Spin nematics, valence-bond solids and spin liquids in SO(N) quantum spin models on the triangular lattice

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We introduce a simple model of SO(N) spins with two-site interactions which is amenable to quantum Monte-Carlo studies without a sign problem on non-bipartite lattices. We present numerical results for this model on the two-dimensional triangular lattice where we find evidence for a spin nematic at small N, a valence-bond solid (VBS) at large N and a quantum spin liquid at intermediate N. By the introduction of a sign-free four-site interaction we uncover a rich phase diagram with evidence for both first-order and exotic continuous phase transitions.

The destruction of magnetic order by quantum fluctuations in spin systems is frequently invoked as a route to exotic condensed matter physics such as spin liquid phases and novel quantum critical points [1–3]. The most commonly studied spin Hamiltonians have symmetries of the groups SO(3) and SU(2) which describe the rotational symmetry of 3-dimensional space. Motivated both by theoretical and experimental [4] interest, spin models with larger-N symmetries have been introduced, e.g. extensions of SU(2) to SU(N) [5–8] or Sp(N) [9].

The extension of SO(3) to SO(N) is an independent large-N enlargement of symmetry, with its own physical motivations [10]. While there have been many studies of SO(N) spin models in one dimension [11–13], our understanding of their ground states and quantum phase transitions in higher dimension is in its infancy. To this end, we introduce here a simple SO(N) spin model that surprisingly is sign free on any non-bipartite lattice. This model provides us with a new setting in which the destruction of magnetic order can be studied in higher dimensions using unbiased methods. As an example of interest, we present the results of a detailed study of the phase diagram of the our SO(N) anti-ferromagnet on the two-dimensional triangular lattice.

Models. Consider a triangular lattice, each site of which has a Hilbert state of N states, we will denote the state of site j as |α⟩j (1 ≤ α ≤ N). Define the N(N−1)/2 generators of SO(N) on site i as \( \hat{L}_i^{αβ} \) with α < β; they will be chosen in the fundamental representation on all sites: \( \hat{L}_i^{αβ}|γ⟩ = i\delta_{βγ}|α⟩_i - i\delta_{αγ}|β⟩_i \). Now consider the following SO(N) [14] symmetric lattice model for N ≥ 3,

\[
\hat{H}_J = -\frac{J}{N^2-2N} \sum_{\langle ij \rangle} (\hat{L}_i \cdot \hat{L}_j)^2, \tag{1}
\]

where the “\( \langle \rangle \)" implies a summation over the N(N−1)/2 generators and (ij) is the set of nearest neighbors. To see that \( \hat{H}_J \) does not suffer from the sign problem, define a “singlet” state on a bond, \( |S_{ij}⟩ = \frac{1}{\sqrt{N}} \sum_α |α⟩_i |α⟩_j \) and the singlet projector \( \hat{P}_{ij} = |S_{ij}⟩⟨S_{ij}| \). Using these operators and ignoring a constant shift we find the simple form [15],

\[
\hat{H}_J = -J \sum_{\langle ij \rangle} \hat{P}_{ij}, \tag{2}
\]

We make four observations: First, it is possible to create an SO(N) spin singlet with only two spins for all N (in contrast to SU(N) where N fundamental spins are required to create a singlet); Second Eq. (1) being a sum of projectors on this two-site singlet is the simplest SO(N) coupling, despite it being a biquadratic interaction in the generators \( \hat{L}_i^{αβ} \); Third, since the singlet has a positive expansion, \( \hat{H}_J \) is Marshall positive on any lattice; Fourth, on bipartite lattices \( \hat{H}_J \) is equivalent to the familiar SU(N) anti-ferromagnet [6], i.e. the obvious SO(N) of Eq. (1) is enlarged to an SU(N) symmetry. Since the bipartite SU(N) case has been studied in great detail in past work on various lattices [7, 16–23], we shall concern ourselves here with the non-bipartite SO(N) case which is relatively unexplored.

Phases of \( \hat{H}_J \): Starting at N = 3, Eq. (1) becomes

\[
\hat{H} = -\frac{J}{4} \sum_{\langle ij \rangle} \left( \vec{S}_i \cdot \vec{S}_j \right)^2 \]
Since $\hat{H}_J$ has SN order for $N = 3$ and is expected to have a non-magnetic VBS at large-$N$, it is interesting to ask what the nature of the transition at which SN magnetism is destroyed. The answer to this question is unclear based on current theoretical ideas and is best settled by unbiased numerical simulations. Exploiting that $\hat{H}_J$ has no sign problem we study it as a function of $N$ on $L \times L$ lattices at temperatue $\beta$ by unbiased stochastic series expansion [29] quantum Monte Carlo simulations, with a previously described algorithm [24]. The SN state is described by the matrix order parameter $Q_{\alpha \beta} = |\alpha\rangle\langle\beta| - \frac{1}{N}$. The static structure factor, $S_{SN}(k) = \frac{1}{N_{sites}} \sum_{ij} e^{ik \cdot (r_i - r_j)} \langle \hat{Q}^{\dagger}_{\alpha \alpha}(i) \hat{Q}_{\alpha \alpha}(j) \rangle$ is used to detect SN order. For the VBS order, we construct the $k$ dependent susceptibility of dimer-dimer correlation functions in the usual way from imaginary time-displaced operators: $\chi_{VBS}(k) = \frac{1}{N_{sites}} \sum_{ij} e^{ik \cdot (r_i - r_j)} \frac{1}{\beta} \int d\tau \langle \hat{P}_{r_i, r_j + \tau} \hat{P}_{r_i, r_j + \tau}(0) \rangle$.

As shown in Fig. 1, a peak in $S_{SN}(k)$ is found at the $\Gamma$ point. Comparing the data at $N = 10$ and $N = 14$, already qualitatively it is possible to see the peak in $S_{SN}(k)$ softens as $N$ is increased. In contrast $\chi_{VBS}(k)$ develops sharp peaks at the $X$ and $M$ points as $N$ is increased. These are precisely the momenta at which previous numerical studies of the triangular lattice quantum dimer model Eq. (3) have observed Bragg peaks [28], validating the large-$N$ mapping to Eq. (3) made earlier. To detect at which $N$, the magnetic order is destroyed and the VBS order first sets in, we study the ratio, $R_{SN} = 1 - \frac{S_{SN}(\Gamma + a_2 \pi/L)}{S_{SN}(\Gamma)}$ (where $a \equiv x - y/\sqrt{3}$) as a function of $L$. $R_{SN}$ must diverge in a phase in which the Bragg peak height scales with volume and becomes infinitely sharp. On the other hand it must go to zero in a phase in which the correlation length is finite and the height and width of the Bragg peak saturate with system size. At a critical point standard finite size scaling arguments imply that the ratio, $R_{SN}$ becomes volume independent. All of these facts together imply a crossing in this quantity for different $L$. Fig. 2 shows the $R_{SN}$ and $R_{VBS}$ ratios (an analogous quantity constructed for the VBS order from $\chi_{VBS}(k)$ close to the $M$-point) as a function of the discrete variable $N$ for different $L$. The data for $R_{SN}$ shows that the magnetic order is present for $N \leq 10$. The $R_{VBS}$ data shows that the long-range VBS order is present for $N > 12$. From Fig. 2 we find that $N = 12$ is on the verge of developing VBS order; from the system sizes accessible we are unable to reliably conclude whether $N = 12$ has long range VBS order or not from our study. However, taken together the data show definitively that $N = 11$ has neither VBS nor SN order. As we shall substantiate below, at $N = 11$, $\hat{H}_J$ is a quantum spin-liquid (QSL).

**J-Q models:** In order to clarify the global phase diagram of SO($N$) anti-ferromagnets and access the quantum phase transitions between the SN, VBS and QSL phases found in $\hat{H}_J$, it is of interest to find an interaction that can tune between these phases at fixed $N$. In order to be meaningful, the new coupling must preserve all the symmetries of $\hat{H}_J$. To this end, we introduce and study a generalization of the four-site $Q$ term of SU(2) spins [30],

$$\hat{H}_Q = -Q \sum_{\langle ijkl \rangle} \left( \hat{P}_{ij} \hat{P}_{kl} + \hat{P}_{il} \hat{P}_{jk} \right)$$

where the sum includes elementary plaquettes of length four on the triangular lattice (with periodic boundary
conditions on an \( L \times L \) system there are \( 3L^2 \) such plaquettes). For a fixed-\( N \), \( \mathcal{H}_Q \) provides a tuning parameter which preserve both the internal and lattice symmetries of \( \mathcal{H}_J \) and hence allows us to study the generic phase diagram of \( \text{SO}(N) \) magnets. A summary of the phase diagram of \( \mathcal{H}_JQ \) in the \( N-Q/J \) plane is in Fig. 3: The \( Q \)-interaction destroys the SN order and gives way to VBS order only for \( N \geq 6 \). We have found evidence for direct first-order SN-VBS transitions for \( 6 \leq N < 10 \) and exotic continuous SN-VBS transitions for \( N = 10 \) and \( N = 11 \).

As an example of our observed first-order behavior we present in Fig. 4, our study of the \( N = 7 \) QMC data for the spin stiffness \( \rho_s \equiv \langle W_x^2 \rangle / L \) (where \( W_x \) is the winding number of the spin world lines), which acts as a sensitive order parameter for the SN phase, and the VBS order parameter \( O_{\text{VBS}} \equiv \langle \chi_{\text{VBS}}(\mathbf{M}) \rangle / N_{\text{site}} \). Clear evidence for a direct first order SN-VBS transition at \( N = 7 \) is found.

The nature of the transition changes at \( N = 10 \), where evidence for two phase transitions is found. As shown in Fig. 5 the SN order vanishes at a \( Q/J \) smaller than the value at which VBS order develops. Although the difference is small for \( N = 10 \), it is significant. The data for \( N = 11 \) in Fig. 5 shows that the SN and VBS orders do not vanish at the same point. In fact \( R_{\text{SN}} \) indicates that the SN order has vanished already at \( Q/J = 0 \), consistent with our previous analysis of \( \mathcal{H}_J \). As illustrated by the dashed and solid lines in Fig. 3, the appearance of the QSL phase is consistent with a global phase diagram for the \( \text{SO}(N) \) magnets.

**QSL phase and criticality:** We have identified the ground state between SN and VBS as a QSL, since it does not show evidence for any Landau-order. Were the intermediate phase characterized by a conventional order parameter, we would have expected strong first order transitions of the kind between SN and VBS (see Fig. 4), instead we find continuous transitions.

There are field theoretic reasons to expect a QSL on quantum disordering a spin nematic. The long-distance description of our \( \text{SO}(N) \) models is given by a \( \text{RP}^{N-1} \) theory (in contrast to the \( \text{CP}^{N-1} \) description of \( \text{SU}(N) \) models [31]), which can be described as \( N \) real matter fields coupled to a \( Z_2 \) gauge field. Such a theory is expected to host three phases [32], a symmetry breaking phase in which the matter condenses (which we identify in our spin model as the SN), a stable phase in which the matter gets a gap and the \( Z_2 \) gauge theory is deconfined (identified here as the QSL) and a phase in which matter is gapped and the \( Z_2 \) is confined (identified here as the VBS). Thus, the SN-QSL critical point should be in the universality class of \( O(N)^* \) critical point [3]. The QSL-VBS phase transition should be in the same universality class as the critical point between these identical phases in the quantum dimer model since the magnetic fluctuations are gapped in both the QSL and VBS phases. A previous analysis of this phase transition has predicted an \( O(4)^* \) phase transition [27], where the VBS order parameter is identified with a bilinear of the primary field.

A detailed study of the critical phenomena at \( N = 10 \) and \( N = 11 \) is clearly beyond the scope of the current manuscript. We shall be satisfied here with a brief analysis: At the QSL-VBS critical point, we are able to carry out reasonable data collapses [15] at both \( N = 10 \) and
N = 11 for $O(4)$ models (for both X and M ordering vectors, see Fig. 1) and $R_{\text{VBS}}$, where we find, $\nu_{\text{VBS}} = 1.3(2)$ and $\nu_{\text{VBS}} = 0.65(20)$ for the anomalous dimension of $O(4)$. The unusually large value of $\nu_{\text{VBS}}$ is a direct consequence of fractionalization in the intermediate QSL phase and is often regarded as a smoking gun diagnostic of exotic critical points (see e.g., [33]). More quantitatively, our critical exponents are in rough agreement with the best estimate of $\eta = 1.375(5)$ of the bilinear field and $\nu = 0.7525(10)$ in the $O(4)$ model [34]. We note that the values for $\nu_{\text{VBS}}$ and $\nu_{\text{VBS}}$ agree within the quoted errors for $N = 10$ and $N = 11$. Taken together, this bolsters the case that the intermediate QSL phase has $Z_2$ fractionalization, albeit more work is needed for a definitive identification. Unfortunately, the SN-QSL transition, observed only at $N = 10$, has large corrections to scaling and we are unable to reliably determine its critical exponents or determine whether it is a weakly first order transition (no direct evidence for a first-order transition has been found of the type shown for the $N = 7$ case).

In summary, we have introduced a new family of sign-free SO($N$) spin models, which can be regarded as non-bipartite generalizations of their popular SU($N$) cousins. The triangular lattice model which we have studied thoroughly here hosts a spin nematic, a VBS with a large unit cell, a quantum spin liquid phase and unusual quantum critical points. The absence in the SO($N$) models of a direct continuous “deconfined quantum critical point” [33] is in striking contrast to previous simulations of the related bipartite SU($N$) models [8, 23]. We have offered a plausible field theoretic scenario that naturally explains this difference. It is interesting that the absence (presence) of a QSL in bipartite SU($N$) (non-bipartite SO($N$)) spin models seems to track the absence or presence of this phase in the kind of quantum dimer models that our model maps to at large-$N$ [35].

While the study in this paper has focused on the triangular lattice, our family of models, Eq. (2.4) may be constructed sign free on any two or three dimensional non-bipartite lattice. Because of the larger degree of frustration, the kagome system may provide a wider swath of the QSL phase and hence could possibly allow a more detailed study of this phase, even if the phase diagram is of the same form found here. Exploring the phase diagram and quantum phase transitions of the three dimensional pyrochlore system is an exciting open direction for future work.

The author is grateful to J. Chalker, T. Lang, M. Levin, R. Mong, G. Murthy, A. Nahum, A. Sandvik, T. Senthil and M. Zaanen for helpful discussions. This research was supported in part by NSF DMR-1056536.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{Crossings of $R_{\text{SN}}$ (above) and $R_{\text{VBS}}$ (below) signaling the location of the onset of long-range SN and VBS orders at $N = 10$ (left) and $N = 11$ (right). At $N = 10$, $R_{\text{SN}}$ and $R_{\text{VBS}}$ cross at close but significantly different couplings, $Q_s = 0.100(5)$ and $Q_c = 0.117(2)$ respectively. At $N = 11$, $R_{\text{SN}}$ appears to have crossed at $Q/J < 0$ (we cannot study this region because of the sign problem), whereas $R_{\text{VBS}}$ crosses at $Q_c = 0.042(3)$. From the location of the crossings, for both $N = 10$ and $N = 11$, we can infer an intermediate phase which is neither SN nor VBS, as shown in Fig. 3(b). We present arguments that this phase is a QSL. No direct evidence for first order behavior is found at either of the transitions, though a weakly first order SN-QSL cannot be ruled out. The QSL-VBS transitions show good scaling behavior with unconventional critical exponents.}
\end{figure}

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Strictly speaking the symmetry of our model is an SO($N$) for odd-$N$ and an O($N$)/$Z_2$ for even $N$. This point is discussed further in the supplementary materials.

Please refer to supplementary materials for more details on the model and the numerical simulations.
SUPPLEMENTARY MATERIALS

Model and Symmetries

Here we provide some additional details of the models introduced in Eq. (1) and Eq. (2).

Mapping between Eqs. (1) and (2)

To see the connection between the two Hamiltonians Eq. (1) and Eq. (2). We consider two SO(N) spins. We can combine them into three representations: a singlet (S), symmetric (χ) and anti-symmetric (Φ) representations of dimensions: 1, $N^2 - N + 1$ and $N^2 - N$. Now construct projectors on these representations, $P_S$, $P_\chi$ and $P_\Phi$. Clearly $P_S + P_\chi + P_\Phi = 1$ and $P_S^2 = P_S$, $P_\chi^2 = P_\chi$, $P_\Phi^2 = P_\Phi$. It is straightforward to show that, $(L_i \cdot L_j) = -(N-1)P_S - P_\chi + P_\Phi$ by explicitly acting on the symmetrized wave-functions. From this it follows that $(L_i \cdot L_j)^2 = (N-1)^2 P_S + P_\chi + P_\Phi$. From which it follows that $(L_i \cdot L_j)^2 = ((N-1)^2 - 1) P_S + 1$, which proves as claimed that for $N \geq 3$, Eq. (1) and Eq. (2) are equivalent up to a constant.

$N = 2$

Although not studied in this manuscript, for the sake of completeness, we discuss our model at $N = 2$. Even though Eq. (1) is trivial for $N = 2$ (since squaring the only SO(2) generator is just an identity operator), Eq. (2) is a well defined non-trivial model. Identifying the two colors with $\uparrow$ and $\downarrow$ spins, Eq. (2) becomes $\hat{H} = \sum_{(ij)} -J(S_i^+ S_j^- + S_i^- S_j^+) + J S_i^x S_j^x$. Previous work on the triangular lattice $N = 2$ model has found clear evidence for SO(2) symmetry breaking superfluid order [1-3].

Symmetries

We now discuss the symmetries of the model Eq. (2). We begin by observing that this model is invariant under uniform O(N) rotations where we multiply each basis state by an orthogonal matrix (one that satisfies $O^2 = 1$), since this leaves the singlet state invariant, i.e.

$$\sum_\alpha |\alpha\alpha\rangle \rightarrow \sum_\alpha O_{\alpha\gamma} O_{\alpha\eta} |\gamma\eta\rangle = \sum_\alpha |\alpha\alpha\rangle.$$  

However we should identify rotations that only differ by changing all the local basis states by the same phase (in this case a sign). Here it becomes necessary to distinguish between even and odd $N$. This is because the matrix $-1$ has determinant 1 for even $N$ and -1 for odd $N$. Thus for odd-$N$ the symmetry is simply SO(N), since the rest of O(N) is obtained from SO(N) by multiplying by -1. For even-$N$ however SO(N) has pairs of elements that cause the same basis transformation up to a sign, e.g. 1 and -1. On the other hand unlike the case of odd-$N$, the O(N) matrices with determinant -1 are independent symmetries, so the symmetry realized for even-$N$ is an $O(N)/Z_2$.

| size | $N$ | $Q$ | $\beta_{QMC}$ | $E_{ex}$ | $E_{QMC}$ |
|------|-----|-----|---------------|---------|-----------|
| $2 \times 2$ | 4 | 0 | 16 | $-1.5$ | $-1.49997(3)$ |
| $2 \times 2$ | 4 | 1 | 16 | $-4.5$ | $-4.5000(1)$ |
| $2 \times 2$ | 5 | 0 | 16 | $-1.4$ | $-1.40000(5)$ |
| $2 \times 2$ | 5 | 1 | 16 | $-4.2$ | $-4.2001(1)$ |
| $2 \times 3$ | 3 | 2 | 16 | $-6.0657499233$ | $-6.0656(1)$ |
| $3 \times 3$ | 2 | 0 | 16 | $-1.7026987262$ | $-1.70269(2)$ |
| $3 \times 3$ | 2 | 1 | 16 | $-3.7290340614$ | $-3.72900(3)$ |
| $3 \times 3$ | 2 | 2 | 16 | $-5.7639923092$ | $-5.76402(5)$ |

TABLE I. Test comparisons of ground state energies from exact diagonalization and average energies from finite-T QMC studies of the SO(N) model introduced here. Note that $J = 1$ always. The energies reported here are per site and on triangular lattices with periodic boundary conditions such that there are always 3$L^2$ bonds and 3$L^2$ plaquettes in Eqs. (2,4). This causes some terms to be appear more than once for the $2 \times 2$ and $2 \times 3$ systems.

Symmetry on Bipartite Lattices

On bipartite lattices the orthogonal rotation symmetry, Eq. (5) gets extended to a unitary symmetry (with $U^\dagger U = 1$) so long as the singlet is defined between sites on opposite sub-lattices, and A sub-lattice spins are rotated by $U$ and B sub-lattice spins are rotated by $U^*$.

$$\sum_\alpha |\alpha\alpha\rangle \rightarrow \sum_\alpha U^*_{\alpha\gamma} U_{\alpha\eta} |\gamma\eta\rangle = \sum_\alpha |\alpha\alpha\rangle.$$  

(6)

Since a uniform phase change of the all the states locally does not have physical consequences, the model is said to have an SU(N) symmetry, as has been discussed and extensively studied previously in such models, see e.g. Ref. [4] for a review.

Ground state theorems

Marshall’s sign theorem guarantees that the ground state of $H_{Q} = H_J + H_Q$ is an SO(N) singlet. In addition, on the triangular lattice, which is the focus of our study here, there is no simple translationally invariant covering of two-site singlets, leading us to suspect that a generalization of the SU(2) square lattice Lieb-Schultz
Mattis (LSM) theorem [5] applies to $H_{JQ}$ on this lattice, i.e. in the thermodynamic limit there must be a degeneracy in the ground state, so that a simple gapped paramagnet is not possible – either a symmetry is broken or the ground state is exotic. A rigorous proof of this intuitive assertion is expected to be at least as technical as the proof for the bipartite $N = 2$ case [5] and is beyond the scope of this work. As we saw above, on a one-dimensional chain, which is bipartite, our model is equivalent to the SU($N$) model studied by Affleck [6] and is hence expected to have an LSM degeneracy.

### Numerical Simulations

**QMC energy tests**

Here we provide the results of some QMC tests on small lattices for the total energy per spin of our models, $\hat{H}_J + H_Q$, Eqs. (2,4) on the triangular lattice, for completeness and future comparisons.

#### Choice of $\beta = L$

In Fig. 6 we show the dependence of the fluctuations of the temporal and spatial winding numbers on the “aspect ratio” of our simulation cell. $\beta$ is a measure of the extent of the imaginary time and $L$ is an estimate for the linear spatial extent. We study the fluctuations of the temporal and spatial winding numbers as the ratio $\beta/L$ is varied for two different sizes, $L = 32$ and $L = 48$ at $N = 10$ in the model $\hat{H}_J$. We find that both quantities are balanced at a value of $\beta/L$ which is of the order of one (close to 1.42) and that the crossing point does not move much with system size. Thus for simplicity we have chosen $\beta/L = 1$ throughout the paper.

![FIG. 6. Estimation of optimal $\beta/L$ ratio for our simulations by comparison of the fluctuations of the temporal ($\langle W^2_t \rangle$) and spatial ($\langle W^2_s \rangle$) winding numbers. Data shown is for $H_J$ at $N = 10$.](image)

![FIG. 7. Finite size scaling of spin nematic order parameter and spin stiffness for the model $H_J$, in Eq. (1) with $10 \leq N \leq 14$. Shown on the left is the square of the spin nematic order parameter, $O_{SN}^2$ (the height of the Bragg peak in Fig. 1), and on the right is the spin stiffness, $\rho_s$, plotted as a function of $1/L$. The data confirms that the system is magnetically ordered for $N \leq 10$ and non-magnetic for $N \geq 11$.](image)

![FIG. 8. Finite size scaling of VBS order parameter for the model $H_J$, in Eq. (1) with $10 \leq N \leq 14$. For $N \geq 13$ we encounter difficulties in equilibrating the system for sizes larger than $L = 48$ due to formation of long-range VBS order. Rather than extrapolating $O_{VBS}^2$, we study the crossing of the ratio $R_{VBS}$, which provides a reliable way to detect the onset of long-range VBS order on moderate system sizes [see Fig. 2].](image)
Extrapolation of order parameters

The simplest estimate for long range order is to study whether the height of the Bragg peak per unit volume extrapolates to a finite quantity in the thermodynamic limit. Unfortunately, this method becomes increasingly unreliable when the measured order is weak, e.g., close to a critical point. In such cases, results from extrapolations will depend on the form of the extrapolation used. A thorough discussion of these difficulties in quantum spin systems may be found in the literature [7]. It is for this reason that we prefer to work with the $R$ ratios defined in the text. The disadvantage is that we do not know the order parameter in the thermodynamic limit, but the advantage is we can calculate the critical coupling reliably by studying the crossing of the $R$ ratio. For completeness we present here the data required for extrapolation of both SN and VBS order parameters for $\tilde{H}_J$. To test quantitatively for long range order we study the scaling of the height of the peak in $S_{SN}(k)$, $O_{SN}^2(k) = S_{SN}(k = 0)/N_{\text{site}}$ and the spin stiffness $\rho_s$ on finite size systems with $N_{\text{site}} = L \times L$. Both quantities are expected to be finite in the M state and zero when the $O(N)$ symmetry is restored. Fig. 7 shows finite size data for both quantities for different values of $N$. From these plots we conclude that the M symmetry is broken up to $N = 10$ and is restored for $N \geq 11$, because $O_{SN}^2$ scales to zero for these $N$. This behavior is mirrored in $\rho_s$, albeit for intermediate $L$ there is some non-monotonic behavior for $N = 11$. This is consistent with our conclusions in the main text made from the analysis of $R_{SN}$.

Finite size scaling for the VBS order parameter is shown in Fig. 8. Notice for the cases where there is VBS order ($N = 13, 14$) we only have data for $L \leq 48$. For system sizes larger than this we face serious equilibration issues with QMC as is expected, since the simulation gets locked into a symmetry broken VBS state. The plot serves to illustrate the ambiguity faced by making direct extrapolations. On the other hand, a study of the $R$ ratios shown in Fig. 2 provides a more clear cut way to locate the critical point.

QSL-VBS and SN-QSL phase transitions

Here we present some details of the study of the both the QSL-VBS ($N = 10, 11$) and SN-QSL ($N = 10$) phase transitions found in our model.

We obtain critical exponents at the QSL-VBS critical point by attempting a data collapse, see Fig. 9, 10. We use the standard finite size scaling ansatz for the order parameter and the crossing ratio,

$$\langle O_{VBS}^2 \rangle = L^{-(1+\nu_{VBS})} F_O(g L^{1/\nu_{VBS}})$$

$$R_{VBS} = F_R(g L^{1/\nu_{VBS}})$$

where $g = (Q - Q_c)/J$. We continue to work with $\beta = L$ as discussed. No attempt is made to make use of corrections to this leading scaling behavior. Our main objective is to determine the universal number $\eta_{VBS}$ for the QSL-VBS transition for $N = 10$ and $N = 11$. We find acceptable collapses for our data sets over a wide range of $\nu_{VBS}$. On the other hand, the estimate for $\eta_{VBS}$ is relatively stable over our various fits. The values and errors of the critical exponents quoted in the main text are based on the variation observed by using different data.
sets. A higher precision study should be possible with access to more accurate data and larger system sizes. In order to carry out the collapse numerically, we make use of a recently developed Bayesian approach to scaling [8]. We note that difficulties in obtaining accurate values of the critical exponents at exotic transitions in quantum spin models is a well-documented difficulty [9].

Another quantum phase transition takes place between SN and QSL. In our model this transition appears only at \( N = 10 \). In Fig. 11 we study the drift of various crossing quantities at the critical points. Presumably the significant drift for the crossing at the SN-QSL transition are due to corrections to scaling. We have looked for signs of first order behavior as we found for smaller-\( N \) and not found them here, though the possibility of a very weak first order transition cannot be ruled out. The corrections to scaling hamper efforts to extract critical exponents at this phase transition. In contrast the QSL-VBS transition shows a reasonably converged crossing point with a nice scaling regime, where the crossing points do not depend significantly on \( L \).

FIG. 11. Crossing of \( L \) and \( L/2 \) for various dimensionless quantities for \( N = 10 \). The dashed line is a quantity (\( R_{\text{VBS}} \)) whose crossing locates the VBS transitions and the solid lines are for two independent quantities (\( \rho_s \) and \( R_{\text{SN}} \)) that locate the SN transition. The blue and red semi-circle shows the range of critical couplings based on the extrapolation of this data. Note that (1) there is clear evidence for an intermediate phase. (2) the errors in the SN transition are significantly larger than those for the VBS transition.

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