A quantum spin liquid phase in the Kitaev-Hubbard model

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The quantum spin liquid (QSL) state has been searched intensively in Kitaev-like materials, such as the Iridium oxides $A_2\text{IrO}_3$ and $\alpha$-RuCl$_3$. The half-filled Kitaev-Hubbard model with bond dependent hopping terms is used to describe the Kitaev-like materials, which is calculated using the state-of-the-art fermionic projected entangled pair states (fPEPS) method. We find a QSL phase near the Mott insulator transition, which has a strong first-order transition to the semi-metal phase with the decrease of Hubbard $U$. We suggest that a promising routine to find the QSL is to find the Iridium oxides that are near the Mott insulator transitions.

A quantum spin liquid (QSL) [1–3] state is a quantum state that lacks any long range magnetic order even down to zero temperature. QSLs have nontrivial topological properties that may host exotic excitations with fractional statistics, such as spinons, and vortons, etc., which may have important applications in quantum computing[4, 5] and may play a crucial role in high-temperature superconductivity.

The Kitaev model[5] is an exactly solvable model on a 2D honeycomb lattice, which hosts a QSL ground state. Several Iridium oxides $A_2\text{IrO}_3$, as well as $\alpha$-RuCl$_3$, have been proposed to realize the Kitaev QSL [6–14]. These materials have a honeycomb structure and the strong spin-orbit coupling leads to an effective $J_{\text{eff}} = \frac{1}{2}$ spin model with bond dependent anisotropic exchange interactions[8, 15], which are the essential ingredients of the Kitaev model. In addition to the Kitaev exchange interactions, there are also Heisenberg interactions in these materials [16]. The Kitaev-Heisenberg model has been intensively studied, and it has been shown that the QSL can only survive in a rather small parameter space [16–20]. Indeed, $\text{Na}_2\text{IrO}_3$ and $\alpha$-RuCl$_3$ were found to have a zigzag antiferromagnetic (AFM) order by resonant X-ray magnetic scattering and inelastic neutron scattering experiments. Tremendous efforts have been made to find the QSL in these materials, and yet no evidence of QSL has been found so far[6, 9, 21, 22]. An important question is that given the extremely small parameter space for the QSL in the Kitaev-Heisenberg model, is it even possible to find the Kitaev QSL in real materials?

The Kitaev-Hubbard model is a more realistic model to describe the Iridium oxides. When the Hubbard $U$ is small, higher order interactions become important, which may introduce exotic states. The Kitaev-Hubbard model has been studied by mean-field theories [23–25]. It has been shown that there exists a QSL phase in the region of $t' < t$ when $U$ is small, where $t$ and $t'$ are the isotropic and spin-dependent hopping terms respectively. A further decrease in $U$ results in a semi-metal (SM) phase. However, these calculations were based on mean-field approximations [23–25], which need to be examined by more rigorous methods. Furthermore, these studies focus on the $t' < t$ region, and the phase diagram for $t' > t$ was missing. Experimentally, the Iridium oxides materials, e.g., $\text{Na}_2\text{IrO}_3$ and $\alpha$-RuCl$_3$, are believed to have strong spin-dependent hopping terms[9, 26–28], and in the $t' > t$ region.

The projected entangled pair states method (PEPS) [29–34], and its generalization to fermionic systems (fPEPS) [35–39] provide systematically improvable variational wave functions for the many-body problems, which allow more rigorous treatment of the Kitaev-Hubbard model. In this Letter, we apply this recently developed and highly accurate fPEPS method to explore the phase diagram of the half-filled Kitaev-Hubbard model. The results show that the QSL state is absent in the $t' < t$ region in contrast to previous mean-field results [23–25]. Instead, we find a QSL phase in the $t' > t$ region when $U$ is small. We show that the phase transition from the SM phase to the QSL phase is a first-order transition, whereas the QSL-zigzag transition is a continuous transition. Given that the Iridium oxide materials and $\alpha$-RuCl$_3$ are in the $t' > t$ region, it is possible to find suitable materials that may host the QSL.

The Hubbard-Kitaev model reads,

$$H = \sum_{\langle i, j \rangle, s} \{\hat{c}_{i,s}^\dagger (\frac{t + t' \sigma^a}{2}) \hat{c}_{j,s} + H.c.\} + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}, \tag{1}$$

where $\hat{c}_{i,s}$ is the annihilation operator that destroys an electron with spin $s$ at site $i$, and $\hat{n}_{i,s} = \hat{c}_{i,s}^\dagger \hat{c}_{i,s}$ is the number operator. $\sigma^a$, with $a=x, y, z$ are the pauli matrices. $\langle i, j \rangle, \alpha$ denotes the nearest-neighbor pairs in the three hopping directions of the lattice, as sketched in Fig. 1. The $t$ and $U$ terms are the hopping and the on-site Coulomb interaction terms in the normal Hubbard model, whereas the $t'$ is the spin-dependent hopping due to spin-orbit coupling.
The bond dimension results fully converge \([34, 35, 40]\). In our calculations, optimized using the stochastic gradient method until the method, and the fPEPS wave functions are further op-
tain the quantum wave functions with the simple update
independent and subject to optimization. We first ob-
converged results for large finite systems.

All the parameters in the fPEPS wave functions are
optimized via a stochastic gradient method, whereas the
wave functions are estimated with the so called fPEPS++ method developed in our
group \([34, 35, 40]\), i.e., the fPEPS wave functions are
optimized via a stochastic gradient method, whereas the
energy and energy gradients are calculated using a Monte
Carlo sampling method. This method significantly re-

All the parameters in the fPEPS wave functions are
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method, and the fPEPS wave functions are further op-
timized using the stochastic gradient method until the
results fully converge \([34, 35, 40]\). In our calculations,
the bond dimension \(D=14\) and the truncation bond di-
mension \(D_c=42\) are used, which show good convergence.
The magnetic phase is determined by the spin struc-
ture factor,

\[
S(\{ \mathbf{k}_\alpha \}) = \sum_{i,j,\alpha} e^{-i \mathbf{k}_\alpha \cdot (\mathbf{r}_i - \mathbf{r}_j)} S_i^\alpha \cdot S_j^\alpha , \tag{2}
\]

where \(r_i\) is the coordinate of the honeycomb lattice and
\(S_i^\alpha\) is the spin operator at site \(r_i\), with \(\alpha = x, y, z\). The
AFM order is characterized by the non-zero value of the
spin structure factor at \(k_x = k_y = k_z = (\frac{\pi}{2}, 0)\), whereas
the zigzag order is detected by the spin structure at \(k_x =
(\frac{\pi}{3}, 0), k_y = (\frac{\pi}{3}, \frac{\sqrt{3}}{3})\) and \(k_z = (\frac{\pi}{3}, \frac{\sqrt{3}}{3})\). The QSL
states are distinguished when all these spin orders vanish
but still have finite charge gaps,

\[
\Delta = E_{N+1} + E_{N-1} - 2E_N , \tag{3}
\]

where \(E_N\) is the total energy of the system with \(N\) elec-
trons.

We first discuss the Kitaev-Hubbard model Eq. (1)
in the large-\(U\) limit. Without loss of generality, we take
\(t = 1\) throughout the paper. At half-filling, the model
can be reduced to the Kitaev-Heisenberg spin model to
the leading order of \(1/U\) \([23, 25]\),

\[
H_{\text{eff}} = \sum_{\langle i,j \rangle} \left( \frac{1 - t'^2}{U} S_i \cdot S_j + \frac{2t'^2}{U} S_i^\alpha S_j^\alpha \right) , \tag{4}
\]

where \(S_i^\alpha, \alpha = x, y, z\) are the spin operators at site \(i\) the
\(S_i = (S_i^x, S_i^y, S_i^z)\) , and the \(\langle i, j \rangle\) denotes the nearest-
neighbor pairs in the three hopping directions of the lattice (see Fig. 1). The Kitaev-Heisenberg model has been studied intensively, and the phase diagram of the model
is well known \([16, 18, 19, 41–49]\). In Ref. 17, the authors
extended the original model to its full parameter space, i.e.,

\[
H_{KH} = \sum_{\langle i,j \rangle} \left[ J S_i \cdot S_j + K S_i^\alpha S_j^\alpha \right] , \tag{5}
\]

where \(J = \cos \phi\) is the Heisenberg coupling strength, and
\(K = 2 \sin \phi\) is the Kitaev coupling strength. The phase angle
\(\phi\) may vary from 0 to \(2\pi\). The phase boundaries have
been obtained by exact diagonalization of the Hamiltonian
on a 24-site hexagonal lattice with periodic boundary
conditions. Compared with the large-\(U\) effective Hamil-
tonian of Eq. 4, the angle \(\phi\) can be related to the \(t'\) as
\(\cot \phi = \frac{1 - t'^2}{t'^2} > -1\) and \(\sin \phi = \frac{t'^2}{t'^2} > 0\), and therefore
we have a constrain of \(0 \leq \phi < 3\pi/4\) for Eq. 5. In
this parameter region, there does exit a QSL phase on \(\phi \in (88^\circ, 92^\circ)\), corresponding to \(t' \sim (0.99970, 1)\) in Eq.
4, which is almost a single point in the parameter space.
It has been shown that when \(t' < 1\), the ground state
is an AFM phase and is the zigzag phase for \(t' > 1\). Therefore,
in the large \(U\) limit, the AFM phase and the zigzag phase are separated by a QSL state that survives
(almost) only at the \(t' = 1\) line.

The decrease in \(U\) may introduce higher order spin in-
teractions \([23]\), which may stabilize the QSL phase in a
larger region. Several studies have shown some insight
into this problem, where the authors claim that an al-
gebraic QSL lies between \(t' \sim 0.7\) and \(t' = 1\), when \(U\) is
small \([23–25]\). However, these calculations were based
FIG. 2. (Color online) The ground state phase diagram of the Kitaev-Hubbard model on the \( t'-U \) plane, where we have set \( t=1 \). Four phases have been identified including a SM phase, an AFM phase, a zigzag phase and a QSL phase. The scatters represent the parameters that are calculated using the fPEPS method.

FIG. 3. (Color online) The charge gaps \( \Delta \) on different lattice sizes for (a) \( t'=0.95 \) and (b) \( t'=1.05 \).

on mean-field approximations [23–25], which need to be examined by more rigorous method. Furthermore, the studies focused on the \( t' < 1 \) region, and the phase diagram for \( t' > 1 \) was not studied.

We calculate the phase diagram of the Kitaev-Hubbard model in the \( t'-U \) plane, using the fPEPS method, and the results are shown in Fig. 2. Four phases have been identified in the phase diagram. On the left side of the diagram, where \( U \) is small, there is a large SM phase that adiabatically connects to the phase at \( t'=0 \), and \( U=0 \), i.e., the electronic structure of graphene. In the large \( U \) limit, the system is in an AFM phase for \( t' < 1 \) and a zigzag phase, when \( t' > 1 \). Remarkably, there is a QSL phase in the parameter range \( t' \in (1,1.2) \) and \( U \in (4.5,7) \). For \( U > 7 \), the QSL phase reduces into the \( t'=1 \) line, consistent with the results of the Kitaev-Heisenberg model [17].

The SM phase is accompanied by the vanishing of the charge gap. Figure 3(a), (b) depict the charge gaps at \( t'=0.95 \) and 1.05, on the honeycomb lattices of 126, 198, 286 sites. The charge gaps decrease with decreasing \( U \). For both \( t'=0.95 \) and \( t'=1.05 \), the charge gaps become zero at approximately \( U \sim 4.5 \), which are the phase boundaries between the SM and Mott insulator phases. The SM phase is further ensured with the vanishing of the local magnetic moment.

We now focus on the insulating region. To determine the magnetic order, we calculate the AFM and zigzag order parameters in the thermodynamic limit via finite size scaling. Figure 4(a), (c) depict AFM and zigzag order parameters for \( U=5 \), with \( t'=0.95 \), 1, 1.05 and 1.2 as functions of the square root of the number of lattice sites used in the calculations, whereas Fig. 4(b), (d) show the results for \( U=8 \). To reduce the boundary effects, the order parameters are calculated using only the central region of the lattice [34, 40, 50]. For \( U=5 \) and \( t'=0.95 \), the system shows a finite AFM order in the thermodynamic limit, and when \( t'=1.2 \), the system shows a zigzag order. However, for \( t'=1 \) and \( t'=1.05 \), both AFM and zigzag orders vanish in the thermodynamic limit. In contrast, for \( U=8 \) and \( t'=0.95 \), the system also has an AFM order, and for \( t'=1.05 \) and \( t'=1.2 \), the system shows a zigzag order. Only when \( t'=1 \), do both AFM and zigzag orders vanish, as expected from the Kitaev-Heisenberg model [17].

Figure 5(a) depicts the AFM order parameter (in the thermodynamic limit) as a function of \( U \) for \( t'=0.95 \). The AFM order disappears at approximately \( U \sim 4.5 \), which is coincident with the disappearance of the charge gap \( \Delta \). This result suggests that there is no other phase between the SM and AFM phases. The calculated phase boundary between the SM and AFM phases is in agreement with the mean field results [23–25] for \( t' < 0.8 \). However it shows a distinguishable difference for \( t' > 0.8 \). Mean field calculations suggest that there is a QSL in this region [23–25], which is absent in more rigorous fPEPS calculations.

Figure 5(b) depicts the AFM and the zigzag order parameters along the line of \( U = 5 \). The system has an AFM order when \( t' < 1 \), and a zigzag order when \( t' > 1.15 \). Both orders disappear in between, which suggests that it is possibly a QSL phase.

To determine the order of the phase transitions, we calculate the first-order energy derivative with respect to \( U \), \( \frac{dE}{dU} \), using the Hellmann-Feynman theorem, i.e.,

\[
\frac{dE}{dU} = \langle \Psi \mid \frac{1}{N} \sum_{i} \frac{\partial H}{\partial U} \mid \Psi \rangle = \langle \Psi \mid \frac{1}{N} \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \mid \Psi \rangle, \tag{6}
\]

where \( \mid \Psi \rangle \) is the ground state fPEPS wave function and \( N \) is the total number of lattice sites that are used to
calculate the total energy. To reduce the boundary effects, only the central region of lattice is used to calculate the total energies [34, 40, 50]. The results are shown in Fig. 6(a) for \( t' = 1.05 \), and the second derivative of the energy with respect to \( U \) (by the finite difference method) are shown in Fig. 6(b). Clearly, there is a sharp discontinuity of \( \frac{dE}{dU} \) at the SM-QSL transition around \( U = 4.5 \), which suggests that this is a strong first-order transition. In contrast, the transition between the QSL and zigzag phases is continuous. Note that, \( \langle \hat{n}_i, \hat{n}_i \rangle \) also characterizes the electron double occupancy on site \( i \). The QSL-SM transition is driven by the sudden increase of the double occupancy. The QSL phase also benefits from the increase in electron double occupancy.

The values of the Heisenberg coupling \( J \) and the Kitaev coupling \( K \) in real materials, such as \( \text{Na}_2\text{IrO}_3 \) and \( \alpha\)-\( \text{RuCl}_3 \), have been estimated in Ref.9, 26–28. It has been suggested that in these materials, \( |J| < |K| \) and \( J/K < 0 \), i.e., \( t' > t \). We find a large region of zigzag phase in \( t' > t, U > 4.5 \), which is consistent with the zigzag phase in \( \text{Na}_2\text{IrO}_3 \) and \( \alpha\)-\( \text{RuCl}_3 \), determined by the resonant x-ray magnetic scattering and inelastic neutron scattering experiments[6, 9, 21, 22]. However, since the Iridium oxides are in the \( t' > t \) region, it is a promising routine...
to find the QSL in Iridium oxides that are close to the Mott insulator transitions.

To summarize, we calculate the ground state phase diagram of the Kitaev-Hubbard model at half-filling using the recently developed, highly accurate fPEPS method. We obtain the SM phase, AFM phase, and zigzag phase. Remarkably, we find a QSL phase near the Mott insulator transition in the strong bond-dependent hopping region. Our calculations suggest that it is possible to find the QSL in Iridium oxides that have strong spin-dependent hopping and are close to the Mott insulator transitions.

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