Tensor network wave function of $S = 1$ Kitaev spin liquids

Hyun-Yong Lee, Naoki Kawashima, and Yong Baek Kim

1Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8581, Japan
2Department of Applied Physics, Graduate School, Korea University, Sejong 30019, Korea
3Division of Display and Semiconductor Physics, Korea University, Sejong 30019, Korea
4Department of Physics, University of Toronto, Toronto, Ontario, Canada M5S 1A7

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The spin-1/2 Kitaev model offers the exactly solvable example of quantum spin liquids. Possible material realizations of the spin-1/2 Kitaev systems and the prospect of using the Majorana fermion excitations for quantum computations have revolutionized quantum spin liquids research. Recently it has been suggested that higher-spin, especially spin-1, Kitaev exchange interactions can be realized in a variety of materials. Numerical computations on small clusters indicate that the ground state of the spin-1 Kitaev model may also be a quantum spin liquid. On the other hand, the nature of the ground state remains elusive since the spin-1 model is not exactly solvable in contrast to the spin-1/2 model. In this work, using the quantum-entanglement based tensor network approach, we construct an explicit ground-state wave function for the spin-1 Kitaev model, which is written only in terms of physical spin operators. We establish the existence of distinct topological sectors on a torus by constructing the minimally entangled states in the degenerate ground-state manifold and evaluating topological entanglement entropy. Our results suggest that the ground state of the spin-1 Kitaev model is a gapped quantum spin liquid with $Z_2$ gauge structure and Abelian quasiparticles. We explain the subtle differences between the spin-1/2 and spin-1 Kitaev quantum spin liquids.

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1. INTRODUCTION

The exact solution of the $S = 1/2$ Kitaev model on the honeycomb lattice, i.e., the Kitaev spin liquid (KSL), is an important milestone in theoretical research on quantum spin liquids [1]. It has firmly established the existence of quantum spin liquids in systems with local spin interactions and opened the door to possible quantum spin liquid states arising from the bond-dependent competing interactions. Both aspects lead to recent intensive experimental and theoretical explorations of the Kitaev materials [2–23], where the Kitaev interaction is dominant and the bond-dependent interactions originate from strong spin-orbit coupling.

On the other hand, the nature may also allow the Kitaev's bond-dependent interactions for higher-spin magnitudes, as recently suggested by electronic structure computations [24]. While the large-spin limit would simply correspond to the classical limit, the ground state of the Kitaev model for relatively small spin magnitudes, especially for $S = 1$, has not been fully understood as the higher-spin Kitaev models on honeycomb lattice do not have exact solutions. It was pointed out early on that there exists a flux operator, $W_p$, made of six spin operators on each plaquette for an arbitrary spin $S$, which commutes with the Hamiltonian [25]. Hence the ground state must have a definite eigenvalue of the flux operator, just like the case of the $S = 1/2$ model. Exact diagonalization of the $S = 1$ Kitaev model on small system sizes shows that the ground state is nonmagnetic [26]. The thermal pure quantum state approach at finite temperatures on small system sizes finds an entropy plateau, similar to the $S = 1/2$ model [27]. All of these indicate the possibility of a quantum spin liquid in the $S = 1$ Kitaev model, while the precise nature of the ground state is not known.

In this paper, we provide the tensor network (TN) representation of the ground-state wave function for the $S = 1$ Kitaev model, with both ferromagnetic and antiferromagnetic interactions between the $S = 1$ local moments. Our approach is inspired by the recent construction of the TN ground-state wave function of the $S = 1/2$ Kitaev model [28], where the wave function is written in terms of physical spin variables, instead of the Majorana fermion operators in the exact solution. We start from the bond dimension $D = 2$ TN representation of the wave function, which is an explicit eigenstate of the flux operator via the projector $Q_{LG}$, or the loop gas (LG) operator. The resulting wave function can be regarded as the sum over loop gas configurations made of a series of local actions of $Q_{LG}$ along a loop of lattice sites. We show that the $Z_2$ gauge structure is automatically built in the wave function. Using the mapping between the norm of the wave function and the partition function of the classical loop gas, it is shown that the wave function is in a gapped state, which is corroborated by the direct computation of the correlation length from the transfer matrix. This wave function is further
on the ground states of the construction, we contrast the difference between the degenerate entangled states in the ground-state manifold. Using this construction of minimally variational energy.

improved by applying an additional dimer gas (DG) operator [28] and imaginary time evolution (ITE), resulting in excellent variational energy.

Our approach also allows us to understand some partial information about topological properties of the ground-state wave function on a torus via the construction of minimally entangled states in the ground-state manifold. Using this construction, we contrast the difference between the degenerate ground states of the \( S = 1 \) and \( S = 1/2 \) systems, elucidating the nature of the quantum spin liquid ground state in the Kitaev model.

II. MODEL AND SYMMETRY

The Hamiltonian of the Kitaev model on the honeycomb lattice [1] is defined as

\[
H_\gamma = - k \sum_{(ij)} S_i^\gamma S_j^\gamma, \tag{1}
\]

where \( (ij)_\gamma \) stands for the nearest-neighboring sites, \( i \) and \( j \), on the \( \gamma \) bond with \( \gamma = x, y, z \) as depicted in Fig. 1(a), and \( S^\gamma \) is the spin-1 operator. One can verify that the Hamiltonian commutes with a flux operator \( W_\gamma = U_x^\gamma U_y^\gamma U_z^\gamma \) having eigenvalues \( \pm 1 \) where \( U^\gamma = e^{i S^\gamma} \) is the 180° spin-rotation operator along the \( \gamma \) direction, and sites 0–5 are defined in Fig. 1(a). It indicates that the spin-1 model also exhibits the Z2 gauge redundancy [29], and thus the Hilbert space can be sectorized by the combination of the flux number.

A. Loop gas states

In a similar fashion to the spin-1/2 model [28], one can define the DG operator \( Q_{\gamma LG} \) for the spin-1 model in a bond dimension \( D = 2 \) TN representation with a local tensor \( Q_{\lambda \mu \nu} = t_{\lambda \mu \nu}(U^\gamma)^{1-\lambda}(U^\gamma)^{1-\mu}(U^\gamma)^{1-\nu}, \) where \( \lambda, \mu, \nu = 0, 1 \) are the virtual indices. Here nonzero elements of the tensor \( \tau \) are only \( t_{\lambda \mu \nu} = 1 \) for \( \lambda + \mu + \nu = 1 \). The operator \( Q_{\gamma LG} \) generates loop configurations made of local actions represented in Fig. 1(b). One can examine the physical symmetries of \( Q_{\gamma LG} \) at the local tensor level as done in Ref. [28] and derive the \( Z_2 \) gauge symmetry: \( \sum_{\lambda, \mu, \nu} \sigma^\lambda_{\lambda} \sigma^\mu_{\mu} \sigma^\nu_{\nu} Q_{\lambda \mu \nu} = Q_{\lambda \mu \nu}. \) Furthermore, it is straightforward to show that the local operator obeys the following equations:

\[
\begin{align*}
U^\gamma Q_{\lambda \mu \nu} & = \sum_{\lambda', \mu', \nu'} \sigma^{\lambda}_{\lambda'} \sigma^{\mu}_{\mu'} \sigma^{\nu}_{\nu'} Q_{\lambda' \mu' \nu'}, \\
U^\gamma Q_{\lambda \mu \nu} & = \sum_{\nu', \lambda', \mu'} \sigma^{\lambda}_{\lambda'} \sigma^{\mu}_{\mu'} \sigma^{\nu}_{\nu'} Q_{\lambda' \mu' \nu'}, \\
U^\gamma Q_{\lambda \mu \nu} & = \sum_{\lambda', \mu', \nu'} \sigma^{\lambda}_{\lambda'} \sigma^{\mu}_{\mu'} \sigma^{\nu}_{\nu'} Q_{\lambda' \mu' \nu'}, \tag{2}
\end{align*}
\]

This is the equal weight superposition of all possible loop configurations where the local state depends on the direction of the local loop as depicted in Fig. 1(b). Using the identity \( \langle 0 | U^\gamma | 0 \rangle = -1/3, \) one can map the norm of \( |\psi_{\gamma LG}\rangle \) into the partition function of the classical \( O(1) \) LG model with the fugacity \( \xi = 1/3, \) which is in the gapped phase of the model [30]. It is worth noting that the \( S = 1/2 \) LG maps to the critical point \( \xi = 1/\sqrt{3} \) [28].

Utilizing the corner transfer matrix renormalization group (CTMRG), we have computed the energy expectation value (per site) of \( |\psi_{\gamma LG}\rangle \), \( E_{LG} = -0.50562, \) which is far from the previous ones \( E_{24site}^{24site} = -0.648 \) obtained on a 24-site system [31] and \( E_{DMRG} = -0.644 \) obtained by the density matrix renormalization group method on a \( (48 \times 3) \)-cylinder system [33]. In what follows, we present two different ways to vary the LG state to obtain better variational energies while most physical properties remain intact: (1) applying the so-called DG operator onto the LG state and optimizing its variational parameters as proposed in Ref. [28] and (2) evolving the LG state through the imaginary time evolution (ITE) operator [34].

B. String gas states

The DG operator \( K_{DG} \) is obtained by summing over all possible dimer operators, made by the direct product of the
on every bond and updating the site tensors using the simple nearest neighbor bonds as follows:

\[ T_{\text{ITERATE}}(\phi) = \sum_{\text{all configurations}} \sum_{\text{site tensors}} - \sum_{\text{nearest neighbors}} \delta(\phi - \psi) \]

where the dimer stands for \( S^x_j S^x_i \) depending on the bond and the empty site for the identity. It is also represented in a \( D = 2 \) TN with the local tensor \( R_{\lambda \mu \nu}(\phi) = \zeta_{\lambda \mu \nu} (S^x)_{\lambda} (S^y)_{\mu} (S^z)_{\nu} \), where the nonzero elements of the \( \zeta \) tensor are simply \( \zeta_{000} = \cos \phi \) and \( \zeta_{001} = \zeta_{010} = \sin \phi \). Applying the DG operators onto the LG state results in the string gas (SG) state with variational parameters \( \{\phi_i\} \), i.e., \( |\psi_{\text{SG}}(\{\phi_i\})\rangle = \prod_{i=1}^n R_{\text{DG}}(\phi_i) |\psi_{\text{LG}}\rangle \), which can be optimized to have the lowest energy [28]. Here \( n \) is referred to as the order of the SG state, and the bond dimension grows as \( D = 2^{n+1} \). The variational energy of the first-order ansatz \( D = 4 \) is shown in Fig. 2(a) as a function of the variational parameter \( \phi \). The lowest energy is found to be \( E_{\text{SG}} = -0.6167 \), which is still significantly higher than the ones obtained by ED and DMRG. Note that the efficiency of the DG operator is not as good as the case of the \( S = 1/2 \) model. We believe that this is because the \( S = 1 \) DG operator cannot be written as the polynomial function of the Hamiltonian in contrast to the spin-1/2 model, where the first-order SG state already gives 99.8% accuracy to the exact one energetically [28]. We have also optimized the second-order ansatz \( |\psi_{\text{SG}}(\phi_1, \phi_2)\rangle \) and obtained the best energy \( E_{\text{SG}} = -0.6366 \). See the Supplemental Material [32] for more details.

C. Imaginary time evolution

We perform the ITE by applying the two-site gate \( e^{ix S^z_i S^z_j} \) on every bond and updating the site tensors using the simple update (SU) iteratively [34]. Note that it is almost impossible to find a KSL-like spin liquid, e.g., \( W_p = 1 \), with an SU from a random initial state. To be more precise, the resulting states are mostly magnetically ordered and not vortex-free, \( (W_p) < 1 \), and even exhibit the strong initial state dependence. However, the initial LG state with a careful choice of \( D \) makes the ITE quite stable and reliable. For instance, the ITE operator commutes with the LG operator, i.e., \( [x^{KS} S^y, Q_{GC}] = 0 \), so that the ITE does not spoil the vortex freeness. While the truncated singular value decomposition in the SU may destroy the vortex-free condition, it can be avoided by keeping the degenerate singular values. Figure 2(b) presents the energy flow as a function of the ITE step. The zeroth step denotes the LG state, and the energy drops quickly and converges already in a few hundred steps. Throughout the ITE, the flux expectation value keeps unity, \( W_p = 1 \), while the state remains nonmagnetic, \( \langle \hat{S} \rangle = 0 \) up to the machine precision. See the Supplemental Material [32] for more details. The variational energy decreases monotonically with increasing \( D \) and the lowest energy obtained by the ITE is \( E_{\text{ITE}}^{D=12} = -0.6453 \), which is comparable to the ones predicted by ED and DMRG. Comparing to the energies of the SG states, the ITE energies are lower at the same \( D \). However, this is not so surprising since the tensors of the SG states are quite sparse, i.e., many of elements are zero. To estimate the infinite-\( D \) variational energy, we have extrapolated the energies \( E_{\text{SG}} \) and \( E_{\text{ITE}} \), and both seem to converge to almost the same one \( E_{D=\infty} \approx -0.6464 \) as shown in Fig. 2(c). Finally, to see how the gapped nature of the LG state is affected by the ITE, we have directly computed the largest correlation length \( \xi \) from the largest and second largest eigenvalues, \( \lambda_0 \) and \( \lambda_1 \), of the transfer matrix in the CTRMG algorithm: \( \xi = 1/\log(\lambda_1/\lambda_0) \). The result from the \( D = 12 \) ansatz is presented in Fig. 2(d) as a function of the CTM dimension \( \chi \). It clearly indicates a finite correlation length in contrast to the case of the spin 1/2 where \( \xi \) diverges as increasing \( \chi \) [28]. Its bond dimension dependence is discussed in the Supplemental Material [32]. While the correlation length with the largest bond dimension \( D = 12 \) is larger than that of \( D = 10 \) so that it does not saturate even in \( D = 12 \), the wave function with \( D = 12 \) is still adiabatically connected to those in smaller bond dimensions. See the Supplemental Material [32] for more details. In this sense, the nature of the wave function remains essentially the same as the gapped spin liquid state of the LG state. On the other hand, with the current set of data, we cannot completely rule out the possibility of a gapless spin liquid in the infinite bond dimension limit, which cannot be obtained or extrapolated with the existing numerical resource.

D. Topological property

On a compact geometry, one should consider not only the local fluxes but also the global fluxes defined on non-contractible paths in the system. For instance, we are able to define a global flux operator on the cylinder, e.g., \( W_T = \prod_{i=1}^{2\pi} U_{\gamma}^i \) wrapping the cylinder. Then, one can sectorize the Hilbert space further using the global flux \( W_T = \pm 1 \). It has been found that, in the case of the spin-1/2, naive LG and SG states on the compact geometry are not the eigenstate of
the global flux operators [36]. Instead it requires a careful manipulation, i.e., the linear superposition of the LG (SG) state and its gauge-twisted one to have the well-defined global flux [36]. On the other hand, one can verify using Eq. (2) that the \( S = 1 \) LG (SG) state is already the eigenstate of the global flux operators with \((W_{\gamma y}, W_{\gamma y}) = (+1, +1)\). Furthermore, the different sector can be obtained by twisting the gauge. The details about the global flux sector are provided in the Supplemental Material [32]. Additionally, in the case of the spin 1/2, the sector is characterized by the parity of the number of loops connecting two edges of the cylinder [36]. For instance, the parity of the number of loops connecting two edges of the cylinder determines the sector. On the other hand, the \( S = 1 \) LG state in each sector is characterized in a completely different way. Namely, all loop configurations are allowed regardless of the sector, whereas the sign of the configurations with the odd number of the loops winding the cylinder depends on the sector:

\[
\begin{align*}
|\psi^{+}_{\text{LG}}\rangle &= \sum_{\text{even}} \pm \sum_{\text{odd}} |\psi_{\text{LG}}\rangle, \\
|\psi^{+}_{1/2,\text{LG}}\rangle &= \sum_{\text{even}} |\psi_{\text{LG}}\rangle, \\
|\psi^{+}_{2,\text{LG}}\rangle &= \sum_{\text{odd}} |\psi_{\text{LG}}\rangle.
\end{align*}
\]

This qualitative difference between the \( S = 1/2 \) and \( S = 1 \) LG states comes from Eq. (2) which is different from the \( S = 1/2 \) case. See the Supplemental Material [32] for more details. It can be shown that the (−) sector is obtained by twisting the gauge of the LG operator using the nontrivial element of the \( Z_2 \) invariant gauge group. Then one can construct the minimally entangled states (MESs) on the infinite cylinder (say, \( L_x \to \infty, L_y : \text{finite} \)) using the degenerate states in the different flux sector [37]. The explicit definition of the MES is presented in the Supplemental Material [32]. It is worth noting that one can construct all the MESs in the \( S = 1 \) model in contrast to the \( S = 1/2 \) model where only the trivial and vortex sectors are accessible [36]. Using the boundary theory of TN [38], we have calculated the entanglement entropy (EE) and then extracted the topological entanglement entropy (TEE) to identify the nature of each anyon sector. The result is shown in Fig. 3(a), where the EE scales as \( S_{\text{EE}} = (\log 2) \times L_y - \gamma \), and TEE is \( \gamma = 0 \) for \((+, +)\) and \( \gamma = \log 2 \) for all other MESs. It indicates that all topological excitations are Abelian so that the ground state possesses the \( Z_2 \) topological order.

Figure 3(b) presents the \( \phi \) dependence of the TEE of \(|\psi_{\text{SG}}\rangle\). When the SG state is close to the LG state (near \( \phi = 0 \)), the TEE is almost perfectly log 2. As \( \phi \) increases, the TEE deviates from log 2, which might come from the stronger finite-size effect \( L_y \).

### E. Antiferromagnetic model

Remarkably, the relation in Eq. (2) allows us to construct the ansatz for the antiferromagnetic model \((K < 0)\) without much effort. First, we prepare a TN operator, say, \( \tilde{Q}_{\text{LG}} \), by inserting \( \sigma^z \) matrix into every bond in the \( Q_{\text{LG}} \) operator as illustrated in Fig. 4. Then, using Eq. (2), one can show that the \( \tilde{Q}_{\text{LG}} \) operator also guarantees the vortex-free condition, i.e., \( W_{\gamma y} \tilde{Q}_{\text{LG}} = \tilde{Q}_{\text{LG}} \), and is related to the \( Q_{\text{LG}} \) by \( \tilde{Q}_{\text{LG}} = V Q_{\text{LG}} V^\dagger \) where \( V \) is a unitary transformation flipping the overall sign of the Hamiltonian, i.e., \( V^\dagger HV = -H \). A detailed derivation and proofs are provided in the Supplemental Material [32]. It implies that the deformed LG state \(|\tilde{\psi}_{\text{LG}}\rangle \equiv \tilde{Q}_{\text{LG}}|0\rangle\) gives exactly the same variational energy as that of the original LG state for the antiferromagnetic model: \(|\tilde{\psi}_{\text{SG}}\rangle = \tilde{Q}_{\text{LG}}|\tilde{\psi}_{\text{SG}}\rangle\). Also, since the DG operator commutes with both \( \tilde{Q}_{\text{LG}} \) and \( \tilde{Q}_{\text{LG}} \), one can also deform the SG state to have the same energy for the antiferromagnetic model; that is, the variational energy of \(|\tilde{\psi}_{\text{SG}}\rangle\) is simply \(|\tilde{\psi}_{\text{SG}}\rangle = \tilde{Q}_{\text{LG}}|\tilde{\psi}_{\text{SG}}\rangle\). Therefore, once the variational parameters are optimized for the ferromagnetic model, one can use the same ones for the antiferromagnetic model with insertion of the \( \sigma^z \)-matrix in the TN state. As will be shown below, this simple transformation comes in handy when we consider a weak perturbation, e.g., the magnetic field, in the antiferromagnetic model. It is also worth noting that such a TN deformation for the \( S = 1/2 \) model exists but requires a larger unit cell in the TN state. See the Supplemental Material [32] for more details.

**FIG. 3.** (a) The entanglement entropy \( S_{\text{EE}} \) of the LG state as a function of the circumference \( L_y \) in the \((+, +)\) flux and the MES sectors. (b) The extracted topological entanglement entropy of the first-order SG state \(|\psi_{\text{SG}}(\phi)\rangle\). The definition and construction of four MESs, |\( I \rangle\), |\( e \rangle\), |\( m \rangle\), and |\( e \rangle\), are presented in the Supplemental Material [32].

**FIG. 4.** Schematic figure of the TN state for the antiferromagnetic model, where the green square denotes the Pauli \( \sigma^z \) matrix, and the original TN state (without green squares) is either the LG state or the SG state.
The results are obtained by the ITE with $D = 12$.

F. Magnetic field

Here we discuss how the $S = 1$ KSL is affected by the (111)-direction magnetic field,

$$H_{\text{field}} = -\frac{h}{\sqrt{3}} \sum_i \left( S_i^x + S_i^y + S_i^z \right).$$

To this end, we perform the ITE from the LG and the deformed LG states for the ferromagnetic and antiferromagnetic models, respectively, in the presence of the magnetic field. We have found that the response to the field resembles the ones of the $S = 1/2$ model [39,40]. That is, the ferromagnetic KSL is easily driven to the polarized phase, in which the spins are aligned in the (111) direction, and at a weak field $h = 0.013$ as shown in Fig. 5(a), where the $D = 12$ TN is optimized to determine the critical field. The other hand, Fig. 5(b) indicates that the antiferromagnetic KSL is much more robust than the ferromagnetic KSL against the field. We believe that our construction is applicable to the general spin-$S$ Kitaev model and may provide insights into the physics of the possible $S = 1$ Kitaev materials proposed in Ref. [41] such as the single-layer NiI$_2$ or layered A$_3$Ni$_2$XO$_6$ ($A = Li, Na, X = Bi, Sb$).

III. CONCLUSION

We have studied the ground-state properties of the $S = 1$ Kitaev model employing the LG and SG ansatz and the ITE optimization. The ground state is found to be a gapped $Z_2$ spin liquid which differs from the $S = 1/2$ model hosting the gapless KSL ground state [1]. The gapped nature has been shown by mapping the LG state into the partition function of the classical $O(1)$ LG model in the gapped phase and by directly computing the largest correlation length of the optimized ansatz. By constructing the MESs, we have identified the topological nature of the excitations, i.e., the Abelian anyons. The TN representation allows us to understand the qualitative difference between the $S = 1$ and $S = 1/2$ LG and SG states including the topological property. In addition, we have found a simple transformation between the tensor network wave functions of the ferromagnetic and antiferromagnetic models, leading to exactly the same variational energy. Therefore, once one optimizes the variational parameters with the ferromagnetic model, the ansatz for the antiferromagnetic model is obtained without additional optimization (or vice versa). The magnetic field effect on the KSL is similar to that of the $S = 1/2$ model. That is, the antiferromagnetic KSL is much more robust than the ferromagnetic KSL against the field. We believe that our construction is applicable to the general spin-$S$ Kitaev model and may provide insights into the physics of the possible $S = 1$ Kitaev materials proposed in Ref. [41] such as the single-layer NiI$_2$ or layered A$_3$Ni$_2$XO$_6$ ($A = Li, Na, X = Bi, Sb$).

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