Topological Characterization of Quantum Phase Transitions in a Spin-1/2 Model

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We have introduced a novel Majorana representation of $S = 1/2$ spins using the Jordan-Wigner transformation and have shown that a generalized spin model of Kitaev defined on a brick-wall lattice is equivalent to a model of noninteracting Majorana fermions with Z_2 gauge fields *without* redundant degrees of freedom. The quantum phase transitions of the system at zero temperature are found to be of topological type and can be characterized by *nonlocal* string order parameters (SOP). In appropriate dual representations, these SOP become *local* order parameters and the basic concept of Landau theory of continuous phase transition can be applied.

The Landau theory of second order phase transitions has fertilized modern statistical and condensed matter physics. It is essential to use local order parameters to describe the continuous phase transition between a disordered and an ordered phase associated with symmetry breaking [1]. However, quantum phase transitions (QPT) driven entirely by quantum fluctuations at zero temperature can occur between two disordered phases without any symmetry breaking [2,3]. A typical example is the topological phase transition between two neighboring quantum Hall plateaus in the fractional quantum Hall effect [4]. As no conventional Landau-type order parameters can be used, a comprehensive characterization of this kind of QPT has become one of the most challenging issues in physics.

In this work, we present a theoretical analysis of QPT in a $S = 1/2$ spin model first introduced by Kitaev [5]

$$H = \sum_{j+l=\text{even}} (J_1 \sigma_{j,l}^x \sigma_{j+1,l}^x + J_2 \sigma_{j-1,l}^y \sigma_{j,l}^y + J_3 \sigma_{j,l}^z \sigma_{j,l+1}^z),$$

(1)

where j and l denote the column and row indices of the lattice. This model is defined on a brick-wall lattice [Fig. 1(c)], which is an alternative representation of a honeycomb lattice [Fig. 1(d)]. The one- and two-row limits of the brick-wall lattices with periodic boundary conditions are simply a single spin chain [Fig. 1(a)] and a two-leg ladder [Fig. 1(b)], respectively. In these limits, the analysis of the model is greatly simplified, while the results obtained are highly nontrivial and can be extended with proper modification to other brick-wall lattices. In the work of Kitaev [5], the two-dimensional phase diagram of the ground state was studied. Here we will concentrate more on the analysis of QPT in an arbitrary brick-wall lattice. Our studies reveal many generic features of topological QPT in this system. It also sheds light on the understanding of more general systems, where analytic solutions are not available.

To solve this model, let us first introduce the following Jordan-Wigner transformation to represent spin operators along each row with spinless fermion operators:

$$\sigma_{jl}^+ = 2a_{jl}^\dagger e^{i\pi(\sum_{i,k<l} a_{ik}^\dagger a_{ik} + \sum_{i<j} a_{il}^\dagger a_{il})}.$$

(2)

For each pair of fermion operators $(a, a^\dagger)$, we can further define two Majorana fermion operators (c, d): $c_{jl} = i(a_{jl}^\dagger - a_{jl})$ and $d_{jl} = a_{jl}^\dagger + a_{jl}$ when $j + l = $ even, and $c_{jl} = a_{jl}^\dagger + a_{jl}$ and $d_{jl} = i(a_{jl}^\dagger - a_{jl})$ when $j + l = $ odd. With these definitions, it is straightforward to show that at each given row only the c type of Majorana fermions are present and the Hamiltonian can be expressed as

$$H = -i \sum_{j+l=\text{even}} (J_1 c_{j,l} c_{j+1,l} - J_2 c_{j-1,l} c_{j,l} + J_3 D_{jl} c_{j,l} c_{j,l+1}),$$

(3)

where $D_{jl} = id_{j,l} d_{j,l+1}$ is defined on each vertical bond. Since there are no direct connections between any two vertical bonds, all D_{jl} are *good quantum numbers*. Each D_{jl} acts like a local static Z_2 gauge field. They commute with each other and with the Hamiltonian.
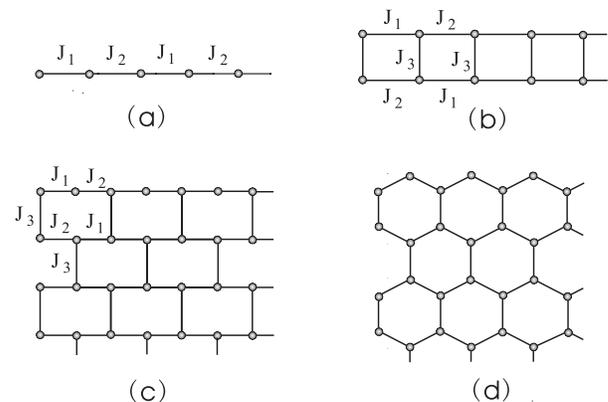

FIG. 1. A brick-wall lattice (c) with its equivalent honeycomb lattice (d). (a) and (b) are the one- and two-row limits of the brick-wall lattices, respectively.

Equation (3) is simply a model of free Majorana fermions [6] with local Z_2 gauge fields. In fact, a similar Majorana fermion representation of the Hamiltonian was first used by Kitaev [5] to solve rigorously the ground state in the two-dimensional limit. However, in the work of Kitaev, [5] a $S = 1/2$ spin operator is represented by *four* Majorana operators, which introduces two redundant degrees of freedom at each site and many important properties of the system, especially those involving excitation states, are blurred by those unphysical states. To remove these redundant degrees of freedom, a complicated projection on the wave function has to be imposed.

In Eq. (3), D_{jl} for a given l can be all changed into $-D_{jl}$ by a unitary transformation. For example, the unitary operator $U_{2l} = \prod_j c_{2j,2l}$ can effectively convert all $D_{2j,2l}$ on the $(2l)$th ladder to $-D_{2j,2l}$, and $U_{2l-1} = \prod_j c_{2j-1,2l-1}$ converts all $D_{2j-1,2l-1}$ on the $(2l-1)$th ladder to $-D_{2j-1,2l-1}$. Therefore, all the eigenstates of the Hamiltonian are at least 2^M-fold degenerate for a M-leg ladder ($M = 0$ for a single chain). In the discussion below, without loss of generality, we will assume all three coupling constants (J_1, J_2, J_3) to be positive.

For a single spin chain, the Hamiltonian can be readily diagonalized. The eigenspectra contain two bands of quasiparticle excitations: $\varepsilon_k^\pm = \pm\sqrt{J_1^2 + J_2^2 + 2J_1J_2\cos k}$, where k is the momentum. In the ground state, one of the bands is fully occupied while the other is empty. When $J_1 \neq J_2$, there is an energy gap in the low-lying excitations. By varying J_1/J_2, we find that the second derivative of the ground state energy density E_0 diverges logarithmically at $J_1 = J_2$ where the gap vanishes [Fig. 2(a)]. Furthermore, by applying the renormalization group (RG) analysis to this model, it can be shown that J_1/J_2 will flow to infinity if $J_1 > J_2$ or to zero if $J_1 < J_2$, and $J_1/J_2 = 1$ is a quantum critical point [Fig. 2(b)].

The transition between the two gapped fermionic states at $J_1/J_2 = 1$ does not involve any change of symmetry. Instead it manifests as a change of topological order. To see this, let us introduce a spin duality transformation [7]

$$\sigma_j^x = \tau_{j-1}^x \tau_j^x, \qquad \sigma_j^y = \prod_{k=j}^{2N} \tau_k^y, \qquad (4)$$

to rewrite the Hamiltonian (1) as

$$H_d = \sum_{j=1}^{N}(J_1\tau_{2j-2}^x\tau_{2j}^x + J_2\tau_{2j}^y). \qquad (5)$$

This is nothing but a one-dimensional Ising model with a transverse field defined in the dual lattice. When $J_1 > J_2$, it is known that a long-range order exists in the dual spin correlation function of τ_{2j}^x [8]:

$$\lim_{j\to\infty}\langle\tau_0^x\tau_{2j}^x\rangle \sim [1 - (J_2/J_1)^2]^{1/4}. \qquad (6)$$

Thus τ_{2j}^x can be regarded as an order parameter characterizing the phase transition from $J_1 > J_2$ to $J_1 < J_2$ in the dual space. In the original spin representation, $\tau_0^x\tau_{2j}^x$ is a string product of σ_j^x:

$$\hat{\Delta}_x(j) = \tau_0^x\tau_{2j}^x = \prod_{k=1}^{2j}\sigma_k^x = (-1)^j\prod_{k=1}^{2j}c_k. \qquad (7)$$

Equation (6) then indicates that H has a hidden topological order in the $J_1 > J_2$ phase with $\Delta_x = \lim_{j\to\infty}\langle\hat{\Delta}_x(j)\rangle$.

When $J_1 < J_2$, the dual spins τ_{2j}^x become disordered and Δ_x vanishes [8]. However, by swapping the J_2 with the J_1 term in Eq. (1) and applying a similar duality argument, it can be shown that a string order of σ_n^y

$$\Delta_y = \lim_{j\to\infty}\left\langle\prod_{k=2}^{2j+1}\sigma_k^y\right\rangle = (-1)^j\lim_{j\to\infty}\left\langle\prod_{k=2}^{2j+1}c_k\right\rangle, \qquad (8)$$

is finite in the $J_1 < J_2$ phase and zero otherwise.

The above discussion indicates that in the single-chain limit, the model is in disordered phases, but it contains two *hidden* string order parameters (SOP). The QPT at $J_1/J_2 = 1$ corresponds to a continuous change of Δ_x or Δ_y from zero to a finite value from one side of the critical point to another. In the dual space, however, these *nonlocal* SOP become *local*. This suggests that Landau-type concepts of continuous phase transition can still be applied to this simple model, but in the dual space.

For a two-leg spin ladder, the ground state is in a π-flux phase [9]. The eigenspectra contain four branches of fermionic quasiparticle excitation bands $\pm\varepsilon_k^\pm$ with $\varepsilon_k^\pm = \sqrt{(J_3 \pm J_-\sin^2\frac{k}{2})^2 + J_+^2\cos^2\frac{k}{2}}$, where $J_\pm = J_1 \pm J_2$. At zero temperature, two bands are fully occupied and the other two are completely empty. In general, there is also an energy gap between the ground and excited states. But this gap vanishes along both $J_- = J_3$ and $J_- = -J_3$ lines. As shown in Fig. 3(b), the second derivative of the ground state energy density diverges logarithmically on these two lines.

To clarify the topological nature of these three gapped phases as shown in Fig. 3(a), let us first relabel all the sites along a special path as shown in Fig. 3(c) to express the original spin Hamiltonian as an effective single-chain model with the third nearest neighbor couplings:

$$H = \sum_j(J_1\sigma_{2j-1}^x\sigma_{2j}^x + J_3\sigma_{2j}^z\sigma_{2j+1}^z + J_2\sigma_{2j}^y\sigma_{2j+3}^y). \qquad (9)$$
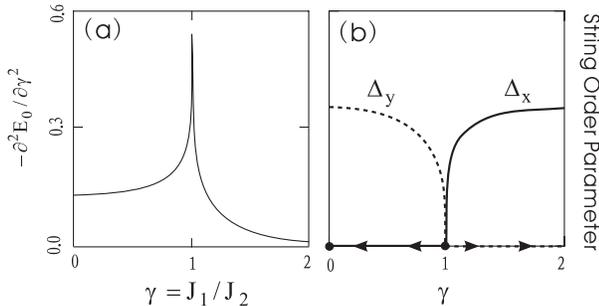

FIG. 2. The second derivative of the ground state energy density E_0 (a) and the nonlocal SOP (b) for a single chain. The arrows in (b) indicate the RG flow.
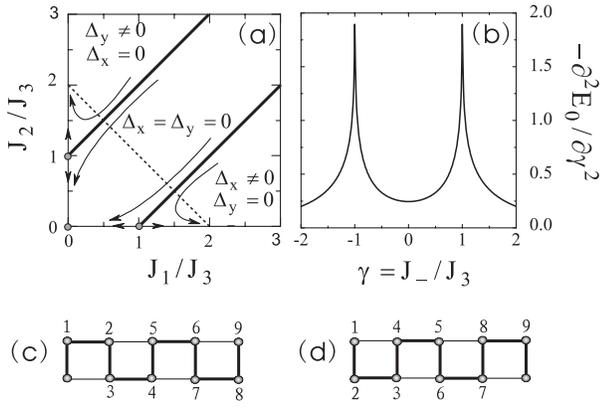
FIG. 3.   (a) The phase diagram with RG flows for the two-leg ladder. (b) The second derivative of E_0 along the dotted line in (a). (c) and (d) are two deformed single-chain representations of the two-leg ladder.

By applying the similar duality transformation (4) to this Hamiltonian, we find that this model is equivalent to an anisotropic *XY* spin chain with a transverse field in the dual space:

$$H_D = \sum_j (J_1 \tau^x_{2j-2}\tau^x_{2j} + J_2 W_{2j}\tau^y_{2j-2}\tau^y_{2j} + J_3 \tau^z_{2j}), \quad (10)$$

where $W_{2j} = \tau^x_{2j-3}\tau^z_{2j-1}\tau^x_{2j+1}$ is the plaquette operator defined in the dual space. It is a good quantum number.

In the ground state, $W_{2j} = -1$, corresponding to the π-flux phase. It is known that the system is in a long-range ordered state of τ^x_{2j} when $J_- > J_3$ and in a disordered state otherwise [10]. Thus, $\langle \tau^x_{2j} \rangle$ is an effective order parameter characterizing the QPT across the critical line $J_- = J_3$. Back to the original spin model, there exists a SOP Δ_x defined by Eq. (7) but in the deformed lattice [Fig. 3(c)] in the $J_- > J_3$ phase. Using the results given in Ref. [10], we find that

$$\Delta_x \sim \frac{\sqrt{J_+/J_-}}{2(1 + J_+/J_-)}\left[1 - \left(\frac{J_3}{J_-}\right)^2\right]^{1/4}. \quad (11)$$

In the other two phases ($J_- < J_3$), $\Delta_x = 0$.

The above duality argument can be generalized to clarify the QPT across the line $J_- = -J_3$ by swapping J_1 with the J_2 term in the original Hamiltonian. In the ground state, it can be also shown that the nonlocal SOP Δ_y defined by Eq. (8), but now in a deformed lattice where σ^y_j is labeled according to Fig. 3(d), is finite in the phase $J_- < -J_3$, and vanishes in the other two phases. Thus the phase diagram of the two-leg ladder system can be classified by the two nonlocal SOP: Δ_x and Δ_y. They are finite in the $J_- > J_3$ and $J_- < -J_3$ phases, respectively. The QPT at each critical line $J_- = \pm J_3$ corresponds to a continuous change of one of the SOP from zero to a finite value.

For a 2*M*-row brick-wall lattice with $M > 1$, the ground state of the model is in a zero-flux phase [9] and all D_{jl} for a given l have the same value. The ground state is thus

2^{2M}-fold degenerate, and this massive degeneracy leads to an extensive zero temperature entropy. In what follows, we will focus on the case $D_{jl} = (-1)^l$. The resulting conclusions can be easily generalized to other degenerate states by unitary transformations.

To elucidate the topological nature of the quantum criticality in this system, let us first follow what we have done for the two-leg ladder to map a 2*M*-row lattice to a *M*-row lattice by chaining all neighboring sites along the stair paths of $J_1 - J_3$ links with periodic boundary conditions. An example of such mappings is displayed in Fig. 4 for a six-row brick-wall lattice. In the new lattice system, the Hamiltonian (3) can be expressed as

$$H = -i\sum_{j=1}^{2N}\sum_{\alpha=1}^{M}(J_1 c_{2j-1,\alpha}c_{2j,\alpha} - J_2 c_{2j,\alpha}c_{2j+3,\alpha+1}$$
$$+ J_3(-1)^j c_{2j,\alpha}c_{2j+1,\alpha}). \quad (12)$$

By transforming the second index of $c_{j,\alpha}$ into its momentum form $c_{j,q}$, Eq. (12) then becomes $H = \sum_q H_q$, where

$$H_q = -i\sum_j [J_1 c_{2j-1,-q}c_{2j,q} - J_2 e^{iq}c_{2j,-q}c_{2j+3,q}$$
$$+ J_3(-1)^j c_{2j,-q}c_{2j+1,q}], \quad (13)$$

and $q = 2\pi m/M$ and $m = 0 \cdots M - 1$. This Hamiltonian is now block diagonalized according to the value of $|q|$. When $q = 0$ or π, $-q$ is equal or equivalent to q, and $c_{j,q}$ is still a Majorana fermion. In other cases, $c_{j,-q}$ and $c_{j,q}$ are conjugate pairs of standard fermion operators, i.e., $c_{j,-q} = c^\dagger_{j,q}$.

The quasiparticle eigenspectra can be obtained by diagonalizing the Hamiltonian at each $|q|$ sector ($|q| \leq \pi$).
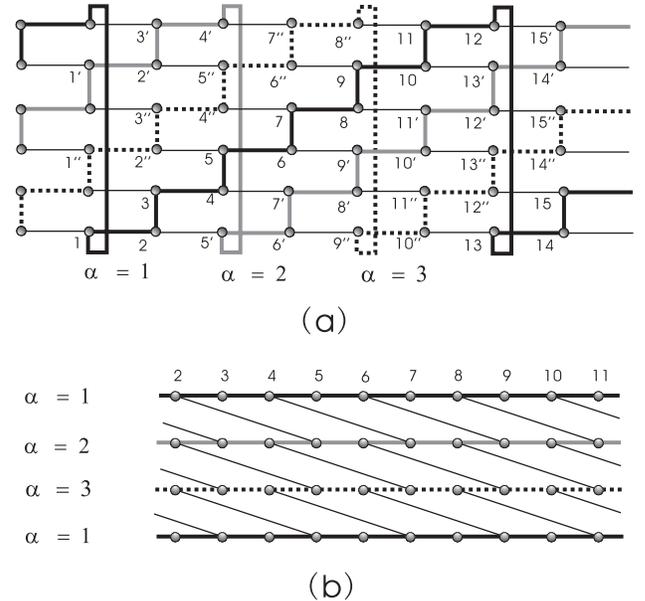

FIG. 4.   (a) The six-row brick-wall lattice and (b) its equivalent three-row lattice.
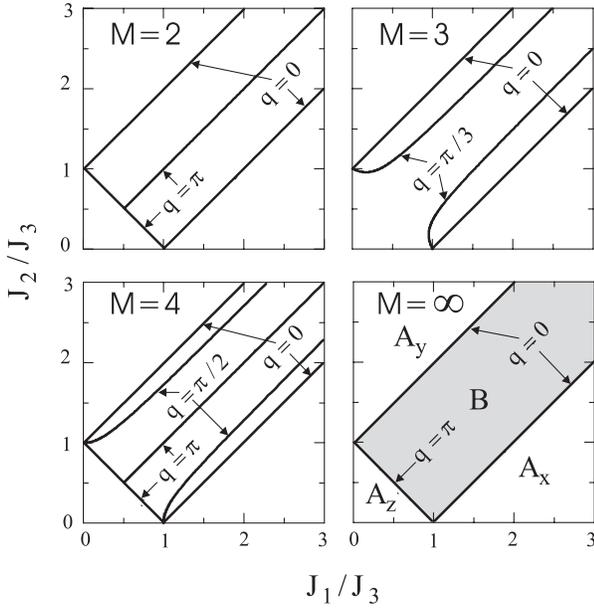
FIG. 5.   The phase diagram with quantum critical lines of the 2M-row brick-wall lattice. In the $M = \infty$ panel, the four phases are, respectively, labeled by (A_x, A_y, A_z) and B following the notation of Kitaev [5].

Figure 5 shows the phase diagram of the multirow lattices with $M = 2, 3, 4$, and ∞. For a $2M$-row lattice, there are $M + 2$ $(M + 1)$ critical lines if $M =$ even ($M =$ odd). These critical lines correspond to the vanishing gap lines, where the second derivatives of the ground state energy in the direction perpendicular diverge logarithmically.

When $q = 0$, H_q has exactly the same form as the Hamiltonian of a two-leg ladder with a π-flux, represented in the deformed lattice in Fig. 3(c). As discussed before, the critical excitation gives rise to two QPT at the lines $J_- = \pm J_3$. The corresponding topological order parameters, $\Delta_{x,0}$ and $\Delta_{y,0}$, can be defined from Eqs. (7) and (8) by replacing c_j with $c_{j,q=0}$. $\Delta_{x,0}$ is finite in the phase $J_- > J_3$, while $\Delta_{y,0}$ is finite in the phase $J_- < -J_3$.

When $q = \pi$ ($M =$ even only), H_q is also equivalent to the Hamiltonian of a two-leg ladder, but with a minus J_2 term. The ground state of H_q is effectively in zero flux. Two critical lines are now located at $J_+ = J_3$ and at $J_- = 0$ with $J_+ > J_3$. Correspondingly, one can also define two topological SOP, $\Delta_{x,\pi}$ and $\Delta_{y,\pi}$, from Eqs. (7) and (8), by replacing c_j with $c_{j,q=\pi}$. $\Delta_{x,\pi}$ ($\Delta_{y,\pi}$) is finite in the $J_+ > J_3$ and $J_1 > J_2$ ($J_1 < J_2$) phase.

When $q \neq 0$ or π, $c_{j,\pm q}$ are no longer Majorana fermions. By considering the limiting cases of $J_1 \gg J_2$ and $J_1 \ll J_2$, it can be shown that two SOP defined from the combinations of $c_{j,q}$ and $c_{j,-q}$ exists. However, as H_q is coupled with H_{-q}, we are still unable to write down accurately the expressions of the SOP.

In the two-dimensional limit ($M = \infty$), all the critical lines inside the regime enclosed by the three curves, $J_- = \pm J_3$ and $J_+ = J_3$, merge together and form a continuum

gapless phase. Therefore, the whole phase space contains three gapped phases and one gapless phase, in agreement with the phase diagram of Kitaev [5]. The gapless phase may have a complicated non-Abelian topological structure [5]. However, the phase transition from any gapped phase to the gapless phase can be characterized by a SOP, since the phase boundaries of the gapless phase are fully determined by the phase transition lines of the decoupled fermionic chains with $q = 0$ and π.

In summary, using the Jordan-Wigner transformation, we have shown that the Hamiltonian defined by Eq. (1) is mapped onto a model of free Majorana fermions with local Z_2 gauge fields *without* any redundant degrees of freedom. By solving this model *exactly* at zero temperature, we find that the system undergoes a number of continuous phase transitions. These QPT are not induced by spontaneous symmetry breaking and there are no conventional Landau-type local order parameters. However, each transition corresponds to a continuous change of a topological SOP from a finite value to zero. This reveals that the QPT in this system can not only be indexed by a topological quantum number, but also be characterized by a topological order parameter. In the dual space, the SOP actually corresponds to a *local* order parameter and the basic concepts of Landau theory of continuous phase transition are still applicable.

The above conclusion is drawn based on the analysis of a specific model (1). However, we believe it might be valid generically since a topological QPT corresponds to a condensation of certain nonlocal operators [4] and these nonlocal operators span a dual space at which the order parameters become local. Similar topological SOP has been found, for example, in the Haldane gapped spin chains [11,12]. Further exploration of this problem is desired, which may lead to a unified description of convention and topological QPT.

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