Spin Liquids and their Transitions in Spin-1/2 XXZ Kagome Antiferromagnets

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By using the density matrix renormalization group, we study the spin-liquid phases of spin-1/2 XXZ kagome antiferromagnets. We find that the emergence of the spin-liquid phase does not depend on the anisotropy of the XXZ interaction. In particular, the two extreme limits—Ising (strong $S^z$ interaction) and XY (zero $S^z$ interaction)—host the same spin-liquid phases as the isotropic Heisenberg model. Both the time-reversal-invariant spin liquid and the chiral spin liquid with spontaneous time-reversal symmetry breaking are obtained. We show they evolve continuously into each other by tuning the second- and third-neighbor interactions. At last, we discuss the possible implication of our results on the nature of spin liquid in nearest neighbor XXZ kagome antiferromagnets, including the most studied nearest-neighbor spin-1/2 kagome anti-ferromagnetic Heisenberg model.

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Ever since Anderson proposed the concept of spin liquid [1] and showed its relevance to high-$T_c$ superconductivity [2], hunting for exotic spin liquids in frustrated magnets has become a long and challenging journey in condensed-matter physics [3–31]. The gapped spin liquid is also a prominent example of topological order [32], which hosts fractionalized quasiparticles obeying fractional statistics that in principle can be used to implement topological quantum computation [13]. Among the many frustrated systems, the spin-1/2 kagome antiferromagnet and its realization in materials such as Herbertsmithite is considered to be the most promising candidate as a spin liquid; the neutron scattering experiment in particular has provided smoking-gun evidence for the existence of spinons [31].

Theoretically, the difficulty in studying spin liquid lies in the fact that there is no exact analytical, numerical or controlled approximation method to generally solve the two-dimensional frustrated models. Approximation methods, like the slave-particle approach, the construction of a variational wave-function ansatz, and the artificial solvable models, have given many insights into spin-liquid physics. However, it is unclear whether these methods might provide reliable results for real systems. One famous example is the minimal model of spin-1/2 kagome antiferromagnets, i.e., nearest-neighbor kagome antiferromagnetic Heisenberg model (NNKAH), for which the ground state is still controversial after more than twenty years of research [6–9, 16–23, 33, 34]. Among various studies, the recent density matrix renormalization group (DMRG) [36] results provide strong evidence for a gapped spinLiquid ground state [19] with topological order [20, 21]. Recently infinite DMRG [35] has been proven powerful in studying topological order by calculating topological degenerate ground states and the corresponding modular matrix [28, 29, 37–39]; however, it fails for kagome spin liquids [39], making their nature remain elusive.

In this Letter, we use the DMRG to study the spin-liquid phases in kagome antiferromagnets, where the SU(2) Heisenberg-type spin-spin exchange interactions are extended into the XXZ type:

$$JS_i \cdot S_j \rightarrow J_z S^z_i S^z_j + J_{xy}(S^{x}_i S^{y}_j + S^{y}_i S^{x}_j).$$  \hspace{1cm} (1)

Besides the most studied SU(2) limit ($J_z = J_{xy}$), we investigate two other limiting cases: Ising ($J_x \gg J_{xy}$) and XY ($J_z = 0$) limits. The underlying physics associated with these three limiting cases are very different: the Ising limit can be mapped into a quantum dimer model or compact $U(1)$ gauge field theory coupled with charge-2 matter [40]; the XY limit can be considered as a hard-core boson system, a spin liquid in which may be realized in an exotic way by fractionalizing vortices [41, 42]; the spin liquid in the SU(2) limit is a resonating valence bond (RVB) state. Although these three limits are physically different, we find the emergent spin-liquid phases are almost the same (see Fig. 1): (1) with only first-neighbor interactions (NNKAXXZ), the system hosts a time-reversal-invariant spin liquid that lies in the same phase as the spin liquid found in NNKAH (SU(2) limit) [19]; (2) similar to recent numerical results in the SU(2) limit [29, 30], the Kalmeyer-Laughlin (KL) chiral spin liquid (CSL) emerges if we add second- and third-neighbor interactions; and (3) we show that the KL-CSL evolves continuously into the spin-liquid state of the NNKAXXZ.

Our results expose some new aspects of spin liquid physics in kagome antiferromagnets. First, a very controlled approximation may be implemented in the Ising limit to solve the spin-liquid phases analytically, which will help to settle the debate over the nature of spin-liquid phases realized in NNKAH. Second, a candidate spin-liquid phase in NNKAXXZ is narrowed down with its continuous transition into KL-CSL. Furthermore, it will be interesting to construct a general theory to describe the spin-liquids and their transitions in three dif-
different limits, which may be beyond the description of RVB states.

Model Hamiltonian.—Our model is a $J_1$-$J_2$-$J_3$ XXZ antiferromagnetic model defined on a kagome lattice, for which the Hamiltonian is:

$$H = J_1 \sum_{\langle ij \rangle} S_i^z S_j^z + J_2^{xy} \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) + J_3^{xy} \sum_{\langle \langle ij \rangle \rangle} (S_i^x S_j^x + S_i^y S_j^y),$$

where $\langle ij \rangle$ denotes first-neighbor, $\langle \langle ij \rangle \rangle$ second-neighbor, and $\langle \langle \langle ij \rangle \rangle \rangle$ third-neighbor interactions (see Fig. 1(a)), and we take $J_1 = \cos \theta$, $J_2^{xy} = \sin \theta$, $J_3^{xy} = \tau \sin \theta$. $\theta$ controls the anisotropy of the XXZ interaction: for $\theta \sim 0$, the system is in the Ising limit; for $\theta = \pi/4$, the system is in the SU(2) limit; for $\theta = \pi/2$, the system corresponds to the XY limit. $\tau$ controls the relative magnitude of the second- and third-neighbor interactions.

We use the infinite DMRG algorithm [35] to study the system wrapped on a cylinder with YC or XC geometry [29]. We use a code with complex variables (KL-CSL spontaneously breaks time-reversal symmetry), and keep 6000 states in the DMRG simulation (near the critical point, we have kept 10000 states). We obtain a generic phase diagram (Fig. 1(b)) based on the calculations on the YC8 ($L_y = 4$ unit cells) cylinder. Except for the KL-CSL phase, all other phases are time-reversal invariant: (1) with intermediate $\tau$ (second- and third-neighbor interactions), we have a KL-CSL with spontaneous time-reversal symmetry breaking, as similarly studied in previous work [29, 30]; (2) for small $\tau$, we obtain a time-reversal-invariant spin liquid which lies in the same phase as the spin-liquid state found by Yan, et al. [19] (NNKAH); (3) with $\theta < 0$ (ferromagnetic XY interaction), we get a superfluid phase, in agreement with quantum Monte Carlo results [43]; (4) for large $\tau$, an ordered phase is obtained [44].

**FIG. 1:** (Color online). (a) Kagome model with first- (XXZ), second-, and third- (XY) neighbor interactions. (b) Phase diagram of the kagome XXZ model.

Chiral spin liquid.—As shown in the phase diagram, the Hamiltonian hosts a KL-CSL with spontaneous time-reversal symmetry breaking in certain parameter region, similar to previous findings [29, 30]. The KL-CSL is a gapped spin liquid state that supports a fractionalized spinon-type quasiparticle—semion. The KL-CSL has two-fold topologically degenerate ground states, which differs from each other in the presence or absence of a semion line. Using the technique developed in Ref. [39], we have obtained these two ground states. The symmetry pattern of the entanglement spectrum (Fig. 2(b)) shows that $\psi_s$ has a semion line threaded in. The degeneracy pattern $(1,1,2,3,5 \cdots)$ of the leading entanglement spectra also agrees with the expectation of KL-CSL state [45]. The energy splitting between the two topological degenerate ground states decay exponentially fast (Fig. 2(c)), supporting the idea that the two states are exactly degenerate in the thermodynamic limit.

![FIG. 2:](Color online). (a) Two topological degenerate states of KL-CSL. (b) Entanglement spectrum of KL-CSL on YC12 cylinder, here $\theta = 0.016\pi$, $\tau = 1$: (I) $\psi_1$ (II) $\psi_s$. The horizontal axis is the momentum along the $y$ direction, $p_y = 0, 2\pi/6, \ldots, 5 \times 2\pi/6$ (up to a global shift). (c) Energy splitting between two topological degenerate ground states. (d) Transition from KL-CSL ($\theta > 0$) to superfluid ($\theta < 0$), here we show results for the YC8 cylinder, $\tau = 1$. I: Scalar chirality order $\chi$; II: log-plot of correlation length $\xi$ (unit cells) from the transfer matrix; III: The fidelity $F$ (defined in Eq. 5) between all pairs of neighboring points.

Furthermore, using these two topological degenerate ground states, we calculate the modular matrix [32, 37,
which gives:

\[
S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} + o(10^{-2}) \tag{3}
\]

and

\[
U = e^{-i(2\pi/24)} \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \times o(10^{-2}) \tag{4}
\]

From the modular matrix, we conclude that the system hosts a KL-CSL spin liquid. For example, from the S matrix, we know the fractional statistics obeyed by the semion: one semion encircling another semion will give rise to a non-trivial phase factor −1.

To show spontaneous time-reversal symmetry breaking, we measure the scalar chirality order, \(\chi = \langle S_x \rangle \times \langle S_y \rangle\). As shown in Fig. 2(d)-I, the system has a large scalar chirality order when \(\theta > 0\). For \(\theta < 0\), the system is in the superfluid phase, which is time-reversal invariant with a vanishing chirality order. From Fig. 2(d)-II, we find the correlation length (from the transfer matrix) [35] is extremely large when \(\theta < 0\), indicating a gapless superfluid state. In contrast, the correlation length for the KL-CSL phase is very small signifying a gapped state. Finally, we calculate the “one column” fidelity, \(F(\theta)\), for a \(L_x \times L_y\) cylinder (or torus) defined as:

\[
|\langle \psi(\theta + \delta \theta)|\psi(\theta) \rangle| = [F(\theta)]^{L_z} \tag{5}
\]

This fidelity \(F(\theta)\) can be easily calculated from transfer matrix [35], and can serve as a good criterion for the nature of phase transition. From the fidelity between \(\theta > 0\) and \(\theta < 0\) (Fig. 2(d)-III), we conclude the phase transition between the superfluid phase and the KL-CSL is first order.

Time-reversal-invariant spin liquid.—In the following, we consider the case \(\tau = 0\), where the Hamiltonian only has nearest-neighbor interactions. If \(\theta = \pi/4\), the interaction is the Heisenberg SU(2) interaction (NNKAH), which is a time-reversal-invariant gapped spin liquid by DMRG simulations [19, 20].

The ground state does not break any lattice symmetry, in particular, the nearest-neighbor spin-spin correlations along XY direction \((S^x_i S^x_j + S^y_i S^y_j)\) is very homogenous (Fig. 3(a) plots two limiting case—Ising \((\theta = 0.016 \pi)\) and XY \((\theta = \pi/2)\) limit). When \(\theta > 0\), the correlation length [35] shown in Fig. 3(b) is very small, and the fidelity (Eq. 5) between all pairs of neighboring points (Fig. 3(c)) is approximately 1. This result proves that there is no phase transition in the whole region of \(\theta > 0\), both the Ising limit and XY limit are adiabatically connected to the spin liquid phase in the NNKAH [19]. When \(\theta < 0\) (unfrustrated XY interactions), the system is in the gapless superfluid phase with a large correlation length; the transition between superfluid phase and spin liquid phase in NNKAXXZ is first order.

Transitions between two spin liquids.—Next, we study how the KL-CSL evolves into the spin-liquid ground state in NNKAXXZ. Our results are based on the YC8 cylinder, the critical point may shift as the system gets larger or more states are retained in the DMRG simulation. However, the nature of the phase transition does not change. The spin liquid has topological degenerate sectors; here we focus only on the vacuum sector (lowest energy state), which has a smaller finite-size effect [29].

The KL-CSL has spontaneous time-reversal symmetry breaking with finite scalar chirality order \(\chi = \langle S_x \rangle \times \langle S_y \rangle\) (on each triangle); hence, we use \(\chi\) as an order parameter to distinguish the KL-CSL and the time-reversal-invariant spin liquid. As shown in Fig. 4(a), for each \(\theta\) there is a transition point after which the system enters into the time-reversal-invariant spin-liquid phase with vanishing chirality order. In the whole process, there is no spin rotational or lattice symmetry breaking, so we conclude there is no intermediate phase between the KL-CSL and spin liquid in NNKAXXZ. The correlation length [35] in Fig. 4(b) also reaches the peak at the critical point; it is consistent with the direct phase transition between KL-CSL and spin liquid in NNKAXXZ. We remark that correlation lengths shown here have not been extrapolated with truncation error or the number of kept states. We find that near the critical point, the correlation lengths keep growing as more states are kept (see supplementary materials). They are supposed to be much larger, even infinite, if one retains more and more states.

To show unambiguously the continuous transition between the two spin liquids, we measure the fidelity \(F(\tau)\) (Eq. 5) between pairs of nearest-neighbor points as \(\tau\) varies progressively (Fig. 4(c)). The overlaps are very large (∼0.99) and hence clearly show that KL-CSL continuously evolves into the spin-liquid state in NNKAXXZ without level crossing.
The continuous transition between KL-CSL and spin liquid in NNKAXXZ actually narrows down the possibility of spin-liquid phase in such system. A recent work [47] has proposed an interesting theory for the continuous phase transition between KL-CSL and double-semion spin-liquid [48, 49]. However, it is argued that [50] double-semion phase cannot be realized in spin-1/2 kagome system (with U(1) charge conservation), unless one enlarges the kagome unit cell or realizes the time-reversal symmetry in a twisted way [51]. Neither of these has been observed in our numerical results, so the spin-liquid state obtained in our simulation appears not to belong to a double-semion phase. If the kagome spin liquid is a Z_2 spin-liquid [20, 21], there will be an exotic phase transition between it and the KL-CSL, which will be very interesting to study.

Besides the gapped topological spin liquid, U(1) Dirac spin liquid [16, 23] is also a promising candidate for the kagome spin liquid ground state. In particular, by adding various mass terms, the U(1) Dirac spin liquid will continuously transit into KL-CSL, valence bond solids, and magnetically ordered state [9, 14], all of which have been found to neighbor the kagome spin liquid. However, this U(1) Dirac spin liquid has a vanishing spin (triplet) gap, which is inconsistent with the large spin gap reported in the DMRG’s results [19, 20]. A possible direction is to construct a new type of spin-liquid such as the fractionalized vortex liquid [42] for the XY kagome antiferromagnets, which might reproduce a critical spin liquid with finite spin gap.

**Note added.**—After we completed this work, we have become aware of a related work [52], which studies nearest-neighbor XXZ kagome model by exact diagonalization and has reached similar conclusions as our own.

**Conclusions.**—We numerically study the spin-liquid phases in spin-1/2 XXZ kagome antiferromagnets, and find both a time-reversal-invariant spin liquid and chiral spin liquid with spontaneous time-reversal symmetry breaking, whose emergence is independent of the anisotropy of XXZ interactions. Furthermore, we show the phase transition between the two spin liquids is continuous. Finally, we discussed possible future directions in understanding the spin liquid phase of kagome antiferromagnets.

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Supplementary Material of “Spin Liquids and their Transitions in Spin-1/2 XXZ Kagome Antiferromagnets”

To calculate the correlation length, we define the transfer matrix $T$ as in Fig. 5. The correlation length is then defined by the first and second largest eigenvalue $\lambda_{1,2}$ of the transfer matrix $T$,

$$\xi_{TM} = -1 / \ln \lambda_2$$  \hspace{1cm} (6)

This correlation length determines the largest correlation in the infinite cylinder [35]. Therefore, instead of calculating various correlation functions, one can simply calculate this single quantity $\xi_{TM}$ to obtain the length scale of the largest possible correlations.

Fig. 6 shows the correlation length as a function of the number of states retained. For the state that lies deeply in the spin liquid phase ($\tau = 0, 1$), the correlation fully converges. However, when the system is near the critical point ($\tau = 0.39$), the correlation length does not converge for the largest number of states that we attempted.

FIG. 5: Definition of transfer matrix and correlation length $\xi$.

FIG. 6: Correlation length versus the number of states kept. Here we show the Heisenberg limit $\theta = 0.25\pi$. 

\begin{itemize}
    \item $\tau = 0.39$ - red
    \item $\tau = 1$ - green
    \item $\tau = 0$ - blue
\end{itemize}