Rotated Ferromagnetic Heisenberg model

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We show that in the strong coupling limit, a spinor boson Hubbard models at integer fillings in the presence of spin-orbit couplings (SOC) leads to a new class of quantum spin models: a Rotated Ferromagnetic Heisenberg (RH) model. We introduce Wilson loops to characterize frustrations and gauge equivalent class in this RH model. For a special equivalent class, we identify a new spin-orbital entangled quantum ground state. The excitation spectrum above the ground state has a continuously changing minimum positions tuned by the SOC strength which is the most striking new feature of the RH model. At high temperatures, the specific heat depends on the SOC strength explicitly. We argue that one special gauge can be very naturally and easily realized in current experiments. It is also possible to realize other gauges in near future experiments. Various experimental detections of the new phenomena are discussed.

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Introduction.— Spin-orbit coupling (SOC) has played important roles in various condensed matter systems \cite{3,4}. Recently the investigation and control of spin-orbit coupling (SOC) have become subjects of intensive research after the discovery of the topological insulators \cite{4}. For example, the SOC is a critical factor leading to a whole new class of correlated electronic states \cite{1,2}. Since the generation of 1D SOC by several experimental groups for neutral atoms \cite{4}, there have been impressive advances in generating artificial gauge fields in optical lattices. Staggered magnetic field along one direction in an optical lattice (See Fig.3a) has been achieved \cite{7,8}. Very recently, two experimental groups \cite{9,10} successfially generated the time-reversal symmetric Hamiltonian underlying the quantum spin Hall effects \cite{1}, namely, two different spin components \cite{12} experience opposite directions of the uniform magnetic field (see Fig.3b). Scaling functions for both gauge-invariant and non-gauge invariant quantities across topological transitions of non-interacting fermions driven by the non-Abelian gauge potentials on an optical lattice have also been derived \cite{13}. However, so far, possible new class of quantum phenomena due to the interplay among the interactions, non-Abelian gauge potentials (or equivalently, SOC) and lattice geometries have not been addressed systematically.

In this paper, we investigate such an interplay systematically by studying the system of interacting spinor bosons at integer fillings hopping in a square lattice in the presence of non-Abelian gauge potentials. At strong interactions, we derive a Rotated Ferromagnetic Heisenberg (RH) model which is a new class of quantum spin models different from any previously known quantum spin models. We introduce Wilson loops to characterize frustrations and gauge equivalent class in this RH model. For the special equivalent class along the dashed line in Fig.1c, we identify a new spin-orbital entangled quantum ground state. At low temperatures, by performing spin wave calculations, we find the excitation spectrum above the ground state has a continuously changing minimum positions tuned by the SOC strength which is the most striking new feature of the RH model. At high temperatures, the specific heat depends on the SOC strength explicitly. We argue that a special gauge can be very naturally and easily realized in current experiments. It is also possible to realize other gauges in near future experiments. Various experimental detections of the new phenomena are discussed.

Rotated spin $S$ Heisenberg model in the strong coupling limit— The pseudo-spin 1/2 boson Hubbard model at integer fillings $\langle b_\uparrow^\dagger b_\uparrow + b_\downarrow^\dagger b_\downarrow \rangle = N$ subject to a non-
Abelian gauge potential is [13]:

\[ H_0 = -t \sum_{\langle i,j \rangle} b^\dagger(i)U_{ij}b(j) + h.c. + \frac{U}{2} \sum_i n_i^2 \]  

where the \( U_1 = e^{i2\alpha} \), \( U_2 = e^{i2\beta} \) are the non-Abelian gauge fields put on the two links in the square lattice (Fig.1a), \( n_i = n_{x_i} + n_{y_i} \) is the total density. In this paper, we focus on spin-independent interaction [14]. Following [13], we find the Wilson loop [13] around one square (1) \( W = Tr[U_1U_2U_1^{-1}U_2^{-1}] = 2 - 4 \sin^2 \alpha \sin^2 \beta \). The \( W = \pm 2 \) (\( |W| < 2 \)) correspond to Abelian (non-Abelian) regimes (Fig.1b). In the following, we focus on the strong coupling limit \( U \gg t \).

In the strong coupling limit \( U \gg t \), to leading order in \( t^2/U \), we get a spin \( S = N/2 \) rotated Ferromagnetic Heisenberg (RH) model:

\[ H_{RH} = -J \sum_i \left[ S_i^a R^{ab}(\hat{x},2\alpha) S_{i+x}^b + S_i^a R^{ab}(\hat{y},2\beta) S_{i+y}^b \right] \]  

with a ferromagnetic (FM) interaction \( J = 4t^2/U \) and the sum is over the unit cell \( i \) in Fig.1a. The \( R(\hat{x},2\alpha), R(\hat{y},2\beta) \) are two \( SO(3) \) rotation matrices around the \( \hat{x}, \hat{y} \) spin axis by angle \( 2\alpha, 2\beta \) putting on the two bonds \( x, y \) respectively (Fig.1a). In fact, when expanding the two \( R \) matrices, one can see that Eq.2 leads to a Heisenberg + Kitaev [16,18] + Dzyaloshinskii-Moriya (DM) interaction: \( H_s = \sum_{(ij)} J_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_{(ij)} J^{ab}_{i} R^{ab}_{ij}(\hat{x},2\alpha) \vec{S}_i \cdot \vec{S}_j + \sum_{(ij)} J^{ab}_{i} R^{ab}_{ij}(\hat{y},2\beta) \vec{S}_i \times \vec{S}_j \). However, as we show in the following, the physics can be best read in the Rotated Heisenberg representation Eqn.2 instead of in the Heisenberg-Kitaev-DM representation.

Classification by Wilson loops in the RH model—It is convenient to introduce the R-matrix Wilson loop around a fundamental square (Fig.1a) \( W_R = Tr[R_x R_y R^{-1}_x R^{-1}_y] = [\cos(2\alpha) + \cos(2\beta) - \cos(2\alpha) \cos(2\beta)][2 + \cos(2\alpha) + \cos(2\beta) - \cos(2\alpha) \cos(2\beta)] \)

\[ = 0 \]  

which characterizes the equivalent class and frustrations in the RH model Eqn.2. The \( W_R = 3 \) (\( W_R \neq 3 \)) stands for the Abelian (non-Abelian) points (Fig.1b) [15]. For example, all the 4 edges and the center belong to Abelian points \( W_R = 3 \). All the other points belong to Non-Abelian points (Fig.1b). Obviously, any RH model with the same set of Wilson loops can be transformed to each other by performing local \( SO(3) \) transformations and belong to the same equivalent class. The classification according to the Wilson loops established connections among seemingly different phases.

In the \( S \rightarrow \infty \) limit, the RH model Eqn.2 becomes classical. Some interesting results on the possible rich classical ground states at general \( (\alpha, \beta) \) in the Heisenberg-Kitaev-DM representation were attempted numerically in [19,20]. Here, we study quantum phenomena in the RH model along the dashed line \( \alpha = \pi/2, 0 < \beta < \pi/2 \) in Fig.1c. Obviously, at \( \alpha = \beta = 0 \), the Hamiltonian becomes the usual FM Heisenberg model \( H = -J \sum_i \vec{S}_i \cdot \vec{S}_j \). At the two ends of the dashed line \( \alpha = \pi/2, \beta = 0 \) (\( \beta = \pi/2 \) in Fig.1c), we get the FM Heisenberg model in the rotated basis \( H = -J \sum_i \vec{S}_i \cdot \vec{S}_j \) where the \( \vec{S}_i \rightarrow \tilde{R}(\vec{x},\pi n_1) \vec{S}_i \). The most frustrated point with \( W_R = -1 \) is located at \( \beta = \pi/4 \). Along the dashed line, it can be shown that \( \sum_i (-1)^i S^y_i \) is a conserved quantity \( [H_0, \sum_i (-1)^i b^\dagger_i \sigma^y_i b_i] = 0 \). This hidden "U(1)" symmetry will become transparent after a local gauge transformation to the "U(1)" basis in Eqn.5. Obviously, this hidden "U(1)" symmetry [21] is kept in the RH model Eqn.2. \( H_{RH}, \sum_i (-1)^i S^y_i = 0 \). It is useful for us to identify the exact quantum ground state, also study the quantum and thermal fluctuations above the exact quantum ground state and their experimental consequences.

It is convenient to make a \( R_x(\pi/2) \) rotation to rotate spin Y axis to Z axis [22], then the Hamiltonian can be written as

\[ H = -J \sum_i \left[ \frac{1}{2} (S_i^a S_{i+x}^a + S_i^a S_{i-x}^a) - S_i^z S_{i+x}^z \right. \]

\[ \left. + \frac{1}{2} (e^{2i\beta} S_{i+y}^z S_{i+y}^z + e^{-2i\beta} S_{i+y}^z S_{i+y}^z) + S_i^z S_{i+y}^z \right] \]  

It is easy to show that the \( Y \rightarrow x \) state (Fig.2a) is the exact ground state with the ground state energy \( E_0 = -2NJS^2 \). The conserved quantity \( \sum_i (-1)^i S_i^y \) reaches its maximum value \( NS \) in the ground state.

Magnetization, specific heat and spin-spin correlation functions at low temperatures—Introducing HP bosons [23,24], \( S^+ = \sqrt{2S} - a\dagger a, S^- = a\dagger \sqrt{2S} - a\dagger a, S^z = S - a\dagger a \) for sublattice A and \( S^+ = b\dagger \sqrt{2S} - b\dagger b, S^- = \sqrt{2S} - b\dagger b, S^z = b\dagger b - S \) for the sublattice B in Fig.2a. The Hamiltonian can be easily diagonalized by a unitary transformation [23] in \( \vec{k} \) space:

\[ H = E_0 + 4JS \sum_k [E_+(k) \alpha^+_k \alpha_k + E_-(k) \beta^+_k \beta_k] \]
where $\vec{k}$ belongs to the Reduced Brillouin Zone (RBZ) and $E_{\pm}(k) = 1 - \frac{1}{2}\cos 2\beta \cos k_y \pm \frac{1}{2}\sqrt{\cos^2 k_x + \sin^2 2\beta \sin^2 k_y}$ are the excitation spectra of the acoustic and optical branches respectively. At the two Abelian points $\beta = 0, \pi/2$, as shown above, the system has SU(2) symmetry in the rotated basis, Eqn.4 reduces to the FM spin wave excitation spectrum $\omega \sim k^2$ at the minima $(0,0)$ $(0,\pi)$. The positions of the minima and the gap at the minima of both branches are shown in Fig.2b. The most striking feature is that there is a continuously changing minima position along the dashed line in Fig.1c which have striking experimental consequences to be discussed in the following.

At the two Abelian points, at any finite $T$, the spin wave fluctuations will destroy the FM order as dictated by the Mermin-Wegner theorem. However, at any non-Abelian points along the dashed line, although the ground state remains a $Y-x$ ground state (Fig.2a), there is a gap $\Delta_{-}(\beta)$ in the excitation spectrum, so the order survives up to a finite critical temperature $T_c \sim \Delta_{-}(\beta)$. At low temperatures $T < T_c$ in Fig.3, one can ignore the optical branch. Expect at $\beta_1(\beta_2 = \pi/2 - \beta_1)$, the acoustic branch can be expanded around the minima $k = k_0 + \mathbf{q}$ as $E_{\pm}(\mathbf{q}; \beta) = \Delta_{-}(\beta) + \frac{q_x^2}{2m_x(\beta)} + \frac{q_y^2}{2m_y(\beta)}$ where the masses $m_x(\beta), m_y(\beta)$ are listed in [27]. We then obtain the magnetization $M(T)$ and specific heat $C(T)$:

$$M(T) = S - \frac{\sqrt{m_x m_y}}{2\pi} T e^{-\Delta/T}$$

$$C(T) = \frac{\sqrt{m_x m_y}}{2\pi} \frac{(\Delta^2/T)}{e^{-\Delta/T}}$$  \hspace{1cm} (5)

where $\Delta = \Delta_{-}(\beta)$. Both quantities can be easily measured in elastic Bragg spectroscopy [30, 31] and specific heat experiments respectively [28].

For the two sublattice structure A and B (Fig.2a), one can define the uniform spin $\vec{M} = (\vec{S}_A + \vec{S}_B)/2$ and the staggered spin $\vec{N} = \vec{S}_A - \vec{S}_B$. Then one can define the uniform $S_{\pm}^m(\bar{k}, t) = \langle M_l(\bar{k}, t)M_m(\bar{k}, 0) \rangle, l = 1, 2, 3$ and staggered $S_{\pm}^m(\bar{k}, t) = \langle N_l(\bar{k}, t)N_m(\bar{k}, 0) \rangle, l = 1, 2, 3$ spin-spin correlation functions [29]. From Eqn.4 one can evaluate the uniform normal and anomalous transverse dynamic spin-spin correlation functions:

$$S_{+}^{-}(\mathbf{k}, \omega) = \pi \left| \frac{\sin^2 \frac{\theta_k}{2}}{1 - e^{-\omega/T}} \right| \left[ \delta(\omega - E_k) - \delta(\omega + E_k) \right]$$

$$S_{-}^{+}(\mathbf{k}, \omega) = \frac{1}{2} \sin \theta_k \left[ \delta(\omega - E_k) - \delta(\omega + E_k) \right]$$

$$S_{+}^{++}(\mathbf{k}, \omega) = \pi \left| \frac{\sin \theta_k}{1 - e^{-\omega/T}} \right| \left[ \delta(\omega - E_k) - \delta(\omega + E_k) \right]$$

where the spectral weights are determined by the coefficients of the unitary transformation [26].

In fact, the hidden "$U(1)$" symmetry dictates the relations between the uniform and staggered correlation functions $S_{\pm}^{-}(\mathbf{k}, \omega) = S_{\pm}^{+}(\mathbf{k}, \omega)$ and $S_{\pm}^{+}(\mathbf{k}, \omega) = -S_{\pm}^{+}(\mathbf{k}, \omega)$. The equal time spin structure factor $S_{\pm}^{m}(\bar{k}) = \int d\omega S_{\pm}^{m}(\bar{k}, \omega)$ follows. As shown explicitly in the SM [31], at $T < \Delta_{-}(\beta)$, the peak positions of $S_{\pm}^{+}(\mathbf{k})$ and $S_{\pm}^{+}(\mathbf{k})$ are precisely determined by the continuously changing minimum positions $k_0 = (0, k_y^0)$ shown in Fig.2b. All these correlation functions can be easily detected by light or atom Bragg scattering experiments [30]. So the continuously changing minimum positions the optical $E_k^+$, the acoustic $E_k^-$ excitation spectra in Fig.2b can be extracted from the peak positions of inelastic scattering cross sections of these experiments.

Specific heat and spin structure factor at high temperatures— It was known that the spin wave expansion only works at low temperature $T \ll T_c$. At high temperatures $T \gg T_c$, one needs to use the high temperature expansion by expanding the spectral weight $e^{-H/T} = \sum_{n=0}^{\infty} \frac{(T/T_c)^n}{n!}$ In this subsection, we focus on $S = 1/2$.

At $T > T_c$, the magnetization vanishes, the symmetry of the Hamiltonian Eqn.4 was restored, so there is no $A$ and $B$ structure anymore. We get the equal-time normal and anomalous transverse spin-structure factors to the

FIG. 2. (a) The exact ground state is the $Y-x$ state where the first capital letter indicates spin polarization along $Y$ direction, the second small letter indicates the orbital ordering along the $x$ bond. (b) The minima position $k_0 = (k_x, 0, k_y^0)$ in the RBZ of the acoustic branch and its gap $\Delta_{-}(\beta)$ at the minima. When $0 < \beta < \beta_1 = \arccos \frac{\sqrt{2}}{2} \approx 0.44\pi$, the minima is at $k_y^0 = 0$ with the gap $\Delta_{-}(\beta) = \sin^2 \beta$. When $\beta_1 < \beta < \beta_2 = \pi/2 - \beta_1$, the minima is at $k_y^0 = \pm \arccos \left( \frac{1 + \sin^2 2\beta}{1 - \sin 2\beta} \right)$ with the gap $\Delta_{-}(\beta) = 1 - \frac{1 + \sin^2 2\beta}{1 - \sin 2\beta}$.

When $\beta_2 < \beta < \pi/2$, the minima is at $k_y^0 = \pm \pi$ with the gap $\Delta_{-}(\beta) = \cos^2 \beta$. The $\Delta_{+}(\beta)$ is the minima gap of the optical branch. When $\beta < \pi/4$, the minimum is at $k_y^0 = (\pi/2,0)$ with the gap $\Delta_{+}(\beta) = 1 - \frac{1}{2}\cos 2\beta$. When $\beta > \pi/4$, the minimum is $k_y^0 = (\pi/2, \pi)$ with $\Delta_{+}(\beta) = 1 + \frac{1}{2}\cos 2\beta$. The position of maxima gap of both branches coincides with the most frustrated point $\beta = \pi/4$ in Fig.1c.
order of \( (J/T)^2 \):

\[
S^{+-}(k) = \left( \frac{J}{4T} - \frac{J^2}{16T^2} \right) \cos(k_y + 2\beta)
+ \frac{J^2}{16T^2} \left[ \cos(2k_x + \cos(2k_y + 4\beta) \right]
\]

\[
S^{++}(k) = \left( \frac{J}{4T} - \frac{J^2}{16T^2} \right) \cos(k_x + \frac{J^2}{8T^2} \cos 2\beta
\times \left[ \cos(k_x + k_y) + \cos(k_x - k_y) \right]
\]

(7)

whose explicit dependence on the gauge parameter \( \beta \) can be easily detected by light or atom Bragg scattering experiments \[30\].

We obtain the high temperature expansion of the specific heat per site to the order of \( (J/T)^4 \):

\[
C_v/N = \frac{3}{8} \frac{J^2}{T^2} - \frac{3}{16} \frac{J^3}{T^3} + \frac{12 \cos 4\beta - 33}{128} \frac{J^4}{T^4}
\]

(8)

which depends on \( \beta \) starting at the order of \( (J/T)^4 \). Obviously, at the two Abelian points \( \beta = 0, \pi/2 \), it recovers that of the Heisenberg model to the same order, reaches the minimum at the most frustrated point \( \beta = \pi/4 \) (Fig.1c). This cosine dependence along the dashed line can be easily detected by cold atom experiments \[28\].

Experimental realizations of the RH models, detections at low and high temperatures— By a local gauge transformation \( \tilde{b}_i = (i\sigma_x)^{\alpha} b_i \) on Eqn.1 along the dashed line in Fig.1c to get rid of the gauge fields on all the \( x^- \) links, then a global rotation \( \tilde{b}_i = e^{-i\tilde{q} \cdot \tilde{x} \cdot \tilde{b}_i} \) to rotate \( S^y \) to \( S^z \), Eqn.1 becomes:

\[
H_{U(1)} = -t \sum_i \left[ \tilde{\sigma}_i \tilde{b}_{i+x} + \tilde{\sigma}_i \tilde{b}_{i+y} + h.c. \right] + \frac{U}{2} \sum_i \tilde{\sigma}_i^2
\]

(9)

where all the remaining gauge fields on the \( y^- \) links commute. Obviously, the hidden \( U(1) \) symmetry in the original basis Eqn.1 becomes explicit in this \( U(1) \) basis with the conserved quantity \( \sum_i \tilde{S}_i^z = \sum_i \tilde{S}_i^y = \sum_i (-1)^i \tilde{S}_i^y \). In Fig.3, we contrast the gauge field configurations in the \( U(1) \) basis with that quantum spin Hall effect realized in recent experiments \[31\]. In the \( U(1) \) basis, for the spin up, the magnetic field is \( \pm 2\beta \) alternating along \( x \) direction, for spin down, the magnetic field is just reversed to keep the Time reversal symmetry. So for the spin up, the staggered magnetic field can be precisely realized in the previous experiments \[7, 8\]. For the spin down, as demonstrated in \[11\], if it carries opposite magnetic moment to the spin up state, then it will experience precisely opposite magnetic field. So the \( U(1) \) basis can be easily realized in a simple combination of previous + recent experiments. As pointed out in \[11\], non-Abelian gauge in Eqn.1 can be achieved by adding spin-flip Raman lasers to induce a \( \sigma_x \) term along the horizontal bond in Fig.1a, or by driving the spin-flip transition with RF or microwave fields. If so, the original basis can also be realized in near future experiments.

It was known \[30\] that for \( V_0/E_r \geq 10 \) where \( V_0 \) is the optical lattice potential and \( E_r \) is the recoil energy, the spinor boson Hubbard model Eqn.1 is well within the strong coupling regime \( J \ll t \ll U \). For \( ^{87} \)Rb atoms used in the recent experiments \[9, 11\], the superfluid-insulator transition is estimated to be \( V_0/E_r \sim 12 \), so the RH model Eqn.2 applies well in the regime. Near the most frustrated point \( \beta = \pi/4 \), the critical temperature \( T_c \sim J \sim 0.2nK \). It remains experimentally challenging to reach such low temperatures \[36\]. However, in view of two recent advances of new cooling techniques \[37, 38\] to reach \( 0.35nK \), the obstacles maybe overcome in the near future. Before reaching such low temperatures, the specific heat measurement \[28\] at high temperatures to demonstrate the \( \cos 4\beta \) dependence along the dashed line in Fig.1c could be performed easily.

In the strong coupling limit, the RH model in the \( U(1) \) basis was written in the SM \[31\]. Many physical quantities such as the gap, Density of states, \( T_c \), specific heat \( C_v \) and magnetization \( M(T) \) are independent of gauge choices. However, all the spin-spin correlation functions Eqn.7 are gauge-dependent \[12\] and computed in the \( U(1) \) basis in the SM \[31\].

Conclusions and perspectives— In this paper, we show that the Rotated Heisenberg model Eqn.2 is a new class of quantum spin models which display a new class of spinorbital correlated quantum phases, excitation spectra and quantum phase transitions. The RH model along the dashed line in Fig.1c in a special gauge can be easily and naturally realized in current experiments. The RH model in other gauges may inspire new experiments to generate various kinds of interpaly between SOC and interaction to observe these fantastic phenomena. They should also shed considerable lights to explore new class of states in strongly correlated electron materials also with strong SOC \[5\]. Extensions to general \( (\alpha, \beta) \) in Fig.1c, other bipartite lattices or frustrated lattice geometries, higher dimensions are being investigated by various analytic and numerical methods. Rotated Anti-ferromagnetic Heisenberg model which show dramatically different quantum phenomena will be presented elsewhere \[39\].

We thank Yi-Xiang Yu and Ruquan Wang for very helpful discussions. This research is supported by NSF-
There are other strong coupling models, for example: Stephan Rachel and Karyn Le Hur, Phys. Rev. B 82, 075106 (2010); These authors studied the effects of $U$ on Kane-Lee model \cite{18} (called Kane-Mele-Hubbard model with the $S^z$ conserving SOC). Raniel Cocks, et.al, Phys. Rev. Lett. 109, 205303 (2012) which studied Time-reversal invariant Hofstadter-Hubbard model of spin $1/2$ fermions hopping on a square lattice subject to an Abelian flux $\alpha = p/q$. This is the quantum spin Hall effects model in Fig.3b. S. R. Hassan, et.al, Phys. Rev. Lett. 110, 037201 (2013) which discussed a model whose hopping terms break time-reversal, to the leading order in the strong coupling expansion, it leads to the Heisenberg-Kitaev model in \cite{17}. Our RH model Eqn.\ref{2} is completely different than these models.

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The unitary transformation is

\[
\left( \begin{array}{c} a_k \\ b_k \end{array} \right) = \frac{1}{\sqrt{\cos^2 k_x + \sin^2 k_x}} \left( \begin{array}{c} \sin \theta_k \\ \cos \theta_k \end{array} \right) \left( \begin{array}{c} \alpha_k \\ \beta_k \end{array} \right) = \frac{1}{\sqrt{\cos^2 k_x + \sin^2 k_x}} \left( \begin{array}{c} \sin k_x \\ \cos k_x \end{array} \right) \left( \begin{array}{c} \sin k_z \\ \cos k_z \end{array} \right) \left( \begin{array}{c} \sin \beta_k \\ \cos \beta_k \end{array} \right)
\]

\[
\sin \beta_k = \frac{\sqrt{\cos^2 k_x + \sin^2 k_x} \sin^2 k_z}{\sqrt{\cos^2 k_x + \sin^2 k_x}} \sin \beta_k
\]

\[
\cos \beta_k = \frac{\sqrt{\cos^2 k_x + \sin^2 k_x} \sin^2 k_z}{\sqrt{\cos^2 k_x + \sin^2 k_x}} \sin \beta_k
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\[
\cos \beta_k = \frac{\sqrt{\cos^2 k_x + \sin^2 k_x} \sin^2 k_z}{\sqrt{\cos^2 k_x + \sin^2 k_x}} \sin \beta_k
\]
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Supplementary material for "Rotated Ferromagnetic Heisenberg model"

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In this Supplementary material, we use M to stand for the figures and equations in the main text.

I. SPIN-SPIN CORRELATION FUNCTIONS IN THE ORIGINAL BASIS

The dynamic transverse spin-spin correlation functions have been discussed in the main text. The crucial conclusion that the continuously changing minimum positions of the excitation spectrum can be mapped out by the peak positions of equal-time transverse spin structure factors at low temperatures is also stated in the main text. Here, we give some details and also calculate the longitudinal correlation functions.

A. Symmetry breaking analysis

Along the dashed line ($\alpha = \pi/2, \beta$), the bosonic model Eqn.M1 has Time reversal $\vec{k} \rightarrow -\vec{k}, \vec{S} \rightarrow -\vec{S}$ (but the position is kept fixed), translational symmetry and a $Z_2$ symmetry $k_y \rightarrow -k_y, S^y \rightarrow -S^y, S^x \rightarrow S^x, S^z \rightarrow -S^z$. Of course, at the two Abelian points, the symmetry is enlarged to $SU(2)$ symmetry in the corresponding rotated basis. The $Y - x$ ground state in the Fig.M2(a) breaks all these discrete symmetries. But it still keeps the hidden $U(1)$ symmetry.

In the strong coupling limit, along the dashed line ($\alpha = \pi/2, \beta$), after rotating spin axis from $Y$ to $Z$, the RH model Eqn.M2 has the Time reversal symmetry $S^z \rightarrow -S^z, S^+ \leftrightarrow -S^-, i \rightarrow -i$ (here $i$ is the imaginary unit, not the site index). Translational symmetry and the $Z_2$ symmetry $S_j^z \rightarrow -S_j^z, S_j^+ \leftrightarrow S_j^-$ where $j$ is the image of the site $j$ reflected with respect to $x$ axis. Of course, at the two Abelian points, the symmetry is enlarged to $SU(2)$ symmetry in the corresponding rotated basis. The $Y - x$ ground state in the Fig.M2(a) breaks all these discrete symmetries. But it still keeps the hidden $U(1)$ symmetry.

As shown in I-C-1, the magnetization $M(T)$ Eqn.M5 in the $Y - x$ ground state can be determined by elastic Bragg spectroscopy in the longitudinal staggered spin-spin correlation function at low temperatures.

B. Peak positions of the Equal-time transverse spin structure factors at low temperatures

From Eqn.M6, we obtain equal-time spin structure factor $S_{u,s}^{lm}(\vec{k}) = \int \frac{d\omega}{2\pi} S_{u,s}^{lm}(\vec{k}, \omega)$:

$$
S_{u}^{+-}(k) = S_{s}^{+-}(k) = \frac{1}{2} + \frac{\cos^2 \theta_k}{e^{E_k^L/T} - 1} + \frac{\sin^2 \theta_k}{e^{E_k^L/T} - 1},
$$

$$
S_{u}^{++}(k) = -S_{s}^{++}(k) = \frac{1}{2} \sin \theta_k \left( \frac{1}{e^{E_k^L/T} - 1} - \frac{1}{e^{E_k^L/T} + 1} \right) \quad (1)
$$

One can see that at $T \ll T_C \sim \Delta_{-}(\beta)$ (Fig.M2b), the acoustic branch dominates over the optical branch, then the peak position of $S_{u}^{+-}(k)$ and $S_{s}^{++}(k)$ are completely determined by the minimum position $k_0 = (0, k_y^0)$ of the acoustic branch shown in Fig.M2b. As said in the main text, expect at $\beta_1 (\beta_2 = \pi/2 - \beta_1)$, the excitation spectrum can be expanded around the minima $k = k_0 + q$ as $E_{-}(q; \beta) = \Delta_{-}(\beta) + \frac{q_x^2}{2m_x(\beta)} + \frac{q_y^2}{2m_y(\beta)}$ where the masses $m_x(\beta), m_y(\beta)$...
are given in the main text. We reach simplified and physically transparent expressions:

\[ S_{u}^{+−}(k) = S_{s}^{+−}(k) \sim \frac{1}{2} + \cos^{2} \frac{\theta k}{2} e^{−\Delta_{−}(β)/T} e^{−(\frac{g^{2}}{m_{u}(β)} + \frac{g^{2}}{m_{s}(β)})/T} \]

\[ S_{u}^{++}(k) = −S_{s}^{++}(k) \sim \frac{1}{2} \sin \theta k e^{−\Delta_{+}(β)/T} e^{−(\frac{g^{2}}{m_{u}(β)} + \frac{g^{2}}{m_{s}(β)})/T} \]

(2)

where \( k \) belongs to Reduced Brillouin Zone (RBZ).

Therefore, the peak positions of the structure factors \( S_{u}^{+−}(k) \) and \( S_{u}^{++}(k) \) are precisely determined by the continuously changing minimum position \( k_0 \) tuned by the SOC strength, which can be measured by the inelastic Bragg spectroscopy at low temperatures.

Here it is instructive to compare with the equal-time spin structure factors of some well-known models. For the Heisenberg Ferromagnetic, Anti-Ferromagnetic or Kitaev model. The peak positions should be at \((0,0)\) or \((π,π)\), a broad continuous spectrum respectively. For the Heisenberg-Kitaev model, in some parameter space, the peak positions should be at the corresponding momentum for the FM state, Stripy state (which is a FM state in a rotated basis), then broad continuous spectrum in the spin liquid state sandwiched between the two FM state. For the other parameter space, the peak positions should be at the corresponding momentum for the AFM state, Zigzag state (which is a AFM state in a rotated basis), then broad continuous spectrum in the spin liquid state sandwiched between the two AFM state. So the continuously changing peak position \( k_0 \) tuned by the SOC strength is the most striking new and unique feature of the RH model.

C. Longitudinal spin-spin correlation functions

In the main text, we evaluated the uniform, staggered transverse spin-spin correlation functions. Here, we will compute the longitudinal spin-spin correlation functions.

1. Magnetization and ground state detection at low temperatures: Spin wave expansions—

One can also evaluate the uniform and staggered connected dynamic longitudinal spin-spin correlation functions at low temperatures:

\[ S_{u}^{zz}(k,ω) = \frac{2π}{N} \sum_{q} \left\{ \cos^{2} \frac{θ q + θ q+k}{2} [n_{q}^{+} (1 + n_{q+k}^{-}) δ(ω + E_{q}^{+} − E_{q+k}^{-}) + n_{q}^{-} (1 + n_{q+k}^{+}) δ(ω + E_{q}^{-} − E_{q+k}^{+})] \right\} \]

\[ \quad + \sin^{2} \frac{θ q + θ q+k}{2} [n_{q}^{+} (1 + n_{q+k}^{-}) δ(ω + E_{q}^{+} − E_{q+k}^{-}) + n_{q}^{-} (1 + n_{q+k}^{+}) δ(ω + E_{q}^{-} − E_{q+k}^{+})] \]

\[ S_{s}^{zz}(k,ω) = \frac{2π}{N} \sum_{q} \left\{ \cos^{2} \frac{θ q - θ q+k}{2} [n_{q}^{+} (1 + n_{q+k}^{-}) δ(ω + E_{q}^{+} − E_{q+k}^{-}) + n_{q}^{-} (1 + n_{q+k}^{+}) δ(ω + E_{q}^{-} − E_{q+k}^{+})] \right\} \]

\[ \quad + \sin^{2} \frac{θ q - θ q+k}{2} [n_{q}^{+} (1 + n_{q+k}^{-}) δ(ω + E_{q}^{+} − E_{q+k}^{-}) + n_{q}^{-} (1 + n_{q+k}^{+}) δ(ω + E_{q}^{-} − E_{q+k}^{+})] \]

(3)

which include both the intra-band transitions and the inter-band transition between the optical \( E_{k}^{+} \) and the acoustic \( E_{k}^{-} \).

It is easy to see that due to the summation over the momentum transfer in Eqn.3, so the dynamic connected longitudinal spin-spin correlation functions will just show a broad distribution, in sharp contrast to the transverse dynamic correlation functions Eqn.M6 discussed in the main text.

The equal-time longitudinal spin structure factors follow \( S_{u,s}^{zz}(k) = \int \frac{dω}{2π} S_{u,s}^{zz}(k,ω) \):

\[ S_{u}^{zz}(k) = \frac{1}{N} \sum_{q} \left\{ \cos^{2} \frac{θ q + θ q+k}{2} [n_{q}^{+} (1 + n_{q+k}^{-}) + n_{q}^{-} (1 + n_{q+k}^{+})] + \sin^{2} \frac{θ q + θ q+k}{2} [n_{q}^{+} (1 + n_{q+k}^{-}) + n_{q}^{-} (1 + n_{q+k}^{+})] \right\} \]

\[ S_{s}^{zz}(k) = \frac{1}{N} \sum_{q} \left\{ \cos^{2} \frac{θ q - θ q+k}{2} [n_{q}^{+} (1 + n_{q+k}^{-}) + n_{q}^{-} (1 + n_{q+k}^{+})] + \sin^{2} \frac{θ q - θ q+k}{2} [n_{q}^{+} (1 + n_{q+k}^{-}) + n_{q}^{-} (1 + n_{q+k}^{+})] \right\} \]
which, at low temperatures $T < \Delta_-(\beta)$, can be simplified to:

\begin{align}
S_{u}^{zz}(k) &= \frac{1}{N} \sum_{q} (n_{q}^{+} + n_{q}^{-}) + \frac{1}{N} \sum_{q} \cos^{2} \frac{\theta_{q} + \theta_{q+k}}{2} n_{q}^{-} n_{q+k}^{-} + \cdots \\
S_{s}^{zz}(k) &= \frac{1}{N} \sum_{q} (n_{q}^{+} + n_{q}^{-}) + \frac{1}{N} \sum_{q} \cos^{2} \frac{\theta_{q} - \theta_{q+k}}{2} n_{q}^{-} n_{q+k}^{-} + \cdots
\end{align}

where \cdots mean the sub-leading terms at low temperatures. Again, due to the the summation over the momentum transfer in Eqn4 so the longitudinal spin structure factors will just show a broad distribution, in sharp contrast to the transverse spin structure factors in Eqn1.

Note that in the staggered connected dynamic (equal-time) longitudinal spin-spin correlation function $S_{u}^{zz}(k, \omega)$ in Eqn3 (in Eqn1), we have subtracted the magnetization part $M^{2}(T)\delta_{k,0}2\pi\delta(\omega)$ ( $M^{2}(T)\delta_{k,0}$) due to the symmetry breaking in the quantum ground state in Fig.M2a. The magnetization $M(T)$ is given by Eqn.M5. The symmetry breaking can be detected easily by elastic longitudinal Bragg spectroscopy peak at momentum $(\pi,0)$ ( $(0,0)$ in the RBZ) at low temperatures.

2. High temperatures: high temperature expansions—

One can also evaluate the equal-time longitudinal spin structure factor at high temperatures:

\begin{equation}
S^{zz}(k) = \left( \frac{J}{8T} + \frac{J^{2}}{32T^{2}} \right) [\cos k_{x} - \cos k_{y}] + \frac{J^{2}}{32T^{2}} [\cos 2k_{x} + \cos 2k_{y}] - \frac{J^{2}}{16T^{2}} [\cos(k_{x} + k_{y}) + \cos(k_{x} - k_{y})]
\end{equation}

which is independent of $\beta$ to the order of $(J/T)^{2}$. In fact, it can be shown that Eqn6 coincides with that of the Heisenberg model to the same order.

In order to make comparisons with the low temperature expressions Eqn3 also contrast with the corresponding expressions in the $U(1)$ basis to be discussed in the following section, we split Eqn4 into sublattice A and B in Fig.M2a, then form a uniform and staggered spin structure factors:

\begin{align}
S_{u}^{zz}(k) &= \left( \frac{J}{8T} + \frac{J^{2}}{32T^{2}} \right) [\cos k_{x} - \cos k_{y}] + \frac{J^{2}}{32T^{2}} [\cos 2k_{x} + \cos 2k_{y}] - \frac{J^{2}}{16T^{2}} [\cos(k_{x} + k_{y}) + \cos(k_{x} - k_{y})] \\
S_{s}^{zz}(k) &= \left( \frac{J}{8T} - \frac{J^{2}}{32T^{2}} \right) [\cos k_{x} + \cos k_{y}] + \frac{J^{2}}{32T^{2}} [\cos 2k_{x} + \cos 2k_{y}] + \frac{J^{2}}{16T^{2}} [\cos(k_{x} + k_{y}) + \cos(k_{x} - k_{y})]
\end{align}

which will be compared to those in the $U(1)$ basis below.

II. SPIN-SPIN CORRELATION FUNCTIONS IN THE $U(1)$ BASIS

As shown in the main text, the $U(1)$ basis can be realized in current experiments easily, so it is important to work out various experimental measurable quantities in this basis explicitly. As first stressed in\footnote{This is a footnote.} that in contrast to condensed matter experiments where only gauge invariant quantities can be measured, both gauge invariant and non-gauge invariant quantities can be measured by experimentally generating various non-Abelian gauges corresponding to the same set of Wilson loops. Some quantities such as the the magnetization, specific heat gaps and density of states are gauge invariant, so are the same in both basis. However, the spin-spin correlations functions are gauge dependent\footnote{Another footnote.}, so will be explicitly computed here.

We first make a local rotation $\hat{S}_{n} = R(\hat{x}, \pi n_{1})\hat{S}_{n}$ to get rid of the $R$-matrix on the $x$-links in Fig.M1a, then just as in the original basis, we make a global rotation\footnote{This is another footnote.} $\hat{S}_{n} = R_{x}(\pi/2)\hat{S}_{n}$ to rotate the spin quantization axis from $Y$ to $Z$, we reach the Hamiltonian in the $U(1)$ basis:\footnote{This is yet another footnote.}

\begin{equation}
H_{U(1)} = -J \sum_{j \in A} \left[ \frac{1}{2} (S_{i}^{z} S_{i+1}^{z} + S_{i}^{z} S_{i-1}^{z}) + S_{i}^{z} S_{i+1}^{z} + \frac{1}{2} (e^{i2\beta} S_{i}^{z} S_{i+1}^{z} + e^{-i2\beta} S_{i}^{z} S_{i+1}^{z}) + S_{i}^{z} S_{i+1}^{z} \right] \\
- J \sum_{j \in B} \left[ \frac{1}{2} (S_{i}^{z} S_{j+1}^{z} + S_{i}^{z} S_{j-1}^{z}) + S_{j}^{z} S_{j+1}^{z} + \frac{1}{2} (e^{i2\beta} S_{j}^{z} S_{j+1}^{z} + e^{-i2\beta} S_{j}^{z} S_{j+1}^{z}) + S_{j}^{z} S_{j+1}^{z} \right]
\end{equation}
where A and B are the two sublattices in Fig. M2a.

By comparing with the Hamiltonian in the original basis Eqn. M3 in the main text, we can see that in the $U(1)$ basis, due to the absence of the anomalous terms like $S^+S^+$ or $S^-S^-$, the $U(1)$ symmetry with the conservation $\sum_i S_i^z$ is explicit, but at the expense of the translational symmetry explicitly broken due to the local spin rotation $\hat{S}_n = R(\hat{x}, \pi n_1)\vec{S}_n$. It is easy to see the exact ground state $Y - x$ (Fig. M2a) in the original basis becomes simply a Ferromagnetic state along $Y$ direction in the $U(1)$ basis.

A. Spin-spin correlation functions at low temperatures: Spin wave expansions—

In the $U(1)$ basis Eqn.8 introducing two sets of HP bosons $S^+ = \sqrt{2S - a^\dagger a}$, $S^- = a^\dagger \sqrt{2S - a^\dagger a}$, $S^z = S - a^\dagger a$ for the sublattice A and $S^+ = \sqrt{2S - b^\dagger b}$, $S^- = b^\dagger \sqrt{2S - b^\dagger b}$, $S^z = S - b^\dagger b$ for the sublattice B, we find the Hamiltonian in terms of the HP bosons becomes identical to that in the original basis, so the excitation spectra in Eqn. M4 follow, the unique and salient features of the continuously changing minimum positions, the gaps of the acoustic and optical branches shown in Fig. M2b remain in the $U(1)$ basis.

1. Peak positions of dynamic transverse spin-spin correlation functions: excitation spectrum

Using the HP bosons, we find the uniform and staggered transverse dynamic spin-spin correlation functions:

$$S_{u,U(1)}^{+-}(k, \omega) = \frac{1}{2} \frac{1 - \sin \theta_k}{1 - e^{-E_k/T}} \delta(\omega - E_k^+) + \frac{1 + \sin \theta_k}{1 - e^{-E_k/T}} \delta(\omega - E_k^-)$$

$$S_{s,U(1)}^{+-}(k, \omega) = \frac{1}{2} \frac{1 + \sin \theta_k}{1 - e^{-E_k/T}} \delta(\omega - E_k^+) + \frac{1 - \sin \theta_k}{1 - e^{-E_k/T}} \delta(\omega - E_k^-)$$

which is indeed different from Eqn. M6 in the original basis, but can be achieved from Eqn. M6 by the local spin rotation $\hat{S}_n = R(\hat{x}, \pi n_1)\vec{S}_n$. Note that the $U(1)$ symmetry dictates that there is no anomalous spin-spin correlation functions $S_{u,U(1)}^{+-}(k, \omega) = S_{s,U(1)}^{+-}(k, \omega) = 0$.

Similar to the original basis Eqn. M6, the uniform and staggered transverse dynamic spin-spin correlation functions in Eqn. [10] can be easily detected by light or atom Bragg scattering experiments. So both the optical $E_k^*$ excitation spectra can be extracted from the peak positions of scattering cross sections of these experiments.

2. Peak positions of equal-time transverse spin structure factors: continuously changing minimum positions $k_0$.

The equal time spin structure factors $S_{u,s,U(1)}^{+-}(\k, \omega) = \int \frac{d^2k}{4\pi} S_{u,s,U(1)}^{+-}(\k, \omega)$ follow:

$$S_{u,U(1)}^{+-}(k) = 1 + \frac{1 + \sin \theta_k}{e^{E_k^-/T} - 1} + \frac{1 - \sin \theta_k}{e^{E_k^+/T} - 1}$$

$$S_{s,U(1)}^{+-}(k) = 1 + \frac{1 - \sin \theta_k}{e^{E_k^-/T} - 1} + \frac{1 + \sin \theta_k}{e^{E_k^+/T} - 1}$$

which has a very similar structure as Eqn. [10] in the original basis. So the same manipulations following Eqn. [10] apply here also. We conclude that in the $U(1)$ basis, the continuously changing minimum position $k_0$ in Fig. M2b will be precisely mapped out by the continuously changing peak position $k_0$ of the structure factors $S_{u,U(1)}^{+-}(k)$ and $S_{s,U(1)}^{+-}(k)$, which can be measured by the Bragg spectroscopy at low temperatures.$^5$

3. Magnetization and ground state detection in longitudinal connected spin correlation functions and spin structure factors

We can also obtain the longitudinal spin-spin correlation functions. They are again related to Eqn. [8] by the local spin rotation $\hat{S}_n = R(\hat{x}, \pi n_1)\vec{S}_n$ which leads to a very simple relation between the two basis: $S_{u,U(1)}^{zz}(k, \omega) = S_{s,U(1)}^{zz}(k, \omega)$, $S_{s,U(1)}^{zz}(k, \omega) = S_{s,U(1)}^{zz}(k, \omega)$, namely, there is an exchange between uniform and staggered components. So they just show a broad distribution, in sharp contrast to the transverse dynamic correlation functions. Eqn. [9]

Similarly, the equal-spin longitudinal structure factors $S_{u,U(1)}^{zz}(k) = S_{s,U(1)}^{zz}(k)$, $S_{s,U(1)}^{zz}(k) = S_{s,U(1)}^{zz}(k)$ in Eqn. [9] also display a broad distribution.

Note that in contrast to the original basis discussed in Sec. III-A, now the magnetization part $M^2(T)\delta_{k,0}2\pi\delta(\omega)$ ( $M^2(T)\delta_{k,0}$) due to the quantum ground state in Fig. M2a appear in the the uniform connected dynamic (equal-time) longitudinal spin-spin correlation function $S_{u,U(1)}^{zz}(k, \omega)$ ( $S_{s,U(1)}^{zz}(k)$) which can be detected easily by elastic longitudinal Bragg spectroscopy peak at momentum $(0,0)$ in the RBZ at low temperatures.$^5$
B. Spin structure factors at high temperatures: high temperature expansions

At high temperature, even the magnetization vanishes, the Hamiltonian Eqn.8 in the $U(1)$ basis still breaks the lattice into two sublattices A and B shown in Fig.M2a, so one still need to calculate the uniform and staggered spin structure factors separately. We get the uniform and staggered structure factors upto the order of $(J/T)^2$:

\[
\begin{align*}
S_{u,U(1)}^+(k) &= \left( \frac{J}{4T} - \frac{J^2}{16T^2} \right) \left[ \cos k_x + \cos 2\beta \cos k_y \right] + \frac{J^2}{16T^2} \left[ \cos 2k_x + \cos 4\beta \cos 2k_y \right] \\
&\quad + \frac{J^2}{8T^2} \cos 2\beta \left[ \cos(k_x + k_y) + \cos(k_x - k_y) \right] \\
S_{s,U(1)}^+(k) &= \left( \frac{J}{4T} - \frac{J^2}{16T^2} \right) \left[ - \cos k_x + \cos 2\beta \cos k_y \right] + \frac{J^2}{16T^2} \left[ \cos 2k_x + \cos 4\beta \cos 2k_y \right] \\
&\quad - \frac{J^2}{8T^2} \cos 2\beta \left[ \cos(k_x + k_y) + \cos(k_x - k_y) \right] \\
\end{align*}
\]

which are indeed different from Eqn.M7 in the original basis, but can be achieved from Eqn.M7 by the local spin rotation $\tilde{S}_n = R(\hat{x}, \pi n_1)S_n$. Both depend on $\beta$ explicitly and can be measured by Bragg spectroscopy experiments.

We can also obtain the longitudinal spin structure factors which is related to Eqn.6 by the local spin rotation $\tilde{S}_n = R(\hat{x}, \pi n_1)S_n$. Then just similar to the low temperatures, we find again there is a exchange between uniform and staggered components in the two basis: $S_{u,U(1)}^{zz}(k) = S_{s,U(1)}^{zz}(k), S_{s,U(1)}^{zz}(k) = S_{u,U(1)}^{zz}(k)$ listed in Eqn.7. So they are also independent of the gauge parameter $\beta$ upto the second order of $(J/T)^2$.

1. Jinwu Ye, et. al, Phys. Rev. A 83, 051604 (R) (2011); Ann. Phys. 328 (2013), 103-138.
2. Fadi Sun, Xiao-Lu Yu, Jinwu Ye, Heng Fan, W. M. Liu, Scientific Reports 3, 2119 (2013).
3. Ji Chaloupka, George Jackeli, and Giniyat Khaliullin, Phys. Rev. Lett. 110, 097204 (2013).
4. More directly, one can just put $\beta \sigma_x$ along the $y$ bonds in Fig.M1a. If one still put $\beta \sigma_y$ along the $y$ bonds in Fig.M1a, then the longitudinal spin-spin correlation function $S_{u,s}^{zz}$ should be understood as $S_{u,s}^{yy}$.
5. For simplicity, we drop the $\tilde{\cdot}$ on top of $S_n$.
6. Compared to the HP bosons introduced in the original basis in the main text, one can see the reverse of $S^z \rightarrow -S^z, S^+ \leftrightarrow S^-$ in the sublattice B.