Spin-1 Kitaev-Heisenberg model on a two-dimensional honeycomb lattice

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We study the Kitaev-Heisenberg model with spin-1 local degree of freedom on a two-dimensional honeycomb lattice numerically by density matrix renormalization group method. By tuning the relative value of the Kitaev and Heisenberg exchange couplings, we obtain the whole phase diagram with two spin liquid phases and four symmetry broken phases. We identify that the spin liquid phases are gapless by calculating the central charge at the pure Kitaev points without Heisenberg interaction. Comparing to its spin-1/2 counterpart, the position and number of gapless modes of the spin-1 case are quite different. Due to the approximate $Z_2$ local conservations, the expectation value of Wilson loop operator measuring the flux of each plaquette stays near to 1, and the static spin-spin correlations remain short-range in the entire spin liquid phases.

\section*{Introduction.} Ever since it was first proposed by Alexei Kitaev in 2006 \cite{Kitaev2006}, the two-dimensional (2D) Kitaev model and its various extensions have drawn extensive attention from both theoretical and experimental side \cite{Chen2006, Xiao2007}. The Kitaev model with spin-1/2 local degree of freedom on a honeycomb lattice could be solved exactly by representing the spin operators with Majorana fermions in extended space, and then the system decouples into a free Majorana fermion system and a static $Z_2$ gauge field. Depending on the relative relations between the exchange couplings in different spatial directions, the system could be a gapless spin liquid or a gapped $Z_2$ topologically ordered spin liquid. Under a small external magnetic field, the gapless spin liquid will open a gap and change to a non-Abelian topological phase \cite{Fradkin2013}, while under a strong magnetic field, the system will be in a fully polarized phase with chiral magnon edge states \cite{Chen2007}. The existence of a $U(1)$ gapless quantum spin liquid phase is also proposed in an intermediate magnetic field \cite{Li2010, Li2011, Lee2012}. The other extensions, for example, the addition of Heisenberg exchange terms, may lead to different magnetically ordered phases with spontaneous symmetry breaking \cite{Fedele2014, Parameswaran2016, Lee2017}. Some candidate materials with signatures of Kitaev physics have also been found \cite{Gierz2013, Xiao2013, Hsu2015, Li2016, Liu2017, Kato2017, Xiao2018, Xia2018}, such as, $\alpha$-RuCl\textsubscript{3} \cite{Kotegawa2016, Xiao2017, Xiao2018a, Xiao2018b, Xiao2019}, $\text{H}_2\text{LiIr}_2\text{O}_6$ \cite{Aguirre2017}, and $\text{A}_2\text{IrO}_3$($\text{A} = \text{Na, Li}$) \cite{Xiao2016, Liao2017, Xiao2018a, Xiao2018b, Xiao2019}, which motivate more studies on various extended Kitaev models with additional couplings as the effective Hamiltonians for realistic materials.

Despite the numerous studies on spin-1/2 Kitaev model, the spin-1 case is still less explored and has not been fully understood. The examples of spin-1 spin liquid are quite rare in Heisenberg-like spin models, and the Hamiltonian terms giving rise to frustration need to be strong enough to overcome the tendencies of magnetic ordering or other spontaneous symmetry breaking. However, with increasing of local spin, quantum fluctuation is reduced while the Hilbert space is enlarged. This combined effect makes spin-1 models interesting and the underlying physics of spin-1 systems may be richer. Most of the current understandings of spin-1 Kitaev model are based on the symmetry analysis, such as the existence of $Z_2$ Wilson loop operators and the vanishing of spin-spin correlations beyond nearest neighbors \cite{Wen1992, Wen1993}. Small sizes numerical calculations \cite{Savary2019} using exact diagonalization suggested that the ground state of the spin-1 Kitaev model is possibly gapless and vortex-free. Unlike the spin-1/2 Kitaev model, there is no exact solution to such a model, and the nature of the quantum state is far from understood. A recent theoretical paper \cite{Kong2020} proposed the relevance of the spin-1 Kitaev spin model to 2D Mott insulators with strong spin-orbit coupling on lattices with edge-shared octahedra, which may be realized in layered transition metal oxides. This work opens the possibility to find spin-1 spin liquid phase in real materials and makes the theoretical understanding of spin-1 Kitaev model more urgent and important.

In this work, we numerically study the spin-1 Kitaev-Heisenberg model on a 2D honeycomb lattice using density matrix renormalization group (DMRG) method. We obtain the whole phase diagram with different relative values of the Kitaev and Heisenberg exchange couplings. Two spin liquid phases exist around the anti-ferromagnetic and ferromagnetic pure Kitaev points (with no Heisenberg term), respectively. The other four phases are magnetically ordered with different patterns of spontaneous symmetry breaking. The entanglement spectrum of the spin liquid phases has a degeneracy with different momentum around a cylinder, while the spectrum of the magnetically ordered phases is dominated by the largest Schmidt value. Furthermore, we find that the ground states of the pure Kitaev points are gapless with a non-zero central charge. However, the position and number of the gapless modes are different from its spin-1/2 counterpart. The expectation value of Wilson loop operator measuring flux of each plaquette stays near to 1, and the static spin-spin correlations remain short-range in the entire spin liquid phases.

\section*{Phase diagram.} We consider the spin-1 Kitaev-Heisenberg model on a 2D honeycomb lattice with the
gram with the ground state energy per site and the von symmetry broken phases. Fig. 1(a) shows the phase dia-

The black line is the energy of the ground state per site, and respectively, the Kitaev and Heisenberg exchange couplings, respec-

We use an infinite DMRG (iDMRG) method \[41, 42\] on an infinite cylinder with circumference \(L_y = 4\), where \(L_y\) is the number of unit cells of a honeycomb lattice around the cylinder, to get the phase diagram with respect to the parameter \(\alpha\). The translational invariant building block of the infinite cylinder we use has two unit cells in \(x\)-directions along the cylinder to be compatible with the symmetry broken phases. Fig. 1(a) shows the phase dia-

Hamiltonian:

\[
\hat{H} = K \sum_{\langle i, j \rangle_\gamma} \hat{S}_i^\gamma \hat{S}_j^\gamma + J \sum_{\langle i, j \rangle} \hat{S}_i \cdot \hat{S}_j
\]

where \(K = 2 \sin(\alpha)\) and \(J = \cos(\alpha)\) with \(\alpha \in [0, 2\pi]\) are the Kitaev and Heisenberg exchange couplings, respectively, \(\hat{S}_i^\gamma\) is the \(\gamma = x, y, z\) component of spin-1 operators on site \(i\), and \(\langle i, j \rangle_\gamma\) denotes the nearest neighbor coupled by \(\gamma\)-link.

We use an infinite DMRG (iDMRG) method \[41, 42\] on an infinite cylinder with circumference \(L_y = 4\), where \(L_y\) is the number of unit cells of a honeycomb lattice around the cylinder, to get the phase diagram with respect to the parameter \(\alpha\). The translational invariant building block of the infinite cylinder we use has two unit cells in \(x\)-directions along the cylinder to be compatible with the symmetry broken phases. Fig. 1(a) shows the phase dia-

Neumann entanglement entropy \(S = -\sum \lambda_\beta^2 \log \lambda_\beta^2\), where \(\lambda_\beta\)s are the Schmidt values on the bond of matrix product state (MPS) cutting the infinite cylinder into two half along a ring. There are four magnetic or-

![FIG. 1. (a) Phase diagram of the spin-1 Kitaev-Heisenberg model with \(\alpha \in [0, 2\pi]\) on an infinite cylinder with \(L_y = 4\). The black line is the energy of the ground state per site, and the blue line is the entanglement entropy by cutting the cylinder along a ring. The bond dimension used in iDMRG is \(\chi = 1000\). (b) and (c) are the zoom-in plots of the spin liquid phases around \(\alpha = 0.5\pi\) and 1.5\(\pi\), respectively. The black solid lines are the ground state energy per site with calculations initialized in the spin liquid phases, and the black dashed lines are the ground state energy per site with calculations initialized in the corresponding nearby symmetry broken phases. The blue lines are the entanglement entropy with similar meaning. The phase boundaries are determined by the discontinuous points of the first-order derivatives of the energy of the lowest energy state at each \(\alpha\) with respect to \(\alpha\). (insets) The spin-spin correlations \(\langle S_i^x S_j^x \rangle\) of each phase in real space with 0 sites denoted by the red squares.](https://example.com/fig1.png)
we will focus on the pure Kitaev model with $\alpha = 1.485\pi$ in ferromagnetic phase, (b) $\alpha = 1.486\pi$ in spin liquid, (c) $\alpha = 1.513\pi$ in spin liquid and (d) $\alpha = 1.514\pi$ in stripy phase. All of these $\alpha$ points are the nearest points to the phase transitions in the order of 0.001$\pi$.

In the ordered phases, the entanglement spectrum has a non-degenerate dominate value, while in the spin liquid the entanglement spectrum has approximate four-fold degeneracies with different $k_y$. The abrupt changes of the spectrum structure at the phase transition points are consisted with the first-order phase transitions. At the pure Kitaev points ($K = 2$), when the ground state is represented by an MPS with bond dimension $\chi = 1000$, the four-fold degeneracy exists with the splitting in the order of 0.01 (the lowest four $\epsilon_\beta$ are $[1.6672, 1.6676, 1.6676, 1.6681]$), while at the phase boundary as shown in Fig. 2(b) the four-fold degeneracy splitting increases to the order of 0.1 (the lowest four $\epsilon_\beta$ are $[1.6551, 1.6553, 1.6734, 1.6737]$). This degeneracy indicates that there is a non-trivial operator $\hat{O}$ that commutes with the entanglement Hamiltonian, which also gives rise to the degeneracy in the edge spectrum. We have checked that the spin liquid phases of spin-1/2 Kitaev model also have similar entanglement structures indicating strong superposition nature of the spin liquid state.

**Pure Kitaev model and spin liquid.** In this part we will focus on the pure Kitaev model with $K = \pm 2$ and $J = 0$, and the corresponding spin liquid phases. Let’s now review some symmetry properties of the pure Kitaev model. The general Wilson loop operator for spin-$S$ on sites $\{1,2,\ldots,n\}$ of a loop $L$ is defined by

$$W_L = e^{i\pi \hat{S}_{12}^{\gamma_1}} e^{i\pi \hat{S}_{23}^{\gamma_2}} e^{i\pi \hat{S}_{34}^{\gamma_3}} \cdots e^{i\pi \hat{S}_{n1}^{\gamma_n}} e^{i\pi \hat{S}_{12}^{\gamma_{n+1}}}$$

where $\gamma_{n+1}(= x, y, z)$ denotes the directions of the link between site $i$ and $i + 1$. It can be verified that $[\hat{W}_L, \hat{H}_K] = 0$ and $[\hat{W}_L, \hat{W}_L'] = 0$, where $\hat{H}_K$ denotes the pure Kitaev Hamiltonian. Since $(\hat{W}_L)^2 = 1$, the eigenvalues of $\hat{W}_L$ are $\hat{W}_L = \pm 1$. It can be checked that this general definition reduces to the correct form in the spin-1/2 case. We rename $\hat{W}_L$ as $\hat{W}_p$ if the loop is around a single hexagonal plaquette of the honeycomb lattice ($\hat{W}_p$ is also called as the $Z_2$ flux operator of a plaquette), and as $\hat{W}_y$ if the loop winds once around the cylinder.

To examine the nature of the spin liquid, we first check if the spin liquid is gapless. We choose two sizes of infinite cylinders with $L_y = 3$ and $L_y = 4$ and consider $\alpha = 1.5\pi$ ($\alpha = 0.5\pi$ is equivalent). We initialize the iDMRG calculations by complex random MPSs with bond dimension $\chi_{ini} = 100$. A random initial state may give a random bias to help selecting states in different sectors with different $\hat{W}_y$ after updating variationally, thus we have a chance to get the lowest energy state in each sector. We name the state with a lower energy of these two states as the ground state and the other one as an excited state.

**FIG. 3.** (a) Finite entanglement scaling of the lowest energy state with $\hat{W}_y = -1$ on an infinite cylinder with $L_y = 3$. The lower right inset is the same plot for the corresponding gapped ground state with $\hat{W}_y = 1$. (b) Finite entanglement scaling of the ground state with $\hat{W}_y = -1$ on an infinite cylinder with $L_y = 4$. The lower right inset is the same plot for the gapped ground state of spin-1/2 Kitaev model with $\hat{W}_y = 1$ on an infinite cylinder with $L_y = 4$. The slope of the black lines in (a) and (b) give the central charge $c = 1$. The upper left insets of (a) and (b) are the Brillouin zone of the honeycomb lattice with $L_y = 3$ and 4, respectively, in which the dashed lines are the momentum lines with periodic boundary condition in $y$-direction, and orange dots show the possible positions of gapless Majorana cones.
For $L_y = 3$, the ground state is gapped with $W_y = 1$, while the lowest energy state with $W_y = -1$ (an excited state) is gapless. As an indication to a gapless state modeled from finite dimension MPSs, both the entanglement entropy $S$ and correlation length $\xi$ of the variational-optimized MPS will increase with its bond dimension, and the scaling relation between them $S = (c/6) \log \xi$ gives the central charge $c$ of the gapless state. Fig. 3(a) shows the finite entanglement scaling for this gapless excited state. The black linear line has the central charge $c = 1$. The same plot for the gapped ground state is given in the lower right inset of Fig. 3(a). The entanglement entropy of the gapped ground state converges quickly and does not grow with the bond dimension. This observation is quite similar to the spin-1/2 case. In spin-1/2 case, although with $L_y = 3$ and periodic boundary condition in $y$-direction the momentum lines cut through the positions of the gapless Majorana cones at $\pm (1/4, 1/2)$ in momentum space (see the upper left inset of Fig. 3(a)), the free fermion degree of freedom will adjust to the anti-periodic boundary condition (due to the gauge flux) to give a gapped ground state with lower energy. While there is no analytical solution in the spin-1 case, we conjecture that similar effect may also play an important role in spin-1 case as we have seen different flux state ($W_y = \pm 1$) have different central charges in finite size system. To identify the pattern of gapless models, we consider $L_y = 4$ in the following.

For $L_y = 4$, the ground state of spin-1 case is already gapless and have a central charge $c = 1$ as shown in Fig. 3(b). This gapless ground state has $W_y = -1$, which is the same as the gapless excited state of $L_y = 3$. The lowest energy state with $W_y = 1$ is also gapless, but has a larger central charge. This is different from the spin-1/2 case, in which $L_y = 4$ is not compatible with the position of the Dirac cones, so we always get a gapped ground state as shown in the lower right inset of Fig. 3(b). One possible explanation of the central charge 1 here is that there are two gapless Majorana cones in the spin-1 case, and they may locate at the $\Gamma = (0, 0)$ point, which is protected by some symmetries, or around a small Fermi-Sea, which are consistent with both $L_y = 3$ and $L_y = 4$ results.

Beside $\hat{W}_p$, the eigenvalue of local flux operator $\hat{W}_p$ is also a good quantum number of the eigenstates of the pure Kitaev Hamiltonian. The ground states we obtained is vortex-free, i.e., eigenvalues of $\hat{W}_p$ are $+1$ for all of the plaquettes. The flux $W_p$ in each plaquette is near to 1 in the spin liquid phase with $J \neq 0$ around the pure Kitaev points, and drops abruptly to near 0 at the phase transition point as shown in Fig. 4(d).

By direct calculation, we know that $\{\hat{S}_i^z, \hat{W}_p\} = 0$ if site $i$ is on the plaquette $p$ and $\gamma$ corresponds to one of the two links on $p$ which is connected to site $i$. On the other hand, $[\hat{S}_i^z, \hat{W}_p] = 0$ if site $j$ has no overlap with the plaquette $p$ or $\gamma'$ does not correspond to the two links on $p$ connecting to site $j$. Therefore, if we apply a local spin operator, for example, $\hat{S}_i^z$ on site $i$ of the lattice, two of the plaquettes which share the site $i$ and link $x$ will reverse their flux $W_p$ as schematically shown in Fig. 4(a) and (b). This property leads to the vanishing of the spin-spin correlations beyond the nearest neighbors, since the eigenstates with different quantum number $W_p$ will be orthogonal to each other and thus have zero overlap. This correlation remains short-ranged in the entire spin liquid phase, and changes to long-range once the symmetry-breaking happens. In Fig. 4(c), the spin-spin correlation $\langle S_n^x S_n^x \rangle$ is plotted with sites $n = 0, 1, \ldots, 5$ as marked in Fig. 4(a), in which $\alpha = 1.5\pi$ is a pure Kitaev point, $\alpha = 1.513\pi$ and $\alpha = 1.514\pi$ are adjacent to the phase transition point between spin liquid and stripy phase. We could see that the change of the spin-spin correlation is very sharp crossing the phase transition.

**Discussion.** We identify the gapless spin liquid phases
in spin-1 Kitaev-Heisenberg model, and find that the gapless modes are very different from the corresponding spin-1/2 model. The extensive numerical studies in this work give some insight about the nature of the gapless excitations and could motivate more theoretical studies to fully understand the spin-1 Kitaev model. There are still many open questions about extended spin-1 Kitaev model for future works. We list a few here: (1) If the Kitaev coupling coefficients are anisotropic, is there a gapped region and what is the topological nature of the gapped phase? Since the local Hilbert space has a dimension three, it may go beyond the physics of the $\mathbb{Z}_3$ toric code. (2) If we apply a magnetic field, will the spin liquid open a gap and become a non-Abelian phase? Is it still the Ising type non-Abelian phase? (3) The real materials which realize spin-1 Kitaev coupling may have many other complicated interactions like the spin-1/2 case, so the phase diagram could be much richer. Therefore, more theoretical studies with different coupling terms added to the pure Kitaev model are also interesting.

Note added: While completing this manuscript, we became aware of a related work [44] based on tensor network approach for spin-1 Kitaev model. Some conclusions of their work on the nature of spin liquid does not agree with our work, and we believe that further theoretical and numerical studies are demanded to resolve the full nature of the spin liquid.

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