Signatures of quantum spin liquids in small lattices

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Quantum spin liquids remain one of the most challenging subjects of quantum magnetism. Characterized by massive degenerate ground states that have long range entanglement and are locally indistinguishable, highly demanding numerical techniques are often needed to describe them. Here we propose an easy computational method based on exact diagonalization with engineered boundary conditions to unveil their most significant features in small lattices. We derive the quantum phase diagram of diverse antiferromagnetic Heisenberg models in the triangular lattice. For all studied cases, our results are in accordance with the previous results obtained by means of sophisticated variational methods.

I. INTRODUCTION

Some entangled ground states of spin systems do not order even at zero temperature. The lack of order, which is originated by strong quantum fluctuations on the spin orientations, prevents their characterization by means of local order parameters. Such quantum disordered states, termed generically quantum spin liquids (QSL), are linked to a highly degenerated ground state and contain long range entanglement. Moreover, they are locally indistinguishable [1–3], meaning that they cannot be detected or distinguished using local measurements.

QSL are often caricatured as a liquid of singlets, where the singlets formed between nearby spins strongly fluctuate from one configuration to another. Due to such fluctuations, the ground state of the system is far from a product state, implying that entanglement in QSL plays a crucial role. Ground states of local spin Hamiltonians are normally short range entangled, as evidenced by the fact that the entanglement entropy, \( S \), of any bipartite cut of the system follows an area law: \( S(L) \sim L^{D-1} \), where \( D \) is the dimension of the system and \( L \) the linear size of the boundary separating both regions. Corrections to this law appear, for instance, in critical gapless quantum phases or in topologically ordered states. In 2D, the latter fulfill \( S(L) \sim L + b L^\gamma \), where \( \gamma \) is a universal correction, independent of the lattice size that signals topological order [4–6].

The combination of the above features makes unfeasible the description of QSL in terms of effective mean field approaches with fluctuation corrections over the mean field ansatz. Hence, finding the eigenstates of the corresponding Hamiltonians mostly relies, for the time being, in numerical approaches and/or complex variational ansatzes in very large lattice systems. The numerical methods are, of course, severely hindered by the requirement of large lattices.

Here we show, however, that the relevant signatures of QSL in frustrated disordered 2D systems can be correctly obtained in surprisingly small lattices by properly engineering the boundary conditions.

With this aim, we analyze several anisotropic spin 1/2 antiferromagnetic (AF) Heisenberg models in the triangular lattice, where quantum fluctuations and frustration compete. The effect of frustration, which is, the impossibility to simultaneously minimize the Hamiltonian locally, can be further tuned by introducing different spin couplings along all lattice directions. This model, sometimes denoted as the spatially completely anisotropic triangular lattice (SCATL) has been scarcely addressed in the literature. It is a generalization of the model with anisotropy just between horizontal and diagonal bonds (SATL), which has been extensively addressed in the literature using different methods such as tensor networks, quantum Monte Carlo, 2D DMRG, exact diagonalization (ED) or modified spin wave theory (MSWT) [7–19]. We also investigate here the \( J_1 - J_2 \) model, with anisotropy between nearest-neighbor (NN) and next-to-nearest neighbor (NNN) couplings, also addressed recently in [20–25]. The above models give room to both, gapless and highly nontrivial gapped QSL.

Before proceeding further we summarize here our main results. We derive the quantum phase diagram of the above models using ED with engineered boundary conditions in lattices of only \( N = 12, 16 \) or 24 spins. Our results reproduce both, the ordered and disordered quantum phases previously reported for such models and show explicitly that massive superpositions of almost quasi-degenerated ground states are at the heart of QSL. Despite we cannot calculate the topological entanglement entropy in such small lattices, geometric entanglement —quantifying how far an entangled state is from its closest separable one—, shows that the predicted gapped QSL have a large entanglement as compared to their surrounding ordered phases. Remarkably enough our method puts at reach the study and detection of new QSL in complex systems with a simple numerical approach.

The paper is organized as follows: in Sec. II, we explain the main features of our numerical method together with the relevant figures of merit used along. In Sec. III, we derive the quantum phase diagram of the SCATL model, with anisotropic couplings along all lat-
tice directions. For this model, to the best of our knowledge, only a study based in a MSWT exist [14]. Therefore, alternative methods are clearly needed to settle the presence of conjectured QSL. In Sec. IV, we move onto another paradigmatic frustrated model, the so-called $J_1 - J_2$. We analyze it also in the presence of chiral interactions which helps to elucidate the nature of the predicted QSL and compare our results with the quantum phase diagram obtained recently in [25] using 2D DMRG. Finally, in Sec. V, we conclude and present some open questions.

II. RANDOM TWISTED BOUNDARY CONDITIONS

Twisted boundary conditions (TBC) were introduced in the seminal contributions of [26, 27], and can be thought of as periodic boundary conditions (PBC) under a twist. Since then, they have been often used to calculate properties of quantum magnets, as they provide better access to momentum space and help to mitigate finite size effects, see e.g. [17, 28–31]. However, here we use TBC in a conceptually different approach. In Fig. 1, we sketch our philosophy. Consider a generic AF Heisenberg model in the triangular lattice. For the ordered phases of the Hamiltonian, the relative orientation of the spins is fixed due to a broken symmetry, as depicted for example in the cartoon of a 2D Néel phase in Fig. 1 (top left). If the lattice is large, the bulk spins dominate over the boundary ones imposing the order expected in the thermodynamical limit, independently of the chosen boundaries. However, for small lattices this is not anymore the case. The boundaries must be properly chosen—in accordance to the lattice geometry—to recover the underlying symmetries of the ordered phase, Fig. 1 (bottom left). For quantum disordered phases that are not associated to a symmetry breaking, we expect the ground state of the system to be spanned over a large superposition of states, as schematically shown in Fig. 1. Presumable, for small lattices different boundary configurations should be compatible with the ground states of the system in the thermodynamic limit. We cannot predict a priory which are the right boundaries configurations since there is not an underlying local symmetry in the phase. This feature is illustrated with the symbols “?” in Fig. 1 (bottom right). Nevertheless, we can count how many random TBC lead to the same ground state energy and post-select only those to calculate physical quantities of interest. This post-selection is the key point to engineer our boundary conditions [19].

Specifically, for 2D spin 1/2 AF Heisenberg models, the spins lay in the XY plane and TBC correspond to adding a phase in the spins $i, j$ interacting through the boundaries:

$$S_i^+ S_j^- \rightarrow S_i^+ S_j^- e^{-i\phi},$$  \hspace{1cm} (1)

$$S_i^- S_j^+ \rightarrow S_i^- S_j^+ e^{i\phi}. \hspace{1cm} (2)$$

To twist the lattice simultaneously in two directions requires two different phases $\phi_1 (\phi_2)$, for left-right (top-bottom) boundaries, as depicted in the bottom panels of Fig. 1. The spins of the lattice laying at both boundaries acquire a phase $\phi = \phi_1 + \phi_2$. Notice that conventional PBC favor order commensurate with the lattice dimensions, $N = L \times W$, since in the reciprocal lattice, momentum is selected at $k_i = 2\pi n_i / L$ and $k_j = 2\pi n_j / W$ for $n_i, n_j \in \mathbb{N}$. In contrast, TBC allow to test all possible momenta in the first Brillouin zone [17, 26, 27]

$$k_1 = \frac{2\pi n_1}{L} \pm \frac{\phi_1}{L},$$

$$k_2 = \frac{2\pi n_2}{W} \pm \frac{\phi_2}{W}. \hspace{1cm} (3)$$

Let us briefly review our approach [19]. First, we fix the lattice size, $N$, and geometry. Here, we use $N = 4 \times 3$ or $N = 4 \times 4$, but to ensure convergence, some of the results are also calculated for $N = 6 \times 4$ and $4 \times 6$. Then, we generate a set $p$ of two randomly chosen phases, $\{\phi_1, \phi_2\}_p$, with $\phi_i \in [0, 2\pi)$ and $p = 1, 2, \ldots, 200$. For each configuration, we diagonalize the Hamiltonian, generating a ground state $|\psi_p\rangle$ with energy $E_p$, and denote by $|\psi_0\rangle$ the ground state with the lowest energy, $E_0$. We post-select those configurations whose ground state energy fulfills: $\epsilon_p = (E_p - E_0)/E_0 < \alpha$. The election of the energy bias, $\alpha$, is somehow arbitrary as it depends on the lattice size and the ratio between bulk and boundary interactions. Nevertheless, our results are independent of it, if the set $p$ is sufficiently large. Notice, however, that for small lattices the bias cannot be vanishingly small.

Consequently, one relevant figure of merit is the number of configurations, $N_c$, laying in the interval $0 \leq \epsilon_p < \alpha$. Typically, we choose $\alpha = 0.01$ meaning that only configurations whose ground state energies are less than 1% than $E_0$ are retained. Actually, for ordered phases just very few random TBC accommodate the symmetry of the phase, and the ones which do not, correspond to large $E_p$ and are automatically discarded in our approach. In contrast, we find regions in the Hamiltonian parameters where $N_c$ increases dramatically. The corresponding ground states, $|\psi_p\rangle$, strongly differ one from each, as observed by computing the overlap $O_p = \langle \psi_p | \psi_0 \rangle$. Finally, as it is standard in disordered systems, we calculate the quantities of interest for each post-selected configuration and perform afterwards the corresponding average which we denote by $\langle \ldots \rangle_d$. The average washes out the spurious symmetries introduced by TBC. In ED, one quantity which can be easily obtained is the static spin structure factor

$$S(k) = \frac{1}{N} \sum_{i,j} e^{-i\vec{k} \cdot \vec{r}_{ij}} \langle S_i S_j \rangle,$$

where the expectation value is taken over the corresponding ground state $|\psi_p\rangle$. From the spin structure factor, one can extract the following order parameter

$$M = \sqrt{S(\vec{Q}_{\text{max}})/N}.$$
where $\mathcal{Q}_{\text{max}}$ are the k-vectors corresponding to the maxima of the spin structure factor in the first Brillouin zone. This parameter signals long range order (LRO), and helps to identify possible QSL. Regarding entanglement, it is well known that local entanglement measures cannot detect QSL, but they help to identify the underlying ordering of the phases. We choose the concurrence, $C$, as a measure of bipartite entanglement between any two spins $i, j$ in the mixed state $\rho_{ij} = \text{Tr}_{k \neq i,j} (|\psi_p\rangle \langle \psi_p|)$ which can be easily computed in ED methods [32]. For local Hamiltonians, the concurrence cannot capture long range entanglement. To go beyond NN entanglement, we calculate the geometrical entanglement. It "measures" the distance of a state to its closest separable one

$$\Lambda_{\text{max}} = \max_{|\psi_{\text{prod}}\rangle} |\langle \psi_p | \psi_{\text{prod}} \rangle|$$

(6)

where $|\psi_{\text{prod}}\rangle = \otimes_{i=1}^{N} |\phi_i\rangle$ and we maximize over the set of all separable (non entangled) states. The larger $\Lambda_{\text{max}}$ is, the lower the entanglement of $|\psi_p\rangle$ is since it is closer to a product state. It makes sense to define the geometric entanglement [33] as:

$$E_G = 1 - \Lambda_{\text{max}},$$

(7)

which clearly goes beyond bipartite entanglement.

III. SPATIALLY COMPLETELY ANISOTROPIC TRIANGULAR LATTICE (SCATL)

Our starting point is AF Heisenberg spin 1/2 model in a triangular lattice whose Hamiltonian reads:

$$H = \sum_{i<j} t_{ij} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z),$$

(8)

where $S_i^x$ are the spin 1/2 Pauli matrices for site $i$, the sum runs over all NN pairs, and all coupling constants $t_{ij} > 0$. We restrict ourselves to the cases $\lambda = 0$ ($\lambda = 1$) which correspond to XY (Heisenberg) interactions. The anisotropy of the model is given by the different interaction strengths $(t_1, t_2, t_3)$ along the lattice directions (see Fig. 1 (bottom)). Without loosing generality, we consider $t_1 = 1$ and leave as free parameters $t_2$ and $t_3$. The case $t_2 = t_3$ has been extensively studied [9, 11, 14, 19]. For the sake of completeness, it is instructive to reproduce first its classical phase diagram. The reader familiar with it can skip this part.

**Classical Phase Diagram.**

The classical phase diagram provides an estimate on the location and nature of the ordered phases. Order is signaled by the points in the reciprocal space that maximize correlations or, equivalently, the ones that minimize the Hamiltonian energy. The classical ordering vector, $\mathcal{Q}^{cl}$, is obtained replacing the spin operators in Eq.(8) by a classical rotor laying in the XY plane, $S_i = S \cdot (\cos (\mathcal{Q}^{cl} \cdot \vec{r}_i), \sin (\mathcal{Q}^{cl} \cdot \vec{r}_i))$, up to a global phase. Energy minimization yields a region in the phase diagram with continuously varying ordering vector, described by the following equations:

$$\mathcal{Q}_x^{cl} = \pm \arccos \left[ \frac{t_2 t_3}{2} - \frac{t_1^2 + t_3^2}{2t_2 t_3} \right] \quad \text{if} \quad \frac{t_2 t_3}{2} - \frac{t_1^2 + t_3^2}{2t_2 t_3} \leq 1$$

$$\mathcal{Q}_y^{cl} = \pm \frac{2}{\sqrt{3}} \arccos \left[ \frac{(t_2 + t_3)}{2t_2 t_3} \sqrt{t_2 t_3 + 2 - \frac{t_1^2 + t_3^2}{t_2 t_3}} \right],$$

(9)

where the argument of $\mathcal{Q}_y^{cl}$ is negative if the correspond-
FIG. 2: Classical phase diagram for the SCATL for both XY ($\lambda = 0$) and Heisenberg ($\lambda = 1$) interactions, obtained by plotting $Q_x$ in Eq. (9) as a function of the anisotropy (top left). The other panels show the spin structure factor and a sketch of the spin order for each classical phase.
in Fig. 3, because in them, the spins are ordered along the corresponding dominant direction and totally disordered along the other two. This constrain strongly restricts the number of random TBC which are quasi degenerate in energy. However, an inspection on the corresponding ground states shows that indeed they are 1D disordered quantum phases. All our results apply both for the XY and the Heisenberg model, but for the sake of concreteness we refer from now on the XY model.

In Fig. 4, we depict the averaged order parameter $\langle M \rangle_d$ for the parameters along the vertical line displayed in Fig. 3 which goes from the 2D Néel (5) to the 2D Néel (7). We observe that between the two 2D Néel ordered phases – faithfully identified by the average spin structure factor –, there is a region with lower LRO, signaled by the decrease of $\langle M \rangle_d$. The corresponding spin structure shows 1D Néel order. We identify this region as a trivial gapless QSL. The same features are observed in the two other limiting cases (1) and (3).

To further explore the nature of the truly quantum disordered phase, we restrict now our analysis to the quantum phase diagram along the diagonal line depicted in Fig. 3 which crosses several quantum phases including the putative QSL (8). In the top row of Fig. 5, we display $\langle S(\vec{k}) \rangle_d$ for some selected points along this line. Its inspection allows for an easy identification of two 2D Néel phases at the extrems of this quantum phase diagram, the first one exemplarized at $t_2 = 0.2$, $t_3 = 0.6$ and the second one at $t_2 = 2.6$, $t_3 = 1.65$. Between them, we find the expected spiral phase at $t_2 = 1$, $t_3 = 0.95$. Finally, between the 2D Néel phases and the spiral one, there are two regions (circa $t_2 = 0.65$, $t_3 = 0.8$ and $t_2 = 1.5$, $t_3 = 1.15$) whose spin structure factor does not correspond to any order. In the middle row of the same figure, we plot the corresponding overlap $O_p = |\langle \psi_p | \psi_0 \rangle|$ for all config-
Oppland also signals the two preferred directions in the 2D study in Fig. 5. As expected, the spiral phase has an 0.5 \text{th}\text{ phase (2D Néel–QSL–spiral–QSL–2D Néel) under the figures point out the location of the different quantum phases have a very small dispersion of the order parameter, the dispersion becomes much more significant for the putative gapped QSL making its average meaningless. 

The vertical lines limit the region $\epsilon_p < 0.01$, where the average is done.

FIG. 5: Quantum phase diagram along the diagonal white line in Fig. 3 for the 4 \times 4 lattice with XY interactions. Top: averaged structure factor $\langle S(\mathbf{k}) \rangle_p$. Center: overlap, $O_p$, versus normalized energy $\epsilon_p$. Bottom: order parameter, $M_p$ (see text). The dashed vertical lines limit the region $\epsilon_p < 0.01$, where the average is done.

In this section, we extend our work to the AF Heisenberg model with nearest (NN) and next-nearest-neighbours (NNN) interactions,

$$H_{J_1–J_2} = J_1 \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j,$$

(10)

where we fix $J_1 = 1$ leaving $J_2$ as the free parameter and the sums run over all NN and NNN pairs respectively.

Before proceeding further, let us mention that finite size effects are now further enhanced by the presence of
quantum fluctuations are taken into account [36, 37]. For \( J_2 > 1 \), there is non-commensurate spiral order.

**Quantum phase diagram.**

Recent studies have analyzed the quantum phase diagram of the model with special attention in the surroundings of the classical phase transition point, at \( J_2 = 1/8 \), with 2D DMRG [20, 21], variational quantum Monte Carlo [22], exact diagonalization [24] and Schwinger boson mean-field [38]. A consensus has been reached in identifying a QSL phase for \( 0.08 \leq J_2 \leq 0.15 \). The nature of this phase, though, is still under debate. To shed more light in the issue, an extra chiral term in the Hamiltonian has been proposed [23–25, 39, 40],

\[
H_k = H_{J_1 - J_2} + J_k \sum_{i,j,k \in \Lambda} \langle S_i \times S_j \rangle,
\]

where the sum runs to all the up and down triangles of the lattice clock-wisely.

In Fig. 7 (left panel), we show an sketch of the quantum phase diagram taken from Refs. [23–25]. For \( J_1 = 0 \), we recover the \( J_1 - J_2 \) model. As \( J_k \) is turned on, there is a phase transition from the QSL under debate into a chiral spin liquid (CSL) which lies between the ordered spiral, the 2D Néel collinear and the tetrahedral phase. In Fig. 7 (right panel), we show our schematic quantum phase diagram obtained by counting the number of post-selected configurations, \( N_c \), for \( \epsilon_p < 0.005 \), as a function of the parameters of the model, \( J_2 \) and \( J_1 \) for a lattice of just \( 4 \times 4 \) spins. For this model, in contrast with the analysis of previous models (Sec. III), we choose a smaller energy bias, \( \epsilon_p \), for post-selection of quasi-degenerate states, because the number of inner bonds is much increased as compared to the Heisenberg model. For \( J_1 = 0 \), we observe a region with a large number of quasi degenerate ground states that extends approximately from 0.05 \( \leq J_2 \leq 0.10 \). As \( J_2 \) increases, this region is continuously enlarged and at \( J_2 = 0 \), it expands approximately between 0.1 \( \leq J_1 \leq 0.40 \). It is interesting to compare both figures. Despite that the boundaries we obtain are clearly different from those sketched in Fig. 7 (left panel), our results show a large increase of compatible configurations in a region reconcilable with the location of both, the CSL present in the model described above (Eq.11) and the QSL of the J1-J2 model (Eq. 10).

Finite size effects can be spotted by calculating the quantum phase diagram in larger lattices. In Fig. 8 (top), we display, \( N_c \) as function of \( J_2 \) (\( J_1 = 0 \)) for different lattice sizes and geometries; \( N = 4 \times 4; 4 \times 6; 6 \times 4 \). As expected, by increasing the lattice size, the localization of the maximum of \( N_c \) shifts to larger values of \( J_2 \) in accordance to the quantum phase diagram of the system. To deepen further in the nature of the possible phases observed in Fig. 7 (right panel), we explore other physical quantities, like the averaged spin structure factor to determine the corresponding orders for a lattice of \( N = 6 \times 4 \). Our results are depicted in Fig. 8 and agree quite closely.
FIG. 7: Left, sketched quantum phase diagram of the $J_1 - J_2$ model with chiral interactions obtained from Refs. [24, 25]. Right, $N_c$ for the same model using a $4 \times 4$ lattice. The area with large $N_c$ is a signature of putative gapped QSL phase.

with the expected orders. For $0 \leq J_2 \leq 0.05$, spiral order is dominant. As $J_2$ further increases, there is a region with large number of random configurations, $N_c$, which lead to a ground state energy $E_p$ quasi degenerate with the smallest one $E_0$. These configurations correspond to different ground states, as demonstrated by all possible values the overlap $O_p$ takes. In this region, the averaged structure factor, $\langle S(\vec{k}) \rangle$, is blurred, showing that there are no clear preferable $k$-vectors. This indicates disorder and, consequently, a decrease of LRO.

Again, it is instructive to compare our results with the results of the quantum phase diagram obtained with more sophisticated methods for larger lattices. In the bottom row of Fig. 8, we attach for comparison, $S(\vec{k})$ obtained with 2D DMRG from Ref. [21]. For the values where the putative QSL is predicted, both $S(\vec{k})$ obtained from the 2D DMRG simulations and our $\langle S(\vec{k}) \rangle_d$ are impressively similar. For $J_2 = 0.2$, the 2D DMRG shows collinear order corresponding to the 2D Néel order along two lattice directions (see Fig. 2) while our results show a superposition of two of the 2D Néel collinear orders. This is not relevant, as all collinear orders are degenerate and of course any superposition of them as well. Finally, let us remark that in the same spirit, we have also analyzed the nature the quantum phases that appear when the chiral term is included for a lattice of $N = 4 \times 4$. The results in this case suffer from strongly finite size effects but ordered phases can be easily identified by $\langle S(\vec{k}) \rangle_d$.

V. CONCLUSIONS

We have shown that with a simple numerical method, based in exact diagonalization with engineered random twisted boundary conditions, it is possible to find clear signatures of QSL phases in small lattice sizes. In particular, we have analyzed with this method the anisotropic

FIG. 8: $J_1 - J_2$ model without chiral interactions ($J_\chi = 0$). Top panel, number of configurations, $N_c$, with $\epsilon_p < 0.05$ for different lattice sizes and geometries. First row $O_p$ and energy bias $\epsilon_p$ for a $6 \times 4$ lattice. Bottom rows, our averaged spin structure factor, $\langle S(\vec{k}) \rangle_d$ and $S(\vec{k})$ obtained with 2D DMRG taken from Ref. [21].
spin 1/2 triangular lattice with AF Heisenberg interactions and the J1-J2 model. Our results closely reproduce in both cases the quantum phase diagram obtained with other methods. We have found regions which display massive ground state degeneracy, large entanglement and ill defined spin structure factors. We have identified these regions as QSL. Our method provides a feasible tool for the study and detection of novel quantum disordered phases in frustrated systems, as it unveils explicitly the underlying properties of quantum spin liquids.

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Appendix

In this Appendix we show how TBC are implemented for the next-nearest-neighbours and chirality terms present in the model studied in sect IV. We show the scheme for both cases in Fig. A.1. In the same way than in the next neighbours interactions (Fig. 1) when a interaction term crosses the left-right (up-down) boundary the external spin gets twisted by a phase $\phi_1$, blue colour ($\phi_2$, red color). The external spins in the top-left corner of the figures, are twisted by $\phi_2$ because the interaction crosses both boundaries. In the next-nearest-neighbours case, there is, as well, an external spin in the bottom-left corner which crosses the left-right down-up border. Note that crossing the down-up border is the opposite as crossing the up-down one. Therefore, the spin in the bottom-left corner gets twisted by a phase $\phi_4 = \phi_1 - \phi_2$ (green colour).

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FIG. A.1: Scheme of twisted boundary conditions in a $4 \times 3$ triangular lattice with next-nearest-neighbours interactions (top panel) and chiral interactions (bottom panel). In every interaction term in the periodic boundary, depicted by a black oval, the coloured spin is twisted by an angle $\phi_1$ (blue), $\phi_2$ (red) for the left-right and top-bottom boundaries respectively. Interaction terms which cross two boundaries get twisted by both phases, $\phi_3 = \phi_1 + \phi_2$ (pink) for the left-top boundary, and $\phi_4 = \phi_1 - \phi_2$ (green) for the left-bottom one. The inner bounds are not depicted for clarity.