sequel, we will treat two distinct operations for time reversal (TR).

First, if the local Hilbert space is interpreted as describing a spin-3/2 particle, the natural TR operation Θ is given by $\Theta=\eta e^{-i\pi S_y^{3/2}}K$, where η stands for an arbitrary phase (will be set to one henceforth), $S_y^{3/2}$ is a four by four matrix representing the y component of spin with $S=3/2$, and K implements the complex conjugation, $KiK^{-1}=-i$. If we take $|\sigma\tau\rangle$ to be the basis that diagonalizes S^z (magnetic basis, $|3/2,m\rangle$), then

$$\Theta=-i\sigma^y\otimes\tau^x K. \tag{6}$$

This is nothing but the charge-conjugation matrix $C=i\gamma^2\gamma^0$ for the gamma matrices in the Dirac representation. As Θ is TRS for half-integer spin, $\Theta^2=-1$. Note also that

$$\Theta\alpha^\mu\Theta^{-1}=-\alpha^\mu, \quad \Theta\zeta^\mu\Theta^{-1}=+\zeta^\mu. \tag{7}$$

Second, if the local Hilbert space is interpreted as describing two spin-1/2 degrees of freedom, we can consider a TR operation T defined by

$$T=(i\sigma^y)\otimes(i\tau^y)K,$$

$$T\sigma^a T^{-1}=-\sigma^a, \quad T\tau^a T^{-1}=-\tau^a, \tag{8}$$

with $a=1,2,3$. Note that $T^2=+1$. Under T, α and ζ are transformed as

$$T\alpha^\mu T^{-1}=-\alpha_\mu, \quad T\zeta^\mu T^{-1}=-\zeta_\mu,$$

$$Ti\gamma^5\gamma^0T^{-1}=-i\gamma^5\gamma^0, \tag{9}$$

where covariant and contravariant vectors are defined as $\alpha^\mu=(\beta,\alpha^a)$ and $\alpha_\mu=(\beta,-\alpha^a)$.

As we will see later, while the σ part of our Hamiltonian is fully anisotropic in σ space, the τ part of the Hamiltonian is invariant under a rotation around τ^y axis. In particular, it is invariant under a rotation R by $\pi/2$ around τ^y axis,

$$R\begin{pmatrix}\tau^x\\ \tau^y\\ \tau^z\end{pmatrix}R^{-1}=\begin{pmatrix}\tau^z\\ \tau^y\\ -\tau^x\end{pmatrix}, \quad R=(\tau^0+i\tau^y)/\sqrt{2}. \tag{10}$$

Under R, α and ζ are transformed as

$$R\alpha^\mu R^{-1}=-\zeta^\mu, \quad R\zeta^\mu R^{-1}=+\alpha^\mu,$$

$$Ri\gamma^5\gamma^0R^{-1}=+i\gamma^5\gamma^0. \tag{11}$$

By combining T with R we can define yet another antiunitary operation, $T'=RT$,

$$T'=RT=(i\tau^y-\tau^0)i\sigma^yK/\sqrt{2},$$

$$T'\sigma^aT'^{-1}=-\sigma^a, \quad T'\begin{pmatrix}\tau^x\\ \tau^y\\ \tau^z\end{pmatrix}T'^{-1}=\begin{pmatrix}-\tau^z\\ -\tau^y\\ +\tau^x\end{pmatrix}. \tag{12}$$

Below, with a slight abuse of language, we will call this operation T' TR operation. When applied to α and ζ,

$$T'\alpha^\mu T'^{-1}=+\zeta_\mu, \quad T'\zeta^\mu T'^{-1}=-\alpha^\mu,$$

$$T'i\gamma^5\gamma^0T'^{-1}=-i\gamma^5\gamma^0, \tag{13}$$

i.e., TRS T' exchanges α and ζ, and covariant and contravariant vectors. Notice that

$$T'^2=i\tau^y, \quad T'^4=-1. \tag{14}$$

III. HAMILTONIAN

In the two-dimensional Kitaev model, different types of interactions (represented by three 2×2 Pauli matrices) are assigned to three distinct types of bonds that are defined by their different orientation in the honeycomb lattice. It is this anisotropic nature of the interaction that makes the Kitaev model exactly solvable. This construction can be extended to the diamond lattice where there are four distinct types of bonds with different orientation.

The diamond lattice is bipartite and consists of two interpenetrating fcc lattices shifted by $a(-1,1,-1)/4$ along the body diagonal, where a is the lattice constant. We label sites r_A and r_B on the two sublattices A and B of the diamond lattice as

$$r_A=\sum_{i=1}^{3}m_ia_i, \quad r_B=r_A+s_0, \quad m_i\in\mathbb{Z}, \tag{15}$$

where the primitive vectors a_i are given by

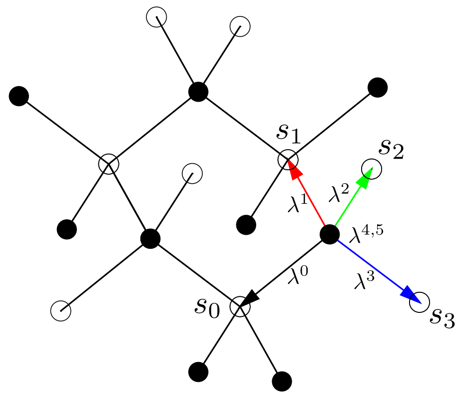

FIG. 1. (Color online) The diamond lattice and the six Majorana fermions $\lambda^{0,\ldots,5}$. Sites on the sublattice A (B) are denoted by an open (filled) circle.

$$a_1 = \frac{a}{2}\begin{pmatrix}1\\1\\0\end{pmatrix}, \quad a_2 = \frac{a}{2}\begin{pmatrix}0\\1\\1\end{pmatrix}, \quad a_3 = \frac{a}{2}\begin{pmatrix}1\\0\\1\end{pmatrix}. \tag{16}$$

We have also introduced the three-component vectors

$$s_1 = \frac{a}{4}\begin{pmatrix}1\\1\\1\end{pmatrix}, \quad s_2 = \frac{a}{4}\begin{pmatrix}-1\\-1\\1\end{pmatrix},$$
$$s_3 = \frac{a}{4}\begin{pmatrix}1\\-1\\-1\end{pmatrix}, \quad s_0 = \frac{a}{4}\begin{pmatrix}-1\\1\\-1\end{pmatrix}, \tag{17}$$

which connect the nearest-neighbor sites (Fig. 1).

The Hamiltonian we study in this paper is defined by

$$H = -\sum_{\mu=0}^{3} J_\mu \sum_{\mu-\text{links}} (\alpha_j^\mu \alpha_k^\mu + \zeta_j^\mu \zeta_k^\mu). \tag{18}$$

Here, the sites j and k are end points of a link of type μ. There are four types of links $\mu=0,1,2,3$ in the diamond lattice since they can be distinguished by their orientations. Hamiltonian (18) can also be written in terms of σ^μ and τ^μ as

$$H = -\sum_{\mu=0}^{3} J_\mu \sum_{\mu-\text{links}} \sigma_j^\mu \sigma_k^\mu (\tau_j^x \tau_k^x + \tau_j^z \tau_k^z). \tag{19}$$

This Hamiltonian is invariant under discrete symmetries, T, R, T', and Θ, and enjoys a U(1) symmetry for rotation around τ^y axis.

IV. MAJORANA FERMION REPRESENTATION

Let us consider the (local) Hilbert space in which we have six Majorana fermions $\{\lambda^p\}_{p=0,\ldots,5}$ per site, which satisfy[20,27]

$$\{\lambda^p, \lambda^q\} = 2\delta^{pq}, \quad p,q = 0,\ldots,5. \tag{20}$$

To construct four-dimensional Hilbert space out of the eight-dimensional Hilbert space, we introduce the fermion number operator by

$$D \coloneqq i\prod_{p=0}^{5} \lambda^p, \quad D^2 = 1. \tag{21}$$

The eigenvalue of $D=\pm 1$ can then be used to select a four-dimensional subspace of the full Hilbert space, which will be called the physical subspace.

We can construct 15 generators of so(6) from the Majorana fermions as

$$\Gamma^{pq} = i\lambda^p \lambda^q, \quad p \neq q. \tag{22}$$

Within the physical subspace, α^μ can be expressed as

$$\alpha^\mu = \Gamma^{\mu 4}, \quad \mu = 0,1,2,3. \tag{23}$$

Since Γ^{45} anticommutes with α^μ, we make the identification

$$\Gamma^{45} = \alpha^1 \alpha^2 \alpha^3 \alpha^0 = \sigma^0 \otimes \tau^y = i\gamma^5 \gamma^0. \tag{24}$$

The second set of the gamma matrices $\{\zeta^\mu\}$ is

$$\zeta^\mu = i\alpha^\mu \Gamma^{45} = \Gamma^{\mu 5}. \tag{25}$$

The Majorana fermions naturally inherit the symmetry operations on α and ζ. The symmetry conditions are automatically satisfied if we define T, R, and T' operations on Majorana fermions by

$$T\lambda^\mu T^{-1} = \lambda_\mu, \quad T\lambda^s T^{-1} = \lambda^s, \quad s = 4,5,$$
$$R\lambda^\mu R^{-1} = -\lambda^\mu, \quad R\begin{pmatrix}\lambda^4\\ \lambda^5\end{pmatrix}R^{-1} = is^y\begin{pmatrix}\lambda^4\\ \lambda^5\end{pmatrix},$$
$$T'\lambda^\mu T'^{-1} = -\lambda_\mu, \quad T'\begin{pmatrix}\lambda^4\\ \lambda^5\end{pmatrix}T'^{-1} = is^y\begin{pmatrix}\lambda^4\\ \lambda^5\end{pmatrix}. \tag{26}$$

Here, the definitions of the covariant (λ^μ) and contravariant (λ^μ) vectors follow from those of $\alpha^\mu(\zeta^\mu)$ and $\alpha_\mu(\zeta_\mu)$, and we have introduced another set of Pauli matrices $s^{\mu=0,1,2,3}$ acting on $\lambda^{4,5}$ with s^0 being 2×2 unit matrix. The discrete rotation operator R can be written in terms of the Majorana fermions λ as $e^{i\pi\lambda^4\lambda^5/4}$.

V. SOLUTION THROUGH A MAJORANA HOPPING PROBLEM

In terms of the Majorana fermions the Hamiltonian can be written as

$$H = i\sum_{\mu=0}^{3} J_\mu \sum_{\mu-\text{links}} u_{jk}(\lambda_j^4 \lambda_k^4 + \lambda_j^5 \lambda_k^5), \tag{27}$$

where we have introduced a link operator by

$$u_{jk} \coloneqq i\lambda_j^{\mu_{jk}} \lambda_k^{\mu_{jk}}, \tag{28}$$

with $\mu_{jk}=0,1,2,3,4$ depending on the orientation of the link ending at sites j and k. Note that TR (T or T') operation flips the sign of a link operator,

$$Tu_{jk}T^{-1} = -u_{jk}, \quad Ru_{jk}R^{-1} = +u_{jk},$$
$$T'u_{jk}T'^{-1} = -u_{jk}. \tag{29}$$

(This is also the case for TRS on the link operators in the spin-1/2 honeycomb lattice Kitaev model.) When necessary, this sign flip can be removed by a subsequent gauge transformation for Majorana fermions $\lambda^{4,5}$ on either one of sublattices if the underlying lattice structure is bipartite (see below).

What is essential to observe is that all u_{jk} appearing in the Hamiltonian commute with each other and with the Hamiltonian. They can thus be replaced by their eigenvalues $u_{jk} = \pm 1$, and the interacting Hamiltonian reduces to, for a fixed configuration of the $\mathbb{Z}_2$ gauge field $\{u_{jk}\}$, a simple hopping model of Majorana fermions. Observe that both λ^4 and λ^5 Majorana fermions feel the same $\mathbb{Z}_2$ gauge field. The ground state of the Hamiltonian can then be obtained by first picking up the $\mathbb{Z}_2$ gauge-field configuration that gives the lowest ground-state energy for the Majorana hopping problem, and then projecting the resulting fermionic ground state onto the physical Hilbert space. According to Lieb's theorem,[31] the $\mathbb{Z}_2$ gauge-field configuration that gives the lowest ground-state energy has zero $\mathbb{Z}_2$ vortex for all hexagons, and hence we can take $u_{jk}=1$ for all links.

For notational convenience, for a Majorana fermion at the jth site located at r_A (r_B) on the sublattice A (B), we denote $a^s_{r_A} := \lambda^s_j$ ($b^s_{r_B} := \lambda^s_j$). With periodic boundary condition and with the Fourier transformation, $a^s_{r_A} = \sum_k e^{ik\cdot r_A} a^s_k / \sqrt{|\Lambda_A|}$ and $b^s_{r_B} = \sum_k e^{ik\cdot r_B} b^s_k / \sqrt{|\Lambda_B|}$, where $|\Lambda_{A,B}|$ is the total number of sites on the sublattice A,B, respectively, the Majorana hopping Hamiltonian in the momentum space is

$$H_{\mathrm{MH}} = \sum_s \sum_k (a^s_{-k}, \quad b^s_{-k}) \mathcal{H}(k) \begin{pmatrix} a^s_k \\ b^s_k \end{pmatrix}, \tag{30}$$

where we have defined

$$\mathcal{H}(k) := \begin{pmatrix} & i\Phi(k) \\ -i\Phi^*(k) & \end{pmatrix}, \quad \Phi(k) := \sum_{\mu=0}^{3} J_\mu e^{ik\cdot s_\mu}, \tag{31}$$

and noted $a_{-k} = a^\dagger_k$ when $k \neq 0$. The energy spectrum $E(k)$ is given by $E(k) = \pm\sqrt{|\Phi(k)|^2}$, with twofold degenerate for each k.

Symmetries and topology of the Majorana hopping Hamiltonian

We have reduced the interacting bosonic model to the Majorana hopping problem. This auxiliary Majorana hopping Hamiltonian is, in the terminology of Altland and Zirnbauer, in symmetry class D,[12,13] i.e., the ensemble of quadratic Hamiltonians describing Majorana fermions. (See Appendix.) In more general situations (which we will consider below), the auxiliary Majorana hopping Hamiltonian is given by

$$H_{\mathrm{MH}} = \sum_k (a^4_{-k}, \quad a^5_{-k}, \quad b^4_{-k}, \quad b^5_{-k}) \mathcal{X}(k) \begin{pmatrix} a^4_k \\ a^5_k \\ b^4_k \\ b^5_k \end{pmatrix}, \tag{32}$$

where $\mathcal{X}$ describes a Hamiltonian for Majorana fermions, and satisfies

$$\mathcal{X}^\dagger(k) = \mathcal{X}(k), \quad \mathcal{X}^T(-k) = -\mathcal{X}(k). \tag{33}$$

This is the defining property of symmetry class D. Below, to describe the 4×4 structure of the single-particle Majorana hopping Hamiltonian $\mathcal{X}(k)$, we introduce yet another set of Pauli matrices $c^{\mu=0,1,2,3}$ acting on sublattice indices.

If our bosonic model further satisfies TRS T', the Hamiltonian $\mathcal{X}$ for the auxiliary Majorana hopping problem respects

$$c^z(is^y)\mathcal{X}^T(-k)(-is^y)c^z = \mathcal{X}(k), \tag{34}$$

where the factor c^z can be thought of as a gauge transformation, adding a phase factor $e^{i\pi}$ for Majorana fermions on B sublattice b^s, and can be removed by a unitary transformation $b^s \to -b^s$. With this further condition arising from T', the relevant Altland-Zirnbauer symmetry class is class DIII. (See Appendix.)

In Ref. 14, it has been shown that the space of all possible quantum ground states in class DIII in three spatial dimensions is partitioned into different topological sectors, each labeled by an integer topological invariant ν. To uncover this topological structure and introduce the winding number, we observe that all Hamiltonians in symmetry class DIII can be brought into a block-off-diagonal form. For $\mathcal{X}$, this is done by a unitary transformation

$$U = U_2 U_1, \quad \mathcal{X} \to \tilde{\mathcal{X}} = U_2 U_1 \mathcal{X} U_1^\dagger U_2^\dagger, \tag{35}$$

where the first unitary transformation rotates $s^y \to U_1 s^y U_1^\dagger = -s^z$,

$$U_1 = (s^0 - is^x)/\sqrt{2}, \tag{36}$$

whereas the second unitary transformation exchanges second and fourth entries,

$$U_2 = (s^0 + s^z)c^0/2 + (s^0 - s^z)c^x/2. \tag{37}$$

The combination of U_1 and U_2 diagonalizes $s^y c^z$ as

$$U_2 U_1 s^y c^z U_1^\dagger U_2^\dagger = -\mathrm{diag}(1,1,-1,-1). \tag{38}$$

After the unitary transformation, we find

$$\tilde{\mathcal{X}}(k) = \begin{pmatrix} 0 & D(k) \\ D^\dagger(k) & 0 \end{pmatrix}. \tag{39}$$

This block-off-diagonal structure is inherited to the spectral projector $P(k)$, $P^2=P$, which projects onto the space of filled Bloch states at each k,

$$2P(k) - 1 = \begin{pmatrix} 0 & q(k) \\ q^\dagger(k) & 0 \end{pmatrix}, \quad q^\dagger q = 1. \tag{40}$$

The integer topological invariant is then defined, from the off-diagonal block of the projector, as[14]

$$\nu[q] = \int_{\mathrm{BZ}} \frac{d^3k}{24\pi^2} \epsilon^{\mu\nu\rho}\, \mathrm{tr}[(q^{-1}\partial_\mu q)\cdot(q^{-1}\partial_\nu q)\cdot(q^{-1}\partial_\rho q)], \tag{41}$$

where $\mu,\nu,\rho = k_x,k_y,k_z$, and the integral extends over the first Brillouin zone (BZ).[32] The nonzero value of the winding number signals a nontrivial topological structure, an observable consequence of which is the appearance of gapless surface Majorana fermion modes.

VI. STRONG PAIRING PHASE

When one of the coupling J_μ is strong enough compared to the others, the spectrum for the Majorana fermions is gapped. In this phase, the winding number ν is zero. This phase can be called "strong pairing phase," following the similar phase in the BCS pairing model. Because of the trivial winding number, there is no surface stable fermion mode in the auxiliary Majorana hopping Hamiltonian when it is terminated by a surface. The properties of this phase can be studied by, say, taking the limit $J_0 \gg J_{a=1,2,3} > 0$ and then developing a degenerate perturbation theory. In this limit of isolated links, there are four degenerate ground states for each link ending at the two sites $(r_A, r_B) = (r_A, r_A + s_0)$,

$$\frac{1}{\sqrt{2}}(|\uparrow\rangle^{\tau}_{r_A}|\uparrow\rangle^{\tau}_{r_B} + |\downarrow\rangle^{\tau}_{r_A}|\downarrow\rangle^{\tau}_{r_B})|\sigma_{r_A}\rangle^{\sigma}_{r_A}|\sigma_{r_B}\rangle^{\sigma}_{r_B}, \tag{42}$$

with $\sigma_{r_{A,B}} = \pm 1$ where $|\cdots\rangle^{\sigma,\tau}_r$ represents the state for σ_r and τ_r, respectively. The effective Hamiltonian acting on these degenerate ground states is defined on the cubic lattice since each J_0 link at $(r_A, r_A + s_0)$ is connected to six neighboring links at $r_A \pm a_i$, where $a_i = s_0 + s_i$ with $i = 1,2,3$, up to the fourth order in the degenerate perturbation theory. If we use notations $\sigma^\mu_A \to \rho^\mu$ and $\sigma^\mu_B \to \mu^\mu$, the effective Hamiltonian up to the fourth order in the degenerate perturbation theory is (up to constant terms)

$$H_{\rm eff} = \frac{5}{64} \sum_{\substack{(i,j,k)=(x,y,z),\\ (y,z,x),(z,x,y)}} \frac{J_i^2 J_j^2}{J_0^3} \sum_p F_p, \tag{43}$$

where p stands for a plaquette surrounded by r, $r + a_i$, $r + a_j$ and $r + a_i + a_j$, and

$$F_p = (\rho^k \mu^0)_r (\rho^j \mu^i)_{r+a_i} (\rho^i \mu^j)_{r+a_j} (\rho^0 \mu^k)_{r+a_i+a_j}. \tag{44}$$

A similar model on the cubic lattice was discussed in Refs. 20, 27, and 28.

VII. WEAK PAIRING PHASE

When all J_μ are equal, $J_\mu = J$, the energy spectrum of the Majorana hopping Hamiltonian [Eq. (30)] has lines of zeros (line nodes) in momentum space. This gapless nature is, however, not stable against perturbations that respect TRS T'. This can be illustrated by taking a four "spin" perturbation in the gapless phase, defined on three sites j,k,l, where sites j and k are two different nearest neighbors of site l. Let us take, as an example,

$$\begin{aligned}\alpha^0_j (i\alpha^0\alpha^1)_l \alpha^1_k &= \alpha^0_j \alpha^2_l \zeta^3_l \alpha^1_k = -\alpha^0_j \alpha^3_l \zeta^2_l \alpha^1_k = \Gamma^{04}_j \Gamma^{24}_l \Gamma^{35}_l \Gamma^{14}_k \\ &= i u_{jl} \lambda^4_j \times D_l \times u_{lk} \lambda^4_k,\end{aligned} \tag{45}$$

where we take the link emanating from sites j (k) and l to be parallel to s_0 (s_1). If perturbations of this type are small enough, relative to the excitation energy of a $\mathbb{Z}_2$ vortex loop (line), i.e., an excitation which flips the sign of $\mathbb{Z}_2$ flux threading hexagons, we can contain ourselves in the vortex-free sector where $u_{jk} = +1$. Thus, the above four spin perturbation leads to next-nearest-neighbor hopping terms of the Majorana fermions. To respect TRS T', Eq. (45) can be supplemented with its TRS partner, $\zeta^0_j \alpha^3_l \zeta^2_l \zeta^1_k = T' \alpha^0_j \zeta^3_l \alpha^2_l \alpha^1_k T'^{-1}$, leading to a perturbation

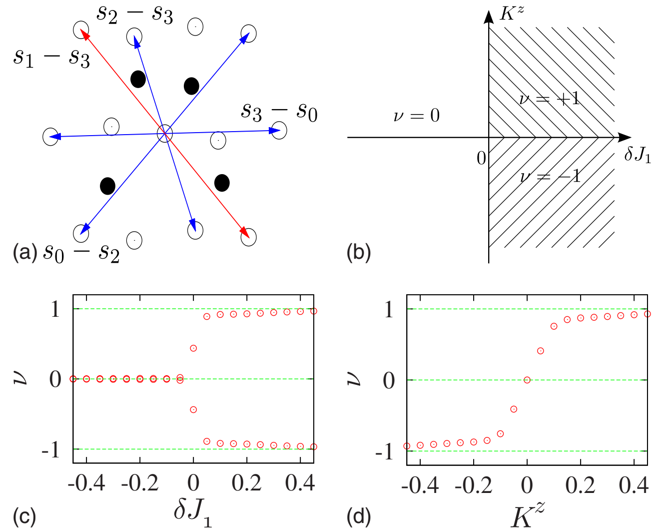

FIG. 2. (Color online) (Top left) The choice of the second-nearest-neighbor couplings K^x_{jlk} (blue links) and K^z_{jlk} (red links). (Top right) The phase diagram in terms of K^z and δJ_1 with $J_{2,3,4} = J = 2$ and $K^x = 1$. (Bottom) The numerical evaluation of the winding number as a function of the second-neighbor coupling K^z and the distortion δJ_1. In the left panel, the winding number is computed for $K^z = \pm 1$ with changing δJ_1 continuously, whereas in the right panel δJ_1 is fixed, $\delta J_1 = 1$. For $K^z = 1$ $(K^z = -1)$, $\nu = 1$ $(\nu = -1)$ when $\delta J_1 > 0$.

$$\begin{aligned}H^z_{\rm nnn} &= \sum_{\langle\langle jlk \rangle\rangle} K^z_{jlk} [i\alpha^\mu_j \alpha^\mu_l \alpha^\nu_l \alpha^\nu_k - (\alpha \leftrightarrow \zeta)] \\ &= i \sum_{\langle\langle jlk \rangle\rangle} K^z_{jlk} u_{jl} u_{lk} (\lambda^4_j \lambda^4_k - \lambda^5_j \lambda^5_k),\end{aligned} \tag{46}$$

where the summation extends over all sites labeled by l and their nearest neighbors j and k, with the link emanating from sites j (k) and l parallel to s_μ (s_ν), and $K^z_{jlk} \in \mathbb{R}$. Similarly, the following perturbation defined on three sites j,l,k is also allowed by TRS T',

$$\begin{aligned}H^x_{\rm nnn} &= \sum_{\langle\langle jlk \rangle\rangle} K^x_{jlk} [\alpha^\mu_j (\alpha^\mu i\gamma^5 \gamma^0 \zeta^\nu)_l \zeta^\nu_k + (\alpha \leftrightarrow \zeta)] \\ &= i \sum_{\langle\langle jlk \rangle\rangle} K^x_{jlk} u_{jl} u_{lk} (\lambda^4_j \lambda^5_k + \lambda^5_j \lambda^4_k),\end{aligned} \tag{47}$$

with $K^x_{jlk} \in \mathbb{R}$. We choose $K^{x,z}_{jlk}$ in such a way that these perturbations lead to the following next-nearest-neighbor terms in the Majorana hopping Hamiltonian (see Fig. 2)

$$H^z_{\rm nnn} = \frac{K^z}{2i} \sum_r \lambda^T_r s^z \lambda_{r+s_1-s_3} + \text{H.c.},$$

$$H^x_{\mathrm{nnn}} = \frac{K^x}{2i}\sum_r \lambda^T_r s^x[\lambda_{r+s_0-s_2} + \lambda_{r+s_2-s_3} + \lambda_{r+s_3-s_0}] + \text{H.c.}, \tag{48}$$

where $\lambda^T=(\lambda^4,\lambda^5)$ and $K^{x,z}\in\mathbb{R}$.

With these perturbations, the Majorana hopping Hamiltonian in momentum space is given by

$$\mathcal{X}(k) = \begin{pmatrix} \Theta(k) & i\Phi(k) \\ -i\Phi^*(k) & -\Theta(k) \end{pmatrix}, \tag{49}$$

where $\Phi(k)$ comes from nearest-neighbor hopping (27), whereas the off-diagonal part $\Theta(k)$ comes from next-nearest-neighbor hopping term (48) and is given by

$$\Theta(k) = \Theta^x(k)s^x + \Theta^z(k)s^z,$$

$$\Theta^x(k) = K^x\left[\sin\frac{k_x-k_y}{2} + \sin\frac{k_y-k_z}{2} + \sin\frac{k_z-k_x}{2}\right],$$

$$\Theta^z(k) = K^z \sin\frac{k_y+k_z}{2}. \tag{50}$$

Observe that this Hamiltonian indeed satisfies class DIII conditions (33) and (34). It can then be made block-off diagonal by the unitary transformation U, with the off-diagonal block being given by

$$D(k) = -\,\mathrm{Im}\,\Phi(k)s^0 + \Theta^z(k)is^x + \Theta^x(k)is^y + \mathrm{Re}\,\Phi(k)is^z. \tag{51}$$

The energy spectrum at momentum k is given by $E(k) = \pm\sqrt{|\Phi(k)|^2+[\Theta^x(k)]^2+[\Theta^z(k)]^2}$.

With these perturbations, we can indeed lift the degeneracy except at three points $k=Q_{x,y,z}$ in the BZ, where

$$Q_x = \frac{2\pi}{a}\begin{pmatrix}1\\0\\0\end{pmatrix}, \quad Q_y = \frac{2\pi}{a}\begin{pmatrix}0\\1\\0\end{pmatrix}, \quad Q_z = \frac{2\pi}{a}\begin{pmatrix}0\\0\\1\end{pmatrix}. \tag{52}$$

The dispersion around these points is Dirac type,

$$\mathcal{X}(Q_a+q) \sim Jq_a c^y + K^x(q_b-q_c)s^x c^z + \frac{K^z}{2}(q_y+q_z)s^z c^z, \tag{53}$$

where (a,b,c) is a cyclic permutation of (x,y,z). These three-dimensional Dirac fermions can be made massive by, say, further adding a slight distortion in the nearest-neighbor hopping, $J_1\to J_1+\delta J_1$. This gives rise to, at $Q_{x,y,z}$, a perturbation to $\mathcal{X}(k)$ which takes the form of a mass term to Dirac fermions, $-\delta J_1 c^x$.

For definiteness, we now set $J_{\mu=2,3,4}=J=2$, $K^x=1$, $J_1=J+\delta J_1$, and vary K^z and δJ_1. In the $(\delta J_1,K^z)$ plane, there are phase boundaries represented by $\delta J_1=0$ and the half-line $K^z=0$ with $\delta J_1>0$ (Fig. 2). On the line $\delta J_1=0$, the spectrum is Dirac type except at the origin $(\delta J_1,K^z)=(0,0)$ where the band gap closes at $Q_{x,y,z}$ quadratically in one direction in momentum space (a similar gapless point is discussed in Ref. 30). To determine the topological nature of the three gapped phases, the first and second quadrants in $(\delta J_1,K^z)$ plane, and the region $\delta J_1<0$, we computed the winding number by numerically integrating the formula [Eq. (41)]. Integral (41) quickly converges to a quantized value $\nu=0,\pm1$ as we increase the number of mesh in momentum space. While the winding number is identically zero when $\delta J_1<0$, it takes either $\nu=+1$ or $\nu=-1$ in the phases $\delta J_1>0$, depending on the sign of K^z. The complete structure of the phase diagram including the value of the winding number is presented in Fig. 2. In the phases with nonzero winding number, there appears a gapless and stable surface Majorana fermion mode when the Majorana hopping Hamiltonian is truncated by a boundary, signaling nontrivial topological character in the bulk.

VIII. DISCUSSIONS

We have constructed a three-dimensional interacting bosonic model which exhibits a topological band structure for emergent Majorana fermions. We thus take a first step to explore topological superconductors arising from interactions rather than giving some external parameters at the single-particle level, such as external magnetic field or spin-orbit coupling. Although the Kitaev model does not look particularly realistic as it is anisotropic both in real and spin spaces, it has played an important role in deepening our understanding of two-dimensional topological order. (See, for example, Refs. 33–41.) Also, there has been a proposal to realize the Kitaev model in terms of cold polar molecules on optical lattices[42,43] and superconducting quantum circuits.[44] Interactions which are anisotropic both in real and internal spaces can appear in systems with orbital degrees of freedom, such as the orbital compass model. Indeed, it is worth emphasizing that our model, in the absence of four spin interactions, possesses a U(1) rotation symmetry unlike the original Kitaev model and its variants. Thus, identifying, say, τ as a spin-1/2 degree of freedom and σ as an orbital degree of freedom, it might be realized as a XY analog of the Kugel-Khomskii model. Finally, while our model is designed to have a Gutzwiller-type projected wave function as its exact ground state, such ground-state wave functions can appear in much wider context, which can be explored, e.g., in terms of a variational approach with slave particle mean-field theories.[45]

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APPENDIX: CLASS DIII SYMMETRY CLASS

In this appendix, we review the symmetry classification of the Bogoliubov-de Gennes (BdG) Hamiltonians by Altland and Zirnbauer, which is relevant to our auxiliary Majorana hopping problems. We consider the following general form of a BdG Hamiltonian for the dynamics of fermionic quasiparticles deep inside the superconducting state of a superconductor

$$H=\frac{1}{2}(\boldsymbol{c}^{\dagger},\quad \boldsymbol{c})\mathcal{H}\begin{pmatrix}\boldsymbol{c}\\ \boldsymbol{c}^{\dagger}\end{pmatrix},\quad \mathcal{H}=\begin{pmatrix}\Xi & \Delta\\ -\Delta^{*} & -\Xi^{T}\end{pmatrix},\qquad (A1)$$

where $\mathcal{H}$ is a $4N\times 4N$ matrix for a system with N orbitals (lattice sites), and $\boldsymbol{c}=(\boldsymbol{c}_{\uparrow},\boldsymbol{c}_{\downarrow})$ is a $2N$ component vector. ($\boldsymbol{c}$ and $\boldsymbol{c}^{\dagger}$ can be either column or row vector depending on the context.) Following the notations in Ref. 14, we use two sets of 2×2 Pauli matrices $t_{0,x,y,z}$ and $s_{0,x,y,z}$, which act on particle-hole and spin indices, respectively. Because of

$$\Xi=\Xi^{\dagger}\quad (\text{hermiticity}),$$

$$\Delta=-\Delta^{T}\quad (\text{Fermi statistics}),\qquad (A2)$$

the BdG Hamiltonian (A1) satisfies particle-hole symmetry (PHS)

$$(a):\quad \mathcal{H}=-t_{x}\mathcal{H}^{T}t_{x},\quad (\text{PHS}).\qquad (A3)$$

The presence or absence of TRS and SU(2) spin rotation symmetry are represented by

$$(b):\quad \mathcal{H}=is_{y}\mathcal{H}^{T}(-is_{y}),\quad (\text{TRS}),\qquad (A4)$$

and

$$(c):\quad [\mathcal{H},J_{a}]=0,\quad J_{a}:=\begin{pmatrix}s_{a} & 0\\ 0 & -s_{a}^{T}\end{pmatrix},$$

$$a=x,y,z,\quad [\text{SU}(2)\ \text{symmetry}],\qquad (A5)$$

respectively.

The ensemble of BdG Hamiltonian (A1) with PHS condition (a) defines symmetry class D of Altland and Zirnbauer.[13] With additional TRS condition (b), the resulting ensemble of BdG Hamiltonians is called symmetry class DIII. For both symmetry classes, spin rotation symmetry (c) is not necessary.

The Hamiltonian in symmetry class D can be thought of as, because of PHS (a), a single-particle Hamiltonian of Majorana fermions. The Majorana structure of the BdG Hamiltonians can be revealed by

$$\begin{pmatrix}\boldsymbol{c}\\ \boldsymbol{c}^{\dagger}\end{pmatrix}\to\frac{1}{\sqrt{2}}\begin{pmatrix}\boldsymbol{\eta}\\ \boldsymbol{\chi}\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}\boldsymbol{c}+\boldsymbol{c}^{\dagger}\\ i(\boldsymbol{c}-\boldsymbol{c}^{\dagger})\end{pmatrix},\qquad (A6)$$

where η and χ are Majorana fermions satisfying

$$\eta_{i}\eta_{j}+\eta_{j}\eta_{i}=2\delta_{ij},\quad \eta^{\dagger}=\eta,\quad (i=1,\ldots,2N),\quad \text{etc.}\qquad (A7)$$

Then, in this Majorana basis, the BdG Hamiltonian can be written as

$$H=(\boldsymbol{\eta},\quad \boldsymbol{\chi})\mathcal{X}\begin{pmatrix}\boldsymbol{\eta}\\ \boldsymbol{\chi}\end{pmatrix},\qquad (A8)$$

where

$$\mathcal{X}=\frac{1}{2}\begin{pmatrix}P+S & -i(Q-R)\\ i(Q+R) & P-S\end{pmatrix},\qquad (A9)$$

and

$$P=\Xi-\Xi^{T}=-P^{T},\quad Q=\Xi+\Xi^{T}=+Q^{T},$$

$$R=\Delta+\Delta^{*}=-R^{T},\quad S=\Delta-\Delta^{*}=+S^{T}.\qquad (A10)$$

Then, the $4N\times 4N$ matrix $\mathcal{X}$ satisfies

$$\mathcal{X}^{\dagger}=\mathcal{X},\quad \mathcal{X}^{T}=-\mathcal{X}.\qquad (A11)$$

These conditions define symmetry class D. On the other hand, symmetry class DIII is defined by, in addition,

$$is_{y}\mathcal{X}^{T}(-is_{y})=\mathcal{X}.\qquad (A12)$$

While it is always possible to cast the BdG Hamiltonians into a form of a single-particle Hamiltonian of Majorana fermions by rewriting the BdG Hamiltonian in terms of the "real" and "imaginary" parts of the electron operator, $\boldsymbol{\eta}$ and $\boldsymbol{\chi}$, there is no natural way in general to rewrite Majorana hopping problems as a BdG Hamiltonian. In order to do so, the single-particle Majorana Hamiltonian must be an even-dimensional matrix, and we need to specify a particular way to make a complex fermion operator out of two Majorana fermion operator. Still, any single-particle Hamiltonian for Majorana fermions, with its defining properties [Eq. (A11)], can be classified in terms of the presence (class DIII) or absence (class D) of TRS [Eq. (A12)] without referring to complex fermions.

1. Off-diagonal block structure of class DIII Hamiltonians

In combining class DIII conditions (a) and (b), one can see that a member of class DIII anticommutes with a unitary matrix $t_{x}s_{y}$,

$$\mathcal{H}=-t_{x}s_{y}\mathcal{H}s_{y}t_{x}.\qquad (A13)$$

In this sense, class DIII Hamiltonians can be said to have a chiral structure. In order to compute the winding number ν, defined for class DIII Hamiltonians in three spatial dimensions, it is necessary to go to a basis in which the chiral transformation $t_{x}s_{y}$ is diagonal. We can find such a basis as follows: we first rotate $t_{x}\to t_{z}$ and $s_{y}\to s_{z}$ by a unitary transformation

$$W_{1}=\frac{1}{\sqrt{2}}(t_{0}+it_{y})\frac{1}{\sqrt{2}}(s_{0}-is_{x}),\qquad (A14)$$

i.e., $W_{1}t_{x}W_{1}^{\dagger}=-t_{z}$ and $W_{1}s_{y}W_{1}^{\dagger}=-s_{z}$. We then exchange the third and fourth entries by a unitary transformation W_{2},

$$W_{2}W_{1}t_{x}s_{y}W_{1}^{\dagger}W_{2}^{\dagger}=W_{2}t_{z}s_{z}W_{2}^{\dagger}=t_{0}s_{z}.\qquad (A15)$$

Further exchanging the second and third entries by a unitary transformation W_{3}, the combined unitary transformation $W=W_{3}W_{2}W_{1}$ diagonalizes $t_{x}s_{y}$,

$$t_{x}s_{y}\to Wt_{x}s_{y}W^{\dagger}=t_{z}s_{0}.\qquad (A16)$$

Under the transformation W PHS and TRS transformations are transformed as

$$t_x s_0 \to W t_x s_0 W^T = -i t_x s_z, \quad \text{(PHS)},$$

$$t_0 s_y \to W t_0 s_y W^T = t_y s_z, \quad \text{(TRS)}, \tag{A17}$$

respectively. Observe the transformed PHS and TRS pick up the same sign under matrix transposition $[(t_x s_z)^T = +(t_x s_z)^T$ and $(t_y s_z)^T = -(t_y s_z)$, respectively] as the original ones $[(t_x s_0)^T = +(t_x s_0)$ and $(t_0 s_y)^T = -(t_0 s_y)^T$, respectively]. In this basis, the Hamiltonian takes the block-off-diagonal form,

$$\mathcal{H} \to \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix}, \quad D = -s_z D^T s_z. \tag{A18}$$

This can be further simplified by a unitary transformation

$$\mathcal{H} \to \begin{pmatrix} 0 & s_{xy}^\dagger \\ s_{xy} & 0 \end{pmatrix} \begin{pmatrix} 0 & D \\ D^\dagger & 0 \end{pmatrix} \begin{pmatrix} 0 & s_{xy}^\dagger \\ s_{xy} & 0 \end{pmatrix} = \begin{pmatrix} 0 & s_{xy}^\dagger D^\dagger s_{xy}^\dagger \\ s_{xy} D s_{xy} & 0 \end{pmatrix}, \tag{A19}$$

where

$$s_z = -i s_{xy}^T s_{xy}, \quad s_{xy}^T = \frac{1}{\sqrt{2}}(s_x - s_y). \tag{A20}$$

Introducing

$$D' := s_{xy} D s_{xy} = -s_{xy}^T D^T s_{xy}^T = -(D')^T, \tag{A21}$$

we finally arrive at

$$\mathcal{H} \to \begin{pmatrix} 0 & D' \\ D'^\dagger & 0 \end{pmatrix}, \quad D' = -D'^T. \tag{A22}$$

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