Phase diagram of the strongly correlated Kane-Mele-Hubbard model

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The phase diagram of the strongly correlated Hubbard model with intrinsic spin-orbit coupling on the honeycomb lattice is explored here. We obtain the low-energy effective model describing the spin degree of freedom. The resulting model describes the spin degree of freedom. The resulting model describes the spin degree of freedom. The resulting model describes the spin degree of freedom.

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I. INTRODUCTION

The spin-orbit interaction driven topological insulator (TI) phase of matter with gapped bulk and protected gapless edge excitations has spurred a renewed interest in the topological states of matter. Kane and Mele proposed the first and the simplest model exhibiting the TI phase for noninteracting electrons on the two-dimensional (2D) honeycomb lattice.1,2 The topological nature of the TI phase and its $Z_2$ structure due to the time-reversal (TR) invariance protects the edge excitation from Anderson localization.3,4 The absence of localization means these systems should be experimentally realizable as they are.5,6 One crucial question that naturally arises is what happens to the TI starting from interacting electron systems. The simplest interaction term is the onsite Hubbard repulsion that causes strong correlation between electrons. Recently, Rachel and Le Hur7 have studied the phase diagram of the Kane-Mele model in the presence of onsite Hubbard interaction. They concluded that the TI phase is stable against onsite repulsion up to a critical value of the interaction strength. Their result has been verified by several other authors both numerically and analytically.8–15

The phase diagram of the Hubbard model has been extensively studied, and various techniques support the existence of a spin liquid phase proximate to the Mott metal-insulator transition point.16–25 In this paper, we are going to address the issue of the possibility of observing the spin liquid phase in the phase diagram of the Kane-Mele-Hubbard model. Spin liquids may occur when the charge degree of freedom is gapped and as a result frozen due to the interaction (Mott insulator), though the spin degree of freedom can be either gapless or gapped. Consequently, we can integrate out the charge degree of freedom as it is gapped with a gap of the order of onsite repulsion in the strong correlation regime. The resulting model describes the spin degree of freedom only. In the pure Hubbard model, that procedure leads to the derivation of the extended Heisenberg model. Adding spin-orbit interaction to the Hubbard model, through the Kane-Mele term, introduces a new term for the second neighbor that is of the form $g_2[-S_i\cdot S_j - S_i \cdot S_j + S_i \cdot S_j]$, where $g_2 = 4\lambda^2/\lambda$.7 Combining this term with the Heisenberg interactions for the next-nearest neighbor (NNN) yields an anisotropic XXZ model for the second-nearest neighbor, while the nearest-neighbor Heisenberg interaction remains intact. In this paper, we study the rich phase diagram of this model. Using a combination of the mean-field results, gauge theory, instanton effect, and topological arguments, we demonstrate that the phase diagram hosts a region of a chiral gapped spin liquid phase26 up to a critical value of the $g_2/J_2$ and for large enough $J_2/J_1$. An interesting possibility is the emergence of the gapped topological spin liquid phase (topological Mott insulator), which is the same as the TI phase, except that its charge degree of freedom is gapped. For large enough values of the $g_2/J_2$, we show that the in-plane XY magnetic ordering wins over the topological spin liquids after taking the instanton effect into consideration. For small values of $J_2/J_1$ and $g_2/J_1$, we obtain a gapless spin liquid which is shown to be unstable toward Neel order or the valence bond solid (VBS) state.

This paper is organized as follows: in Sec. II, we introduce our model that describes the effective action for the spin degree of freedom in the strongly correlated Kane-Mele-Hubbard model and we derive the Kane-Mele-Heisenberg (KMH) model. Section III aims at studying the KMH model using the Schwinger boson approach. Within the mean-field approximation, we investigate the possibility of the spin liquid phase in the KMH model. Our study yields a phase diagram with (1) Neel order, (2) incommensurate Neel order, and (3) a gapped spin liquid phase within the mean-field level. Then we focus on the spin liquid phase and study it further in Sec. IV using the Schwinger fermion approach. Within the mean-field approximation we study the competition between three different kinds of spin liquids. In Sec. V, we discuss the gauge theory of the Schwinger fermion mean-field states. We argue that the microscopic KMH enjoys an SU(2) gauge degree of freedom. However the SU(2) group may break
down to its $U(1)$ or $Z_2$ subgroup in the mean-field state after the Anderson-Higgs mechanism. Moreover, a mean-field state with nonzero Hall conductance can suppress gauge fluctuations further. We also take the effect of instantons into consideration to have a more accurate accounting of gauge fluctuations. Using topological arguments and gauge theory, in Sec. VI, we argue that among the proposed spin liquids the chiral gapped spin liquid with nonzero Hall conductance for Schwinger fermions is stable against gauge fluctuations, while two other states may undergo transition to spontaneously broken-symmetry phases.

II. MODEL

The Kane-Mele-Hubbard model on the honeycomb lattice is described as

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_i^z n_i^\perp + i\lambda_{SO} \sum_{\langle \langle i,j \rangle \rangle, \sigma} \sigma \nu_{ij} c_{i,\sigma}^\dagger c_{j,\sigma},$$

where $t$, $U$, and $\lambda_{SO}$ are the nearest-neighbor hopping energy, the strength of the on-site repulsion, and the second-neighbor spin-orbit coupling strength, respectively. Here $c_{i,\sigma}$ ($c_{i,\sigma}^\dagger$) annihilates (creates) an electron with spin $\sigma$ on site $i$. $\nu_{ij}$ is introduced so as to obtain a nonzero flux turning around any triangular path and is defined as $\nu_{ij} = \frac{\vec{d}_i \times \vec{d}_j}{|\vec{d}_i \times \vec{d}_j|} \hat{z}$ where $\vec{d}_i$ and $\vec{d}_j$ are the two shortest vectors that connect sites $i$ and $j$, i.e., $\vec{d}_i + \vec{d}_j = \vec{R}_i - \vec{R}_j$ (see Fig. 1). Since we are interested in studying the interplay between the strong correlation and the topology of the band structure, we only consider the intermediate and the large $U/t$ and $U/\lambda_{SO}$ limit of the Kane-Mele-Hubbard model.

For the parameter space defined above and at half filling (the undoped case), we can use standard techniques such as canonical transformations or the second-order perturbation to obtain an effective Hamiltonian for the spin degree of freedom. Integrating out the hopping to the nearest-neighbor term, we obtain the $J_1 - J_2$ Heisenberg model:

$$H_{1-2} = J_1 \sum_{\langle ij \rangle} S_i^z S_j^z + J_2 \sum_{\langle \langle ij \rangle \rangle} S_i^z S_j^z,$$

where $J_1$ and $J_2$ are related to the parameters of the Hubbard model as follows:

$$J_1 = 4 \frac{t^2}{U} - 16 \frac{t^4}{U^3}, \quad J_2 = 4 \frac{t^4}{U^3}.$$

Integrating out the Kane-Mele term leads to the following effective Hamiltonian:

$$H_{g_2} = g_2 \sum_{\langle ij \rangle} S_i^z S_j^z - S_i^x S_j^x - S_i^y S_j^y,$$

where $g_2 = 4 \frac{\lambda_{SO}^2}{U}$. The effective Hamiltonian is thus the sum of the $H_{1-2}$ and $H_{g_2}$ as follows:

$$H = J_1 \sum_{\langle ij \rangle} S_i^z S_j^z + \sum_{\langle \langle ij \rangle \rangle} \left[ J_{2,\perp} (S_i^x S_j^x + S_i^y S_j^y) + J_{2,\parallel} S_i^y S_j^y \right],$$

where

$$J_{2,\perp} = J_2 - g_2 = 4 \frac{t^4}{U^3} - \frac{\lambda_{SO}^2}{U},$$

$$J_{2,\parallel} = J_2 + g_2 = 4 \frac{t^4}{U^3} + \frac{\lambda_{SO}^2}{U}.$$

In order to obtain the phase diagram of the strongly correlated Kane-Mele-Hubbard model, we can invert the above equations to solve $U/t$ and $\lambda_{SO}/t$ in terms of $J_1 - J_{2,\perp} - J_{2,\parallel}$ parameters as follows:

$$\frac{\lambda_{SO}}{t} = \sqrt{\frac{(J_{2,\parallel} - J_{2,\perp})}{2(J_1 + 2J_{2,\parallel} + 2J_{2,\perp})}},$$

$$\frac{U}{t} = \sqrt{\frac{2J_1 + 2J_{2,\parallel} + 2J_{2,\perp}}{J_{2,\parallel} + J_{2,\perp}}}.$$

Since the above Hamiltonian describes only the spin degree of freedom and is a generalization for the Heisenberg model, we name it the **Kane-Mele-Heisenberg** Hamiltonian. Because of the extra parameter in this model, its phase diagram is expected to be much richer than the phase diagram of the $J_1 - J_2$ Heisenberg model, which is extensively studied in the literature. In this paper, we study the phase diagram of the Kane-Mele-Heisenberg Hamiltonian using several theoretical and numerical approaches. Before presenting formal discussions we would like to comment on the possible phases for the above Hamiltonian based on general arguments. The phase diagram depends on the two ratios $p_1 = J_{1/2}/J_1$ and $p_2 = J_{2,\perp}/J_1$. Naively speaking, the next-nearest-neighbor interaction becomes important when $p_1$ is comparable to one. When $p_1$ is small, we expect a gapless spin liquid phase within the mean-field approximation. On the other hand, for large values of $p_1$, when $p_2 \to 1$ the model is closer to the $J_1 - J_2$...
Heisenberg model and we can neglect the spin-orbit coupling term. For those parameters, we expect a chiral spin liquid phase with a gapped spin excitation spectrum which is described by the Haldane model in the mean-field approximation. In the opposite limit where $p_2 \to -1$, the Heisenberg interaction is negligible and the spin-orbit coupling dominates. In this regime, a topological spin liquid phase with nonzero spin Hall conductance is expected, which is described by the Kane-Mele model within the mean-field level. In the remainder of this paper we present calculations based on the Schwinger boson and fermion approaches to study the KMH model in more detail.

### III. SCHWINGER BOSONS APPROACH

Heisenberg interaction enjoys a global SU(2) spin rotation symmetry. Forgetting about the quantum-mechanical nature of the spin operators, a simple classical analysis of the spontaneous symmetry breaking yields the antiferromagnetic Neel ordering as the ground state of the Heisenberg model. However, taking quantum fluctuations may melt the Neel order with solidlike long-range order (LRO) down to a spin liquid phase by temperature leads to a vanishing expectation value for the spin operators. Subsequently, we obtain a spin liquid phase by definition of the spin operators in terms of these new Schwinger boson quasiparticles, they acquire a nonvanishing expectation value. Forgetting about the quantum-mechanical nature of the spin operators, a simple classical analysis of the symmetry. Forgetting about the quantum-mechanical nature of the spin operators, a simple classical analysis of the symmetry. Forgetting about the quantum-mechanical nature of the spin operators, a simple classical analysis of the symmetry.

Therefore, in the Schwinger boson approach, we decompose the spin operator in terms of two flavors of bosons $S_j = \frac{1}{2} b_j^\dagger \sigma b_j$, where $b_j = (b_{j,\uparrow}, b_{j,\downarrow})^\dagger$. We also assume a uniform spatial pattern of the magnetic is determined by the momentum along with the local constraint that we either have $|\uparrow\downarrow\rangle_i = b^\dagger_i |\uparrow\downarrow\rangle_i$ or $|\downarrow\downarrow\rangle_i = |\downarrow\downarrow\rangle_i$, where $|\downarrow\downarrow\rangle_i$ is an unphysical state which does not host any quasiparticle (neither the empty nor the occupied state by the hardcore boson).

In the following, the Schwinger boson approach, we derive the spin operator in terms of two flavors of bosons $S_j = \frac{1}{2} b_j^\dagger \sigma b_j$. We also assume a uniform spatial pattern of the magnetic is determined by the momentum along with the local constraint $b^\dagger_i b_{i,\uparrow} + b_i^\dagger b_{i,\downarrow} = 1$, to recover the physical Hilbert space. Using the Schwinger boson approach, we come to the following relations:

\begin{align*}
4S_j, S_j &= -2\Delta_{i,j} \hat{\Delta}_{i,j} + 1
= 1 + 2\Delta_{i,j} \hat{\Delta}_{i,j} - \Delta_{i,j},
\end{align*}

\begin{align*}
4S_j, S_j &= -2\Delta_{i,j} \hat{\Delta}_{i,j} + 1
= 1 + 2\Delta_{i,j} \hat{\Delta}_{i,j} - \Delta_{i,j},
\end{align*}

\begin{align*}
\text{in which } \hat{\Delta}_{i,j} &= b^\dagger_{i,\uparrow} b_{j,\downarrow} + b^\dagger_{i,\downarrow} b_{j,\uparrow}, \quad \hat{\Delta}_{i,j} = b^\dagger_{i,\uparrow} b_{j,\downarrow} - b^\dagger_{i,\downarrow} b_{j,\uparrow}, \\
\Delta_{i,j} &= b^\dagger_{i,\uparrow} b_{j,\downarrow} - b^\dagger_{i,\downarrow} b_{j,\uparrow}. & (10)
\end{align*}

Therefore the second term in the Kane-Mele-Heisenberg Hamiltonian, which is $g_2 S_j S_j + J_2 S_j^2$, decouples as

\begin{align*}
-\frac{1}{2} J_2 \Delta_{i,j} \hat{\Delta}_{i,j} - \frac{1}{2} g_2 S_j S_j, & (11)
\end{align*}

It is worth mentioning that $\Delta_{i,j} = -\Delta_{i,j}$, while $\Delta_{i,j} = \Delta_{i,j}$. Wang in Ref. 24 has studied the model at $g_2 = 0$ using the Schwinger bosons. In the following we closely follow him and extend his study to the nonzero $g_2$ values. To study the above model formally, we appeal to the Hubbard-Stratonovic transformation followed by the saddle-point approximation. Let us use the following definitions:

\begin{align*}
\mu &= \langle \lambda_i \rangle, \\
\Delta_{i,j} &= \langle \Delta_{i,j} \rangle, \\
\delta_{i,j} &= \langle \delta_{i,j} \rangle. & (12)
\end{align*}

We also assume $\chi_{i,j} = \langle \chi \rangle_{i,j} = 0$. To obtain the mean-field Hamiltonian we assume the zero flux state pattern for $\Delta_{i,j}$ and $\Delta_{i,j}$ parameters, which is introduced in Ref. 24. We also assume a uniform $s$ wave $\Delta_{i,j}$ in the mean-field state. Accordingly, the mean-field Hamiltonian can be rewritten as

\begin{align*}
S_j^+ \to d_j^\dagger, \quad S_j^- \to d_j, \quad S_j^z \to d_j^\dagger d_j - \frac{1}{2}. & (8)
\end{align*}

where $d_j$ is the annihilation operator of the hardcore boson at site $i$. It is easy to check that the above definition recovers the SU(2) group symmetric relations for the spin generator. The dimension of the Hilbert is also two per site as we used hardcore bosons. However, working with hardcore bosons is hard. An acclaimed method is the slave boson, which employs two types of bosons, $d^\dagger_i$ denoting the creation of the hardcore boson and $b^\dagger_{i,\downarrow}$ representing the empty site. Because we either have an occupied or an empty site, we need to implement the $b^\dagger_{i,\downarrow}$, $b_{i,\downarrow}$ as the slave boson representation of the hardcore boson. It is clear from the definition of the $b_{i,\downarrow}$ along with the local constraint that we either have $|\uparrow\downarrow\rangle_i = b^\dagger_{i,\downarrow} |\uparrow\downarrow\rangle_i$ or $|\downarrow\downarrow\rangle_i = |\downarrow\downarrow\rangle_i$, where $|\downarrow\downarrow\rangle_i$ is an unphysical state which does not host any quasiparticle (neither the empty nor the occupied state by the hardcore boson).
follows:

\[ H_{MF} = \sum_k \Psi_k^\dagger \begin{pmatrix} \mu & 0 & \Delta_{2,k} & \eta_k \\ 0 & \mu & -\eta_k^* & \Delta_{2,k} \\ \Delta_{2,k}^* & -\eta_k & \mu & 0 \\ \eta_k^* & \Delta_{2,k}^* & 0 & \mu \end{pmatrix} \Psi_k 
+ N_s \left( \frac{3}{2} J_1 \Delta_{1,s}^2 + 3 J_2 \Delta_{2,s}^2 + 3 g_2 \Delta_{3,s}^2 + \mu \right). \]  
(13)

where \( N_s \) is the number of sites, \( \Psi_k = (b_{k,A},b_{k,B},b_{k,A}^\dagger,b_{k,B}^\dagger)^T \), and

\[ \eta_k = \frac{J_1}{2} \Delta_{1,s}(\exp(-i k_s) + 2 \exp(i k_s/2) \cos \left( \frac{\sqrt{3}}{2} k_s \right)), \]
\[ \Delta_{2,k} = \xi_{t,k} + i \xi_{s,k}, \]
\[ \xi_{s,k} = 2 J_2 \Delta_{s} \sin(\sqrt{3} k_s/2)[\cos(3k_s/2) - \cos(\sqrt{3} k_s/2)], \]
\[ \xi_{s,k} = g_2 \Delta_{s} [2 \cos(3k_s/2) \cos(3k_s/2) + \cos(\sqrt{3} k_s)]. \]  
(14)

The above Hamiltonian can be diagonalized using the Bogoliubov transformations which reduce to finding the eigenvalues of the \( M_f \) matrix where \( \Delta = \text{diag}(1, -1, -1) \). Accordingly, the energy dispersion has two branches as follows:

\[ E_{k}^\pm = \sqrt{\mu^2 \pm 2|\eta_k|\xi_{s,k} - |\eta_k|^2 - \xi_{s,k}^2 - \xi_{t,k}^2}. \]  
(15)

Minimizing the total energy

\[ E_{tot} = N_s \left( \frac{3}{2} J_1 \Delta_{1,s}^2 + 3 J_2 \Delta_{2,s}^2 + 3 g_2 \Delta_{3,s}^2 + \mu \right) + \sum_k E_{k}^\pm, \]  
(16)

with respect to \( \mu \), \( \Delta_{1,s} \), \( \Delta_{2,s} \), and \( \Delta_{3,s} \), we obtain the phase diagram of the KMH model. Among the self-consistency equations emerging from the minimization with respect to \( \mu \) we have the following constraint:

\[ \sum_k \frac{|\mu|}{E_k^+} + \frac{|\mu|}{E_k^-} = 2 = 0, \]  
(17)

that implements the local constraint on the Hilbert space in the average. To achieve the phase diagram we need to determine whether or not the energy excitation of Schwinger bosons, i.e., \( E_k^\pm \), is gapped. If gapped we obtain the spin liquid phase, while the gapless case corresponds to the magnetic ordering. If bosons condense in site \( i \) such that \( b_{i,\uparrow} = z_{1,i} \) and \( b_{i,\downarrow} = z_{2,i} \), we have

\[ \langle S_i^z \rangle (i) = \Re(\langle z_{1,i}^* z_{2,i} \rangle), \]
\[ \langle S_i^x \rangle (i) = \Im(\langle z_{1,i}^* z_{2,i} \rangle), \]
\[ \langle S_i^y \rangle (i) = \frac{1}{2} \langle |z_{1,i}|^2 - |z_{2,i}|^2 \rangle. \]  
(18)

We also need to find at which momentum Schwinger bosons condense. For example, if we obtain \( \Delta_{2,s} = 0 \) and Schwinger bosons condense at \( K = (0,0) \), i.e., \( E_{0,0} = 0 \), we have \( \mu = -\eta_k = 0 \). The eigenvectors corresponding to the zero mode are given by \( (1,0,0,1) \) and \( (0,1,1,0) \). Assuming that the weight of Schwinger bosons that condense at \( E_{0,0}^+ \) is \( z_1 \) and

\[
\begin{align*}
\langle S_0^z \rangle (i) &= \Re(\langle z_{1,0}^* z_{2,0} \rangle), \\
\langle S_0^x \rangle (i) &= \Im(\langle z_{1,0}^* z_{2,0} \rangle), \\
\langle S_0^y \rangle (i) &= \frac{1}{2} \langle |z_{1,0}|^2 - |z_{2,0}|^2 \rangle.
\end{align*}
\]

The weight of Schwinger bosons that condense at \( E_{0,0}^- \) is \( z_2 \), so we have

\[
\begin{align*}
\langle S_0^z \rangle (i) &= \Re(\langle z_{2,0}^* z_{1,0} \rangle), \\
\langle S_0^x \rangle (i) &= \Im(\langle z_{2,0}^* z_{1,0} \rangle), \\
\langle S_0^y \rangle (i) &= \frac{1}{2} \langle |z_{2,0}|^2 - |z_{1,0}|^2 \rangle.
\end{align*}
\]

that the weight of those at \( E_{0,0}^- \) is \( z_2 \). Therefore, we have presented a schematic phase diagram in Fig. 2 based on our numerical results. Using the Schwinger boson approach, we obtained a gapped spin liquid phase that does not break any lattice symmetry. In this phase, the SU(2) gauge symmetry associated with the redefinition of the spin operator in terms of Schwinger bosons breaks down to \( Z_2 \) symmetry due to the pair condensation of Schwinger bosons. Therefore, we obtained a \( Z_2 \) spin liquid phase whose ground-state degeneracy is four on a 2D torus. Other states that we obtained include the magnetically ordered phases: coplanar AF order (commensurate order) and noncoplanar (incommensurate) AF order.
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IV. SCHWINGER FERMION APPROACH

As we discussed in the previous section, the Schwinger boson approach is a useful tool to identify the spin liquid phase in the phase diagram. The mean-field Schwinger boson method sparks the existence of the gapped spin liquid phase for the intermediate values of $J_2/J_1$ and for small values of $g_2/J_2$. The rest of the phase diagram is prone to exhibit magnetism of either commensurate or incommensurate Neel ordering forms. In this section, we are going to study the spin liquid phase more carefully. To that end, we employ the Schwinger fermion approach to represent the spin operators. The decomposition procedure for the spin operators is the same as that of the Schwinger bosons except that we replace bosonic $b_{i,\sigma}$ operators with fermionic ones $f_{i,\sigma}$. In the following, we consider the competition between spin liquids only as the starting point; i.e., we assume there is no long-range magnetic ordering in the ground state. However, after discussing the gauge theory of the KMH model, we argue that only the gapped spin liquid phase is a chiral spin liquid; i.e., the spin excitation in the bulk is gapped, while it has topologically protected gapless edge modes. This result is consistent with several previous studies.

The spin-1/2 operator can be represented in terms of Schwinger fermions with two flavors subject to a constraint (such that the dimension of the local Hilbert space is twice that of the spin-1/2 operator) as follows:

$$S_{\uparrow,\sigma} = f_{\uparrow,1,\sigma}, \quad S_{\downarrow,\sigma} = f_{\downarrow,1,\sigma}, \quad S_{\uparrow} = \frac{n_{\uparrow,\sigma} - n_{\downarrow,\sigma}}{2},$$  \hspace{1cm} (21)

$$n_{\uparrow,\sigma} + n_{\downarrow,\sigma} = f_{\uparrow,1,\sigma}^\dagger f_{\uparrow,1,\sigma} + f_{\downarrow,1,\sigma}^\dagger f_{\downarrow,1,\sigma} = 1.$$

Due to the constraint the $S_{\uparrow,\sigma}$ operator can also be written as $S_{\uparrow}^\uparrow = n_{\uparrow,\sigma} - 1/2 = 1/2 - n_{\downarrow,\sigma}$. Using the Schwinger fermion redefinition of the spin operator we can rewrite the Kane-Mele-Heisenberg Hamiltonian in the following way:

$$H = -J_1/2 \sum_{\langle i,j \rangle} \hat{\chi}(i,j) \hat{\chi}(i,j)$$

$$- J_{\perp}/2 \sum_{\langle i,j \rangle} [\hat{\chi}(i,j) \hat{\chi}(i,j) + H.c.]$$

$$- J_{||}/2 \sum_{\langle i,j \rangle} [\hat{\chi}(i,j) \hat{\chi}(i,j) + \hat{\chi}(i,j) \hat{\chi}(i,j)],$$  \hspace{1cm} (22)

in which we have defined $\hat{\chi}(i,j) = f_{\uparrow,\sigma}^\dagger f_{\downarrow,\sigma}$ and $\hat{\chi}(i,j) = \hat{\chi}_1(i,j) + \hat{\chi}_2(i,j)$. The constraint can be implemented using the Lagrange multiplier method, though at half filling it can be set to zero at the level of the mean-field approximation. By implementing a Hubbard-Stratonovic transformation, the above Hamiltonian can be approximated by the following effective Hamiltonian:

$$H_{MF} = -\frac{1}{2} \sum_{\langle i,j \rangle,\sigma} J_1 \chi_1(i,j) f_{\uparrow,\sigma}^\dagger f_{\downarrow,\sigma}$$

$$- \frac{1}{2} \sum_{\langle i,j \rangle,\sigma} [J_2 \chi_2(i,j) + J_{||}\chi_2(i,j)] f_{\uparrow,\sigma}^\dagger f_{\downarrow,\sigma},$$  \hspace{1cm} (23)

where $\chi_i(i,j) = \langle \hat{\chi}_i(i,j) \rangle$. To obtain the phase diagram, we assume $\chi_1(i,j) = \chi_1$ and $\chi_2(i,j) = \chi_2$ for simplicity, in which we have followed the convention for $v_i$ used in the Kane-Mele-Hubbard model [see Eq. (1) for example]. Using these assumptions the Hamiltonian becomes quadratic and is described by the following matrix Hamiltonian for each spin degree of freedom:

$$H_{MF} = \sum_{k,\sigma} \left( f_{k,A,\sigma} f_{k,B,\sigma}^\dagger \right) \left( \begin{array}{cccc} \xi_{\uparrow,\sigma} + \tilde{\xi}_{\sigma} & \eta_k & n_k & \xi_{\downarrow,\sigma} \\ \eta_k^* & n_k & \xi_{\uparrow,\sigma} - \tilde{\xi}_{\sigma} \end{array} \right),$$  \hspace{1cm} (24)

where

$$\eta_k = -J_1 \chi_1[\exp(-ik_y) + 2 \cos(\sqrt{3}k_x/2) \exp(ik_y/2)],$$  \hspace{1cm} (25)

$$\tilde{\xi}_k = 2 \sin(\sqrt{3}k_x/2) [\cos(3k_y/2) - \cos(\sqrt{3}k_y/2)],$$  \hspace{1cm} (26)

and the energy spectrum is given by

$$E_k = \xi_{\sigma} \pm \sqrt{\eta_k^2 + \tilde{\xi}_k^2}.$$  \hspace{1cm} (28)

At half filling all energy levels in the lower bands are occupied by Schwinger fermions. There are four parameters in the total energy: $\chi_1, \chi_2, \phi_1$, and $\phi_1$. To obtain their optimum values at half filling, the self-consistency equations for $\chi_{\sigma}(i,j) = \langle f_{\sigma}^\dagger f_{\sigma} \rangle$ should be solved. Alternatively, we can minimize the total energy with respect to those parameters and we obtain the same values. We have solved the self-consistency equations numerically and we obtain three different phases: (1) gapless spin liquid, (2) chiral gapped spin liquid with non-zero Hall conductance and protected gapless edge states, and (3) topological gapped spin liquid, with non-zero spin Hall conductance and protected gapless edge states (see Fig. 3 for the phase diagram). In the following we present more details on the nature of these phases.

FIG. 3. (Color online) Mean-field phase diagram of the KMH within the Schwinger fermion model.
A. Gapless spin liquid phase

Numerical minimization of the total energy shows that, when \( J_{2,\|} \geq |J_{2,\perp}| \leq 1.7J_1 \) (or equivalently \( J_2 > 0.85J_1 \) and \( g_2 < 0.85J_1 \)), the optimum values for \( \chi_2, \phi_1, \) and \( \phi_1 \) are all equal to zero. In this phase, the energy dispersion of Schwinger fermions is identical to the energy dispersion of electrons in noninteracting graphene sheets with \( t_{\text{eff}} = J_1\chi_1 \). Accordingly, the spin excitation (i.e., the excitation energy for Schwinger fermions) is gapless. On the other hand, it is easy to check that at the mean-field level there is no long-range spin or charge ordering. Therefore this gapless phase does not break any lattice symmetry and by definition is a gapless spin liquid phase. This result is, however, a consequence of the mean-field approximation and needs to be more carefully studied under fluctuations around the mean-field ground state which is a result of the strong correlations among Schwinger fermions. For example, fluctuations of mean-field parameters, i.e., \( \chi_1, \phi_1 \), may destroy the properties of the mean-field state. It has been discussed in the literature that the most important fluctuations which should be included in any serious study are compact gauge fluctuations. In the next section we discuss that this state may undergo phase transition to the antiferromagnetic or VBS state.  

B. Chiral gapped spin liquid phase

For \( J_{2,\|} \geq |J_{2,\perp}| \geq 1.7J_1 \) and \( J_{2,\perp} > 0 \) (or equivalently \( J_2 > 0.85J_1 \) and \( g_2 > 0 \)), the minimum of the ground-state energy manifold yields nonzero values for both \( \chi_1 \) and \( \chi_2 \). We obtain \( \phi_1 = \phi_2 = \pm \frac{\pi}{2} \), and the effective Hamiltonian for the Schwinger fermions within the mean-field approximation is given by

\[
H = -J_1\chi_1 \sum_{\langle ij \rangle, \sigma} f^\dagger_{i,\sigma} f_{j,\sigma} + i(J_{2,\|} + J_{2,\perp})\chi_2 \sum_{\langle \|ij\rangle, \sigma} \nu_{ij} f^\dagger_{i,\sigma} f_{j,\sigma,\sigma},
\]

which is identical to the Haldane model for the chiral phase on the honeycomb lattice. Consequently, the magnetic flux penetrating triangulares consisting of three neighboring same-sublattice sites equals \( \Phi_\sigma = \pm 3\phi_1 \neq 0 \) for both \( f_1 \) and \( f_1 \) Schwinger fermions. The above model in the continuum model describes two gapped Dirac cones around \( K = (\frac{\pi}{2\sqrt{3}}1,0) \) and \( K' = -K \) and the Chern of each band equals \( C^\sigma = \sigma C = \sigma \text{sgn}(\phi_1) \) depending on the spin of the Schwinger fermions. Therefore the Hall conductance of the system is \( \sigma_{xy}^{\chi_1} = \frac{e}{2\pi} \text{sgn}(\phi_1) \frac{\pi}{2} \Phi \) which means that the density of Schwinger fermions changes by \( \Delta n_\sigma = \text{sgn}(\phi_1) \frac{\pi}{2} \Phi \) after inserting \( \Phi \) magnetic flux (which couples to Schwinger fermions). Therefore the total number of fermions \( \Delta n_1 = \Delta n_2 = 0 \), while the spin density \( 1/2(D\Delta n_1 - D\Delta n_2) = \text{sgn}(\phi_1) \frac{\pi}{2} \Phi \) is nonzero. Accordingly, the spin Hall conductance of the system is nonzero while fermions do not transfer across the edge of the system. Since \( C_\alpha = \sigma C \) and \( |C| = 1 \), there is one protected chiral edge mode for each spin degree of freedom with opposite chiralities. The system does not break the time-reversal (TR) symmetry and any TR preserving perturbation cannot destroy them due to Kramer’s degeneracy. Therefore chiral edge modes are robust against nonmagnetic disorder and their chirality is given by their spin and \( C \).

C. Topological gapped spin liquid phase

For \( J_{2,\|} \geq |J_{2,\perp}| \geq 0.85J_1 \) and \( J_{2,\perp} < 0 \) (or equivalently \( g_2 > 0.85J_1 \) and \( g_2 > 0 \)), we obtain both \( \chi_1 \) and \( \chi_2 \) nonzero and \( \phi_1 = \sigma \phi = \pm \frac{\pi}{2} \). The effective Hamiltonian for the Schwinger fermions within the mean-field approximation is given by

\[
H = -J_1\chi_1 \sum_{\langle ij \rangle, \sigma} f^\dagger_{i,\sigma} f_{j,\sigma} + i(J_{2,\|} + J_{2,\perp})\chi_2 \sum_{\langle \|ij\rangle, \sigma} \nu_{ij} f^\dagger_{i,\sigma} f_{j,\sigma,\sigma},
\]

which is identical to the Kane-Mele model for the topological insulator phase on the honeycomb lattice. Consequently, the magnetic flux penetrating triangulares consisting of three neighboring same-sublattice sites equals \( \Phi_\sigma = \pm 3\phi_1 \) for \( f_1 \) and \( f_1 \) Schwinger fermions. The above model in the continuum model reduces to two gapped Dirac cones around \( K = \frac{\pi}{2\sqrt{3}}(1,0) \) and \( K' = -K \) and the Chern of each band equals \( C^\sigma = \sigma C = \sigma \text{sgn}(\phi_1) \) depending on the spin of the Schwinger fermions. Therefore the Hall conductance of the system is \( \sigma_{xy}^{\chi_1} = \frac{e}{2\pi} \text{sgn}(\phi_1) \frac{\pi}{2} \Phi \) which means that the density of Schwinger fermions changes by \( \Delta n_\sigma = \text{sgn}(\phi_1) \frac{\pi}{2} \Phi \) after inserting \( \Phi \) magnetic flux (which couples to Schwinger fermions). Therefore the total number of fermions \( \Delta n_1 = \Delta n_2 = 0 \), while the spin density \( 1/2(D\Delta n_1 - D\Delta n_2) = \text{sgn}(\phi_1) \frac{\pi}{2} \Phi \) is nonzero. Accordingly, the spin Hall conductance of the system is nonzero while fermions do not transfer across the edge of the system. Since \( C_\alpha = \sigma C \) and \( |C| = 1 \), there is one protected chiral edge mode for each spin degree of freedom with opposite chiralities. The system does not break the time-reversal (TR) symmetry and any TR preserving perturbation cannot destroy them due to Kramer’s degeneracy. Therefore chiral edge modes are robust against nonmagnetic disorder and their chirality is given by their spin and \( C \).

V. GAUGE THEORY OF THE KANE-MELE-HEISENBERG MODEL

The Kane-Mele-Heisenberg model at half filling is described in terms of spin operators only. As we showed in Sec. IV, these spin operators can be represented in terms of Schwinger fermions. It is straightforward to check that \( S_i^z, S_i^y, \) and \( S_i^x \) are all invariant under the following local SU(2) gauge transformations:

\[
\begin{align*}
f_i &\rightarrow \alpha f_i, \quad \alpha f_i \rightarrow \beta f_i, \\
\n\end{align*}
\]

\[
\begin{align*}
f_i &\rightarrow -\beta^* f_i, \quad \alpha^* f_i \rightarrow \beta^* f_i, \\
\end{align*}
\]

E_i,j,k implies the breaking of the time-reversal and parity symmetries in the ground state. In this phase, it can be shown that \( E_i,j,k \propto |\Phi| \) when \( i,j,k \) belong to the same sublattice and are nearest neighbors of each other (they belong to a triangle). However, within the mean-field level, the ground state respects the spin rotation, \( C_6 \) (120-deg rotation symmetry) and the translational symmetries. Therefore we name it the chiral gapped spin liquid phase.
One way to see this is to consider the following matrix:
\[ \psi_i = \begin{pmatrix} f_i, \quad f_i, \\ f_i, \quad -f_i, \end{pmatrix}. \tag{32} \]

Spin operators can be described in terms of \( \psi_i \) in the following way:
\[ S_i = \frac{1}{2} \text{Tr}(\psi_i^\dagger \psi_i \sigma^T), \tag{33} \]
where \( \sigma^T \) is the transpose of Pauli matrices, \( \sigma \). From the above definitions, it is obvious that spin operators under \( \psi_i \rightarrow h_i \psi_i \) where \( h_i \) is a SU(2) unitary transformation. This transformation is equivalent to the transformation introduced in Eq. (32) provided \( h_{11} = \alpha_i \) and \( U_{12} = \beta_i \). In addition to the Hamiltonian, the action should also be invariant under SU(2) gauge transformations. To that end, we only need to show that the local constraints on the Hilbert space are also gauge invariant. The SU(2) group has three generators, so there should be three constraints implemented through three temporal gauge fields that can serve as Lagrange multipliers. At half filling, at any site the total number of Schwinger fermions should by exactly one in order to retain the physical Hilbert space with two states per site. Therefore one constraint is \( f_i^\dagger f_i + f_i f_i = 1 \). Two other constraints at half filling can be chosen as \( f_i^\dagger f_i = f_i f_i \), which are direct results of the first constraint. These constraints can be written as \( \psi_i \psi_i^\dagger = 1 \) or equivalently
\[ \text{Tr}(\psi_i^\dagger \sigma \psi_i) = 0. \tag{34} \]

The above constraint is manifestly gauge dependent. These constraints can be implemented using \( A_0 \) gauge fields. Therefore the Lagrangian is
\[ \mathcal{L} = \frac{1}{2} \text{Tr} \left[ \psi_i^\dagger \left( i \frac{d}{dt} + \sigma \cdot A_0 (i) \right) \psi_i \right] - H. \tag{35} \]

It is straightforward to check that the Lagrangian is invariant under the following simultaneous transformations: \( \psi_i \rightarrow h_i \psi_i \), and \( A_0 (i) \cdot \sigma \rightarrow h_i \left[ A_0 (i) \cdot \sigma + i \frac{2}{\sqrt{\pi}} h_i \right] \). This completes our claim of the SU(2) gauge invariance of the Kane-Mele-Heisenberg Hamiltonian.

In the above paragraph, we showed that the original model has local SU(2) gauge symmetry. However, the mean-field solution of the system does not necessarily respect this property and can break the gauge symmetry down to U(1) or Z_2 symmetries by the Anderson-Higgs mechanism. To determine the gauge theory of the mean-field state, we need to identify the invariant gauge group (IGG) of the mean-field solutions. To do so, we investigate the transformation properties of the \( \langle \psi_i \psi_j \rangle \) matrices for every \( i \) and \( j \) site, under the global SU(2) gauge transformations. When gauge particles are massless, these operators are invariant under any global gauge symmetries and the gauge fluctuations around the mean-field state are described by the original compact SU(2) gauge theory. When only a U(1) subgroup of the SU(2) gauge transformations leaves all operators intact, the gauge theory is given by a compact U(1). The Z_2 spin liquid phase is also given by a mean-field ansatz that is invariant under a Z_2 subgroup of the SU(2) gauge transformations only. It is easy to show that the IGG of the gapless spin liquid is SU(2) and the other two spin liquid phases have U(1) IGG, and therefore we need to consider a spin liquid phase coupled to a compact SU(2) or U(1) gauge theory. Compact gauge theories are in principle hard to study as they include nonperturbative phenomena such as instanton effects (monopole configurations). Instantons (anti-instantons) change the value of the gauge potential by \( 2\pi (-2\pi) \) and can potentially cause phase transition to symmetry-breaking phases such as the spin-ordered phase, VBS, or dimerized state.

A. Gauge theory of the gapless spin liquid phase

In this phase, the gapless Dirac fermions at \( K \) and \( K' \) points are coupled to a compact SU(2) gauge fluctuation (QCD_3). The spectrum of the gapless spin liquid phase is similar to the spectrum of the staggered flux phase. The instanton effect on the staggered flux has been extensively studied. Large-N expansions indicate that QCD_3 can be in the deconfined phase and therefore it might not undergo confinement transition.

Therefore the gapless spin liquid phase on the honeycomb lattice can be stable against gauge fluctuations and might remain physical even after the instanton proliferation. It should be noted that it is not clear enough whether the large-N studies are applicable to the physical SU(2) case. If we believe the other scenario where instantons destabilize the mean-field state, instanton condensation spontaneously breaks lattice symmetries. For instance, we may obtain the VBS state or the Neel order as the ground state of the KMH in this regime.

B. Gauge theory of the chiral gapped spin liquid phase

In the chiral gapped spin liquid phase, the mean-field state is described by the gapped Dirac fermions coupled to a compact U(1) gauge field. To obtain an effective action for the gauge field, we can integrate out fermions. Because of the gap in the spectrum of Schwinger fermions, we can easily obtain the Chern number for their energy band. Doing so, we obtain the total Chern number equal to \( C = \pm 2 \) depending on the sign of \( \phi_i \). Therefore, other than instantons, the U(1) gauge field contains a Chern-Simons terms in addition to the Maxwell action as follows:
\[ S_{\text{CS}} = \int d^2x dt \frac{C}{4\pi} e^{i\mu x} a_\mu \partial_\nu a_\nu - \frac{1}{2e^2} (e^{i\mu x} \partial_\mu a_\nu)^2. \tag{36} \]

It is well known that the Chern-Simons term gaps out the gauge particles and, therefore, we can neglect the gauge fluctuations as well as the instanton effect in the low-energy description. Accordingly, the chiral gapped spin liquid is stable against gauge fluctuations and remains physical.

We would like to mention that the ground-state degeneracy of the chiral spin liquid phase is four on the torus. To see why this happens to be true, we should notice that the chiral spin liquid breaks both time-reversal and parity symmetries, so the degeneracy equals \( 2 \times 2 = 4 \). Another way to check this is to note that, fixing the sign of the spin chirality, e.g., \( E_{i,j,k} > 0 \), the ground-state degeneracy on the 2D torus is given by the value of the Chern number. Since \( |C| = 2 \), the ground-state degeneracy for each \( E_{i,j,k} > 0 \) sector is two. Similarly the ground-state degeneracy for the other sector is two as well. Therefore the total degeneracy is four on the torus. This topological invariant serves as good probe to identify the spin
liquid phase in numerical techniques such as the quantum Monte Carlo method.

C. Gauge theory of the topological gapped spin liquid phase

In the topological gapped spin liquid phase, Schwinger fermions are gapped in the bulk and the only low-energy excitation is the compact gauge field. Since spin-up Schwinger fermions and spin-down Schwinger fermions have opposite Hall conductances, the total Chern number vanishes as a result of the time-reversal invariance of the ground state. Accordingly, the Chern-Simons action is absent in the low-energy physics. Therefore, the gauge fluctuation is controlled by the gapless Maxwell term. However, the instanton effect should also be taken into account due to the compact nature of the gauge symmetry.

In this phase, monopole insertion (instanton effect) adds a flux quantum of the gauge field to the system. Assuming $C_1 = -C_1 = +1$, a monopole insertion will increase the number of spin-up Schwinger fermions by plus one and decreases the number of spin-down fermions by minus one. Therefore, the flux quantum of the gauge field carries a charge of the spin operator $S_z = 1$ and flips the spin of Schwinger fermions. This means the density fluctuation of $S_z$ generates a magnetic flux quantum of the gauge field. Since the gauge fluctuation is gapless and linearly dispersed, it can be viewed as the Goldstone mode of the system. Consequently, there should be a spontaneous XY ordering in the system with a nonzero $(S_z^+)^2$.\(^{35}\)

To conclude this subsection, at the mean-field level we obtained a topological gapped spin liquid phase that does not break any lattice symmetry. The spectrum of fermions is gapped and so their fluctuations are suppressed. However, the gauge fluctuation is still gapless and should be taken into account. Among those fluctuations the most relevant one is that of the instanton effects. Instantons proliferate condensate $S_z^+$ and $S_z^-$ operators, and as a result there is an in-plane (XY) spin ordering in the ground state. Therefore we finally end up with a state that is not a spin liquid, and instead it breaks the spin rotational symmetry spontaneously.

VI. SUMMARY AND DISCUSSION

We have studied the strongly correlated limit of the Kane-Mele-Hubbard model. We derived the Kane-Mele-Heisenberg interaction as the effective model for the spin degree of freedom. Using the Schwinger boson approach we derived the phase boundary between the spin liquid and the magnetically ordered phases. The spin liquid phase happens to be a $Z_2$ gapped state. Therefore, both charge and spin degrees of freedom are gapped in the spin liquid phase. To have a better insight into the spin liquid phase nature, we studied the Kane-Mele-Heisenberg model through the Schwinger fermion approach. We went beyond the mean field by taking the instanton effect into account. We discussed that instanton proliferation spoils the spin liquid phases except the chiral spin liquid phase. However, it is not completely clear whether or not instantons will proliferate. Strong gauge fluctuations may generate pairing terms as well as hop to farther neighbors. These terms can stabilize the spin liquid phase of matter. Moreover, large-$N$ limit studies of the SU(N) gauge fields yield the stability of the spin liquid phase. Further investigation of the fate of the spin liquids is needed to determine what happens to the proposed topological spin liquid and the gapless spin liquid phases. Based on a combination of the Schwinger boson and fermion study, gauge theory, and topological arguments, we suggest that the phase diagram of the KMH is as depicted in Fig. 4. It is worth mentioning that the Schwinger boson study yields a $Z_2$ spin liquid phase, while within the Schwinger fermion approach chiral spin liquid is more favorable. A more careful study of the ground-state energy can elucidate further the nature of the spin liquid phase.

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\(^{35}\)C. Gauge theory of the topological gapped spin liquid phase

FIG. 4. (Color online) Our proposal for the phase diagram of the KMH model. $Z_2$ and CSL stand for $Z_2$ and chiral spin liquid phases, respectively, and AF denotes out-of-plane Neel ordering. XY ordering refers to the Neel order along an axis in the plane, e.g., along the $x$ direction.
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