Entanglement Entropy and Entanglement Spectrum of the Kitaev Model

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In this Letter, we obtain an exact formula for the entanglement entropy of the ground state and all excited states of the Kitaev model. Remarkably, the entanglement entropy can be expressed in a simple separable form $S = S_G + S_F$, with S_F the entanglement entropy of a free Majorana fermion system and S_G that of a Z_2 gauge field. The Z_2 gauge field part contributes to the universal "topological entanglement entropy" of the ground state while the fermion part is responsible for the nonlocal entanglement carried by the Z_2 vortices (visons) in the non-Abelian phase. Our result also enables the calculation of the entire entanglement spectrum and the more general Renyi entropy of the Kitaev model. Based on our results we propose a new quantity to characterize topologically ordered states—the capacity of entanglement, which can distinguish the states with and without topologically protected gapless entanglement spectrum.

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Exotic phases such as fractional quantum Hall (FQH) states, which are not in the paradigm of conventional symmetry breaking, were termed as topologically ordered [1] since they have robust ground state degeneracy which is protected against all local perturbations, but sensitive to the topology of the system [2]. A topologically ordered state has a nonlocal pattern of quantum entanglement, which is essential for the proposal of topological quantum computation [3–5].

By bipartitioning a system spatially, the entanglement entropy (EE) measures how closely entangled the two subsystems are. For a gapped system, EE is usually proportional to the area of the interface between the two subsystems in the thermodynamic limit. However, as discovered by Levin and Wen [6] as well as Kitaev and Preskill [7], the entanglement entropy of a topologically ordered state contains a universal constant term, which is uniquely determined by the topological order of the state, named the topological entanglement entropy (TEE). TEE enables a direct characterization of topological ordered states without referring to the Hamiltonian. EE and TEE are properties of a many-body state and are usually hard to compute. EE and/or TEE have been computed exactly or numerically for several models such as toric code model [3,8,9], FQH states [10–12], and quantum dimer models [13–15]. So far there has been no exact result for the EE of topologically ordered states whose quasiparticles obey non-Abelian statistics.

This Letter serves to fill in that gap by providing a simple but exact method to compute the EE for any eigenstate (either ground or excited states) of the Kitaev model [16], which is one of the most important exact solvable models with non-Abelian anyons. The essence of our method is a rigorous proof that the EE of the Kitaev model is equal to that of two decoupled systems: a sourceless Z_2 gauge field and a free Majorana fermion system. Although the TEE of the ground state comes only from the Z_2 gauge field, the fermionic part is responsible for all nontrivial entanglement properties of the non-Abelian phase. Besides the EE, our method also enables the computation of the whole entanglement spectrum (ES), i.e., the eigenvalue spectrum of the reduced density matrix [17]. We show that the entanglement spectrum is gapless or gapped in the non-Abelian and Abelian phase of the Kitaev model, respectively. We propose a new quantity, the capacity of entanglement, which can be used to distinguish different topological states with gapped and gapless entanglement spectrum.

Kitaev model is a spin-$1/2$ model originally proposed on the honeycomb lattice [16] with the Hamiltonian

$$H = -\sum_{x\ \mathrm{link}} J_x \sigma_i^x \sigma_j^x - \sum_{y\ \mathrm{link}} J_y \sigma_i^y \sigma_j^y - \sum_{z\ \mathrm{link}} J_z \sigma_i^z \sigma_j^z, \quad (1)$$

where x, y, and z link stand for the three types of links. It has a non-Abelian phase when the time-reversal symmetry is broken either explicitly by magnetic field [16] or three-spin couplings [18] or spontaneously by decorating the honeycomb lattice [19]. For simplicity, hereafter we will present our exact results of EE and entanglement spectrum for the Kitaev model on honeycomb lattice, but our approach can be generalized straightforwardly to a broad class of Hamiltonians, including the Kitaev model on any trivalent lattice and Gamma matrix models [20–24].

The Kitaev model can be solved by introducing the Majorana representation of the Pauli matrices [16]: $\sigma_i^\alpha = i\gamma_i^\alpha \eta_i$ ($\alpha = x, y, z$), where γ_i^α and η_i are Majorana fermion operators. γ_i^α and η_i on each lattice site define a four-dimensional Hilbert space, so that the Majorana representation of a spin-$1/2$ is redundant. The physical Hilbert space is defined by a constraint

$D_i = -i\sigma_i^x\sigma_i^y\sigma_i^z = \gamma_i^x\gamma_i^y\gamma_i^z\eta_i = 1$. In other words, a state $|\Psi\rangle$ is physical only if $D_i|\Psi\rangle = |\Psi\rangle$ for every i. In the Majorana representation we have $\sigma_i^\alpha\sigma_j^\alpha = \gamma_i^\alpha\gamma_j^\alpha\eta_i\eta_j = -i\hat{u}_{ij}\eta_i\eta_j$, in which the link operators $\hat{u}_{ij} = i\gamma_i^\alpha\gamma_j^\alpha$ mutually commute and also commute with the Hamiltonian. Since $\hat{u}_{ij}^2 = 1$, $\hat{u}_{ij}$ can be considered as c numbers with values $u_{ij} = \pm 1$, so that the Kitaev model is equivalent to a free model of η Majorana fermions coupled to static Z_2 gauge fields [16,18,19,24–27]. The ground state of such a model is given by the direct product of a Z_2 gauge configuration $|u\rangle$ and the corresponding Majorana fermion ground state $|\phi(u)\rangle$. Here the configuration u is determined by minimizing the fermion ground state energy. There is a macroscopic ground state degeneracy in the enlarged Hilbert space, because each state $|u\rangle \otimes |\phi(u)\rangle$ is degenerate with all the states $|u'\rangle \otimes |\phi(u')\rangle$ with u' gauge equivalent to u. However, such a degeneracy is removed when the constraint $D_i = 1$ is applied. The physical ground state is the "gauge" average of the degenerate states, implemented by the projection [16]

$$|\Psi\rangle = \frac{1}{\sqrt{2^{N+1}}}\sum_g D_g|u\rangle \otimes |\phi(u)\rangle, \tag{2}$$

where N is the total number of lattice sites, g denotes a set of lattice sites, and $D_g = \prod_{i\in g} D_i$. We define $D = \prod_{i\in\mathcal{L}} D_i$ with $\mathcal{L}$ the set of all lattice sites. The sum $\sum_g$ is taken over all possible subsets g of $\mathcal{L}$. Note that, in Eq. (2), we implicitly assumed that $D|u\rangle \otimes |\psi(u)\rangle = |u\rangle \otimes |\psi(u)\rangle$ because states with $D = -1$ will be annihilated by the projection. Consequently, we have $D_g = DD_{\bar{g}}$ for the complement $\bar{g} = \mathcal{L} - g$, so that $D_g|u\rangle \otimes |\phi(u)\rangle = D_{\bar{g}=\mathcal{L}-g}|u\rangle \otimes |\phi(u)\rangle$. In other words there are only 2^{N-1} inequivalent gauge transformations, as expected.

We define the Kitaev model on a torus and bipartite the lattice into subsystems A and B, as shown in Fig. 1. The EE between A and B is defined as $S = -\mathrm{Tr}_A[\rho_A \log\rho_A]$, where $\rho_A = \mathrm{Tr}_B\rho = \mathrm{Tr}_B|\Psi\rangle\langle\Psi|$ is the reduced density matrix of A. To calculate the EE, we will follow the "replica trick" introduced in Ref. [28]:

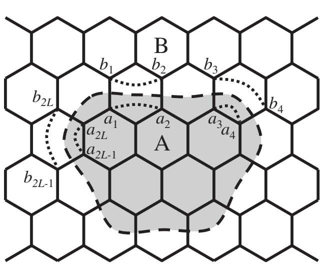

FIG. 1. The schematic honeycomb lattice is bipartitioned into two parts A and B. The partition boundary (dashed line) cuts the links $\overline{a_n b_n}$, $n = 1, \ldots, 2L$. New Z_2 gauge variables (see the supplementary material [29]) $\hat{w}_{A,n}$ and $\hat{w}_{B,n}$ are introduced on the new (dotted) links $\overline{a_{2n-1}a_{2n}}$ and $\overline{b_{2n-1}b_{2n}}$, $n = 1, \ldots, L$, respectively.

$$S = -\mathrm{Tr}_A[\rho_A \log\rho_A] = -\frac{\partial}{\partial n}\mathrm{Tr}_A[\rho_A^n]|_{n=1}. \tag{3}$$

The entanglement entropy can be obtained if we can compute $\mathrm{Tr}_A[\rho_A^n]$ for arbitrary positive integer n and then extrapolate the result to $n \in \mathbb{R}$.

To obtain ρ_A, we trace out the spin degrees of freedom in B, which normally can be carried out in terms of fermions and gauge fields. However, the gauge fields on the partition boundary are shared by A and B, so we regroup those gauge fields on the boundary links to introduce new Z_2 gauge variables which live in A and B exclusively, as shown in Fig. 1. (See supplementary material [29] for details.) The calculation of $\mathrm{Tr}[\rho_A^n]$ requires some careful treatment of the gauge transformation but is a well-defined mathematical procedure. Thus, we will leave the details involved in obtaining ρ_A and $\mathrm{Tr}[\rho_A^n]$ to the supplementary material [29] and present only the final result here:

$$\mathrm{Tr}_A[\rho_A^n] = \mathrm{Tr}_{A,G}[\rho_{A,G}^n] \cdot \mathrm{Tr}_{A,F}[\rho_{A,F}^n], \tag{4}$$

for any positive integer n. Here $\rho_{A,F} = \mathrm{Tr}_B[|\phi(u)\rangle\langle\phi(u)|]$ is the reduced density matrix for the free Majorana fermion state $|\phi(u)\rangle$ and $\rho_{A,G} = \mathrm{Tr}_B[|G(u)\rangle\langle G(u)|]$ is that of a pure Z_2 gauge field [9]; the ground state of the Z_2 gauge field $|G(u)\rangle$ is given by a equal weight superposition of all the 2^{N-1} gauge field configurations $|\tilde{u}\rangle$ that are gauge equivalent to $|u\rangle$, i.e., $|G(u)\rangle = 2^{-(N-1)/2}\sum_{\tilde{u}\simeq u}|\tilde{u}\rangle$.

Combining Eqs. (4) and (3), it is now obvious that the EE S can be separated into the gauge field part S_G and the fermion part S_F as follows:

$$S = S_G + S_F. \tag{5}$$

Equations (4) and (5) are among the central results of this work. From $\mathrm{Tr}_{A,G}[\rho_{A,G}^n] = 2^{-(L-1)(n-1)}$ (see supplementary material [29] for details), it is clear that $S_G = (L - 1)\log 2$. As will be shown below, the fermion part has the form $S_F = \alpha L + o(1)$, where α is a positive constant and $o(1)$ represents terms which vanish as $L \to \infty$. In the thermodynamic limit, the total entanglement entropy is given by

$$S = (\alpha + \log 2)L - \log 2, \tag{6}$$

from which we conclude that the TEE is $S_{\mathrm{topo}} = -\log 2$. Our derivation is valid for all phases of the Kitaev model, including the Abelian (Z_2 gauge theory), non-Abelian (Ising anyon) phases, and also gapless phases. Thus our result directly proves that the TEE for the Abelian and non-Abelian phases are identical, as expected from the total quantum dimensions of their quasiparticles [30].

Despite its trivial contribution to TEE, the fermion sector S_F is responsible for all the essential differences between the Abelian and non-Abelian phase of the Kitaev model in their quantum entanglement properties. The EE of a free fermion system can be computed by the method introduced in Ref. [31]. To obtain an explicit understanding of the fermion EE, we consider a torus divided by two parallel circles into A and B regions, as shown in Fig. 2(a). The boundary circle is along the $\hat{y}$ direction. On the torus, the free Majorana fermion Hamiltonian can be block diagonalized in the basis of k_y: $H = \sum_{i,j} \eta_i \eta_j h_{ij} = \sum_{x,x',k_y} \eta_x^\dagger(k_y) h_{xx'}(k_y) \eta_{x'}(k_y)$. Thus the system consists of decoupled one-dimensional subsystems of each k_y. The EE is given by [31]

$$S_F = -\frac{1}{2}\sum_{n,k_y} [\lambda_n \log\lambda_n + (1-\lambda_n)\log(1-\lambda_n)](k_y), \quad (7)$$

where $\lambda_n(k_y)$ are the eigenvalues of the single-particle correlation function $C_{xx'}(k_y) = \langle \eta_x^\dagger(k_y)\eta_{x'}(k_y)\rangle$ for each k_y. λ_n plays the role of Fermi-Dirac distribution $1/(e^{\beta\epsilon_n}+1)$ in thermal entropy, so that $\lambda_n = 0(1)$ corresponds to fully unoccupied (occupied) states, respectively. The "entanglement spectrum" $\lambda_n(k_y)$ has been computed numerically for both non-Abelian and Abelian phases, as shown in Fig. 2(b), for the Kitaev model with three-spin terms J' [18]. The ES is gapped for the Abelian phase, and gapless for the non-Abelian phase, similar to the edge states in the energy spectrum. Similar observations have been made in topological insulators and superconductors [32–35] and in FQH systems [17]. The two gapless branches in the ES come from the two boundaries between A and B. Since $\lambda_n(k_y)$'s are smooth functions of k_y, we see from Eq. (7) that in the continuum limit $S_F = \sum_{k_y} S(k_y) \simeq L \int S(k_y)\frac{dk_y}{2\pi}$

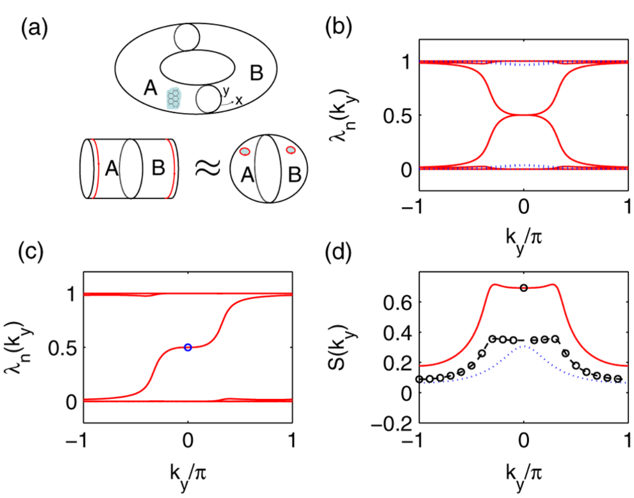

FIG. 2 (color online). (a) Schematic picture of a torus and a cylinder, each split to two regions A and B. The cylinder is equivalent to a sphere with two quasiparticles. (b) The entanglement spectrum $\lambda_n(k_y)$ vs k_y for non-Abelian (red solid lines) and Abelian (blue dotted lines) states on the torus. Here and below, we take the parameters $J_x = J_y = J_z = 1$ and next-nearest neighbor coupling $J' = 0.2$ for the non-Abelian state and $J_x = J_z = 1$, $J_y = 2.5$, $J' = 0.2$ for the Abelian state. (c) The entanglement spectrum for the non-Abelian state on cylinder. The blue circle marks an additional state with $\lambda = 1/2$ at $k_y = 0$. (d) The entropy $S(k_y)$ vs k_y for non-Abelian (red solid line) and Abelian (blue dotted line) states on the torus and for non-Abelian state on cylinder (black dashed line with circles).

satisfies the area law. It is interesting to note that a "gap" always exists between the edge states and other bulk states with $\lambda_n(k_y)$ close to 0 or 1, which is analogous to the "entanglement gap" studied in Ref. [36] for FQH system.

The situation becomes more interesting when we consider a cylinder with periodic boundary condition (PBC) for fermions and the partition shown in Fig. 2(a). As shown in Fig. 2(c), in the non-Abelian phase the numerical calculation gives only one branch of "gapless" states in the entanglement spectrum. Physically, this is because the coupling through the other boundary between A and B is removed by the open boundary condition. However, at $k_y = 0$ there is one isolated additional state with $\lambda = 1/2$, as shown by the blue circle in Fig. 2(c), which is due to the nonlocal entanglement between the two Majorana zero modes at the open boundary. Consequently, the entropy $S(k_y)$ is not a smooth function of k_y but has an additional $\log\sqrt{2}$ contributed by $k_y = 0$, as shown in Fig. 2(d). Compared with the torus case, in the thermodynamic limit we get $S_F = \alpha L + \log\sqrt{2}$, which shows explicitly that in the non-Abelian phase a cylinder with PBC for fermions is topologically equivalent to a sphere with two non-Abelian quasiparticles (usually named as σ particles), as illustrated in Fig. 2(a). Each particle carries a $\log\sqrt{2}$ entropy which is solely contributed by the fermion sector.

In addition to the EE, more information is contained in our result. The fact that Eq. (4) holds for any positive integer n indicates that the many-body entanglement spectrum—the eigenvalue spectrum of ρ_A—is the direct product of the ones of $\rho_{A,G}$ and $\rho_{A,F}$. From $\mathrm{Tr}_{A,G}[\rho_{A,G}^n] = 2^{-(L-1)(n-1)}$, one can know that $\rho_{A,G}$ has 2^{L-1} nonzero eigenvalues, all of which are degenerate and have the value of $2^{-(L-1)}$. Consequently, all nonvanishing eigenvalues of ρ_A are given by those of the Majorana fermion reduced density matrix $\rho_{A,F}$ times $2^{-(L-1)}$. Thus the low "energy" (i.e., close to the maximal eigenvalue of ρ_A) feature in the entanglement spectra of ρ_A can be entirely characterized by its fermionic part, which is gapped in the Abelian phase and gapless in the non-Abelian phase, as shown in Fig. 2(b).

Such a qualitative difference in the entanglement spectrum can be characterized by the Renyi entropy [37] $S_\alpha = \frac{1}{1-\alpha}\log\mathrm{Tr}\rho^\alpha$, which reduces to the EE (or von Neumann entropy) at $\alpha \to 1$. According to Eq. (4) the Renyi entropy of the Kitaev model is given by $S_\alpha = S_{F\alpha} + S_{G\alpha}$ for any α, with $S_{G\alpha}$ and $S_{F\alpha}$ the contribution from Z_2 gauge fields and fermions, respectively. From $\mathrm{Tr}_{A,G}[\rho_{A,G}^n] = 2^{-(L-1)(n-1)}$, one can see that $S_{G\alpha} = S_G = (L-1)\log 2$. Thus the TEE in $S_{G\alpha}$ is α independent, which is a generic property of the string-net models [38,39]. The α dependence of $S_{F\alpha}$ in the Abelian and non-Abelian phases has qualitative difference due to their different entanglement spectra. If we define $\rho = e^{-\mathcal{H}}$, the quantity $S_\alpha(1-1/\alpha) = -\frac{1}{\alpha}\log\mathrm{Tr}e^{-\alpha\mathcal{H}}$ is the same as the free energy

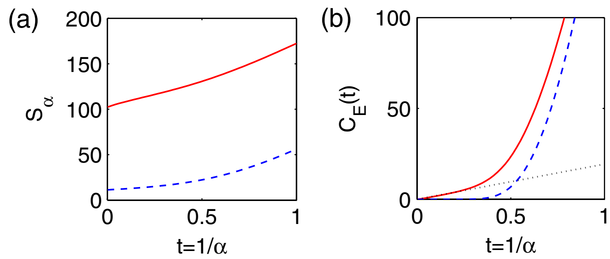

FIG. 3 (color online). (a) Renyi entropy S_α and (b) capacity of entanglement C_E defined by Eq. (8) of non-Abelian (red solid line) and Abelian (blue dashed line) states. The black dotted line is a linear fitting. The parameters are the same as those in Fig. 2.

of a thermal system with Hamiltonian $\mathcal{H}$ and temperature $t = 1/\alpha$. The behavior of the low energy spectrum of $\mathcal{H}$ can be obtained from the following quantity:

$$C_E(t) = -t\frac{\partial^2}{\partial t^2}[(1-t)S_{1/t}], \tag{8}$$

which is termed the "capacity of entanglement" and is the analog of heat capacity C_v in a thermal system. The explicit expression of S_α and $C_E(t)$ is given in the supplementary material [29], which leads to the numerical results shown in Fig. 3. As expected, in the limit of $t \rightarrow 0$, $C_E(t)$ vanishes exponentially for the Abelian phase but linearly for the non-Abelian phase, since the latter has a gapless entanglement spectrum with constant density of state. More generically, if the entanglement Hamiltonian $\mathcal{H}$ describes a $(1+1)$-dimensional conformal field theory (CFT) in the long wavelength limit [7,17], the capacity of entanglement is given by $C_E(t) = (\pi c L/3v)t$ for $t \rightarrow 0$, with L the length of the boundary and c and v the central charge and velocity of the CFT, respectively [40]. Moreover, if $\mathcal{H}$ describes a critical theory with dynamical exponent z, from dimensional analysis one can obtain the asymptotic behavior $C_E(t) \propto Lt^{1/z}$ for $t \rightarrow 0$. Thus we see that the capacity of entanglement characterizes some important qualitative behavior of the entanglement spectrum in generic systems.

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