

Time reversal symmetry breaking chiral spin liquids: Projective symmetry group approach of bosonic mean-field theories

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Projective symmetry groups are the mathematical tools which make it possible to list and classify mean-field spin liquids (SLs) based on a parton construction. The seminal work of Wen [Phys. Rev. B **65**, 165113 (2002)] and its subsequent extension to bosons by Wang and Vishwanath [Phys. Rev. B **74**, 174423 (2006)] concerned the so-called *symmetric* SLs; i.e., states that break neither lattice symmetries nor time reversal invariance. Here we generalize this tool to *chiral* (time reversal symmetry breaking) SLs described in a Schwinger boson mean-field approach and illustrate it on the triangular lattice, which can harbor nine different weakly symmetric SLs (two *symmetric* SLs and seven *chiral* SLs) with nearest neighbor bond operators only. Results for other lattices (square and kagome) are given in the Appendixes. Application of this new approach has recently led to the discovery of two chiral ground states on the kagome lattice [Messio *et al.*, Phys. Rev. Lett. **108**, 207204 (2012); Fåk *et al.*, Phys. Rev. Lett. **109**, 037208 (2012)]. The signature of a time reversal symmetry breaking SL is the presence in the ground state of nontrivial fluxes of loop operators that break some lattice point group symmetries. The physical significance of these gauge invariant quantities is discussed both in the classical limit and in the quantum SL and their expressions in terms of spin observables are given.

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I. INTRODUCTION

Symmetry breaking is a ubiquitous feature of the low temperature behavior in condensed matter physics. Solids or Néel antiferromagnets are phases that break some essential symmetries of the physical laws: translational symmetry or rotational spin symmetry. Understanding the nature of the broken symmetries, discrete or continuous, allows to understand the nature of the elementary excitations and to predict the low-energy behavior of the materials (Goldstone modes, Mermin-Wagner theorem, topological defects, etc.). In some phases, at first glance, the symmetry content may be hidden: as, for example, in helium liquids. The first obvious character is the absence of translation symmetry breaking and the absence of a solid phase at zero temperature. It was very early understood (F. London) that this absence of solidification is due to the many-body quantum dynamics and the helium phases have been named quantum liquids to be contrasted to the more “classical liquids.” It was only decades after the discovery of the ⁴He superfluidity that the nature of the order parameter was unveiled. The understanding of the ³He order parameter has also been heavily dependent on group symmetry considerations.

A parallel can be developed between this distinction of quantum liquids versus classical solids and that of spin liquids (SLs) versus Néel ordered phases. Néel ordered phases at least break the translational symmetry of the lattice and rotational symmetry of the spins. They can be described by a local order parameter and a Landau theory, whereas SL do not break any lattice symmetries nor spin rotation symmetry and cannot be described by a *local* order parameter. Similarly to ⁴He, SLs can be characterized by an internal hidden, more or less complex order.

In this paper we are mainly concerned with topological SL. These SLs are characterized at $T = 0$ by exponentially

decaying correlations for all local observables (spins, dimers, or spin nematic operators) and a spin gap to bulk excitations. They contrast to critical SLs which have algebraic correlations and gapless excitations. It has been understood very early^{1,2} that the elementary excitations of these resonating valence bond (RVB) SLs carry a spin- $\frac{1}{2}$ contrarily to the spin-1 magnons of the Néel antiferromagnets. These emergent excitations are called spinons. A natural framework to describe the SL physics is the use of effective theories with the fractional particles as elementary building blocks (parton construction). Going from the original spins to these fractionalized spinons implies the introduction of gauge fields in which the spinons are deconfined (SL) or glued (Néel order). At first glance these approaches introduce via the gauge fields a considerable (infinite) number of degrees of freedom. In fact, the number of possible distinct SLs is limited by the requirement that their physical observables do not break any lattice or spin symmetry and the enumeration of the different classes of distinct SLs can be done through group theory analysis.

This was understood 10 years ago by Wen, who developed a classification of symmetric SLs using projective symmetry group (PSG) technique.³ The analysis of Wen for fermionic spinons on the square lattice was extended by Wang and Vishwanath to bosonic spinons.⁴ In these works, the definition of a SL is limited to spin systems that do not break any symmetry, neither SU(2) spin symmetry nor lattice symmetries nor time reversal symmetry. These SLs have been dubbed by Wen *symmetric* SLs. This definition excludes *chiral* SLs, which break time reversal symmetry (and some minimal amount of lattice symmetry) but which do not break SU(2) and do not have long range order in spin-spin or dimer-dimer correlations.

In the wake of Laughlin theory of FQHE, chiral SLs have been very popular at the end of the 1980s,⁵⁻⁸ but, in the absence

of indisputable candidates, this option has nearly disappeared from many discussions in the last decade.

Nonplanar structures are quite ubiquitous in classical frustrated magnetism⁹ and are associated to scalar chirality: $\vec{S}_1 \cdot (\vec{S}_2 \times \vec{S}_3) \neq 0$. In some cases where the ground state is nonplanar this chirality can persist at finite temperature,^{10,11} although the magnetic order itself is absent for $T > 0$ (Mermin-Wagner). A similar phenomenon may take place in quantum systems at $T = 0$. There, the usual scenario is that of a gradual reduction of the Néel order parameter when the strength of the quantum fluctuations is increased. At some point the sublattice magnetization vanishes and the SU(2) symmetry is restored (leading to a SL). Now, if the ordered magnetic structure is *chiral*, the time reversal symmetry \mathcal{T} may still be broken at the point where the magnetic order disappears, hence leading to a time reversal symmetry breaking (TRSB) SL.¹² All models with classical chiral ground states (not so rare, as can be seen in Refs. 9, 13 and 14) are putative TRSB SL candidates. It is the case of the famous problem of the Heisenberg Hamiltonian on the kagome lattice. A TRSB SL ground state is the best ground state appearing in the framework of the Schwinger Bosons mean-field theory (SBMFT).¹⁵ It breaks time reversal symmetry, is gapped for moderate spin fluctuations and is in this acceptance a chiral SL.¹⁶ In a J_1 - J_2 model on the same lattice (with ferromagnetic J_1) a chiral phase is present in a large range of parameters but in this framework it remains gapless and Néel ordered even in the presence of large fluctuations.¹⁷

The goal of this paper is to revisit the PSG analysis by relaxing the time reversal symmetry constraint in order to include chiral SLs. The framework used here is the SBMFT.¹⁸ However, as for the symmetric PSG, the symmetry considerations we use here should also be valid to classify SL in the presence of moderate fluctuations beyond mean field.

The paper is organized as follows. Sections II and III are reviews, to keep this article self-contained. Section II is a description of SBMFT to fix the notations and make more precise the present understanding of this approach. Section III starts by recalling the gauge invariance of SBMFT and then describes how the PSG is used to enforce the SL symmetries on mean-field theories.

In Sec. IV, the concept of PSG is extended to include all chiral SLs. In Sec. V all the chiral and nonchiral SL theories with explicit nearest neighbor gauge fields on the triangular lattice are derived. As an example of application we propose a chiral SL as the ground state of a ring-exchange model on the triangular lattice. The physical meaning of the fluxes and their expressions in terms of spin operators is developed in Sec. VI, as well as the question of topological loops on finite size samples. Section VII is the conclusion. Appendixes contain proofs of some statements in the main text, technical details, and further applications to the square and kagome lattices.

II. SCHWINGER BOSON MEAN-FIELD THEORY

We consider a spin Hamiltonian $\widehat{H}_0(\{\widehat{\mathbf{S}}_i\}_{i=1,\dots,N_s})$ on a periodic lattice with N_s spins, each of length S . \widehat{H}_0 can contain Heisenberg interaction or more complicated terms such as cyclic exchange, all invariant under global spin rotations [SU(2) symmetry] and by time reversal transformation \mathcal{T}

($\widehat{H}_0(\{\widehat{\mathbf{S}}_i\}) = \widehat{H}_0(\{-\widehat{\mathbf{S}}_i\})$). We insist on these symmetries since they are the basis of our construction.

Finding the ground state (GS) of a quantum spin problem is a notoriously difficult problem and the SBMFT provides an approximate way to treat the problem. This approach can be summarized by the following steps: (i) The spin operators (hence the Hamiltonian) are expressed using Schwinger bosons. (ii) A suitable rotationally invariant mean-field decoupling leads to a quadratic Hamiltonian H_{MF} . (iii) H_{MF} is diagonalized using a Bogoliubov transformation and solved self-consistently.

A. Bosonic operators and bond operators

Let m be the number of sites per unit cell in the lattice and N_m the number of unit-cells, so that $N_s = N_m m$ is the total number of sites. We define the two bosonic operators $\widehat{b}_{i\sigma}^\dagger$ that create a spin $\sigma = \pm 1/2$ (or $\sigma = \uparrow$ or \downarrow) on site i . The spin operators read

$$\widehat{S}_i^z = \sum_{\sigma} \sigma \widehat{b}_{i\sigma}^\dagger \widehat{b}_{i\sigma}, \quad (1a)$$

$$\widehat{S}_i^+ = \widehat{b}_{i\uparrow}^\dagger \widehat{b}_{i\downarrow}, \quad (1b)$$

$$\widehat{S}_i^- = \widehat{b}_{i\downarrow}^\dagger \widehat{b}_{i\uparrow}. \quad (1c)$$

The Hamiltonian is thus a polynomial of bosonic operators with only even degree terms. These relations imply that the commutation relations $[\widehat{S}_i^\alpha, \widehat{S}_i^\beta] = i\epsilon^{\alpha\beta\delta} \widehat{S}_i^\delta$ are verified.

As for the total spin, it reads $\widehat{S}_i^2 = \frac{\widehat{n}_i}{2}(\frac{\widehat{n}_i}{2} + 1)$, where $\widehat{n}_i = \widehat{b}_{i\uparrow}^\dagger \widehat{b}_{i\uparrow} + \widehat{b}_{i\downarrow}^\dagger \widehat{b}_{i\downarrow}$ is the total number of bosons at site i . To fix the ‘‘length’’ of the spins, the following constraint must therefore be imposed on physical states:

$$\widehat{n}_i = \sum_{\sigma} \widehat{b}_{i\sigma}^\dagger \widehat{b}_{i\sigma} = 2S. \quad (2)$$

In traditional MF theories, the MF parameter is the order parameter (as, for example, the magnetization $\langle \widehat{\mathbf{S}}_i \rangle$) and the MF Hamiltonian consequently breaks the initial Hamiltonian symmetries, except in the high temperature phase where the MF parameter is zero. Here, we would like to describe SLs that do not break any symmetry. Thus, we express \widehat{H}_0 using quadratic bosonic operators, requiring their invariance by global spin rotations.

The expectation value of these operators is then used as mean-field parameters, ensuring that the MF Hamiltonian respects the rotational invariance. Only linear combinations of the two following operators and of their hermitian conjugates obey this property:

$$\widehat{A}_{ij} = \frac{1}{2}(\widehat{b}_{i\uparrow}^\dagger \widehat{b}_{j\downarrow} - \widehat{b}_{i\downarrow}^\dagger \widehat{b}_{j\uparrow}), \quad (3a)$$

$$\widehat{B}_{ij} = \frac{1}{2}(\widehat{b}_{i\uparrow}^\dagger \widehat{b}_{j\uparrow} + \widehat{b}_{i\downarrow}^\dagger \widehat{b}_{j\downarrow}). \quad (3b)$$

i and j are lattice sites and these operators are thus bond operators. They are linked by the relation

$$:\widehat{B}_{ij}^\dagger \widehat{B}_{ij} : + \widehat{A}_{ij}^\dagger \widehat{A}_{ij} = \frac{1}{4} \widehat{n}_i (\widehat{n}_j - \delta_{ij}), \quad (4)$$

where $:\cdot : \widehat{\cdot}$ means normal ordering.

Any Hamiltonian invariant by global spin rotation can be expressed in terms of these operators only. For example, a

Heisenberg term $\widehat{\mathbf{S}}_i \cdot \widehat{\mathbf{S}}_j$, where $i \neq j$ can be decoupled as

$$\widehat{\mathbf{S}}_i \cdot \widehat{\mathbf{S}}_j = : \widehat{B}_{ij}^\dagger \widehat{B}_{ij} : - \widehat{A}_{ij}^\dagger \widehat{A}_{ij}, \quad (5a)$$

$$= 2 : \widehat{B}_{ij}^\dagger \widehat{B}_{ij} : - S^2, \quad (5b)$$

$$= S^2 - 2 \widehat{A}_{ij}^\dagger \widehat{A}_{ij}, \quad (5c)$$

where the first line is true whatever the boson number, but the last two lines use Eq. (4) and suppose that the constraint of Eq. (2) is strictly respected.

To make clear the physical significance of these two bond operators in the case $S = \frac{1}{2}$, we write them in terms of projection operators \widehat{P}_s on the singlet state and \widehat{P}_t on the triplet states:

$$\widehat{A}_{ij}^\dagger \widehat{A}_{ij} = \frac{1}{2} \widehat{P}_s, \quad (6a)$$

$$: \widehat{B}_{ij}^\dagger \widehat{B}_{ij} : = \frac{1}{4} (\widehat{P}_t - \widehat{P}_s). \quad (6b)$$

We see in Eq. (6a), that $: \widehat{B}_{ij}^\dagger \widehat{B}_{ij} :$ represents a ferromagnetic contribution to Eq. (5a), whereas $\widehat{A}_{ij}^\dagger \widehat{A}_{ij}$ gives the singlet contribution.

B. The mean-field approximation

We now need two successive approximations to obtain a quadratic and solvable Hamiltonian. We first relax the constraint on the boson number by imposing it only on *average*,

$$\langle \widehat{n}_i \rangle = \kappa, \quad (7)$$

where κ does not need to be an integer. To implement this constraint, a Lagrange multiplier (or chemical potential) λ_i is introduced at each site i and the term $\sum_i \lambda_i (\kappa - \widehat{n}_i)$ is added to the Hamiltonian. κ can be continuously varied to interpolate between the classical limit ($\kappa = \infty$) and the extreme quantum limit ($\kappa \rightarrow 0$).

It should be recalled, in general, that fixing $\kappa = 2S$ to study a spin- S model is not necessarily the best choice as in the SBMFT $\langle \widehat{\mathbf{S}}_i^2 \rangle = \frac{3}{8} \kappa (\kappa + 2)$.¹⁹ An alternative choice could be to fix κ in such a way that the spin fluctuations and not the spin length have the correct value.²⁰

In a second step, bond operator fluctuations are neglected and a MF Hamiltonian \widehat{H}_{MF} that is linear in bond operators is obtained. For instance,

$$: \widehat{B}_{ij}^\dagger \widehat{B}_{ij} : \simeq \langle \widehat{B}_{ij}^\dagger \rangle \widehat{B}_{ij} + \widehat{B}_{ij}^\dagger \langle \widehat{B}_{ij} \rangle - |\langle \widehat{B}_{ij} \rangle|^2. \quad (8)$$

We replace $\langle \widehat{B}_{ij} \rangle$ and $\langle \widehat{A}_{ij} \rangle$ by complex bond parameters \mathcal{A}_{ij} and \mathcal{B}_{ij} . This MF approximation can be seen as the first term of a large N expansion of a $\text{Sp}(N)$ theory.²¹ The steps are explained in detail in Ref. 19 in the very similar case of an $\text{SU}(N)$ theory. This zeroth order $1/N$ expansion can be pursued to the first order.²² The MF Hamiltonian is now a quadratic bosonic operator. It can be written in terms of a $2N_s \times 2N_s$ complex matrix M and of a real number ϵ_0 depending on the \mathcal{A}_{ij} and \mathcal{B}_{ij} and on the Lagrange multipliers λ_i ,

$$\widehat{H}_{\text{MF}} = \phi^\dagger M \phi + \epsilon_0, \quad (9)$$

where $\phi^\dagger = (\widehat{b}_{1\uparrow}^\dagger, \widehat{b}_{2\uparrow}^\dagger, \dots, \widehat{b}_{N_s\uparrow}^\dagger, \widehat{b}_{1\downarrow}, \dots, \widehat{b}_{N_s\downarrow})$.²³ The expression for M and ϵ_0 depend on \widehat{H}_0 and on the chosen decoupling [for example, using Eqs. (5a)–(5c)].

The set of mean-field parameters $\{\mathcal{A}_{ij}, \mathcal{B}_{ij}\}$ appearing in H_{MF} is called an *ansatz*. Up to an equivalence relation that is described in the next section, an ansatz defines a specific phase (GS and excitations). Depending on the value of κ , this state can either have Néel long range order, or the bosons are gapped (several types of SL are then possible).

In the following, we explain and exploit the relation which exists between regular classical magnetic orders⁹ and SLs.

To enforce self-consistency, the following conditions should be obeyed:

$$\mathcal{A}_{ij} = \langle \widehat{A}_{ij} \rangle \quad \text{and} \quad \mathcal{B}_{ij} = \langle \widehat{B}_{ij} \rangle, \quad (10)$$

which are equivalent to

$$\frac{\partial F_{\text{MF}}}{\partial \mathcal{A}_{ij}} = 0 \quad \text{and} \quad \frac{\partial F_{\text{MF}}}{\partial \mathcal{B}_{ij}} = 0, \quad (11)$$

where F_{MF} is the MF free energy, together with the constraint

$$\langle \widehat{n}_i \rangle = \kappa \Leftrightarrow \frac{\partial F_{\text{MF}}}{\partial \lambda_i} = 0. \quad (12)$$

The next step is to calculate the mean values of the operators \widehat{A}_{ij} and \widehat{B}_{ij} either in the GS of \widehat{H}_{MF} if the temperature is zero or in the equilibrium state for nonzero temperatures. In both cases one needs to use a Bogoliubov transformation to diagonalize H_{MF} . As this transformation is often explained in the simple case of 2×2 matrices (or for particular sparse matrices), we explain the algorithm in a completely general case in Appendix A.

C. Choice of bond fields: \widehat{A}_{ij} and \widehat{B}_{ij} or \widehat{A}_{ij} or \widehat{B}_{ij} only

As in the example of Eqs. (5), the relation (4) can be used to eliminate \mathcal{A}_{ij} or \mathcal{B}_{ij} from \widehat{H}_{MF} . If we choose to keep only the \mathcal{B}_{ij} parameters, M is block diagonal with two blocks of size N_s , and the vacuum of bosons is a GS. To obey the constraint of Eq. (2), we have to adjust the boson densities by filling some zero-energy mode(s), therefore breaking the $\text{SO}(3)$ symmetry. The GS is thus completely classical. On the contrary, we can keep the \mathcal{A}_{ij} only, but then the singlet weight is overestimated, which can introduce some bias on frustrated lattices where short-distance correlations are not collinear. Keeping \widehat{A}_{ij} only is a widespread practice in the literature, but Trumper *et al.*²⁴ have explicitly shown that the bandwidth of the spectrum of excitations of the Heisenberg model on the triangular lattice is twice too large when using \mathcal{A}_{ij} fields only. On the other hand, the use of both \mathcal{A}_{ij} and \mathcal{B}_{ij} restores the correct bandwidth and improves quantitatively the excitation spectrum. Note that even on the square lattice the simultaneous use of both bond operators improves the GS energy.²⁵

From a different point of view Flint and Coleman²⁶ advise the use of both fields in order to have a large- N limit where spin generators are *odd* under the time reversal symmetry, as is the case for $\text{SU}(2)$.

III. THE SEARCH OF SL

Even when considering a Hamiltonian with nearest neighbor interactions only, the dimension of the MF parameter manifold is exponentially large.²⁷ Moreover, the Lagrange multipliers λ_i make the search of the stationary points of the MF free energy difficult (constrained optimization) as for each considered ansatz, all λ_i must be adjusted to calculate the MF free energy. In Ref. 28 this optimization was carried out (without any simplifying/symmetry assumption) on square and triangular lattices with up to 36 sites. In almost all cases the MF GS turned out to be highly symmetric, as expected, but excited mean-field solutions are, however, highly inhomogeneous (and often not understood yet). The problem can be considerably simplified if we restrict our search to states respecting some (or all) the symmetries of \widehat{H}_0 . Such symmetries are divided into global spin rotations, lattice symmetries, and time reversal symmetry. We have assumed from the beginning that \widehat{H}_0 is invariant by global spin rotations and chosen the MF approximation in such a way that it remains true for \widehat{H}_{MF} , but the choice of a specific ansatz may or may not break other discrete symmetries. The following section explains how to find all ansätze such as the physical quantities are invariant by all the lattice symmetries \mathcal{X} , either strictly (for symmetric SLs) or only up to a time reversal transformation (chiral SLs).

We now define some groups specific to an ansatz: the invariance gauge group in Sec. III A and the PSG in Sec. III B. Then, in Sec. III C, we define the algebraic PSG, which is associated to a lattice symmetry group and not specific to a particular ansatz on this lattice.

A. Gauge invariance, fluxes, and invariance gauge group (IGG)

Let $\mathcal{G} \simeq U(1)^{N_s}$ be the set of gauge transformations. A gauge transformation is characterized by an angle $\theta(i) \in [0, 2\pi]$ at each site and the operator \widehat{G} which implements the associated gauge transformation

$$\widehat{b}_{j\sigma} \rightarrow \widehat{b}_{j\sigma} e^{i\theta(j)} = \widehat{G}^\dagger \widehat{b}_{j\sigma} \widehat{G} \quad (13)$$

is given by

$$\widehat{G} = \exp \left(i \sum_j \widehat{b}_{j\sigma}^\dagger \widehat{b}_{j\sigma} \theta(j) \right). \quad (14)$$

A wave function $|\phi\rangle$ respects a symmetry \widehat{F} if all the physical observables measured in the state $\widehat{F}|\phi\rangle$ are identical to those measured in $|\phi\rangle$. It does not mean that $|\phi\rangle = \widehat{F}|\phi\rangle$, but that the two wave functions are equal up to a gauge transformation: $\exists \widehat{G} \in \mathcal{G}, |\phi\rangle = \widehat{G}\widehat{F}|\phi\rangle$.

The action of \widehat{G} on the ansatz is

$$\mathcal{A}_{jk} \rightarrow \mathcal{A}_{jk} e^{i(\theta(j)+\theta(k))}, \quad \mathcal{B}_{jk} \rightarrow \mathcal{B}_{jk} e^{i(-\theta(j)+\theta(k))}, \quad (15)$$

such that \widehat{H}_{MF} remains unaffected by \widehat{G} . We note that $\langle \widehat{A}_{jk} \rangle$ and $\langle \widehat{B}_{jk} \rangle$ are gauge dependent: They are not physical quantities as they do not preserve the on-site boson number. As any such quantity, their mean values calculated using \widehat{H}_0 is zero when the average is taken on all gauge choices. Using \widehat{H}_{MF} , it can be nonzero as the gauge symmetry is explicitly broken by the choice of the ansatz.

We have seen that changing the gauge modifies the ansatz but not the physical quantities. Conversely, if two MF

Hamiltonians give rise to the same physical quantities, then their ansätze are linked by a gauge transformation. In fact, two types of physical quantities are directly related to the ansatz: the MF parameter moduli (related to the scalar product of two spins) and the fluxes. The fluxes are defined as the arguments of Wilson loop operators such as $\langle \widehat{B}_{ij} \widehat{B}_{jk} \widehat{B}_{ki} \rangle$ or of $\langle \widehat{A}_{ij}^\dagger \widehat{A}_{jk} \widehat{A}_{kl}^\dagger \widehat{A}_{li} \rangle$. By construction these quantities are gauge invariant and define the ansatz up to gauge transformations. The physical meaning of fluxes are addressed in Sec. VI.

The gauge transformations that do not modify a specific ansatz form a subgroup of \mathcal{G} called the IGG. It always contains the minimal group \mathbb{Z}_2 formed by the identity and by the transformation Eq. (13) with $\theta(i) = \pi$ for all lattice sites i . In the particular cases where we can divide the lattice in two sublattices such as $\mathcal{A}_{ij} = 0$ whenever i and j are in the same sublattice (bipartite problem), the IGG is enlarged to $U(1)$. The later situation corresponds, for instance, to an ansatz on a square lattice with only first neighbor \mathcal{A}_{ij} . The transformations of the IGG are then given by $\theta(i) = \theta$ on one sublattice and $\theta(i) = -\theta$ on the other, with arbitrary $\theta \in [0, 2\pi]$.

B. The projective symmetry group

Let \mathcal{X} be the group of the lattice symmetries of the Hamiltonian \widehat{H}_0 (translations, rotations, reflections, etc.). From now on, for the sake of simplicity, we discard the hat on the gauge and symmetry operators. The effect of an element X of \mathcal{X} on the bosonic operators is

$$X : \widehat{b}_{j\sigma} \rightarrow \widehat{b}_{X(j)\sigma}. \quad (16)$$

The effect of X on the ansatz is

$$\mathcal{A}_{jk} \rightarrow \mathcal{A}_{X(j)X(k)}, \quad \mathcal{B}_{jk} \rightarrow \mathcal{B}_{X(j)X(k)}. \quad (17)$$

We know that a gauge transformation does not change any physical quantities. What about the lattice symmetries? We know from Sec. III A that if the ansätze before and after the action of X have the same physical quantities, they are linked by a gauge transformation: Thus, at least one gauge transformation G_X such as $G_X X$ leaves the ansatz unchanged. The set of such transformations of $\mathcal{G} \times \mathcal{X}$ is called the PSG of this ansatz. Note that this group only depends on the ansatz and on \mathcal{X} , but not on the details of the Hamiltonian. Thus, an ansatz is said to respect a lattice symmetry X if there is a transformation $G_X \in \mathcal{G}$ such that the ansatz is invariant by $G_X X$.

The IGG of an ansatz is the PSG subgroup formed by the set of gauge transformations G_I associated with the identity transformation I of \mathcal{X} . For each lattice symmetry $X \in \mathcal{X}$ respected by the ansatz, the set of gauge transformations G_X such as $G_X X$ is in the PSG is isomorphic to the IGG: For any G_I in the IGG, $(G_I G_X) X$ is in the PSG. Thus, the condition for an ansatz to respect all the lattice symmetries is that its PSG is isomorphic to $\text{IGG} \times \mathcal{X}$.

C. The algebraic projective symmetry groups

An ansatz is characterized (partially) by its IGG and its PSG. In turn, we know from these groups which lattice symmetries it preserves. Reversely we now want to impose lattice symmetries and find all ansätze that preserve them. To

reach this goal, we proceed in two steps. The first one is to find the set of the so-called algebraic PSGs.^{3,4} They are subgroups of $\mathcal{G} \times \mathcal{X}$ verifying algebraic conditions necessarily obeyed by a PSG. Contrary to the PSG of an ansatz, the algebraic PSGs exist independently of any ansatz and only depend on the lattice symmetry group \mathcal{X} and on the choice of an IGG (chosen as the more general). An algebraic PSG does not depend on the details of the lattice such as the positions of the sites. However, depending on these details, an algebraic PSG may have zero, one, or many compatible ansätze. The second step consists, for a given lattice, of finding all the ansätze compatible with a given algebraic PSG.

Let us detail the algebraic conditions verified by the algebraic PSGs. The group \mathcal{X} is characterized by its generators x_1, \dots, x_p . A generator x_a has an order $n_a \in \mathbb{N}^*$ such as $x_a^{n_a}$ is the identity (if no such integer exists, we set $n_a = \infty$). For any transformation $X \in \mathcal{X}$, there exists a unique ordered product $X = x_1^{k_1} \dots x_p^{k_p}$ with $0 \leq k_a < n_a$ if n_a is finite, $k_a \in \mathbb{Z}$ if not. The rules used to transform an unordered product into an ordered one are the algebraic relations of the group. Each of these rules implies a constraint on the G_{x_a} (chosen as one of the gauge transformation associated with x_a). Basically, it states that if a lattice symmetry X can be written in several ways using the generators, the gauge transformation G_X is independent of the writing (up to an IGG transformation). The subgroups of $\mathcal{G} \times \mathcal{X}$ respecting all these constraints are the algebraic PSGs.

To illustrate the idea, let us consider a basic example where \mathcal{X} is generated by two translations x_1 and x_2 . Both transformations have an infinite order $n_1 = n_2 = \infty$. We have $X \in \mathcal{X}$ written as product of generators $X = x_1^{m_1} x_2^{m_2} x_1^{m_3} x_2^{m_4} \dots$ and we would like to write it as $X = x_1^{p_1} x_2^{p_2}$. The needed algebraic relation is simply the commutation between the two translations: $x_1 x_2 = x_2 x_1$. We then have $p_1 = m_1 + m_3 + \dots$ and $p_2 = m_2 + m_4 + \dots$. We now see that this implies a constraint on G_{x_1} and G_{x_2} . Suppose that we have an ansatz unchanged by $G_{x_1} x_1$ and $G_{x_2} x_2$. Then the inverses $x_1^{-1} G_{x_1}^{-1}$ or $x_2^{-1} G_{x_2}^{-1}$ too are in the PSG. So, the product $G_{x_1} x_1 G_{x_2} x_2 x_1^{-1} G_{x_1}^{-1} x_2^{-1} G_{x_2}^{-1} \in$ PSG. This product has been chosen to make the algebraic relation $x_1 x_2 = x_2 x_1$ ($\Leftrightarrow x_1 x_2 x_1^{-1} x_2^{-1} = I$) appear after the following manipulations:

$$\begin{aligned} & G_{x_1} x_1 G_{x_2} x_2 x_1^{-1} G_{x_1}^{-1} x_2^{-1} G_{x_2}^{-1} \in \text{PSG} \\ \Leftrightarrow & G_{x_1} (x_1 G_{x_2} x_1^{-1}) x_1 x_2 x_1^{-1} x_2^{-1} (x_2 G_{x_1}^{-1} x_2^{-1}) G_{x_2}^{-1} \in \text{PSG} \\ \Leftrightarrow & G_{x_1} (x_1 G_{x_2} x_1^{-1}) (x_2 G_{x_1}^{-1} x_2^{-1}) G_{x_2}^{-1} \in \text{PSG}. \end{aligned}$$

The expressions in parentheses in the last line are pure gauge transformations and the full resulting expression is a product of gauge transformations. Thus, we can more precisely write

$$G_{x_1} (x_1 G_{x_2} x_1^{-1}) (x_2 G_{x_1}^{-1} x_2^{-1}) G_{x_2}^{-1} \in \text{IGG}. \quad (18)$$

If the IGG is \mathbb{Z}_2 , this constraint can be written in terms of the phases $\theta_X(i)$ of the gauge transformation G_X as

$$\theta_{x_1}(i) + \theta_{x_2}(x_1^{-1}i) - \theta_{x_1}(x_2^{-1}i) - \theta_{x_2}(i) = p\pi, \quad (19)$$

with $p = 0$ or 1 . This constraint coming from the commutation relation between x_1 and x_2 must be obeyed by all algebraic PSGs.

It is useless to list all algebraic PSGs for the simple reason that some of them are equivalent and give ansätze with the same physical observables. Two (algebraic or not) PSGs are equivalent if they are related by a gauge transformation G : For any gauge transformation G_X associated with the lattice symmetry X in the first PSG, $G G_X G^{-1}$ belongs to the set of gauge transformations associated with X in the second PSG. We are only interested in equivalence classes of PSGs.

Taking algebraic PSGs in different classes does not imply that they have no common ansätze: A trivial example is the ansatz with only zero parameters, belonging to any algebraic PSGs. However, each class includes ansätze that are in no other class and have specific physical properties.

Once all the algebraic PSGs classes are determined, it remains to find the possible compatible ansätze for one representant of each class. As an example of compatibility condition, let us take the case where X belongs to the considered algebraic PSG (i.e., $G_X = I$). Then an ansatz can be compatible with this algebraic PSG only if, for any couple of sites (i, j) , $\mathcal{A}_{ij} = \mathcal{A}_{X(i)X(j)}$. If such compatible ansätze exist, they respect the lattice symmetries by construction (in the sense that their physical quantities do so). We now want to impose the time reversal symmetry: Among the compatible ansätze, we only keep those that are equivalent to a real ansatz up to a gauge transformation. We call them *strictly symmetric* ansätze (*weakly symmetric* ones are defined in the next section).

To completely define an ansatz, it is sufficient to give the algebraic PSG and the values of the MF parameters on non-symmetry-equivalent bonds. For example, on a square (or triangular or kagome) lattice with all usual symmetries (see Fig. 2) and only first neighbor interactions, the \mathcal{A}_{ij} and \mathcal{B}_{ij} of one bond are enough.

IV. FROM CHIRAL LONG RANGE ORDERS TO CHIRAL SLS

We now show that the zoo of Néel LRO obtained from the strictly symmetric ansätze misses the chiral states which are exact GSs of a large number of frustrated classical models. This will lead us in a straightforward manner to the construction of chiral algebraic PSGs in which time reversal and some lattice symmetries can be broken (Sec. IV B). This generalized framework will then be illustrated on the triangular lattice in Sec. V and on the square and kagome lattice in Appendix D.

A. SU(2) symmetry breaking of symmetric ansätze

To simplify, we suppose that all lattice sites are equivalent by symmetry and only consider ansätze such that the λ_i are all equal to a single λ . Even if an ansatz is strictly symmetric, it does not always represent a SL phase. As is well known in SBMFT, a Bose condensation of zero energy spinons can occur and leads to Néel order. We discuss how the ansätze symmetry constrains the magnetic order obtained after condensation and establish a relation with the *regular states* introduced in Ref. 9.

The Bogoliubov bosons creation operators are linear combinations of the $\hat{b}_{i\sigma}$ and $\hat{b}_{i\sigma}^\dagger$ such that their vacuum $|\tilde{0}\rangle$ is a GS of \hat{H}_{MF} (see Appendix A). If the GS is unique, it must respect all the Hamiltonian symmetries and consequently,

cannot break the global spin rotation invariance. However, when κ increases (we continuously adapt the ansatz to κ so that the self-consistency conditions remains verified and the PSG remains the same), some eigenenergies decrease to zero. The GS is then no more unique as the zero mode(s) can be more or less populated and the phases of each zero mode are free. It is then possible to develop a long-range spin order.

This phenomenon occurs when no λ verifies condition (12). If λ increases the mean number of boson per site increases up to a maximal number κ_{\max} . At this point, some eigenenergies become zero. Increasing λ further is not possible as the Bogoliubov transformation becomes unrealizable [the M matrix of Eq. (9) has nonpositive eigenvalues]. To reach the required number of boson per site, we have to fill the zero energy modes $\hat{b}_1^\dagger, \hat{b}_2^\dagger, \dots$, using coherent states $e^{\alpha_1 \hat{b}_1^\dagger + \alpha_2 \hat{b}_2^\dagger + \dots} |\bar{0}\rangle$, for example. In the thermodynamical limit the fraction of missing bosons is macroscopic and a Bose condensation occurs in each of the soft modes. The choice of the weight α_i of these modes fixes the direction of the on-site magnetization. Detailed examples of magnetization calculations in a condensate are given by Sachdev.²⁹

In the classical limit ($\kappa \rightarrow \infty$), all bosons are in the condensate and contribute to the on-site magnetization \mathbf{m}_i . The modulus $|\mathbf{m}_i|$ should be equal to $\kappa/2$ to satisfy Eq. (9). The $\hat{b}_{i\sigma}$ operators acquire a nonzero expectation value $\langle \hat{b}_{i\sigma} \rangle$ and are (up to a gauge transformation) linked to \mathbf{m}_i by

$$\begin{pmatrix} \langle \hat{b}_{i\uparrow} \rangle \\ \langle \hat{b}_{i\downarrow} \rangle \end{pmatrix} = \begin{pmatrix} \sqrt{|\mathbf{m}_i| + m_i^z} \\ \sqrt{|\mathbf{m}_i| - m_i^z} e^{i \text{Arg}(m_i^x + i m_i^y)} \end{pmatrix}, \quad (20)$$

where Arg is the argument of the complex number and $m_i^{x,y,z}$ are the magnetization components. These values are constrained by the ansatz through

$$A_{ij} = \frac{1}{2} (\langle \hat{b}_{i\uparrow} \rangle \langle \hat{b}_{j\downarrow} \rangle - \langle \hat{b}_{j\uparrow} \rangle \langle \hat{b}_{i\downarrow} \rangle), \quad (21a)$$

$$B_{ij} = \frac{1}{2} (\langle \hat{b}_{i\uparrow} \rangle \langle \hat{b}_{j\uparrow} \rangle + \langle \hat{b}_{i\downarrow} \rangle \langle \hat{b}_{j\downarrow} \rangle). \quad (21b)$$

The supplementary constraint reads

$$|\mathbf{m}_i| \sim \kappa/2. \quad (22)$$

This extra constraint can make the classical limit problem unsolvable: No classical magnetization pattern is then compatible with the ansatz. An example of such a situation was studied by Wang and Vishwanath⁴ (see Appendix C).

We can take the problem of the classical limit from the other side. We begin from a classical state, from which we calculate $\langle \hat{b}_{i\sigma} \rangle$ and the ansatz [using Eqs. (20) and (21)]. What are the conditions on the classical state for the associated ansatz to be strictly symmetric? As we look for an ansatz respecting all lattice symmetries, the rotationally invariant quantities (as the spin-spin correlations) must be invariant by all lattice symmetries, which severely limits the classical magnetization pattern. Such a state is called a SO(3)-regular state. Mathematically, a state is said to be SO(3) regular if for any lattice symmetry X there is a global spin rotation $S_X \in \text{SO}(3)$ such as the state is invariant by $S_X X$. Moreover, the time reversal symmetry (i.e., the ansatz can be chosen to be real) imposes the coplanarity of the spins.³⁰ The set of coplanar SO(3)-regular states can be sent on the set of condensed states of strictly symmetric ansätze. In the same way, we define the

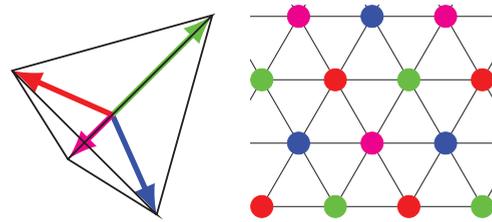


FIG. 1. (Color online) Tetrahedral order on the triangular lattice.

O(3)-regular states by including global spin flips $\mathbf{S}_i \rightarrow -\mathbf{S}_i$ in the group of spin transformations. These O(3)-regular states are listed in Ref. 9 for several two-dimensional lattices. The O(3)-regular states are divided in coplanar SO(3)-regular states and in chiral states. In a chiral state, the global inversion $\mathbf{S}_i \rightarrow -\mathbf{S}_i$ cannot be “undone” by a global spin rotation. Equivalently, there exist three sites i, j, k such as the scalar chirality $\mathbf{S}_i \cdot (\mathbf{S}_j \wedge \mathbf{S}_k)$ is nonzero: The spins are not coplanar. Then a strictly symmetric ansatz, upon condensation, can only give coplanar SO(3)-regular states in the classical limit, therefore missing all chiral O(3)-regular states.

This limitation can seem unimportant as most of the usual long range ordered spin models have planar GSs. However, some new counterexamples have recently been discovered. The first example is the cyclic exchange model on the triangular lattice¹⁰ with a four sublattice tetrahedral chiral GS (see Fig. 1). More recently, two 12 sublattice chiral GSs, with the spins oriented towards the corners of a cuboctahedron, were discovered on the kagome lattice with first and second neighbor exchanges^{11,31} (studied in Appendix D 2). A systematic study of the classical GSs of simple models on different lattices has indeed revealed that the GSs are chiral for large ranges of interaction values.⁹

The theory of symmetric PSG is unable to encompass such chiral states. In the following section, we build TRSB SL ansätze which include, upon condensation, all classical regular chiral states. This method was already applied to the kagome lattice with up to third neighbor interactions, leading to the surprising result of a chiral state even in the purely first neighbor model.¹⁵ If this state is physically relevant or not is still an open question, but independently, it shows that the omission of chiral ansätze has prevented the discovery of more competitive MF solutions.

B. The chiral algebraic PSGs: How to include weakly symmetric states

The time reversal transformation \mathcal{T} acts on an ansatz by complex conjugation of the MF parameters.³ If an ansatz respects this symmetry, it is sent to itself by \mathcal{T} (up to a gauge transformation). So, in an appropriate gauge, all parameters can then be chosen real. In most previous SBMFT studies, the hypothesis of time reversal invariance of the GS was implicit, as only *real* ansätze were considered. In contrast to SU(2) global spin symmetry that can easily be broken through the Bose condensation process, no transition is known to produce a chiral ordered state out of a \mathcal{T} -symmetric ansatz. Indeed, chiral ansätze have loops with complex-valued fluxes which evolve continuously with κ . We do not expect any singular behavior of these (local) fluxes when crossing the condensation point,

so the generic situation is that a chiral LRO phase will give rise to a TRSB SL^{15,17} when decreasing κ . It is, of course, possible that the lowest-energy ansatz changes with κ but such a first-order transition has no reason to coincide with the onset of magnetic LRO.

To obtain all chiral SLs we have to explicitly break time reversal symmetry at the MF level in the ansatz. For SO(3) classical regular states, a lattice transformation from \mathcal{X} is compensated by a global spin rotation (that leaves the ansatz unchanged). For O(3) classical regular states, a lattice transformation $X \in \mathcal{X}$ is compensated by a global spin rotation possibly followed by an inversion $\mathbf{S}_i \rightarrow -\mathbf{S}_i$. This defines a parity ϵ_X to be +1 if no spin inversion is needed and -1 otherwise. In a chiral SL, the parity will be deduced from the effect of X on the fluxes: $\epsilon_X = 1$ if they are unchanged and -1 if they are reversed. With this distinction in mind we call *weakly symmetric* (WS) ansätze the ansätze respecting the lattice symmetries up to \mathcal{T} , whereas the ansätze respecting strictly all lattice symmetries and \mathcal{T} have already been called *strictly symmetric* (SS) ansätze (all lattice symmetries are even).

The distinction between even and odd lattice symmetries (as defined by ϵ_X) is the basis of the construction of all WS ansätze via the chiral algebraic PSGs. Let us consider \mathcal{X}_e the subgroup of transformations of \mathcal{X} that can only be even. Mathematically, \mathcal{X}_e is the subgroup of \mathcal{X} , whose elements are sent to the identity by *all* morphisms from \mathcal{X} to \mathbb{Z}_2 . \mathcal{X}_e contains at least all the squares of the elements of \mathcal{X} as $\epsilon_{X^2} = \epsilon_X^2 = 1$. However, depending on the algebraic relations of \mathcal{X} , it may contain more transformations as we show in the triangular case in Sec. IV C. Once \mathcal{X}_e is known, we define the *chiral* algebraic PSGs of \mathcal{X} as the algebraic PSGs of \mathcal{X}_e . The method described previously to find all algebraic PSGs applies the same way. We define \mathcal{X}_o as the set of transformations which may be odd ($\mathcal{X} - \mathcal{X}_e$). It contains transformations of undetermined parities.

To filter the weakly symmetric ansätze from those compatible with the chiral algebraic PSGs, we have to take care of the transformations of \mathcal{X}_o . This gives two types of extra constraints. First, same type (\mathcal{A} or \mathcal{B}) MF parameters on bonds linked by such transformation must have the same modulus. The second constraint concerns their phases through the fluxes. The phases are gauge dependent, but the fluxes are gauge independent. Fluxes are sent to their opposite by \mathcal{T} , as well as by the odd transformations of \mathcal{X} . They are unchanged by even transformations. To find all WS ansätze we then have to determine a maximal set of independent elementary fluxes and distinguish all possible cases of parities for the transformations of \mathcal{X}_o ($\epsilon_X = \pm 1$).

We can now apply these theoretical considerations to find all WS ansätze on some usual lattices as the triangular, honeycomb, kagome, and square lattice. The calculations are detailed for the triangular lattice in the following subsections and some results for the kagome and square lattice are given in Appendix D.

C. Chiral algebraic PSGs of lattices with a triangular Bravais lattice

The first step is to find all chiral algebraic PSGs. As already mentioned, they only depend on the symmetries of \mathcal{X}_e and on the IGG. We choose the most general case of IGG $\sim \mathbb{Z}_2$ and

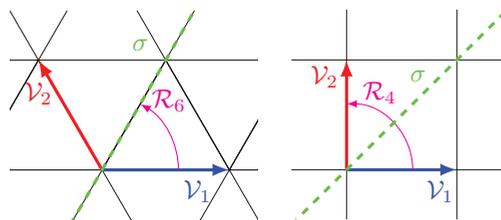


FIG. 2. (Color online) Generators of the lattice symmetries \mathcal{X} for the triangular and square lattices. \mathcal{V}_i is a translation, σ is a reflection, and \mathcal{R}_i is a rotation of order i .

suppose that \widehat{H}_0 respects all the lattice symmetries with the generators described in Fig. 2. These symmetries are those of a triangular lattice, but the actual (spin) lattice of \widehat{H}_0 can be any lattice with a triangular Bravais lattice such as a honeycomb, a kagome, or more complex lattices. The coordinates (x, y) of a point are given in the basis of the translation vectors $\mathcal{V}_1, \mathcal{V}_2$ and the effect of the generators on the coordinates are

$$\mathcal{V}_1 : (x, y) \rightarrow (x + 1, y), \quad (23a)$$

$$\mathcal{V}_2 : (x, y) \rightarrow (x, y + 1), \quad (23b)$$

$$\mathcal{R}_6 : (x, y) \rightarrow (x - y, x), \quad (23c)$$

$$\sigma : (x, y) \rightarrow (y, x). \quad (23d)$$

The algebraic relations in \mathcal{X} are

$$\mathcal{V}_1 \mathcal{V}_2 = \mathcal{V}_2 \mathcal{V}_1, \quad (24a)$$

$$\sigma^2 = I, \quad (24b)$$

$$\mathcal{R}_6^6 = I, \quad (24c)$$

$$\mathcal{V}_1 \mathcal{R}_6 = \mathcal{R}_6 \mathcal{V}_2^{-1}, \quad (24d)$$

$$\mathcal{V}_2 \mathcal{R}_6 = \mathcal{R}_6 \mathcal{V}_1 \mathcal{V}_2, \quad (24e)$$

$$\mathcal{V}_1 \sigma = \sigma \mathcal{V}_2, \quad (24f)$$

$$\mathcal{R}_6 \sigma \mathcal{R}_6 = \sigma. \quad (24g)$$

Let us now determine the subgroup \mathcal{X}_e of transformations which are necessarily even. It evidently includes $\mathcal{V}_1^2, \mathcal{V}_2^2$, and \mathcal{R}_6^2 (noted \mathcal{R}_3). However, there are more even transformations in this subgroup. Using Eq. (24e) we find $\epsilon_{\mathcal{V}_2} \epsilon_{\mathcal{R}_6} = \epsilon_{\mathcal{R}_6} \epsilon_{\mathcal{V}_1} \epsilon_{\mathcal{V}_2}$, so $\epsilon_{\mathcal{V}_1} = 1$. In the same way, using Eq. (24d), we get $\epsilon_{\mathcal{V}_2} = 1$. Thus, \mathcal{X}_e is generated by $\mathcal{V}_1, \mathcal{V}_2$, and \mathcal{R}_3 . The algebraic relations in \mathcal{X}_e are

$$\mathcal{V}_1 \mathcal{V}_2 = \mathcal{V}_2 \mathcal{V}_1, \quad (25a)$$

$$\mathcal{R}_3^3 = I, \quad (25b)$$

$$\mathcal{R}_3 \mathcal{V}_1 = \mathcal{V}_2 \mathcal{R}_3, \quad (25c)$$

$$\mathcal{R}_3 = \mathcal{V}_1 \mathcal{V}_2 \mathcal{R}_3 \mathcal{V}_2. \quad (25d)$$

As explained in Sec. III C, each of these relations gives a constraint on the gauge transformations associated to the corresponding generators. Equations (25) imply that for any site i ,

$$\theta_{\mathcal{V}_2}(\mathcal{V}_1^{-1}i) - \theta_{\mathcal{V}_2}(i) = p_1\pi, \quad (26a)$$

$$\theta_{\mathcal{R}_3}(i) + \theta_{\mathcal{R}_3}(\mathcal{R}_3i) + \theta_{\mathcal{R}_3}(\mathcal{R}_3^2i) = p_2\pi, \quad (26b)$$

$$\theta_{\mathcal{R}_3}(i) - \theta_{\mathcal{R}_3}(\mathcal{V}_2^{-1}i) - \theta_{\mathcal{V}_2}(i) = p_3\pi, \quad (26c)$$

$$\begin{aligned} &\theta_{\mathcal{V}_2}(\mathcal{V}_1^{-1}i) + \theta_{\mathcal{R}_3}(\mathcal{V}_2^{-1}\mathcal{V}_1^{-1}i) \\ &+ \theta_{\mathcal{V}_2}(\mathcal{V}_2\mathcal{R}_3^2i) - \theta_{\mathcal{R}_3}(i) = p_4\pi, \end{aligned} \quad (26d)$$

where p_1 to p_4 can take either the value 0 or 1 (the equations are written modulo 2π). We note $[x]$ the integer part of x and $x^* = x - [x]$ ($0 \leq x^* < 1$). By partially fixing the gauge, we can impose

$$\theta_{\nu_1}(x_i, y_i) = 0, \quad \theta_{\nu_2}(x_i^*, y_i) = p_1 \pi x_i^*. \quad (27)$$

Through a gauge transformation G of argument θ_G , the θ_X of a lattice transformation X becomes

$$\theta_X(i) \rightarrow \theta_G(i) + \theta_X(i) - \theta_G(X^{-1}i) \quad (28)$$

and the algebraic PSG is transformed in an other element of its equivalence class. Using the gauge transformations

$$G_3 : (x, y) \rightarrow \pi x, \quad G_4 : (x, y) \rightarrow \pi y, \quad (29)$$

we see that a change of p_3 or p_4 is a gauge transformation, so we can set them to zero. Solving the set of Eqs. (26) leads to

$$\theta_{\nu_1}(x, y) = 0, \quad (30a)$$

$$\theta_{\nu_2}(x, y) = p_1 \pi x, \quad (30b)$$

$$\theta_{\mathcal{R}_3}(x, y) = p_1 \pi x \left(y - \frac{x+1}{2} \right) + g_{\mathcal{R}_3}(x^*, y^*), \quad (30c)$$

with a supplementary constraint that can only be treated when the spin lattice is defined:

$$g_{\mathcal{R}_3}(x^*, y^*) + g_{\mathcal{R}_3}((-y)^*, (x-y)^*) + g_{\mathcal{R}_3}((y-x)^*, (-x)^*) = p_2 \pi. \quad (31)$$

This constraint only depends on the coordinates of the sites in a unit cell (x^* and y^*).

Equations (30) and (31) define the chiral algebraic PSG on the triangular Bravais lattice. The full determination of the WS ansätze requires the determination of the spin lattice [triangular, honeycomb ($m=2$), or kagome ($m=3$)] and of the number of interactions included in the MF Hamiltonian (first neighbor only or first and second neighbor; \mathcal{A} and \mathcal{B} parameters, or \mathcal{A} only, etc.). The case of the triangular lattice ($m=1$) with nearest neighbor interactions and \mathcal{A} and \mathcal{B} MF parameters is described in the next section.

V. STRICTLY AND WEAKLY SYMMETRIC ANSÄTZE ON THE TRIANGULAR LATTICE WITH FIRST NEIGHBOR INTERACTIONS

A. Construction of WS ansätze on the triangular lattice

The triangular lattice has a single site per unit cell and the values of x^* and y^* are the coordinates of this site in a unit cell, say $(0,0)$. Equation (31) simplifies to

$$6g_{\mathcal{R}_3}(0,0) = 0. \quad (32)$$

The solutions are $g_{\mathcal{R}_3}(0,0) = k\pi/3$, with k integer. Because the IGG is \mathbb{Z}_2 , only the three values $k = -1, 0, 1$ lead to physically different ansätze.

Finally, we have six distinct algebraic PSGs for the reduced set of symmetries \mathcal{X}_e . They are characterized by two integers $p_1 = 0, 1$ and $k = -1, 0, 1$ and defined by

$$\theta_{\nu_1}(x, y) = 0, \quad (33a)$$

$$\theta_{\nu_2}(x, y) = p_1 \pi x, \quad (33b)$$

$$\theta_{\mathcal{R}_3}(x, y) = p_1 \pi x \left(y - \frac{x+1}{2} \right) + \frac{k\pi}{3}. \quad (33c)$$

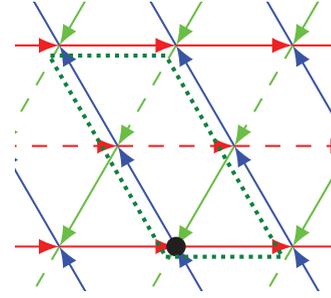


FIG. 3. (Color online) Ansätze respecting the \mathcal{X}_e symmetries on the triangular lattice. All arrows carry \mathcal{B}_{ij} parameters of modulus B_1 and of argument ϕ_{B_1} and \mathcal{A}_{ij} parameters of modulus A_1 and of argument 0 on red arrows (choice of the gauge), $2k\pi/3$ on blue ones, and $4k\pi/3$ on green ones. On dashed arrows \mathcal{A}_{ij} and \mathcal{B}_{ij} take an extra $p_1\pi$ phase.

Now, we have to find all the ansätze compatible with these PSGs.³² The first useful insight is to count the number of independent bonds. Here, one can obtain any bond from any other by a series of rotations and translations (i.e., elements of \mathcal{X}_e). Thus, if we fix the value of \mathcal{A}_{ij} and \mathcal{B}_{ij} on a bond ij , we can deduce all other bond parameters from the PSG. Note that \mathcal{A}_{ij} can be chosen as real by using the gauge freedom. The value of all bond parameters are represented on Fig. 3 as a function of their value on the reference bond. The unit cell of the ansatz contains up to two sites because p_1 may be nonzero.

From now on we can forget about the PSG construction and only retain the definition of the ansatz given by Fig. 3 and its minimal set of parameters: two integers p_1 and k , two moduli A_1 and B_1 , and one argument ϕ_{B_1} .

Until now, we have only considered the subgroup \mathcal{X}_e and we have looked for ansätze strictly respecting these symmetries. We now want to consider all symmetries in \mathcal{X} , but the symmetries in \mathcal{X}_o will be obeyed modulo an eventual time reversal symmetry. This requires supplementary conditions on the ansätze of Fig. 3. As explained in Sec. IV B, the transformations of \mathcal{X}_o imply relations between the modulus and the arguments of the ansatz. Since we are in a very simple case, where all bonds are equivalent in \mathcal{X}_e , no extra relation on the modulus can be extracted from \mathcal{X}_o . However, some conditions can be found by examining how the fluxes $\text{Arg}(\mathcal{A}_{ij}\mathcal{A}_{jk}^*\mathcal{A}_{kl}\mathcal{A}_{li}^*)$ on an elementary rhombohedron and $\text{Arg}(\mathcal{A}_{ij}\mathcal{B}_{jk}\mathcal{A}_{ki}^*)$ on an elementary triangle transform with \mathcal{R}_6 and σ . Assuming that neither A_1 nor B_1 are zero we find

$$2k\pi(1 - \epsilon_{\mathcal{R}_6})/3 = 0, \quad (34a)$$

$$2k\pi(1 + \epsilon_\sigma)/3 = 0, \quad (34b)$$

$$(1 + \epsilon_{\mathcal{R}_6})\phi_{B_1} = p_1\pi, \quad (34c)$$

$$(1 - \epsilon_\sigma)\phi_{B_1} = p_1\pi. \quad (34d)$$

For each set $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma)$, the compatible ansätze are thus limited to

(i) $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (1, 1)$: $k = 0$, $p_1 = 0$ and $\phi_{B_1} = 0$ or π ,

(ii) $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (-1, -1)$: $k = 0$, $p_1 = 0$ and $\phi_{B_1} = 0$ or π ,

(iii) $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (1, -1)$: $\phi_{B_1} = p_1\pi/2$ or $\pi + p_1\pi/2$,

(iv) $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (-1, 1)$: $k = 0$, $p_1 = 0$ and no constraint on ϕ_{B_1} .

A couple $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma)$ does not characterize an ansatz. A given ansatz, can be found for several couples of parities. For

TABLE I. The nine weakly symmetric ansätze families on the triangular lattice, with the notations of Fig. 3. The moduli A_1 and B_1 are not constrained although supposed nonzero.

Ansatz No.	p_1	k	ϕ_{B_1}
1	0	0	0
2			π
3			Any
4	1	1	0
5			π
6	1	0	$\pi/2$
7			$3\pi/2$
8		1	$\pi/2$
9			$3\pi/2$

example, the ansätze obtained for $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (1, 1)$ are also present for all other $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma)$. Indeed, as their MF parameters are real, they are not sensitive to time reversal and any $\epsilon_{\mathcal{R}_6}, \epsilon_\sigma$ can be chosen. From the classical point of view, these ansätze describe coplanar spin configurations, which are invariant under a global spin flip followed by a π rotation around an axis perpendicular to the spin plan.

Finally, there are nine different WS ansätze families, given in Table I. We now conclude this section with a series of remarks concerning the solutions we have obtained.

(i) The number of WS ansätze families is larger than the number of algebraic PSGs of \mathcal{X}_e , because the operators in \mathcal{X}_o can act in different ways on the ansätze.

(ii) Among these nine ansätze families, only the two first are nonchiral, and the seven others are TRSB ansätze (by applying \mathcal{T} , $k = 1$ is changed to $k = -1$ and ϕ_{B_1} to $-\phi_{B_1}$).

(iii) These solutions are called *families* as the moduli A_1 and B_1 can vary continuously without modifying the symmetries. The third ansatz has no fixed value for ϕ_{B_1} and includes the first and second ansätze families (they are kept as distinct as they are nonchiral).

(iv) The fluxes of these ansätze are easily calculated using Fig. 3.

TABLE II. Values of the parameters of Fig. 3 for ansatz families related to regular classical states on the triangular lattice. The states are designed by F for ferromagnetic, Coplanar for the $\sqrt{3} \times \sqrt{3}$ state, and Tetra for tetrahedral. These states are described in more detail in Ref. 9. The question marks mean that the two values $\epsilon = \pm 1$ are possible (coplanar or colinear state). The * means that the parameter value is free; we give its value in the classical limit.

	F	Coplanar	Tetra
p_1	0	0	1
k		0	1
ϵ_R	?	?	1
ϵ_σ	?	?	-1
A_1	0	$\frac{\sqrt{3}}{4}^*$	$\frac{1}{\sqrt{6}}^*$
B_1	$\frac{1}{2}^*$	$\frac{1}{4}^*$	$\frac{1}{\sqrt{12}}^*$
ϕ_{B_1}	0	π	$\frac{\pi}{2}$

(v) The detailed list of compatible ansätze depends on the choice of the mean-field parameters (here, nonzero \mathcal{A}_{ij} and \mathcal{B}_{ij} on first neighbor bonds) as we explain in Appendix C by contrasting these results to those of Wang *et al.* on the same lattice.⁴

B. Condensation of the WS ansätze: The missing tetrahedral state

The SBMFT has already been used to study the anti-ferromagnetic Heisenberg first-neighbor Hamiltonian on the triangular lattice with the \mathcal{A}_{ij} -only decoupling^{4,29} [Eq. (5c)] or with both \mathcal{A}_{ij} and \mathcal{B}_{ij} ²⁴ [Eq. (5a)]. The classical limit of this model gives the well known three sublattice Néel order with coplanar spins at angles of 120° . The bond parameters obtained from this classical order [see Eqs. (21)] lead to a strictly symmetric ansatz [no need to break \mathcal{T} : We can choose to fix $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (1, 1)$] with $p_1 = 0, k = 0$, and $\phi_{B_1} = \pi$ (see Table II). We note that all MF parameters are real in this gauge choice (it is always possible to do so for coplanar states). In this case the restriction to real bond parameters did not prevent obtaining the true MF GS.

The tetrahedral state (Fig. 1) is the unique GS of the multi-spin exchange Hamiltonian in a large range of parameters:^{9,10}

$$\hat{H} = J_2 \sum_{\langle ij \rangle} \hat{P}_{(ij)} + J_4 \sum_{\langle ijkl \rangle} (\hat{P}_{(ijkl)} + \hat{P}_{(ilkj)}), \quad (35)$$

where the second sum runs on every elementary rhombohedra and $\hat{P}_{(ijkl)}$ is a cyclic permutation of the spins and $J_4 > 0$ and $\frac{1}{4} < \frac{J_2}{J_4} < 1$. Moreover, it is one of the GSs of a Heisenberg Hamiltonian with first and second neighbor interactions

$$\hat{H} = \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + \alpha \sum_{\langle\langle ij \rangle\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \quad (36)$$

for $\frac{1}{8} \leq \alpha \leq 1$. In the later situation the GS is, however, degenerate and fluctuations (order by disorder) favor collinear orders.^{33,34}

The bond parameters obtained from this classical order [Eqs. (21)] lead to the weakly symmetric ansatz $((\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (1, -1))$ with $p_1 = 1, k = 1$, and $\phi_{B_1} = \pi/2$ (or opposite k and ϕ_{B_1} for the opposite chirality), as indicated in Table II. The previous SBMFT studies of the ring exchange model [Eq. (35)] have been limited to real parameters³⁵ and it would be interesting to perform a systematic search for a possible chiral MF GS. If the chiral ansatz indeed turns out to have the lowest energy—as suggested by its classical limit—then the spin- $\frac{1}{2}$ might be a chiral SL since exact diagonalizations^{36,37} have shown the absence of Néel long range order in some parameter range.

VI. FLUXES

We have already given a brief definition of the fluxes in Sec. III A; in this section we enlarge this definition and comment on the physical meaning of the various loop operators (local and nonlocal) that can be defined on a lattice.

The gauge invariance of a product of $\hat{A}_{ij}, \hat{A}_{ij}^\dagger, \hat{B}_{ij},$ and \hat{B}_{ij}^\dagger operators on a closed contour requires two conditions:

(i) each site i appears in an even number of terms; (ii) the set of operators containing a site i can be organized into pairs such as the product of each pair is invariant by a local gauge transformation on site i (for example, \hat{A}_{ji} and \hat{B}_{ik}). Such a gauge-invariant operator is the analog of a Wilson loop operator in gauge theory and the complex argument of its expectation value is called a flux. $\text{Arg}\langle\hat{A}_{ij}\hat{A}_{jk}\cdots\hat{A}_{lm}\hat{A}_{mi}\rangle$, $\text{Arg}\langle\hat{B}_{ij}\hat{B}_{jk}\cdots\hat{B}_{li}\rangle$ are examples of fluxes with only \hat{A}_{ij} or \hat{B}_{ij} operators, but it is possible to mix both, as, for example, in $\text{Arg}\langle\hat{A}_{ij}\hat{A}_{jk}^\dagger\hat{B}_{kl}^\dagger\hat{A}_{lm}\hat{A}_{mi}^\dagger\rangle$. In SBMFT we approximate these averages of products by the product of the averages (this can be formally justified in the $N \rightarrow \infty$ limit). For example, $\langle\hat{B}_{ij}\hat{B}_{jk}\cdots\hat{B}_{li}\rangle \rightarrow \mathcal{B}_{ij}\mathcal{B}_{jk}\cdots\mathcal{B}_{li}$.

There is an infinite set of nonindependent fluxes.³⁸ A method to determine the number of independent fluxes for a given set of non zero \mathcal{A}_{ij} and \mathcal{B}_{ij} is given in Appendix E. To characterize a given ansatz, we can limit ourselves to the minimal set of independent parameters that define unequivocally its equivalence class: essentially the nonzero bond field modulus and a minimal set of fluxes.

The first insight on the physical meaning of the fluxes is given in the classical limit (Sec. VIA), where they are simple geometric quantities related to the orientation of the spins. Then we come back to the quantum case and express the fluxes, which are physical quantities, with the exclusive use of spin operators (Sec. VIB).

A. Definition and physical meaning in the classical limit

We first concentrate on the mean-field flux formed by products of \mathcal{B}_{ij} parameters. In the classical limit, the flux of \mathcal{B}_{ij} around a loop $ijk\cdots l$: $\text{Arg}(\mathcal{B}_{ij}\mathcal{B}_{jk}\cdots\mathcal{B}_{li})$ is related to the solid angle associated to the contour described by the spins on the Bloch sphere. We give here a simplified formulation of the calculation given in Ref. 19. Let us suppose that the direction of the magnetization (with a modulus fixed to 1) evolves slowly along the loop and use the gauge of Eq. (20), but in spherical coordinates:

$$\begin{pmatrix} \langle\hat{b}_{i\uparrow}\rangle \\ \langle\hat{b}_{i\downarrow}\rangle \end{pmatrix} = \sqrt{S} \begin{pmatrix} \cos\frac{\theta_i}{2} \\ \sin\frac{\theta_i}{2}e^{i\phi_i} \end{pmatrix}. \quad (37)$$

Then,

$$\text{Arg}(\mathcal{B}_{ij}^*) \simeq S(1 - \cos\theta_i)\frac{\phi_j - \phi_i}{2}. \quad (38)$$

This last quantity (to first order in the variation of the spin) is the half of the solid angle between the three directions defined by the z axis and the spins at sites i and j . By summing such quantities around a closed contour, we obtain the half of the solid angle spanned by the spins along the loop. This illustrates the gauge dependence of a single \mathcal{B}_{ij}^* : By a gauge transformation we change the direction of the z axis and

thus $\text{Arg}(\mathcal{B}_{ij}^*)$, but the total solid angle of the closed loop is independent of the choice of the z .

In a similar approach the flux $\text{Arg}(\mathcal{A}_{ij}(-\mathcal{A}_{jk}^*)\cdots\mathcal{A}_{lm}(-\mathcal{A}_{mi}^*))$ is associated with the half of the solid angle defined by the spins along the loop, but after flipping one spin every two sites (the j spin for \mathcal{A}_{ij} , the i for $-\mathcal{A}_{ij}^*$). The -1 's present in the above expression have their importance as they can lead to a final difference of π .

For more complicated fluxes mixing \mathcal{A}_{ij} and \mathcal{B}_{ij} parameters, we flip one spin every two sites on \mathcal{A}_{ij} and \mathcal{A}_{ij}^* bonds (as previously), we flip all of them for \mathcal{B}_{ij} , and none for \mathcal{B}_{ij}^* . The flux is then half the solid angle associated with these modified spin directions.

We can now reformulate the previously discussed relation between chirality and fluxes. If a classical state is chiral, it has nontrivial fluxes on contours where the spins are noncoplanar. If the corresponding MF parameters are nonzero, we then have found a loop with a nontrivial flux and whatever the gauge choice, at least one MF parameter has to be complex. Now, if a state is coplanar, then all fluxes are trivial and in a gauge where the spin plane is xz , all MF parameters are real.

In the tetrahedral state described on Fig. 1, the flux of the \mathcal{A}_{ij} around a small rhombohedron is $\pm\pi/3$ and the flux of the \mathcal{B}_{ij} around a small triangle is $\pm\pi/2$ (depending on the choice $k = \pm 1$; see Sec. VB).

B. Fluxes in quantum models

In the quantum realm, the fluxes can no longer be expressed in term of solid angles. However, as we have already noted, Wilson loop operators are gauge invariant quantities and, as such, they are physical observables and can be expressed in terms of the spin operators.

1. Spin- $\frac{1}{2}$ formulas

To simplify we start by imposing that the constraint is strictly verified for $S = \frac{1}{2}$, so there is exactly one boson per site. We have noted that in the classical limit, the scalar chiralities are associated with the fluxes. In the quantum case, we can express the flux operators in terms of permutation operators, generalizing some results of Ref. 7. The operator that transports the spins at sites 1,2,3 to sites 2,3,1 is the permutation noted $\hat{P}_{(123)}$. We recall that the permutation operator of spins between two sites can be written as

$$\hat{P}_{(ij)} = \frac{1}{2} + 2\hat{S}_i \cdot \hat{S}_j. \quad (39)$$

This straightforwardly implies that the flux of the \hat{B}_{ij} operators is

$$:\hat{B}_{12}^\dagger\hat{B}_{23}^\dagger\cdots\hat{B}_{n1}^\dagger := \frac{1}{2^n}\hat{P}_{(12..n)}. \quad (40)$$

where the colons denotes the normal ordered form. The formula for the flux of the \hat{A}_{ij} operators is more involved. It reads

$$:\hat{A}_{12}^\dagger\hat{A}_{23}^\dagger\hat{A}_{34}^\dagger\cdots\hat{A}_{2n1}^\dagger := \frac{1}{2^{2n}}\hat{P}_{(12..2n)}(1 - \hat{P}_{(23)})(1 - \hat{P}_{(45)})\cdots(1 - \hat{P}_{(2n1)}). \quad (41)$$

To prove this last assertion, we first note that $\frac{1-\hat{P}_{(ij)}}{2}$ is the projector on the singlet state of the two spins i and j . We then verify this equality in the basis of states $\bigotimes_{i=1}^n \psi_{2i,2i+1}$, where $\psi_{i,j}$ are eigenvectors of $P_{(ij)}$. In the case where at least one bond is in a symmetric state (triplet), both sides of Eq. (41) are zero. The final step is simply to check that the relation holds for the state which is a product of singlets.

2. Fluxes in quantum spin- S models

For $S > 1/2$, Eq. (39) is no more valid and Eqs. (40) and (41) are not more valid either. However, we can still replace the on-site number of bosons by $2S$ and obtain an expression depending only on the spin operators. The expression of the product of four \hat{A}_{ij} operators is

$$\begin{aligned} 8 : \hat{A}_{12}^\dagger \hat{A}_{23}^\dagger \hat{A}_{34}^\dagger \hat{A}_{41}^\dagger := & (\mathbf{S}_1 \cdot \mathbf{S}_2)(\mathbf{S}_3 \cdot \mathbf{S}_4) + (\mathbf{S}_2 \cdot \mathbf{S}_3)(\mathbf{S}_4 \cdot \mathbf{S}_1) - (\mathbf{S}_1 \cdot \mathbf{S}_3)(\mathbf{S}_2 \cdot \mathbf{S}_4) + S^2(\mathbf{S}_1 \cdot \mathbf{S}_3 + \mathbf{S}_2 \cdot \mathbf{S}_4 - \mathbf{S}_1 \cdot \mathbf{S}_2 \\ & - \mathbf{S}_2 \cdot \mathbf{S}_3 - \mathbf{S}_3 \cdot \mathbf{S}_4 - \mathbf{S}_4 \cdot \mathbf{S}_1) + S^4 + iS(\mathbf{S}_4 \cdot (\mathbf{S}_1 \times \mathbf{S}_2) \\ & - \mathbf{S}_1 \cdot (\mathbf{S}_2 \times \mathbf{S}_3) + \mathbf{S}_2 \cdot (\mathbf{S}_3 \times \mathbf{S}_4) - \mathbf{S}_3 \cdot (\mathbf{S}_4 \times \mathbf{S}_1)). \end{aligned}$$

The expression of the product of three \hat{B}_{ij} operators is

$$4 : \hat{B}_{12}^\dagger \hat{B}_{23}^\dagger \hat{B}_{31}^\dagger := S(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_1) + S^3 - i\mathbf{S}_1 \cdot (\mathbf{S}_2 \times \mathbf{S}_3). \quad (42)$$

3. Fluxes in SBMFT

In a state where the on-site number of bosons is not strictly conserved, the previous expressions become a bit more complicated. The number operators can no longer be replaced by $2S$, and we have, for example,

$$4 : \hat{B}_{12}^\dagger \hat{B}_{23}^\dagger \hat{B}_{31}^\dagger := \frac{1}{2}\hat{n}_3\mathbf{S}_1 \cdot \mathbf{S}_2 + \frac{1}{2}\hat{n}_1\mathbf{S}_2 \cdot \mathbf{S}_3 + \frac{1}{2}\hat{n}_2\mathbf{S}_3 \cdot \mathbf{S}_1 + \frac{\hat{n}_1\hat{n}_2\hat{n}_3}{8} - i\mathbf{S}_1 \cdot (\mathbf{S}_2 \times \mathbf{S}_3). \quad (43)$$

C. Finite size calculations lattice symmetries and nonlocal fluxes

For simple lattices as the square or triangular lattice, we can solve analytically the MF Hamiltonian H_{MF} of Eq. (9) directly in the thermodynamical limit. However, in most cases, we have to solve numerically the self-consistency conditions on finite lattices.

To use the chiral PSGs on a finite periodic lattice, we have to be cautious about symmetries. Indeed, all precautions have been taken so that the ansatz (strictly or weakly) respects the lattice symmetries on an infinite lattice. However, we have to verify that the finite periodic lattice has the same symmetry group as the infinite one. This verification is quite usual for local properties, but is more subtle for nonlocal ones and can be most easily understood in term of fluxes on large nonlocal loops.

PSGs impose that fluxes on local loops are preserved by lattice symmetries (or sent to their opposite in the case of a chiral state). However, some additional care has been taken concerning loops which are topologically nontrivial (cannot be shrunk to a point by a succession of local deformations). These loops which “wind” through the boundary conditions do not exist on the infinite lattice. For a symmetric ansatz to remain symmetric on a finite periodic lattice, we have to verify that the fluxes associated with these topologically nontrivial loops also respect the lattice symmetries. The way to treat the problem of the nonlocal loops is detailed in Appendix F, together with several ways of understanding their meaning.

VII. CONCLUSION

In this paper we have extended the PSG construction to include time reversal symmetry breaking states with the SBMFT. These TRSB phases that we describe generically as *chiral*, also break one or many discrete symmetries of the lattice (in the triangular example either σ or \mathcal{R}_6). Using this constructive method we have built all the strictly and weakly symmetric ansätze with two MF parameters on the triangular lattice. All the regular O(3) magnetically ordered phases can be obtained from these ansätze by spinon condensation (the others ansätze have no regular classical limit). The TRSB ansätze have, when they condense, nonplanar magnetic order and nonzero scalar chiralities.

The present formalism has already been used in two different models on the kagome lattice.^{15,17} In each case a specific TRSB ansatz is found to be the GS. In Sec. VB, another TRSB ansatz was discussed in relation to the ring exchange model on the triangular lattice. It could reveal to be the GS in some parameter range.^{10,36,37} More generally, all classical regular nonplanar phases that have been studied in Ref. 9 are putative TRSB SL in the quantum limit. The present paper gives the general method to enumerate and build all candidate SLs, and illustrate it more or less completely for the triangular, the square, and the kagome lattice.

The TRSB SLs have short range spin-spin correlations but nontrivial fluxes on various loops. The simplest of these fluxes are related to the imaginary part of the permutation operator

of three spins that is directly related to their scalar chirality. In some cases the time reversal symmetry breaking fluxes might be more complex, as explained in Sec. VI and illustrated in Appendix D 2 for the kagome lattice. These various fluxes have been initially defined within the SBMFT but Sec. VI has shown how these gauge invariant quantities can be expressed in terms of spin operators, independently of any MF approximation. It should be noticed that in a TRSB SL fluxes other than those deduced from the ansatz may be nonzero and easier to compute. It is the case, for example, in the *cubocl* SL recently proposed for the nearest-neighbor Heisenberg model on the kagome lattice.¹⁵ The flux of the \hat{A} bond operators around the hexagons can be expressed in terms of spin permutation operators but it is relatively involved [Eq. (41)] and has not yet been computed numerically. In fact, in that phase (at least at the MF level), there are simpler fluxes which are nonzero, as, for example, the triple product of second neighbor spins around hexagons, or the triple product of three consecutive spins on an hexagon.

In spite of short range spin-spin correlations the TRSB SL have some local order parameter associated with the fluxes, which can break the lattice point-group symmetry. The finite temperature broken symmetries being discrete symmetries, there are no Goldstone modes and these chiral phases should survive thermal fluctuations in 2D. The phase transition associated with the restoration of the chiral symmetry has been studied in some classical spin models.^{11,39,40} In spite of the Ising-like character of the order parameter, the phase transition was shown to be weakly first order due to interplay of vortices in the magnetic texture with domain walls of the chirality. It has been shown within the SBMFT framework in the *cubocl* phase that large enough thermal fluctuations tend to expel the chiral fluxes¹⁵ (favor coplanar correlations) but a more complete study (beyond MF) of the finite temperature properties of a TRSB SL would be required to understand the specific properties of the chiral transition in these systems.

Finally, it would be useful to clarify the “topological” differences (entanglement, degeneracy, edge modes, etc.) between the present chiral SL described in the SBMFT framework with the chiral SL wave functions related to fractional quantum Hall states (such as the Kalmeyer-Laughlin state⁶ or that of Yang *et al.*⁸ for instance), as well as the difference with conventional (\mathcal{T} -symmetric) \mathbb{Z}_2 liquids. It would also be very interesting to analyze qualitatively the effects of (gauge) fluctuations in the present chiral SL.

APPENDIX A: THE BOGOLIUBOV TRANSFORMATION

This Appendix explains how to obtain the eigenmodes of Eq. (9). New bosonic operators, components of $\tilde{\phi}$, are created by linear combinations of the components of ϕ to obtain a new diagonal matrix \tilde{M} . For the Hamiltonian to possess a GS (spectrum bounded from below), the diagonal elements ($\omega_1, \dots, \omega_{2N_s}$) must all be positive or null. This transformation is called the Bogoliubov transformation and is generally well documented (see, for instance, Ref. 19) when the size of the matrix M is 2×2 (the transformation can then be done analytically), but more rarely for larger sizes (where numerical calculations are sometimes required). When periodic ansätze

are considered, a Fourier transform can block-diagonalize M , with blocks of size $2m \times 2m$, with m the number of sites in the unit cell. As soon as $m > 1$, Bogoliubov transformation of matrices larger than 2×2 are needed.

Note that the choice of an ansatz without any \mathcal{A}_{ij} parameters [for example, using Eq. (5b)] simplifies considerably the Bogoliubov transformation since the total number of boson is conserved and M is block diagonal with two blocks of size N_s . The transformation reduces to the diagonalization of each block by a unitary matrix. The new bosons $\tilde{b}_{i\sigma}$ are then linear combinations of the old $b_{i\sigma}$, without any $b_{i\sigma}^\dagger$ component. The vacuum of the new bosons is the same vacuum as for the old bosons. To respect the constraint on the boson number, we have to create a Bose condensate (see Sec. IV A), which implies long-range magnetic order. This proves that the \mathcal{A}_{ij} parameters are necessary to obtain SL.

Here we describe the general method for the cases where \tilde{M} can have an arbitrary size, as explained in details in by Colpa.⁴¹ The $2N_s \times 2N_s$ matrix P defined such that $\phi = P\tilde{\phi}$ is called the transformation matrix. Let us look at the conditions P should satisfy. The most evident is that \tilde{M} must be diagonal, which gives a first constraint. The second one is that the N_s first components of $\tilde{\phi}$ must be annihilation operators and the last N_s , creation operators. This gives a constraint on their commutation relations. The two resulting conditions are

$$P^\dagger M P = \tilde{M}, \quad P^\dagger J P = J, \quad (\text{A1})$$

where J is the $2N_s \times 2N_s$ diagonal matrix with coefficients -1 for the N_s first terms and 1 for the last N_s elements ($J_{ij} = [\phi_i^\dagger, \phi_j]$). The second constraint makes the Bogoliubov transformation different from a diagonalization (where J would be the identity matrix). It is sometimes called a paradiagonalization.

Here we just recall the main steps of the algorithm⁴¹ to solve these equations.

(i) Verify that M is definite positive. It ensures that the GS is unique (in some cases where M has zero eigenvalues, the GS exists but is not the unique).

(ii) Find a complex upper-triangular square matrix K such as $M = K^\dagger K$ (Cholesky decomposition of M).

(iii) Find a unitary matrix U such that $L = U^\dagger K J K^\dagger U$ is diagonal with its first N_s coefficients positive and the other negative (usual diagonalization of a Hermitian matrix).

(iv) The solution is $\tilde{M} = J L$ and $P = K^{-1} U \tilde{M}^{1/2}$.

Using the rotational invariance, we deduce that the N_s first coefficients ($\omega_1, \dots, \omega_{N_s}$) of \tilde{M} are the same as the N_s last (maybe differently ordered). The energy of the MF Hamiltonian GS writes

$$E_0 = \frac{1}{2} \sum_{i=1}^{N_s} \omega_i + \epsilon_0, \quad (\text{A2})$$

and its elementary excitations are free bosonic spinons with energies ($\omega_1, \dots, \omega_{N_s}$) and spin- $\frac{1}{2}$, from which we can get the free energy at any temperature. We are now able to look for solutions of Eqs. (11) and (12), i.e., the stationary points of the free energy with respect to the MF parameters and with respect to the Lagrange multipliers.

APPENDIX B: BOUNDS ON SELF-CONSISTENT VALUES OF THE MF PARAMETERS IN SBMFT

The moduli $|\mathcal{A}_{ij}|$ and $|\mathcal{B}_{ij}|$ are *a priori* unconstrained real numbers in SBMFT. We prove here that in a self-consistent ansätze, their moduli cannot exceed an upper bound: $|\mathcal{A}_{ij}| \leq \frac{\kappa+1}{2}$ and $|\mathcal{B}_{ij}| \leq \frac{\kappa}{2}$. These inequalities considerably restrict the domain to explore and facilitate the numerical search for solutions.

Let $|\phi\rangle$ be any normalized bosonic state. We denote by $\langle \widehat{O} \rangle$ the expectation value of an operator in this state. Whatever the operators \widehat{u} and \widehat{v} we have

$$|\langle \widehat{u}\widehat{v} \rangle| \leq \frac{\langle \widehat{u}\widehat{u}^\dagger \rangle + \langle \widehat{v}^\dagger\widehat{v} \rangle}{2}. \quad (\text{B1})$$

Applying it to \widehat{A}_{ij} and \widehat{B}_{ij} , we obtain

$$|\langle \widehat{A}_{ij} \rangle| \leq \frac{\langle \widehat{n}_i + \widehat{n}_j + 2 \rangle}{4}, \quad |\langle \widehat{B}_{ij} \rangle| \leq \frac{\langle \widehat{n}_i + \widehat{n}_j \rangle}{4}. \quad (\text{B2})$$

We now take $|\phi\rangle$ as the GS of H_{MF} [Eq. (9)] for some ansatz. If the chemical potential is adjusted, $\langle \widehat{n}_i \rangle = \kappa$ on every lattice site. In the case of self-consistent parameters, $|\mathcal{A}_{ij}| = |\langle \widehat{A}_{ij} \rangle|$, $|\mathcal{B}_{ij}| = |\langle \widehat{B}_{ij} \rangle|$ and Eq. (B2) leads to

$$|\mathcal{A}_{ij}| \leq \frac{\kappa+1}{2}, \quad |\mathcal{B}_{ij}| \leq \frac{\kappa}{2}. \quad (\text{B3})$$

APPENDIX C: THE STRANGE CLASSICAL LIMIT OF THE π FLUX ANSATZ OF WANG AND VISHWANATH⁴

Wang and Vishwanath⁴ explored all the strictly symmetric ansätze ($(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (1, 1)$) with the \mathcal{A}_{ij} decoupling for first neighbor Heisenberg interactions. They found two ansätze. The first one is characterized by a flux $\text{Arg}(\mathcal{A}_{ij}\mathcal{A}_{jk}^*\mathcal{A}_{kl}\mathcal{A}_{li}^*) = 0$ around a rhombohedra for ($p_1 = 0$), giving the 3 sublattice Néel order in the classical limit. The second one has a flux π rhombohedra ($p_1 = 1$). The \mathcal{A}_{ij} parameters they used are those obtained from Fig. 3 with the corresponding value of p_1 and $k = 0$.

Comparing this to our result for the SS ansätze, we may wonder why do they obtain *two* possibilities for p_1 (0 or 1), whereas we found that $p_1 = 0$ was the only solution for $(\epsilon_{\mathcal{R}_6}, \epsilon_\sigma) = (1, 1)$. The difference comes from the absence of the \mathcal{B}_{ij} parameter in their MF approach. The complex phase of \mathcal{B}_{ij} is then ill defined and only the first of our two constraints [Eqs. (34)] remains. They thus impose $k = 0$, but nothing on p_1 . In fact, as this situation is the limit $B_1 \rightarrow 0$ of none of the SS cases we have explored in Sec. V, it appears that the π -flux ansatz is unstable with respect to the introduction of \mathcal{B}_{ij} . In other words, any nonzero value of \mathcal{B}_{ij} will break at least one lattice symmetry. The two WS ansätze described in the sixth and seventh lines of Table I correspond to this limit.

The nature of the spinon condensation in the π -flux ansatz could not be completely clarified in Ref. 4. Our understanding is that it is not consistent to impose $\mathcal{B}_{ij} = 0$ to describe ordered states on a frustrated lattice. The only way to have $|\mathcal{B}_{ij}|^2 = 0$ classically is indeed to have antiparallel spins on all bonds, which is not possible on the triangular lattice.

APPENDIX D: WEAKLY SYMMETRIC ANSATZE ON SOME USUAL LATTICES
1. Lattices with a square Bravais lattices

The first step is to find all chiral algebraic PSGs. We choose the most general case IGG $\sim \mathbb{Z}_2$ and we suppose that \widehat{H}_0 respects all the lattice symmetries whose generators are described in Fig. 2 (right). The coordinates (x, y) of a point are given in the basis of the translation vectors $\mathcal{V}_1, \mathcal{V}_2$ and the action of the generators on the coordinates are

$$\mathcal{V}_1 : (x, y) \rightarrow (x + 1, y), \quad (\text{D1a})$$

$$\mathcal{V}_2 : (x, y) \rightarrow (x, y + 1), \quad (\text{D1b})$$

$$\mathcal{R}_4 : (x, y) \rightarrow (-y, x), \quad (\text{D1c})$$

$$\sigma : (x, y) \rightarrow (y, x). \quad (\text{D1d})$$

The algebraic relations between them are

$$\mathcal{V}_1\mathcal{V}_2 = \mathcal{V}_2\mathcal{V}_1, \quad (\text{D2a})$$

$$\mathcal{V}_2\mathcal{R}_4 = \mathcal{R}_4\mathcal{V}_1, \quad (\text{D2b})$$

$$\mathcal{R}_4^4 = I, \quad (\text{D2c})$$

$$\mathcal{V}_1\mathcal{R}_4\mathcal{V}_2 = \mathcal{R}_4, \quad (\text{D2d})$$

$$\mathcal{V}_1\sigma = \sigma\mathcal{V}_2, \quad (\text{D2e})$$

$$\mathcal{R}_4\sigma\mathcal{R}_4 = \sigma, \quad (\text{D2f})$$

$$\sigma^2 = I. \quad (\text{D2g})$$

To our knowledge, even the nonchiral algebraic PSGs have not been derived previously. Here, we directly derive the chiral ones. From Eqs. (D2), we deduce that the reduced set of symmetries \mathcal{X}_e is generated by $\mathcal{V}_1^2, \mathcal{V}_2^2$, and \mathcal{R}_4^2 (noted $\mathcal{V}'_1, \mathcal{V}'_2$, and \mathcal{R}_2). Moreover, we find that $\epsilon_{\mathcal{V}_1} = \epsilon_{\mathcal{V}_2}$. An ansatz is characterized by the parities $(\epsilon_{\mathcal{V}_1}, \epsilon_{\mathcal{R}_2}, \epsilon_\sigma)$.

The algebraic relations between these generators are

$$\mathcal{V}'_1\mathcal{V}'_2 = \mathcal{V}'_2\mathcal{V}'_1, \quad (\text{D3a})$$

$$\mathcal{R}_2^2 = I, \quad (\text{D3b})$$

$$\mathcal{V}'_1\mathcal{R}_2\mathcal{V}'_1 = \mathcal{R}_2, \quad (\text{D3c})$$

$$\mathcal{V}'_2\mathcal{R}_2\mathcal{V}'_2 = \mathcal{R}_2. \quad (\text{D3d})$$

As explained in Sec. III C, each of these relations gives a constraint on the gauge transformations associated with the generators. The constraints from Eqs. (D3) are then, for all i :

$$\theta_{\mathcal{V}'_2}(\mathcal{V}'_1{}^{-1}i) - \theta_{\mathcal{V}'_2}(i) = p_1\pi, \quad (\text{D4a})$$

$$\theta_{\mathcal{R}_2}(i) + \theta_{\mathcal{R}_2}(\mathcal{R}_2i) = p_2\pi, \quad (\text{D4b})$$

$$\theta_{\mathcal{R}_2}(\mathcal{V}'_1{}^{-1}i) - \theta_{\mathcal{R}_2}(i) = p_3\pi, \quad (\text{D4c})$$

$$\theta_{\mathcal{V}'_2}(\mathcal{V}'_2i) + \theta_{\mathcal{V}'_2}(\mathcal{R}_2i) + \theta_{\mathcal{R}_2}(i) - \theta_{\mathcal{R}_2}(i) = p_4\pi, \quad (\text{D4d})$$

where p_1, \dots, p_4 can take either the value 0 or 1 (the equations are written modulo 2π). We note $[x]$ the integer part of $x/2$ and $x^* = x - 2[x]$ ($0 \leq x^* < 2$). By partially fixing the gauge, we impose

$$\theta_{\mathcal{V}'_1}(x_i, y_i) = 0, \quad \theta_{\mathcal{V}'_2}(x_i^*, y_i) = p_1 \frac{\pi}{2} x_i^*. \quad (\text{D5})$$

Contrary to the triangular lattice, no gauge transformation can here be used to get rid of some p_i .

Solving the previous equations (D4) leads us to

$$\theta_{\nu_1}(x, y) = 0, \quad (\text{D6a})$$

$$\theta_{\nu_2}(x, y) = p_1 \frac{\pi}{2} x, \quad (\text{D6b})$$

$$\theta_{\mathcal{R}_2}(x, y) = p_3 \frac{\pi}{2} x + p_4 \frac{\pi}{2} y + g_{\mathcal{R}_2}(x^*, y^*), \quad (\text{D6c})$$

with a complicated supplementary constraint that can be treated only when the lattice is more precisely defined

$$g_{\mathcal{R}_2}(x^*, y^*) + g_{\mathcal{R}_2}((-x)^*, (-y)^*) = p_2 \pi. \quad (\text{D7})$$

This constraint only depends on the coordinates of the sites in a 2×2 unit cell (x^* and y^*), so it gives at most $4m$ independent constraints.

These general algebraic PSGs can then be used to find the weakly symmetric ansätze on any lattice with a square Bravais lattice (for example, the square, the Shastry-Sutherland lattice, etc.).

2. Weakly symmetric ansätze on the kagome lattice

The Bravais lattice of the kagome lattice is triangular, so we use the algebraic PSGs determined in Sec. IV C. The unit cell contains three sites. We choose to place the origin of the frame at the center of a hexagon and the coordinates of the sites in a unit cell are $(\frac{1}{2}, 0)$, $(0, \frac{1}{2})$, and $(\frac{1}{2}, \frac{1}{2})$.

Since the sites have noninteger coordinates, it is convenient to transform Eqs. (30) using the following gauge transformation [see Eq. (28)]:

$$G_1 : (x, y) \rightarrow -p_1 \pi y x^*. \quad (\text{D8})$$

The new algebraic PSG is

$$\theta_{\nu_1}(x, y) = 0, \quad (\text{D9a})$$

$$\theta_{\nu_2}(x, y) = p_1 \pi [x], \quad (\text{D9b})$$

$$\theta_{\mathcal{R}_3}(x, y) = p_1 \pi [x] \left([y] - \frac{[x] + 1}{2} + [y^* - x^*] \right) + g_{\mathcal{R}_3}(x^*, y^*). \quad (\text{D9c})$$

Even if it seems more complicated than Eqs. (30), it avoids some $p_1 \pi/2$ and simplifies the future ansätze. This gauge transformation is equivalent to a different initial choice of $\theta_{\nu_2}(x_i^*, y_i)$ in Eq. (27):

$$\theta_{\nu_2}(x_i^*, y_i) = 0. \quad (\text{D10})$$

Under the effect of G , Eq. (31) is modified and gives the constraint

$$g_{\mathcal{R}_3}(\frac{1}{2}, 0) + g_{\mathcal{R}_3}(0, \frac{1}{2}) + g_{\mathcal{R}_3}(\frac{1}{2}, \frac{1}{2}) = (p_2 + p_1)\pi.$$

Using the gauge transformations

$$G_2 : (x, y) \rightarrow ax^*, \quad (\text{D11a})$$

$$G_3 : (x, y) \rightarrow by^*, \quad (\text{D11b})$$

$$G_4 : (x, y) \rightarrow [y^* - x^*]\pi, \quad (\text{D11c})$$

with a and b real numbers, we can set $g_{\mathcal{R}_3} = 0$. Finally, we have two distinct algebraic PSGs for the reduced set of symmetries. They are characterized by $p_1 = \pm 1$ and defined by Eqs. (D9) with $g_{\mathcal{R}_3} = 0$.

We have now to find all ansätze compatible with these PSGs. We limit ourselves to first neighbor parameters, but

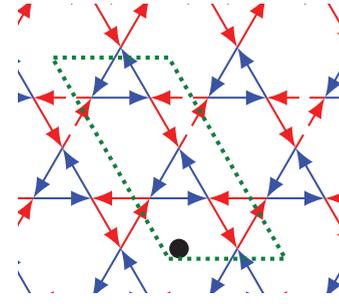


FIG. 4. (Color online) Ansätze respecting the \mathcal{X}_e symmetries on the kagome lattice up to a gauge transformation. Blue arrows carry B_{ij} parameters of modulus B_1 and of argument ϕ_{B_1} and A_{ij} parameters of modulus A_1 and of argument 0. Red arrows are for moduli B'_1 and A'_1 and arguments $\phi_{B'_1}$ and $\phi_{A'_1}$. On dashed arrows A_{ij} and B_{ij} take an extra $p_1 \pi$ phase.

this procedure is easily generalized to further neighbors. Two bonds are needed to generate the whole lattice: one blue and one of red bond of Fig. 4. Using the PSG one obtains the values of A_{ij} and B_{ij} on all other bonds. Note that A_{ij} can be chosen real for say the reference blue bond by using the gauge freedom. The values of all bond parameters are represented in Fig. 4 as a function of their value on the reference bond. The general unit cell of parameters contains six sites because of the possible nonzero p_1 . The simplicity of Fig. 4 ansätze, where phases differ only by π between two bonds of the same color is a consequence of the choice of Eq. (D10).

Finally, we can forget all about the PSG and only retain the parameters needed to completely describe an ansatz with the help of Fig. 4. These parameters consist of one integer p_1 , four moduli A_1 , A'_1 , B_1 , and B'_1 , and three arguments $\phi_{A'_1}$, ϕ_{B_1} , and $\phi_{B'_1}$.

We have now to consider all symmetries in \mathcal{X}_o . As blue and red bonds are related through \mathcal{R}_6 , this implies equality of the modulus: $A_1 = A'_1$ and $B_1 = B'_1$. Phase relationships are obtained by looking at the effect of \mathcal{R}_6 and σ on the flux $\text{Arg}(\mathcal{A}_{ij} \mathcal{A}_{jk}^* \mathcal{A}_{kl} \mathcal{A}_{lm}^* \mathcal{A}_{mn} \mathcal{A}_{ni}^*)$ on an elementary bow tie and $\text{Arg}(\mathcal{A}_{ij} \mathcal{B}_{jk} \mathcal{A}_{ki}^*)$ on an elementary triangle (we suppose that neither A_1 nor B_1 are zero). This leads to the constraints

$$(\epsilon_{\mathcal{R}_6} + \epsilon_{\sigma}) \phi_{B_1} = 0, \quad (\text{D12a})$$

$$\phi_{B'_1} = \epsilon_{\mathcal{R}_6} \phi_{B_1}, \quad (\text{D12b})$$

$$(1 + \epsilon_{\mathcal{R}_6}) \phi_{A'_1} = 0, \quad (\text{D12c})$$

$$(1 + \epsilon_{\sigma}) \phi_{A'_1} = 0. \quad (\text{D12d})$$

For each couple $(\epsilon_{\mathcal{R}_6}, \epsilon_{\sigma})$, the number of compatible ansätze is thus reduced:

(i) $(\epsilon_{\mathcal{R}_6}, \epsilon_{\sigma}) = (1, 1)$: $\phi_{B_1} = \phi'_{B_1} = 0$ or π and $\phi_{A'_1} = 0$ or π ,

(ii) $(\epsilon_{\mathcal{R}_6}, \epsilon_{\sigma}) = (1, -1)$: $\phi_{B_1} = \phi'_{B_1}$ and $\phi_{A'_1} = 0$ or π ,

(iii) $(\epsilon_{\mathcal{R}_6}, \epsilon_{\sigma}) = (-1, 1)$: $\phi_{B_1} = -\phi'_{B_1}$ and $\phi_{A'_1} = 0$ or π ,

(iv) $(\epsilon_{\mathcal{R}_6}, \epsilon_{\sigma}) = (-1, -1)$: $\phi_{B_1} = \phi'_{B_1}$ and $\phi_{B_1} = 0$ or π .

Finally, there are 20 different WS ansätze families, given in Table III. Each regular states of Ref. 9 belongs to one of them: the 2nd for the $\mathbf{q} = 0$, the 6th for the $\sqrt{3} \times \sqrt{3}$, the 17th for the *octahedral*, the 20th for the *cuboc1*, and the 14th for the *cuboc2* state. The parameters of the states in the classical limit are calculated using Eq. (20) and are described in Table IV. In a given family of ansätze, the modulus of the

TABLE III. The 20 weakly symmetric ansätze families on the kagome lattice, with the notations of Fig. 4. The moduli $A_1 = A'_1$ and $B_1 = B'_1$ are not constrained, except that they do not vanish.

Ansatz No.	p_1	ϕ'_{A_1}	ϕ_{B_1}	ϕ'_{B_1}
1	0	0	ϕ'_{B_1}	0
2				π
3				Any
4				$-\phi'_{B_1}$
5		π	ϕ'_{B_1}	0
6				π
7				Any
8				$-\phi'_{B_1}$
9		Any	ϕ'_{B_1}	0
10				π
11	1	Same as for $p_1 = 0$		
⋮				
20				

bonds are free parameters; we give in Table IV their values in the classical limit ($\kappa \rightarrow \infty$). The self-consistent parameters for finite S are different, but generally not far from the classical values. Thus, the classical values can be used as a starting point in numerical optimizations. The phases may (or not) be fixed in a given ansatz: They are fixed in ansätze describing planar nonchiral phases, and there is at least one free phase parameter in the chiral ansätze.

These calculations are easily generalized to further neighbors and have already been used for two studies on the kagome lattice.^{15,17}

TABLE IV. Values of the parameters of Fig. 4 for ansatz families related to regular classical states on the kagome lattice. (The states are designed by F for ferromagnetic, oct for octahedral, and cuboc for cuboctaedron order parameters. These states are described in more detail in Ref. 9.) The moduli verify $A_1 = A'_1$ and $B_1 = B'_1$. The interrogation points mean that the two values $\epsilon = \pm 1$ are possible (coplanar state). The * means that the parameter value is free; we give its value in the classical limit.

	F	$q = 0$	$\sqrt{3}\sqrt{3}$	oct	cuboc1	cuboc2
p_1	0	0	0	1	1	1
ε_R	?	?	?	1	-1	-1
ε_σ	?	?	?	-1	-1	1
A_1	0	$\frac{\sqrt{3}^*}{2}$	$\frac{\sqrt{3}^*}{2}$	$\frac{1^*}{\sqrt{2}}$	$\frac{\sqrt{3}^*}{2}$	$\frac{1^*}{2}$
$\phi_{A'_1}$		0	π	π	$\pi - \text{atan}\sqrt{8}^*$	0
B_1	1*	$\frac{1^*}{2}$	$\frac{1^*}{2}$	$\frac{1^*}{\sqrt{2}}$	$\frac{1^*}{2}$	$\frac{\sqrt{3}^*}{2}$
ϕ_{B_1}	0	π	π	$\frac{-3\pi^*}{4}$	π	$\text{atan}\sqrt{2} - \pi^*$
$\phi_{B'_1}$	0	π	π	ϕ_{B_1}	π	$-\phi_{B_1}$

APPENDIX E: NUMBER OF INDEPENDENT FLUXES ON A LATTICE

We suppose that we have a MF Hamiltonian with $n_A + n_B$ nonzero bond parameters ($\{\mathcal{A}_{ij}\}, \{\mathcal{B}_{ij}\}$) (\mathcal{A}_{ij} and \mathcal{A}_{ji} count as only one parameter, and the same for \mathcal{B}_{ij} and \mathcal{B}_{ji}). As they are complex numbers, we need $2n_A + 2n_B$ self-consistent conditions to solve this MF problem. We already know that the solution is not unique and that two ansätze related by a gauge transformation are equivalent. Thus, by fixing the gauge, we can decrease the number of equations for the complex phases. In fact, the number f of necessary arguments corresponds to the number of independent fluxes on the lattice. In this appendix, we describe a simple method to compute f on a finite cluster.

We define a rectangular matrix M of size $(n_A + n_B) \times N_s$ (N_s is the number of sites), where each line characterizes a MF parameter, and is therefore associated with a pair of sites (ij). As for the column, they correspond to the lattice sites. The coefficients of a line are all zero except for the two entries at columns i and j . Both entries equal 1 for an \mathcal{A}_{ji} bond, whereas these entries are -1 and 1 for a \mathcal{B}_{ji} bond (which site is ± 1 has no importance). Then the result is

$$f = n_A + n_B - \text{rank}(M). \quad (\text{E1})$$

The effect of a gauge transformation on the bond phases is obtained by multiplying M by the vector $(\theta_1, \dots, \theta_{N_s})^t$. By definition, a product of bond parameters defines a flux if the sum of their complex phases is unchanged by a gauge transformation. It means that the sum of associated matrix lines is 0. As the complex conjugate of a bond parameter can be used, the weight of each line in the sum can be ± 1 . As we can imagine using several times the same parameter, the weight of each line in the sum can finally be any relative integer. So, the existence of a flux relating a set of parameters is equivalent to the existence of a vanishing linear combination of their lines.

We can now give the proof of Eq. (E1) by induction. The relation Eq. (E1) is true for one parameter:

$$M = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \text{or} \quad M = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \quad (\text{E2})$$

We suppose now Eq. (E1) is true for $n_A + n_B$ parameter and we add a parameter on a bond (possibly with a new site).

(i) If a new site is added, the matrix gains a column and a line with a 1 at their intersection, so the rank of M increases by 1 and f remains the same. As we can choose the gauge on the new site, the new parameter can be chosen real, and Eq. (E1) remains true.

(ii) If no new site is added and there is new flux using the new parameter, the new line is a linear combination of previous lines, thus, $\text{rank}(M)$ is unchanged and f increases by 1.

(iii) If no new site is added and no new flux exists using the new parameter, the new line cannot be written as a linear combination of previous lines and f remains the same.

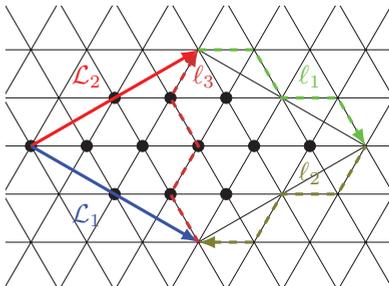


FIG. 5. (Color online) Triangular lattice with 12 sites (solid circles) and periodicity \mathcal{L}_1 and \mathcal{L}_2 , respecting all the lattice symmetries of Fig. 2. Three nonlocal loops ℓ_1 , ℓ_2 , and ℓ_3 are drawn in dashed arrows. The green dotted lines cross the bonds where the MF parameters are multiplied by -1 .

APPENDIX F: EXAMPLE OF NONLOCAL FLUXES BREAKING THE LATTICE SYMMETRIES

We illustrate the possibility for an ansatz to be incompatible with a periodic lattice. The example we give is an ansatz on a 12-site periodic triangular lattice (Fig. 5) that strictly respects the infinite lattice symmetries (Fig. 2). Let us choose for simplicity the ansatz with only first neighbor \mathcal{A}_{ij} MF parameters defined by $k = 0$ and $p_1 = 1$ (already discussed in the classical limit in Appendix C). This ansatz is the simplest illustration of these symmetry issues, but they can be encountered for any other ansatz (as becomes clearer later on).

Periodic boundary conditions defining a finite lattice are defined by the two vectors: \mathcal{L}_1 and \mathcal{L}_2 . Two sites separated by an integer linear combination of the \mathcal{L}_1 and \mathcal{L}_2 vectors (Fig. 5) are identified as the same sites. The three loops ℓ_1 , ℓ_2 , and ℓ_3 are mapped onto each other by rotations and should therefore have the same fluxes in a WS or SS ansatz. However, here their values are 0 for ℓ_2 and ℓ_3 and π for ℓ_1 . This is due to the fact that the unit cell of the ansatz is twice the unit cell of the triangular lattice, and it introduces a distinction between the directions \mathcal{L}_1 and \mathcal{L}_2 . The \mathcal{R}_3 symmetry cannot be restored simply using a gauge transformation. We see in the figure that the combination of the three loops ($\ell_1 + \ell_2 + \ell_3$) is a local loop, with trivial winding numbers. Thus, the flux of this loop is fixed by the ansatz and it is π . If we do not change the local physical properties of the ansatz, which we did not want to do, the sum of the three fluxes should remain equal to π (modulo 2π), and the only way out is to have a π flux on the three nonlocal loops. This can be done by choosing a specific nonlocal contour (here the green ℓ_1 contour, for example) and adding an extra phase π to all MF bond parameters crossing this contour.⁴⁵ Transformation does not affect the local (contractible loops) fluxes since they always contain an even number of altered parameters. However, the fluxes associated to ℓ_2 and ℓ_3 acquire an extra phase factor. The three fluxes around ℓ_1 , ℓ_2 , and ℓ_3 are all equal to π and the symmetries of the infinite lattice are now respected for this finite periodic lattice.

We can see this modification as a change in the boundary conditions (BCs), from periodic in both directions,

$$b_{(i+n_1\mathcal{L}_1+n_2\mathcal{L}_2)\sigma} = b_{i\sigma},$$

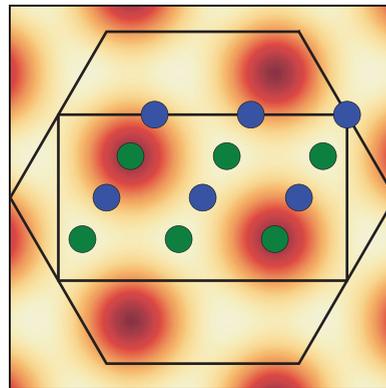


FIG. 6. (Color online) The hexagon is the Brillouin zone of the triangular lattice, the rectangle, this of the ansatz. The wave vectors of the 12-site lattice with PBCs are the blue ones, whereas they are the green ones for PBC in the \mathcal{L}_1 direction and APBC in the \mathcal{L}_2 direction. The background intensity is the value of the spinon energy (dark for minima).

to periodic in the \mathcal{L}_1 direction and antiperiodic in the \mathcal{L}_2 direction,

$$\rightarrow b_{(i+n_1\mathcal{L}_1+n_2\mathcal{L}_2)\sigma} = (-1)^{n_2} b_{i\sigma},$$

where n_1 and n_2 are arbitrary integers. This changes the set of allowed wave vectors \mathbf{k} from

$$\mathbf{k} \cdot \mathcal{L}_1 = 0, \quad \mathbf{k} \cdot \mathcal{L}_2 = 0,$$

to

$$\mathbf{k} \cdot \mathcal{L}_1 = 0, \quad \mathbf{k} \cdot \mathcal{L}_2 = \pi.$$

The wave vectors of the 12-site lattice before and after the transformation are drawn in Fig. 6. The spinon dispersion computed in the thermodynamic limit has two minima (dark red). Periodic BCs (PBCs) for this 12-site sample present evident drawbacks: The pattern of allowed wave vectors (blue points in Fig. 6) does not respect the \mathcal{R}_3 symmetry of the spinon dispersion and the minimum of the spinon dispersion is not reached in the 12 sites samples with these PBCs. We could hastily have supposed that single-spinon states are not physical excitations and as such they do not have to respect the lattice symmetries. However, this statement is incorrect. The vacuum of spinons calculated from the set of wave vectors obtained from PBCs is itself distorted and so are any physical quantities, as, for example, spin-spin correlations that are calculated from this input. On the contrary, the modified BCs restore the \mathcal{R}_6 symmetry of the pattern of authorized wave vectors around the spinon minima.

This can also be understood in a different way. The periodic or antiperiodic BCs (APBC) define the four topological sectors on the torus. To go from one sector to another, we create two vortices,⁴² move one of them around the lattice and annihilate them again. It is equivalent to the sign change of the MF parameters along this loop. The present discussion shows that for the 12-site sample, PBCs do not define the (0,0) topological sector of the model and we have to go to the APBC to describe this fully symmetric sector. In classical terms a change of π in a flux around a loop corresponds to a rotation of 2π of the

spin orientations, thus to a \mathbb{Z}_2 vortex.^{43,44} Translated to the classical limit, the previously used *periodic* BCs correspond

in fact to a twist of 2π of the magnetization around the lattice, and thus to a non trivial vorticity.

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