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Phase Diagram of the Kane-Mele-Hubbard model

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Motivated by recent numerical results, we study the phase diagram of the Kane-Mele-Hubbard (KHM) model, especially the nature of its quantum critical points. The phase diagram of the Kane-Mele-Hubbard model can be understood by breaking the $SO(4)$ symmetry of our previous work down to $U(1)_{\text{spin}} \times U(1)_{\text{charge}} \times \text{PH}$ symmetry. The vortices of the inplane Néel phase carry charge, and the proliferation of the *charged* magnetic vortex drives the transition between the inplane Néel phase and the QSH insulator phase; this transition belongs to the 3d XY universality class. The transition between the liquid phase and the inplane Néel phase is an anisotropic $O(4)$ transition, which eventually becomes first order due to quantum fluctuation. The liquid-QSH transition is predicted to be first order based on a $1/N$ calculation.

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I. INTRODUCTION

Thanks to the discovery of Graphene¹⁻³, a great deal of attention has been devoted to systems with Dirac fermions at low energy. It was demonstrated that many topological states of fermions are related to Dirac fermions, such as the quantum Hall state⁴, quantum spin Hall state^{5,6}, and 3d Topological insulator^{7,8}, etc. Since last year, motivated by the quantum Monte Carlo (QMC) simulation on the Hubbard model on the honeycomb lattice⁹, strongly interacting Dirac fermions have stimulated a lot of interests. Quite unexpectedly, a fully gapped liquid phase was discovered in the phase diagram of the honeycomb lattice Hubbard model at intermediate Hubbard U ⁹, and by increasing U this liquid phase is driven into a Néel phase after a continuous quantum phase transition. This liquid phase has stimulated many theoretical and numerical studies on possible spin liquid phases on the honeycomb lattice¹⁰⁻¹⁷. So far almost all the theoretical proposals about this liquid phase involve nontrivial topological orders^{10-12,15,16}.

The Hubbard model on the honeycomb lattice has the full $SO(4) \sim [SU(2)_{\text{spin}} \times SU(2)_{\text{charge}}]/Z_2$ symmetry^{18,19}, thus a true liquid phase of the Hubbard model should preserve all these symmetries. In Ref. ^{15,16}, a full $SO(4)$ invariant theory of the Hubbard model was developed, and it was proposed that the liquid phase observed in Ref.⁹ is a topological spin-charge liquid phase with mutual semion statistics between gapped spin-1/2 and charge- e excitations. The global phase diagram of this theory is depicted in Fig. 1. We will review this theory in the next section.

In the current work, we will consider perturbations on the Hubbard model that break the $SO(4)$ symmetry down to its subgroups. In particular we will focus on the Kane-Mele-Hubbard (KMH) model that was recently studied numerically²⁰⁻²³:

$$H = \sum_{\langle i,j \rangle, \alpha} -tc_{i,\alpha}^\dagger c_{j,\alpha} + \sum_{\langle\langle i,j \rangle\rangle, \alpha, \beta} \lambda i\nu_{i,j} c_{i,\alpha}^\dagger \sigma_{\alpha\beta}^z c_{j,\beta} + Un_{i,\uparrow} n_{i,\downarrow}. \quad (1)$$

The second term of this Hamiltonian is the spin-orbit coupling introduced in the original Kane-Mele model for the quantum spin Hall effect (QSH)^{5,6}.

So far most of the studies on topological insulator have been focused on noninteracting electron physics. The KMH model is the simplest model that combines both the strong correlation and topological band structure. It is very clear that Topological band insulator cannot be adiabatically connected to a trivial band insulator without going through a phase transition, while it is much less understood how a topological insulator evolves into a strongly correlated phase, for instance an antiferromagnetic insulator, or a more exotic spin liquid phase. In the KMH model, all these phases have been shown to exist in recent numerical works^{9,20-24}, thus the KMH model is a perfect model to study the interplay between topology and interaction. The goal of the current work is to theoretically understand the quantum phase transitions between all the phases in the KMH model.

II. $SO(4)$ INVARIANT THEORY

In Ref.¹⁶, the author used the $SO(4)$ symmetry to classify the order parameters on the honeycomb lattice¹⁶. In particular, the quantum spin Hall (QSH) and triplet-superconductor (TSC) order parameters belong to a $(\mathbf{3}, \mathbf{3})$ matrix representation of the $SO(4)$ group:

$$Q_{ab} = \begin{pmatrix} \text{Im}(\text{TSC})_x, & \text{Im}(\text{TSC})_y, & \text{Im}(\text{TSC})_z \\ \text{Re}(\text{TSC})_x, & \text{Re}(\text{TSC})_y, & \text{Re}(\text{TSC})_z \\ \text{QSH}_x, & \text{QSH}_y, & \text{QSH}_z \end{pmatrix} \quad (2)$$

Since all these order parameters are topological, their topological defects carry nontrivial quantum numbers. For instance, a Skyrmion of the spin vector $(\text{QSH}_x, \text{QSH}_y, \text{QSH}_z)$ carries charge- $2e$ ²⁵, while a Skyrmion of the charge vector $(\text{Im}(\text{TSC})_z, \text{Re}(\text{TSC})_z, \text{QSH}_z)$ carries spin-1 *i.e.*

spin and charge are dual to each other, and view each other as topological defects¹⁶. The liquid phase proposed in Ref.^{15,16} was obtained by proliferating both the spin and charge Skyrmions from the condensate of Q_{ab} .

In the SO(4) invariant theory, the low energy physics of topological defects of the matrix order parameter Q_{ab} is described by the following theory:^{15,16}:

$$\begin{aligned} \mathcal{L}_{cs} = & \frac{2i}{2\pi} \epsilon_{\mu\nu\rho} A_{c,\mu}^z \partial_\nu A_{s,\rho}^z \\ & + |(\partial_\mu - iA_{s,\mu}^z)z_\alpha^s|^2 + r_s |z_\alpha^s|^2 \\ & + |(\partial_\mu - iA_{c,\mu}^z)z_\alpha^c|^2 + r_c |z_\alpha^c|^2 + \dots \end{aligned} \quad (3)$$

The CP(1) fields z_α^s and z_α^c are SU(2)_{spin} and SU(2)_{charge} fundamental doublets. In terms of z_α^s and z_α^c , the order parameter Q_{ab} is represented as

$$Q_{ab} \sim (z^{s\dagger} \sigma^a z^s)(z^{c\dagger} \sigma^b z^c). \quad (4)$$

The two U(1) gauge fields $A_{c,\mu}^z$ and $A_{s,\mu}^z$ in Eq. 3 impose the following constraint: $\delta\mathcal{L}/\delta A_{c,0}^z = \delta\mathcal{L}/\delta A_{s,0}^z = 0$. These two equations identify z_α^s (z_α^c) as the vortex (meron) of charge (spin) sectors of the order parameter Q_{ab} , thus spin and charge are each other's topological defects, which is precisely the effect that we have mentioned above when the system develops the matrix order Q_{ab} . Thus the mutual CS theory precisely describes the duality between spin and charge in this system, which is an important consequence of quantum spin Hall state that has been discussed in previous publications^{26,27}. A rigorous derivation of Eq. 3 was given in Ref.¹⁶.

By tuning the parameters r_s and r_c , a global phase diagram Fig. 1 is obtained. There are in total four phases:

(1). Phase A3 corresponds to the case with z^s and z^c both gapped, and the system is in a topological liquid phase with mutual anyon statistics between spin-1/2 and charge- e excitations. This statistics is guaranteed by the mutual CS fields in Eq. 3. In Ref.¹⁶ it was proposed that this is the liquid phase observed by QMC⁹.

(2). In Phase A2, z^s is condensed while z^c is gapped. The system is in a magnetic ordered phase with both Néel and transverse nematic order. The ground state manifold (GSM) of this phase is SO(3)/Z₂.

(3). In phase A, both z^s and z^c are condensed, the system is described by the condensate of order parameter Q_{ab} , with GSM ($S^2 \times S^2$)/Z₂. One example state of this phase is the QSH_z state, which couples to the fermions in the same way as the spin-orbit coupling introduced in the Kane-Mele model^{5,6}.

(4). Phase A4 is the charge-dual of the phase A2, with the same GSM SO(3)/Z₂.

All the phase transitions in phase diagram Fig. 1 are continuous. For example, the transition between A3 and A2 belongs to the 3d O(4) universality class, while the transition between A and A2 is a CP(1) transition, which is equivalent to the deconfined quantum critical point^{28,29}. The multicritical point in Fig. 1 was studied

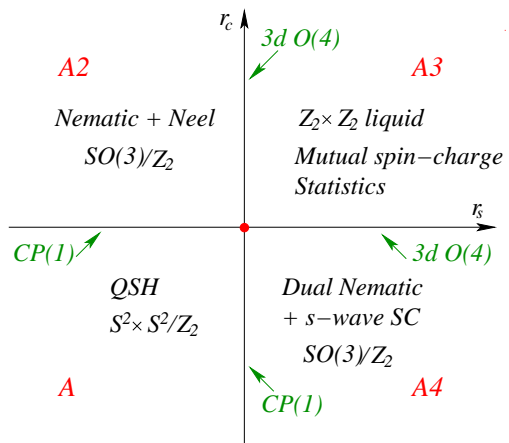


FIG. 1: The global phase diagram for the SO(4) invariant theory Eq. 3 proposed in Ref.¹⁶.

using a $1/N$ expansion in Ref.³⁰, and when N is sufficiently large this multicritical point is a conformal field theory.

The same field theory Eq. 3 was used to describe various phases observed experimentally on the triangular lattice frustrated magnets³⁰, such as κ -(ET)₂Cu₂(CN)₃, EtMe₃Sb[Pd(dmit)₂]₂, EtMe₃P[Pd(dmit)₂]₂, etc. Also, a similar theory without SU(2)_{charge} was applied to the cuprates^{31,32}.

III. THE KANE-MELE-HUBBARD MODEL

A. General formalism

In the Kane-Mele-Hubbard (KMH) model Eq. 1, the symmetry of the Hubbard model is broken down to

$$U(1)_{\text{spin}} \times U(1)_{\text{charge}} \times \text{PH}, \quad (5)$$

where $U(1)_{\text{spin}}$ is the spin rotation around z axis, while $U(1)_{\text{charge}}$ corresponds to the ordinary charge U(1) rotation. The extra particle-hole symmetry (PH) is

$$\text{PH} : c_{i,\alpha} \rightarrow c_{i,\alpha}^\dagger (-1)^i. \quad (6)$$

This PH symmetry is in fact a product of spin and charge π -rotations around the y axis: $\text{PH} = \pi^{y,c} \cdot \pi^{y,s}$. One can verify that $\pi^{y,c}$ and $\pi^{y,s}$ individually changes the KMH model, while their product keeps the model invariant. The definition of PH is not unique. For instance, one can also define PH as $\text{PH} = \pi^{x,c} \cdot \pi^{x,s}$, then fermion operator transforms as $c_i \rightarrow \sigma^z c_i^\dagger (-1)^i$.

The QSH spin-orbit coupling corresponds to Q_{33} of the matrix order parameter Q_{ab} in Eq. 2. Thus a nonzero $\langle Q_{33} \rangle$ in the Hamiltonian will modify the field theory Eq. 3 as follows:

$$\mathcal{L}_{cs} = \frac{2i}{2\pi} \epsilon_{\mu\nu\rho} A_{c,\mu}^z \partial_\nu A_{s,\rho}^z$$

$$\begin{aligned}
& + |(\partial_\mu - iA_{s,\mu}^z)z_\alpha^s|^2 + r_s|z_\alpha^s|^2 \\
& + |(\partial_\mu - iA_{c,\mu}^z)z_\alpha^c|^2 + r_c|z_\alpha^c|^2 \\
& + u\langle Q_{33}\rangle(z^{s\dagger}\sigma^z z^s)(z^{c\dagger}\sigma^z z^c) + \dots \quad (7)
\end{aligned}$$

Notice that terms like $z^{c\dagger}\sigma^z z^c$, $z^{s\dagger}\sigma^z z^s$ etc. are all forbidden by the PH symmetry. The symmetry-breaking introduced by the QSH spin-orbit coupling will not change the nature of the liquid phase (A3 of Fig. 1). However, the other phases with spin and charge orders will be modified. The modified global phase diagram is depicted in Fig. 2a.

B. Néel phase and charged vortex

Let us start with phase A2. With the background QSH order parameter, the phase A2 of Fig. 1 is reduced to a pure inplane Néel phase with GSM S^1 in Fig. 2a.

One very special property of this Néel order is that, the vortex of the Néel order carries unit electric charge due to the “dual” QSH effect, since the vortex of the inplane Néel order carries a magnetic π -flux. This “dual” QSH effect and charged spin-flux was discussed in Ref.^{26,27}. In our formalism, the charge-carrying vortex is transparent in the mutual CS theory in Eq. 7: the constraint $\delta\mathcal{L}/\delta A_{c,0}^z = 0$ leads to the result that the π -flux of $A_{s,\mu}^z$, which is equivalent to a magnetic vortex, carries charge doublet z_α^c . The key question we want to address here is, does the charge carried by the vortex affect the quantum phase transitions around the Néel phase?

This problem can be understood by classifying the charged vortices of the Néel order based on the symmetry of the system. Every charged vortex carries two quantum numbers, charge and vorticity, denoted as (e, v) . There are in total four flavors of charged-vortices:

$$\begin{aligned}
z_1^c &= (e, v), & (z_1^c)^* &= (-e, -v), \\
z_2^c &= (-e, v), & (z_2^c)^* &= (e, -v). \quad (8)
\end{aligned}$$

z_1^c and z_2^c are precisely the $SU(2)_{\text{charge}}$ doublet introduced in Eq. 3. If there is a full $SO(4)$ symmetry, all four flavors of vortices are degenerate. Within the current KMH model, the symmetry guarantees that z_α^c and $(z_\alpha^c)^*$ are degenerate, but z_1^c and z_2^c are *not* necessarily degenerate. This is due to the fact that under the PH transformation in Eq. 6, both e and v are reversed. (Notice that PH defined in Eq. 6 transforms $S^x \rightarrow -S^x$, $S^y \rightarrow S^y$.)

The classification of vortices can also be understood from the general theory Eq. 7. For instance, in phase A2 (condensate of z_α^s), due to the existence of the last term of Eq. 7, the condensate of z_α^s splits the degeneracy between z_1^c and z_2^c .

Without using our formalism Eq. 7, the quantized charge carried by the magnetic vortex can be understood

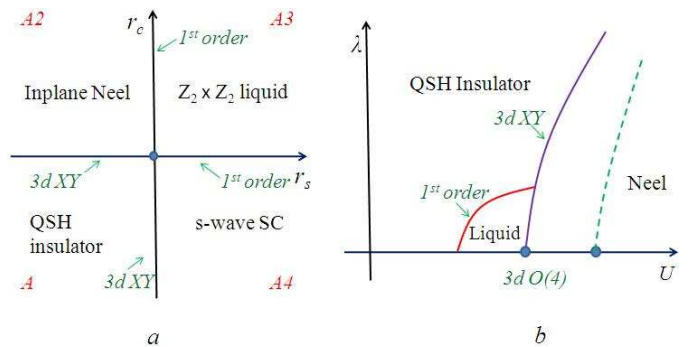


FIG. 2: (a). The global phase diagram of Eq. 7, for models that break $SO(4)$ to $U(1)_{\text{spin}} \times U(1)_{\text{charge}} \times \text{PH}$ symmetry. (b). The phase diagram of the actual KMH model. The theory in Ref.¹¹ would predict an extra transition line inside the Néel phase (dashed line), which corresponds to the order-disorder transition of the CAF order parameter. This dashed line is absent in our theory.

in a more pictorial way: Let us consider a disk geometry with a hole at the origin. Then the system has two boundaries, one internal boundary around the hole, and one external boundary of the disk. Inside the QSH insulator phase, both boundaries have helical edge state, which is equivalent to a one dimensional Dirac fermion:

$$H = iv_f(\psi_L^\dagger \partial_x \psi_L - \psi_R^\dagger \partial_x \psi_R) = iv_f \psi^\dagger \tau^z \partial_x \psi. \quad (9)$$

Now let us develop the inplane Néel order in the system, and create a vortex of the inplane Néel order, with the vortex core located at the hole of the disk. Then the Néel order will gap out the boundary. The one dimensional Dirac fermion at the boundaries has two different mass gaps $\psi^\dagger \tau^x \psi$ and $\psi^\dagger \tau^y \psi$, which can be linearly combined as $\cos(\theta) \psi^\dagger \tau^x \psi + \sin(\theta) \psi^\dagger \tau^y \psi$. A vortex of the inplane Néel order can be viewed as a smooth but quantized domain wall of θ for both boundaries. It is well-known that for a one dimensional Dirac fermion, a quantized smooth domain wall of mass gap will acquire quantized charge $e^{33,34}$, thus the charge carried by the vortex is always quantized.

This inplane Néel order is always accompanied with a background QSH spin-orbit coupling. Since the QSH spin-orbit coupling breaks the reflection symmetry $x \rightarrow -x$ of the honeycomb lattice, one might expect that the following spin order parameter automatically acquires a nonzero expectation value:

$$H' \sim \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} \hat{z} \cdot (\vec{S}_i \times \vec{S}_j). \quad (10)$$

However, H' is **odd** under PH. Thus unless the system further breaks the PH symmetry, H' should *not* have any nonzero expectation value.

C. Néel-QSH transition

Usually the order-disorder transition of inplane XY order is driven by proliferating the vortices of the order parameter. In the previous section we have classified the vortices in the inplane Néel phase. In the Néel phase, since vortices z_1^c and z_2^c are not degenerate, only one component of the vortex doublet z_α^c condenses at the transition. Let us take this vortex to be z_1^c , then the field theory of the transition is

$$\mathcal{L} = |(\partial_\mu - iA_{c,\mu}^z)z_1^c|^2 + r_c|z_1^c|^2 + \dots \quad (11)$$

This is a 2+1d Higgs transition, which belongs to the 3d XY universality class. The gauge field $A_{c,\mu}^z$ is precisely the dual of the Goldstone mode of the inplane Néel phase. The condensate of z_1 has no Goldstone mode due to the Higgs mechanism, thus the condensate has no superconductor order even though z_1^c carries charge. The condensate of z_1^c is precisely the QSH insulator.

If we start with the QSH insulator phase, this QSH-Néel phase transition can be viewed as condensation of magnetic exciton $b_i \sim c_{\uparrow,i}^\dagger c_{\downarrow,i}$ ³⁵. Since $(b_i)^2 = 0$, the magnetic exciton is a hard-core boson. Under PH transformation, b_i transforms as $b_i \rightarrow -b_i^*$. This symmetry rules out the linear time-derivative term in the Lagrangian of b , thus this transition is an ordinary 3d XY transition, which is consistent with the analysis in the previous paragraph.

Ref.³⁶ studied the Néel-QSH transition using a U(1) rotor theory. However, for a particle-hole symmetric system it is usually more adequate to use an SU(2) rotor formalism like Ref.^{37,38}. Our vortex analysis demonstrated that in the KMH model, even if one starts with an SU(2) rotor theory, it will reduce to a U(1) rotor theory.

As a comparison to the KMH model, let us discuss a slightly different kind of symmetry breaking of the Hubbard model. In this case, the SO(4) symmetry of the Hubbard model is broken down to $U(1)_{\text{spin}} \times U(1)_{\text{charge}} \times \pi^{y,c} \times \pi^{y,s}$, *i.e.* both $\pi^{y,c}$ and $\pi^{y,s}$ are symmetries of the system individually (in the KMH case only their product is the symmetry). According to the symmetry $U(1)_{\text{spin}} \times U(1)_{\text{charge}} \times \pi^{y,c} \times \pi^{y,s}$, in the inplane Néel phase (phase A2) all four flavors of charged vortices (merons) with quantum numbers $(\pm e, \pm v)$ are degenerate. Thus the low energy field theory describing these charged vortices is the CP(1) model with easy-plane anisotropy:

$$\mathcal{L} = \sum_{\alpha=1}^2 |(\partial_\mu - iA_{c,\mu}^z)z_\alpha^c|^2 + r_c|z_\alpha^c|^2 + g(\sum_{\alpha=1}^2 |z_\alpha^c|^2)^2 + u|z_1^c|^2|z_2^c|^2 + \dots \quad (12)$$

We keep $u < 0$, thus the $SU(2)_{\text{charge}}$ is broken down to the easy-plane direction, *i.e.* z_1^c and z_2^c both condense at the transition. When z_α^c both condense, the system enters a superconductor state with one Goldstone mode. This superconductor is the triplet superconductor TSC_z

in the matrix order parameter Eq. 2. If we define an O(4) vector $\vec{\phi} = (\text{Neel}_x, \text{Neel}_y, \text{Re}[\text{TSC}_z], \text{Im}[\text{TSC}_z])$, the nonlinear sigma model of $\vec{\phi}$ has a topological Θ -term. A Néel-TSC transition on the honeycomb lattice was discussed in Ref.³⁸. However, this Néel-TSC transition does *not* happen in the KMH model, since in the KMH model z_1^c and z_2^c are nondegenerate.

D. Liquid-Néel transition

In the KMH model, the phase transition between the spin-charge liquid phase and the Néel phase does not involve any low energy charge degrees of freedom, thus this transition can be understood as the condensation of z_α^s , while z_α^c are gapped. When z_α^c are gapped out, they can be safely integrated out from Eq. 7, then z_1^s and z_2^s become degenerate. z_α^s is coupled to a $Z_2 \times Z_2$ gauge field, as was discussed in Ref.^{16,39}. Now the liquid-Néel transition is described by the following Lagrangian

$$\mathcal{L} = \sum_{\alpha=1}^2 |\partial_\mu z_\alpha^s|^2 + r_s|z_\alpha^s|^2 + g(\sum_{\alpha=1}^2 |z_\alpha^s|^2)^2 + u|z_1^s|^2|z_2^s|^2 + \dots \quad (13)$$

The Néel order parameter is a bilinear of z_α^s :

$$N^x \sim \text{Re}[(z^s)^t i \sigma^y \sigma^x z^s] \sim \text{Re}[z_1^2 - z_2^2],$$

$$N^y \sim \text{Re}[(z^s)^t i \sigma^y \sigma^y z^s] \sim \text{Re}[iz_1^2 + iz_2^2]. \quad (14)$$

The first line of Eq. 13 has a full O(4) symmetry, while the second line breaks the O(4) symmetry down to $U(1) \times U(1) \times Z_2$. In this field theory $u > 0$, thus in the condensate of z_α^s there is only one Goldstone mode that corresponds to the inplane Néel order. According to the high order ϵ expansion in Ref.⁴⁰, u is a relevant perturbation at the 3d O(4) universality class, which is expected to drive the transition first order eventually.

E. The s -wave superconductor

The phase A4 in Fig. 1 is reduced to the s -wave superconductor in Fig. 2a. The s -wave SC is the charge-dual of the inplane Néel order in phase A2. Just like the magnetic vortex of the Néel order, the vortex of the SC also carries two quantum numbers: spin- $\pm 1/2$ and vorticity: (s, v) . The symmetry of the KMH model divides the vortices into two groups: $(\frac{1}{2}, v)$ and $(-\frac{1}{2}, -v)$ are degenerate, while $(\frac{1}{2}, -v)$ and $(-\frac{1}{2}, v)$ are degenerate. These two groups of vortices are precisely (z_1^s, z_1^{s*}) and (z_2^s, z_2^{s*}) introduced in Eq. 3.

The quantum phase transition between the s -wave SC (phase A4) and the QSH insulator (phase A) is interpreted as condensing either z_1^s or z_2^s , this transition is a 3d XY transition. The transition between the liquid phase A3 and phase A4 is described by a similar theory as Eq. 13, and it is expected to be a first order transition.

F. Multicritical point

There is a multicritical point in our phase diagrams Fig. 1 for SO(4) invariant systems, which separates the liquid phase from the QSH insulator. In Ref.³⁰, this multicritical point was studied using a large- N generalization, where N is the number of components of z_α^s and z_α^c . It was demonstrated that when N is large enough, this multicritical point is a conformal field theory³⁰. Compared with the theory studied in Ref.³⁰, Eq. 7 has several SO(4) symmetry breaking perturbations, for example the last term in Eq. 7. If we extrapolate the $1/N$ calculation in Ref.³⁰ to our current case with $N = 2$, the last term in Eq. 7 is a relevant perturbation at the multicritical conformal field theory. Thus we expect the transition between the liquid and the QSH insulator in the KMH model to be a first order transition.

IV. COMPARE WITH OTHER THEORIES

Based on our theory discussed in this paper, we propose the phase diagram for the KMH model in Fig. 2b plotted against λ and U . When $\lambda = 0$, there is one extra transition inside the Néel phase, which corresponds to the transition between the pure Néel order with GSM S^2 , and the Néel + nematic order with GSM SO(3)/ Z_2 (phase A2 in Fig. 1). This transition is *absent* once nonzero λ is turned on, this is because the symmetry of the Néel + nematic order is identical to the Néel order with a background QSH spin-orbit coupling.

In Ref.¹¹, the authors proposed a different phase diagram for the Hubbard model on the honeycomb lattice. Instead of a Néel+nematic order, the authors of Ref.¹¹ predicted a chiral antiferromagnetic (CAF) phase with an extra nonzero order $\langle \nu_{ij} \hat{z} \cdot (\vec{S}_i \times \vec{S}_j) \rangle \neq 0$ between next nearest neighbor sites. Unlike the Néel+nematic order, the CAF order has a different symmetry from the pure Néel order even with presence of the QSH spin-orbit coupling in the background. For instance, when the Néel vector is along the y direction, it is still invariant under the PH transformation defined in Eq. 6; but the CAF order breaks this PH transition, as was discussed in section IIIB.

This symmetry analysis leads to the following two conclusions:

(1). If there is a CAF phase with zero λ , there must be a transition line within the inplane Néel phase in Fig. 2b even with finite λ (dashed line of Fig. 2b), which corresponds to the order-disorder transition of the CAF order parameter.

(2). The transition between the QSH insulator and the Néel+CAF phase is *not* a 3d XY transition, because the symmetry breaking at this transition is different from the 3d XY transition.

The different predictions between our theory and Ref.¹¹ can be checked numerically in the future.

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