Global phase diagram and chiral spin liquids in the extended spin-$\frac{1}{2}$ honeycomb XY model

Yixuan Huang,¹ Xiao-yu Dong,²,³ D. N. Sheng,² and C. S. Ting¹

¹Texas Center for Superconductivity, University of Houston, Houston, Texas 77204, USA.
²Department of Physics and Astronomy, California State University, Northridge, California 91330, USA.
³Department of Physics and Astronomy, Ghent University, Krijgslaan 281, 9000 Gent, Belgium

(Dated: December 25, 2019)

The frustrated XY model on the honeycomb lattice has drawn lots of attentions because of the potential emergence of chiral spin liquid (CSL) with the increasing of frustrations or competing interactions. In this work, we study the extended spin-$\frac{1}{2}$ XY model with nearest-neighbor ($J_1$), and next-nearest-neighbor ($J_2$) interactions in the presence of a three-spins chiral ($J_3$) term using density matrix renormalization group methods. We obtain a global phase diagram with both conventional ordered and topological ordered phases. In particular, the long-sought Kalmeyer–Laughlin CSL is shown to emerge under a small $J_3$ perturbation due to the interplay of the magnetic frustration and chiral interactions. The CSL, which is a non-magnetic phase, is identified by the scalar chiral order, the finite spin gap on a torus, and the chiral entanglement spectrum described by chiral $SU(2)_1$ conformal field theory.

Introduction. A spin liquid¹ features a highly frustrated phase with long range ground state entanglement²,³ and fractionalized quasi-particle excitations⁴–⁶ in the absence of conventional order. The exotic properties⁷–⁹ of the spin liquid are relevant to both unconventional superconductivity¹⁰–¹³ and topological quantum computation¹⁴. Among various kinds of spin liquids, the chiral spin liquid (CSL), which has gapped bulk and gapless chiral edge excitations, is proposed by Kalmeyer and Laughlin¹⁵. It has a non-trivial topological order, and belongs to the same topological class with the fractional quantum Hall states.

In recent years, there have been extensive studies to identify the CSL in realistic spin models on different geometries such as Kagome¹⁶–²⁰, triangle²¹,²², square²³, and honeycomb lattices²⁴. Interestingly, for the XY model on honeycomb lattice theoretical studies have suggested the existence of a CSL in the highly frustrated regime that is generated by the staggered Chern-Simons flux with nontrivial topology¹³,²⁵. However, so far there is no direct numerical evidence supporting this claim²⁶–³³, leaving the possible existence of a CSL in the honeycomb XY model as an open question.

Aside from the possible CSL, the XY model itself is expected to have a rich phase diagram because of the frustration induced by the next-nearest-neighbor coupling $J_2$. As the reminiscent of the debated intermediate phase in numerical studies, density matrix renormalization group (DMRG)²⁸,³¹ and coupled cluster method³³ studies suggest an Ising antiferromagnetic state. However, exact diagonalization (ED)²⁶,³⁴ and quantum Monte Carlo method studies²⁷,³⁵ suggest a Bose-metal phase with spinon Fermi surface³⁶. A very recent numerical study using ED reveals an emergent chiral order but the phase remains a topologically trivial chiral spin state³⁷. Up to now, the theoretical understanding of the phase diagram for honeycomb XY model is far from clear.

The aim of this letter is to provide strong numerical evidence of the long-sought CSL in the extended spin-$\frac{1}{2}$ XY model on the honeycomb lattice and clarify the conditions for such a phase to emerge. Based on large scale DMRG²⁸,³⁰ studies, we identify the global quantum phase diagram in the presence of the nearest, next-nearest XY spin couplings and three-spins chiral interactions $\vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k)$. While there are only magnetic ordered phase in the absence of the chiral couplings, the CSL emerges with finite chiral interactions, where the minimum $J_3$ required for the emergence of the CSL appears in the intermediate $J_2$ regime. This suggests a possible multi-degenerate point in the phase diagram, neighboring between Ising antiferromagnetic order, collinear/dimer order, and the CSL.

The CSL is identified in the extended regime above
the XY-plane Neel state and the Ising antiferromagnetic state induced by chiral interactions. We also obtain a chiral spin state at large $J_x$ with finite chiral order. The chiral spin state shows peaks in the spin structure factor that increase with system sizes, indicating a magnetic ordered state. The phases we find without the chiral term agree with previous numerical studies using DMRG.\textsuperscript{28} Our results demonstrate the importance of the interplay between the frustration and chiral interactions, which leads to a rich phase diagram.

**Model and method.** We investigate the extended spin-$\frac{1}{2}$ XY model with a uniform scalar chiral term using both infinite and finite size DMRG methods\textsuperscript{10,41} in the language of matrix product states.\textsuperscript{42} We use the cylindrical geometry with circumference up to 6 (8) unit cells in the finite (infinite) size systems except for the calculations of spin gap, which is based on smaller size toruses.

The Hamiltonian of the model is given as

$$H = J_1 \sum_{\langle i,j \rangle} (S^+_i S^-_j + h.c.) + J_2 \sum_{\langle (i,j) \rangle} (S^+_i S^-_j + h.c.) + J_\chi \sum_{i,j,k\in\Delta} \vec{S}_i \cdot (\vec{S}_j \times \vec{S}_k)$$

(1)

where $\langle i, j \rangle$ refers to the nearest-neighbor sites and $\langle (i, j) \rangle$ refers to the next-nearest-neighbor sites. $\{i, j, k\}$ in the summation $\sum_{\Delta}$ refers to the three neighboring sites of the smallest triangle taken clockwise as shown in Fig.\textsuperscript{1}. The chiral term could be derived as an effective Hamiltonian of the Hubbard model with an additional $\Phi$ flux through each elementary honeycomb.\textsuperscript{17,24,43,44} We set $J_1 = 1$ as the unit for the energy scale, and use the spin U(1) symmetry for better convergence.

**Phase diagram.** The ground state phase diagram is illustrated in Fig.\textsuperscript{1}. We use spin structure factors to identify magnetic ordered phases, and entanglement spectrum to identify the topological ordered CSL. For larger $J_\chi$, a magnetic ordered chiral spin state with nonzero scalar chiral order is also identified.

The static spin structure in the Brillouin zone is defined as

$$S(\vec{q}) = \frac{1}{N} \sum_{i,j} \langle \vec{S}_i, \vec{S}_j \rangle e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)}$$

(2)

For the XY-plane Neel state there are peaks at the Brillouin zone $\Gamma$ points in the static spin structure as shown in the inset of Fig.\textsuperscript{2}(a). The magnitude of the peak is plotted as a function of $J_\chi$ in Fig.\textsuperscript{2}(a). It decreases rapidly as $J_\chi$ increases, and disappears as the system transits into the CSL at $J_\chi \approx 0.15$. Similarly, the peak for the collinear order at various $J_x$ is given in Fig.\textsuperscript{2}(b). The inset of Fig.\textsuperscript{2}(b) shows the spin structure at $J_x = 0.01$ where the phase is dominant by the collinear order. The phase boundary could be identified by the sudden drop and the disappearance of the peak at $J_x \approx 0.06$. In the intermediate regime at $J_2 = 0.3$ and small $J_\chi$, the staggered on-site magnetization serves as the order parameter as shown in Fig.\textsuperscript{2}(c). This quantity shows a sudden drop from the Ising antiferromagnetic state to the CSL at $J_\chi \approx 0.04$, which determines the phase boundary.

Besides the magnetic order parameters, other properties such as the spin correlation, the entanglement entropy and spectrum are also used to identify the phase boundary. We have found consistence in those different measurements. As shown in Fig.\textsuperscript{2}(d), the spin correlat-
tions are strongly enhanced at $J_\chi \approx 0.04$ near the phase boundary between the Ising antiferromagnetic phase and the CSL, while both phases have exponentially decaying spin correlations. The phase boundary determined by the spin correlation is the same as the one by the staggered magnetization.

Both CSL and the chiral spin state in the larger $J_\chi$ regime have a finite scalar chiral order that is defined as

$$\langle \chi \rangle = \frac{1}{3N} \sum_{i,j,k \in \Delta} \sum_{S} \langle \hat{S}_j \times \hat{S}_k \rangle$$  

(3)

As shown by the red curve in Fig.2(c), the chiral order increases monotonically with the increase of $J_\chi$ in the chiral spin liquid and chiral spin state, and saturates around $\langle \chi \rangle \approx 0.177$. The spin correlations in these two states are given in Fig.2(d) as examples at $J_\chi = 0.08$, and $0.14(0.25)$ respectively, where they remain exponentially decay. However, the spin correlation increases generally as $J_\chi$ increases. As shown in Fig.4(b), for the parameters we labeled as chiral spin state, the spin structure factors show sharp peaks, with the magnitudes of the peak values increasing with system sizes, suggesting a magnetic ordered state in the larger $J_\chi$ regime. We also notice that the spin structure of this chiral spin state shares the same peaks as the tetrahedral phase(see Appendix), and we do not rule out the possibility of tetrahedral magnetic order in this regime.

The extended regime of $J_2 > 0.6$ and $J_2 < 0.1$ are not our main focus in this letter because we are interested in the intermediate $J_2$ regime with strong frustration, but we do find that the CSL extends to a relatively large $J_\chi \approx 0.5$ at $J_2 = 0$. This implies that the CSL could survive even without the frustration induced by second nearest neighbor interactions in the XY model, which may be interesting for future study. In the regime labeled as collinear/dimer, we also find a non-magnetic dimer ground state in close competition with the collinear state at $J_1 > 0.55$. As pointed out in Ref.28, the actual ground state depends on the system size and XC/YC geometry, and we will not try to resolve this close competition here.

The phase near the critical point of $J_2 \approx 0.36$, $J_\chi \approx 0.02$ is hard to define numerically because different spin orders are mixed together in the low energy spectrum, thus the spin correlation is generally large. Here the phase boundary is measured by the unique properties of the CSL through the entanglement spectrum as discussed below, and it will be marked by the dash line as a guide to the eye.

**Chiral spin liquid.** The CSL is characterized by the twofold topological degenerate ground states, which are called ground state in vacuum and spinon sectors26,46, respectively. The entanglement spectrum (ES) of the ground state corresponds to the physical edge spectrum that is created by cutting the system in half47. Following the chiral SU(2)$_1$ conformal field theory48, the leading ES of a gapped CSL has a degeneracy pattern of 1,1,2,3,5...49. As shown in Fig.3(a) and (b), the ES in the CSL phase has such quasi-degenerate pattern with decreasing momentum in the y-direction for each spin sector. The ES of the spin ground state has a symmetry about $S_z = 1/2$ which corresponds to a spinon at the edge of the cylinder, while the one of the vacuum ground state has a symmetry about $S_z = 0$. The ES is robust in the bulk part of the CSL phase for various parameters and system sizes, but as we approach the phase boundary, additional eigenstates may also mix in the spectrum(see Appendix).

The main difference between the CSL and the chiral
spin state is the topological edge state that can be identified through the ES. An example of the ES in the chiral spin state is also given in Fig. 3(c), where the quasi degenerate pattern disappears and additional low-lying states emerges, as opposed to the ES of the CSL in Fig. 3(a) and (b). The phase boundary between these two states are determined mainly by the ES.

The finite chiral order represents the time reversal symmetry breaking chiral current in each small triangle, as shown in Fig. 2(c). The chiral order is significantly enhanced as the system undergoes a phase transition from the Ising antiferromagnetic state to the CSL. However, the spin correlation remains following exponential decay, as shown by the line of \( J_\chi = 0.08 \) in Fig. 2(d). We further confirm the vanish of any conventional spin order in the CSL by obtaining the spin structure in Fig. 4(a), and comparing it with the one in the chiral spin state in Fig. 4(b). There is no significant peak in the CSL phase as opposed to other magnetic phases.

In order to identify the excitation properties of the CSL, we obtain the spin-1 excitation gap by the energy difference between the lowest state in \( S = 0 \) and 1 sector. To measure the bulk excitation gap, we use the torus geometry to reduce the boundary effect. We also perform finite size scaling using rectangle like clusters as shown in Fig. 4(c). The spin gap decays slowly as the cluster grows, and remains finite after the extrapolation, suggesting a gapped phase in the thermodynamic limit. In addition, we study the entanglement entropy of the subsystems by cutting at different bonds. As shown in Fig. 4(d), the entropy becomes flat away from the boundary, which corresponds to a zero central charge in the conformal field theory interpretation. This supports a gapped CSL phase that is consistent with the finite spin gap.

**Summary and discussions.** Using large scale DMRG, we identify the long-sought CSL with the perturbation of three-spins chiral interactions in the spin-\( \frac{1}{2} \) XY model on the honeycomb lattice. The CSL extends to the intermediate regime with a small \( J_\chi \), providing evidence of the important interplay between frustration and chiral interactions driving the CSL. Here, we demonstrate that the chiral interactions are essential for the emergence of the CSL, because the minimum critical \( J_\chi \) of the phase transition is around 0.02, which is stable against the increasing of system sizes (see Appendix).

A chiral spin state is also obtained at larger \( J_\chi \), which extends to the wider regime of \( J_2 \). The chiral spin state has a peak value for spin structure factor growing with system sizes. Further studies include finding the exact nature of this chiral spin state, and the nature of the phase transition into the CSL.

Experimentally, of all the honeycomb materials that show a quantum-spin-liquid-like behavior, the Co-based compounds are mostly studied in the context of XY model such as \( \text{BaCo}_2(PO_4)_2 \) and \( \text{BaCo}_2(AsO_4)_2 \), thus it would be extremely interesting to search for the quantum spin liquid in such model. On the other hand, the results of CSL may be tested in cold atoms experiments as the spin XY model could be mapped by the bosonic Kane-Mele model in the Mott regime.

**Acknowledgments.** Y.H and C.S.T was supported by the Texas Center for Superconductivity and the Robert A. Welch Foundation Grant No. E-1146. Work at CSUN was supported by National Science Foundation Grants PREM DMR-1828019. Numerical calculations was completed in part with resources provided by the Center for Advanced Computing and Data Science at the University of Houston.

**Appendix A: The convergence of DMRG results**

We ensure the convergence of our Density Matrix Renormalization Group (DMRG) results by checking the truncation error and other physical quantities such as...
ground state energy, spin correlations, and entanglement entropy, with increasing number of states kept. Here we give one example of the entanglement entropy in the chiral spin liquid (CSL) phase in Fig. 5. For both finite and infinite DMRG the entanglement entropy remains almost unchanged as the states increase, indicating that the results are converged. We keep 3000 (6000) states for finite (infinite) DMRG for most of the calculations and are able to reach the truncation error less than $10^{-7}$ ($10^{-5}$).

Appendix B: The size dependence of the phase boundary

In order to test the finite size effect we study larger systems in both x and y directions. While the CSL is robust in various sizes, the critical $J_2$ of the phase boundary between the Ising antiferromagnetic state and the CSL in the intermediate regime may vary slightly. Here we show one example at $J_2 = 0.3$ in Fig. 6. The critical $J_\chi$ increases by 0.01 as $L_x$ increases from 20 to 30 while keeping $L_y$ fixed, and it increases by 0.02 when $L_y$ increases from $4 \times 2$ to $6 \times 2$ with fixed $L_x$. The finite size scaling indicates that the phase transition into CSL happens at $J_\chi > 0.06$ in the thermodynamic limit. In the mean time, we haven’t found any size dependence of other phase boundaries, suggesting that the CSL identified here has little finite size effect.

Appendix C: The entanglement spectrum near the phase boundary

The entanglement spectrum provides an efficient way to determine the phase boundary between the CSL and the chiral spin state. As shown in Fig. 7(a), the counting of the quasi degenerate states in the CSL is very clear in every spin sector. In Fig. 7(b) we can still identify the counting for $S = 0$ sector near the phase boundary, but additional low-lying eigenstates have already mixed in the the $S = -1$ and $1$ sector. As soon as the system enters the chiral spin state the counting disappears, as shown in Fig. 7(c).

Appendix D: The Spin structure in chiral spin state

The spin structure in the chiral spin state is given in Fig. 8, which is calculated at $J_2 = 0.2, J_\chi = 0.27$ using finite size cylinder of $L_x \times L_y = 20 \times 4 \times 2$. There are 6 moderate peaks at $M$ points, which resembles the spin structure of the tetrahedral phase in the extended Heisenberg model with three-spins chiral interactions on the honeycomb lattice.

---

1. L. Balents, Nature 464, 199 (2010).
2. M. Levin and X.-G. Wen, Physical review letters 96, 110405 (2006).
3. A. Kitaev and J. Preskill, Physical review letters 96, 110404 (2006).
4. T. Senthil and O. Motrunich, Physical Review B 66, 205104 (2002).
5. L. Balents, M. P. A. Fisher, and S. M. Girvin, Phys. Rev. B 65, 224412 (2002).
6. D. N. Sheng and L. Balents, Physical review letters 94, 146805 (2005).
7. R. Moessner and S. L. Sondhi, Phys. Rev. Lett. 86, 1881 (2001).
8. D. F. Schroeter, E. Kapit, R. Thomale, and M. Greiter, Phys. Rev. Lett. 99, 097202 (2007).
9. S. V. Isakov, M. B. Hastings, and R. G. Melko, Nature Physics 7, 772 (2011).
10. P. W. Anderson, science 235, 1196 (1987).
11. D. S. Rokhsar and S. A. Kivelson, Physical review letters 61, 2376 (1988).
12. P. A. Lee, N. Nagaosa, and X.-G. Wen, Reviews of modern physics 78, 17 (2006).
13. R. Wang, B. Wang, and T. A. Sedrakyan, Physical Review B 98, 064402 (2018).
14. C. Nayak, S. H. Simon, A. Stern, M. Freedman, and S.-D. Sarma, Reviews of Modern Physics 80, 1083 (2008).
FIG. 6. (Color online) The staggered magnetization for various length in the x direction (Fig. 6(a)) and the y direction (Fig. 6(b)) in the intermediate regime. The phase transition from the Ising antiferromagnetic state to the CSL is determined by the sudden drop of $\langle S_z \rangle$. For the smallest size in (a) ($L_x \times L_y = 20 \times 3 \times 2$) and (b) ($L_x \times L_y = 6 \times 4 \times 2$) we found that $\langle S_z \rangle = 0$ at zero $J_\chi$ limit due to finite size effect.

FIG. 7. (Color online) The entanglement spectrum in CSL at $J_\chi = 0.09$ (Fig. 7(a)), boundary at $J_\chi = 0.13$ (Fig. 7(b)), and the chiral spin state at $J_\chi = 0.2$ (Fig. 7(c)). All three plots are obtained at $J_2 = 0.26$. The dash red lines are guide to the eye.
FIG. 8. (Color online) The spin structure in the chiral spin state at $J_z = 0.2, J_x = 0.27$, which peaks at the $M$ points in the second Brillouin zone.

15 V. Kalmeyer and R. B. Laughlin, Physical Review Letters 59, 2095 (1987).
16 S. S. Gong, W. Zhu, and D. N. Sheng, Scientific reports 4, 6317 (2014).
17 B. Bauer, L. Cincio, B. P. Keller, M. Dolfi, G. Vidal, S. Trebst, and A. W. W. Ludwig, Nature communications 5, 5137 (2014).
18 A. Wietek, A. Sterdyniak, and A. M. Läuchli, Physical Review B 92, 125122 (2015).
19 Y.-C. He, D. N. Sheng, and Y. Chen, Physical review letters 112, 137202 (2014).
20 W. Zhu, S. S. Gong, and D. N. Sheng, Physical Review B 92, 014424 (2015).
21 P. Nataf, M. Lajkó, A. Wietek, K. Penc, F. Mila, and A. M. Läuchli, Physical review letters 117, 167202 (2016).
22 A. Wietek and A. M. Läuchli, Physical Review B 95, 035141 (2017).
23 A. E. Nielsen, G. Sierra, and J. I. Cirac, Nature communications 4, 2864 (2013).
24 C. Hickey, L. Cincio, Z. Papić, and A. Paramekanti, Physical review letters 116, 137202 (2016).
25 T. A. Sedrakyan, L. I. Glazman, and A. Kamenev, Physical review letters 114, 037203 (2015).
26 C. N. Varney, K. Sun, V. Galitski, and M. Rigol, Physical review letters 107, 077201 (2011).
27 J. Carrasquilla, A. Di Ciolo, F. Becca, V. Galitski, and M. Rigol, Physical Review B 88, 241109 (2013).
28 Z. Zhu, D. A. Huse, and S. R. White, Physical review letters 111, 257201 (2013).
29 A. Di Ciolo, J. Carrasquilla, F. Becca, M. Rigol, and V. Galitski, Physical Review B 89, 094413 (2014).
30 P. H. Y. Li, R. F. Bishop, and C. E. Campbell, Physical Review B 89, 220408 (2014).
31 Z. Zhu and S. R. White, Modern Physics Letters B 28, 1430016 (2014).
32 J. Oitmaa and R. R. P. Singh, Physical Review B 89, 104423 (2014).
33 R. F. Bishop, P. H. Y. Li, and C. E. Campbell, Physical Review B 89, 214413 (2014).
34 C. N. Varney, K. Sun, V. Galitski, and M. Rigol, New Journal of Physics 14, 115028 (2012).
35 T. Nakafuji and I. Ichinose, Physical Review A 96, 013628 (2017).
36 D. N. Sheng, O. I. Motrunich, and M. P. A. Fisher, Physical Review B 79, 205112 (2009).
37 K. Plekhanov, I. Vasić, A. Petrescu, R. Nirwan, G. Roux, W. Hofstetter, and K. Le Hur, Physical review letters 120, 157201 (2018).
38 S. R. White, Physical review letters 69, 2863 (1992).
39 S. R. White, Physical Review B 48, 10345 (1993).
40 Calculations were performed using the iTensor Library http://itensor.org/ and the TEfnPy library (version 0.4.1).
41 P. Calabrese and J. Cardy, Journal of Statistical Mechanics: Theory and Experiment 2004, P06002 (2004).
42 S. Nakatsuji, K. Kuga, K. Kimura, R. Satake, N. Katayama, E. Nishihori, H. Sawa, R. Ishii, M. Hagiwara, F. Bridges, et al., Science 336, 559 (2012).
43 J. G. Cheng, G. Li, L. Balicas, J. S. Zhou, J. B. Goodenough, C. Xu, and H. D. Zhou, Phys. Rev. Lett. 107, 197204 (2011).
44 J. A. Quilliam, F. Bert, A. Manseau, C. Darie, C. Guillot-Deudon, C. Payen, C. Baines, A. Amato, and P. Mendels, Phys. Rev. B 93, 214432 (2016).
45 H. S. Nair, J. M. Brown, E. Coldren, G. Hester, M. P. Gelfand, A. Podlesnyak, Q. Huang, and K. A. Ross, Physical Review B 97, 134409 (2018).
46 H. Hofstetter, R. J. Cava, and C. Xu, P06002 (2004).
47 U. Schollwöck, Annals of Physics 326, 96 (2011).
48 D. Sen and R. Chitra, Physical Review B 51, 1922 (1995).
49 P. Francesco, P. Mathieu, and D. Sénéchal, Conformal field theory (Springer Science & Business Media, 2012).
50 J. Oitmaa and R. R. P. Singh, Physical Review B 73, 155115 (2006).
51 O. I. Motrunich, Physical Review B 89, 014424 (2014).
52 S. Trebst, and A. W. W. Ludwig, Nature Communications 27, which peaks at the $M$ points in the second Brillouin zone.