Twelve sublattice ordered phase in the $J_1 - J_2$ model on the kagomé lattice

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Motivated by recent experiments on an $S = 1/2$ antiferromagnet on the kagomé lattice, we investigate the Heisenberg $J_1 - J_2$ model with ferromagnetic $J_1$ and antiferromagnetic $J_2$. Classically the ground state displays Néel long-range order with 12 noncoplanar sublattices. The order parameter has the symmetry of a cuboctahedron, it fully breaks $SO(3)$ as well as the spin flip symmetry, and we expect from the latter a $Z_2$ symmetry breaking pattern. As might be expected from the Mermin-Wagner theorem in two dimensions, the $SO(3)$ symmetry is restored by thermal fluctuations while the $Z_2$ symmetry breaking persists up to a finite temperature.

A complete study of $S = 1/2$ exact spectra reveals that the classical order subsists for quantum spins in a finite range of parameters. First-order spin wave calculations give the range of existence of this phase and the renormalizations at $T = 0$ of the order parameters associated to both symmetry breakings. This phase is destroyed by quantum fluctuations for a small but finite $J_2/|J_1| \simeq 3$, consistently with exact spectra studies, which indicate a gapped phase.

I. THEORETICAL AND EXPERIMENTAL ISSUES

Whatever the nature of the spin, classical or quantum, the first neighbor Heisenberg antiferromagnet on the kagomé lattice fails to display Néel-like long-range order. Classically, it is characterized by an extensive entropy\(^1,2\) at $T = 0$. Quantum mechanically the spin-1/2 system has an exceptionally large density of low lying excitations\(^3,4\) reminiscent of the classical extensive entropy. It is still debated whether and eventually how this degeneracy is lifted in the quantum limit\(^5,6\).

An essential issue concerns the influence of perturbations: classically the effect of a second neighbor coupling $J_2$ has been very early studied by Harris and co-workers\(^7\). They showed that an infinitesimal $J_2$ is sufficient to drive the system toward an ordered phase with the three spins around a triangle pointing 120° from each other. Antiferromagnetic second-neighbor coupling ($J_2 > 0$) favors the $q = 0$ Néel order of this pattern on the Bravais lattice, whereas there are nine spins per unit cell for $J_2 < 0$ ($q = \sqrt{3} \times \sqrt{3}$ order). The effect of Dzyaloshinsky-Moriya interactions has also been analyzed\(^8\). To our knowledge the reduction of the order parameter by quantum fluctuations has only been studied through exact diagonalizations\(^9\). This approach points to an immediate transition from the "disordered phase" at the pure $J_1 > 0$ point, to the semiclassical Néel phases.

Up until now the $J_1 - J_2$ model on the kagomé lattice has only been studied for antiferromagnetic $J_1$. Many magnetic compounds\(^10-13\) with this geometry have been studied so far, but most of them have spin $S = 3/2$. A few compounds with $S = 1/2$ Cu ions have recently been synthetized\(^14-16\). None of them can be described by a pure isotropic first neighbor antiferromagnetic Heisenberg model. Recent experimental work on an organic compound with copper ions on a kagomé lattice\(^17\) gives indication of competing ferromagnetic and antiferromagnetic interactions.

It is thus the purpose of the present work to extend the previous study of the $J_1 - J_2$ model to ferromagnetic nearest neighbor coupling ($J_1 < 0$). The Hamiltonian reads as

$$H = J_1 \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{<<i,k>>} \mathbf{S}_i \cdot \mathbf{S}_k,$$

(1)

where the first and second sums run, respectively, over pairs of nearest neighbors $<i,j>$ and next-nearest neighbors $<<i,k>>$.

For a pure ferromagnetic $J_1$ coupling the system is indeed in a ferromagnetic phase. For a pure antiferromagnetic $J_2$ interaction the model reduces to three decoupled kagomé lattices with antiferromagnetic interactions and has thus an extensive entropy in the classical limit. The behavior of the model between these two limits is the object of the present study.

In Sec. II the classical ground state of the Hamiltonian (1) is investigated and the phase diagram of the model is given in the classical limit. For competing interactions $J_1 < 0$ and $J_2 > 0$ the model exhibits an ordered phase with 12 sublattices that fully breaks $SO(3)$ as well as a discrete symmetry (chiral symmetry breaking). We show that contrary to the Néel order, which breaks a continuous symmetry and therefore is destroyed down to infinitesimal temperatures, the chiral order survives thermal fluctuations and undergoes a phase transition at finite temperature.

In Sec. III we study the $S = 1/2$ quantum model using
exact diagonalizations and show the premise of the semi-classical ordering on samples up to 36 spins.
In Sec. IV we study the effect of long wavelength quantum fluctuations on this semi-classical order in the spin-wave approximation. It appears that the twelve sublattice Néel order survives quantum fluctuations in an extended range of parameters but is destroyed for a non zero $J_2 > 0$ ($J_2/|J_1| > 3$).
In Sec. V we show that exact diagonalizations in this range of parameters indeed point to (a) gapped phase(s).

II. CLASSICAL APPROACH

In this section we restrict ourselves to classical spins: the spins $S_i$ are usual unit vectors living in a three-dimensional space.

A. Ground state for $J_1 < 0$ and $J_2 > |J_1|/3$

To investigate the nature of the ground state of the Hamiltonian (1), we first Fourier transform it to find its lowest-energy modes. The kagomé lattice having three sites per Bravais cell, we get three branches. For $J_1 < 0$ and $J_2 < 0$ we find a single minimum at $q = 0$ corresponding to the expected ferromagnetic ground state. Upon increasing $J_2 > 0$, we find three degenerate minima at the edge centers of the first Brillouin zone, the classical transition occurring at $J_2 = |J_1|/3$. The three modes $q = X_{1,2,3}$ (Fig. 1) are the only solution as long as $J_2 > |J_1|/3$ and in the limit of pure $J_2 > 0$ one recovers the flat zero-energy branch of the pure $J_1 > 0$ case: we then have three decoupled kagomé lattices with nearest neighbor coupling $J_2$. In the $J_1 < 0$, $J_2 > |J_1|/3$ region, the unit cell compatible with the three edge centers contains 12 sites and the direct minimization of (1) for small samples of size multiple of 12 indeed reveals a Néel long-range order with 12 noncoplanar sublattices pointing toward the 12 centers of edges of a cube (Fig. 2). The apparent complexity of this structure is somewhat lightened when one considers the six spins around an hexagon: they lie in the same plane and make an angle $\pi/3$ with their nearest neighbors. We thus have four hexagons in the unit cell defining four different planes oriented like the faces of a tetrahedron. The polyhedron whose vertices coincide with the directions of the sublattices is named a cuboctahedron, and we will refer to that order parameter as the cuboc phase in the following. Consistently, Monte Carlo simulations with a Metropolis algorithm reveal a local cuboc Néel order with fluctuations increasing with temperature.

We now have a complete picture of the classical phase diagram of the Hamiltonian (1) at $T = 0$ in the entire $J_1 - J_2$ plane (Fig. 3).

B. Discrete symmetry breaking

It is clear that $O(3)$ is fully broken in the cuboc phase at $T = 0$: the point group symmetry of a cuboctahedron is simply that of the cube, i.e., $O_h = O \times \{I, i\}$, where $O$ is the octahedral group containing the 24 rotations leaving a cube or an octahedron invariant, and $I$ and $i$ are, respectively, the identity and the spin inversion, or
An important result arises when one considers the action of the spin flip alone. It is clear that $i$ acting on a cuboctahedron takes it onto another cuboctahedron but the labels of the two cuboctahedra cannot be made to coincide by means of a global rotation. Namely, the order parameter we obtain is the mirror-symmetry image of the previous one (Fig. 4). The order parameter in the cuboc phase thus breaks the spin flip symmetry, and we are able to divide the ground states manifold into two classes. This makes us expect a transition at finite temperature associated with this $\mathbb{Z}_2$ symmetry breaking.

To show that this is indeed the case, we define a variable labeling the two classes of ground states. Consider the normalized scalar chirality on a triangle, namely $\sigma_\triangle = \frac{(S_i \wedge S_j) \cdot S_k}{|S_i \wedge S_j|}$ with $(i,j,k)$ labeling the three sites clockwise. An inspection of the order parameter of Fig. 2 reveals that $\sigma_\triangle$ is alternatively $+1$ on upward triangles and $-1$ on downward triangles (Fig. 5). We naturally define the alternate scalar chirality as

$$m_\sigma = \frac{3}{2N} \sum_\triangle (-1)^{\alpha_\triangle} \sigma_\triangle,$$

where the sum runs over the $2N/3$ triangles of the kagomé lattice, and $\alpha_\triangle$ is, respectively, 0 and 1 on upward and downward triangles. The spin flip trivially changes the sign of $\sigma_\triangle$ so that $m_\sigma = \pm 1$ at zero temperature, depending on the class of the order parameter. Hence, $m_\sigma$ is the order parameter associated with the spin flip symmetry breaking.

Monte Carlo simulations have been performed on samples of up to 1200 spins: they show that $m_\sigma$ vanishes at finite temperature while the associated chiral susceptibility, defined as

$$k_B \chi_\sigma = \frac{2N}{3T} \left( < m_\sigma^2 > - < |m_\sigma| >^2 \right),$$

and the specific heat, seemingly both diverge (Fig. 6). Typical simulations involved $10^6$ Monte Carlo steps per spin. The first results indicate that the transition is not in the two-dimensional Ising universality class. The complexity of the global set of excitations that does not reduce to those of the above-mentioned $\sigma_\triangle$ variable are probably at the origin of a more complex behavior, presumably a weak first-order phase transition. The complete study of this classical phase transition will be published elsewhere.

## III. SPIN-1/2 MODEL

We now turn to the spin-1/2 quantum model. Considering the classical analysis, the question is whether quantum fluctuations are strong enough to wipe out the classical order. If so, we end up with a purely quantum...
phase such as a valence bond solid or a RVB liquid. If not, this means that quantum fluctuations merely dress the classical order parameter, reducing the mean sublattice magnetization while preserving its symmetries. Such states may thus be referred to as semiclassical states.

A. À la Néel SU(2) symmetry breaking

The exact spectra of finite size samples have already been shown to be a powerful tool to find eventual Néel orders in quantum spin systems. Of course they allow for the exact computation of the square of the sublattice magnetization or any relevant structure factor. But mostly, while the extensive use of the symmetries of the Hamiltonian is compulsory in order to diagonalize large enough samples (typically 36 spins today), it also gives a clear signature of SU(2)-breaking phases, even on small samples spectra. Namely, for an SU(2) symmetry breaking we expect a large set of low-lying eigenstates of the Hamiltonian, with different total spin $S$ values, to collapse onto the ground state when the size of the sample $N \to \infty$. These states have been called the quasidegenerate joint states (QDJS) and they have been recently observed experimentally on nanomagnets. If the semiclassical picture is valid, these QDJS are expected to have energies well below the magnon excitations and to scale as $S(S+1)/N$, as expected for a quantum top. Exact spectra are thus displayed versus $S(S+1)$ and the QDJS are often referred to as the Anderson’s tower of states. To have a true SU(2) symmetry breaking in the thermodynamic limit, the QDJS should have total spins up to $S \sim \mathcal{O}(\sqrt{N})$. The breaking of the SU(2) symmetry then occurs with all the QDJS collapsing onto the absolute ground state like $1/N$ when $N \to \infty$, i.e., faster than the softest magnons, whose energies scale as $1/\sqrt{N}$, defining the à la Néel SU(2)-symmetry breaking scheme. This result explains why it is numerically more favorable to look at the QDJS, since order parameters only scale as $1/\sqrt{N}$.

In the thermodynamic limit, the ground state is a superposition of an infinite number of QDJS with different $S$ values, which clearly breaks SU(2).

The crucial point is that in each spin sector the number and symmetries of the QDJS are exactly determined from group representation theory by the symmetry of the expected ground state.

B. Determination of the QDJS

If the thermodynamic ground state exhibits a semiclassical 12-sublattice Néel order then the QDJS, if ever they exist, should be of symmetry compatible with both those of the Hamiltonian (1), since they are eigenstates, and those of the cuboc phase, i.e., $\mathcal{O}_h$. A classical result of group theory is that the number of such states is completely determined by the structures of the two groups. Indeed, if we restrict ourselves to the rotational symmetry breaking, we see that the original SO(3) symmetry of (1) is reduced to its subgroup $\mathcal{O}$ in the Néel-ordered ground state. Thus, while $D_S$ is an irreducible representation (IR) of SO(3) of spin $S$, it is an a priori reducible representation of $\mathcal{O}$ that one can decompose onto the five IRs $\Gamma_\nu$ of $\mathcal{O}$ according to

$$D_S = \sum_{\nu=1}^{5} n_\nu(S) \Gamma_\nu, \quad (4)$$

with

$$n_\nu(S) = \frac{1}{24} \sum_{g \in \mathcal{O}} \chi_\nu^g(g) \chi_\nu^g(g), \quad (5)$$

where $\chi_\nu^g(g)$ and $\chi_\nu^g(g)$ are the characters of $g \in \mathcal{O}$ in the IR $\Gamma_\nu$ of $\mathcal{O}$, and in the IR $D_S$ of SO(3), respectively. The character table of $\mathcal{O}$ is given in Table I and $\chi_\nu^g(g) = \frac{\sin(2S+1)\theta/2}{\sin\theta/2}$ with $\theta$ the angle of the rotation $g$.

For completeness we give the explicit decomposition (4) for spins up to $S=6$ in Table II.

|
| $\nu$ | Id | 8C3 | 3C2 | 6C2 | 6C4 |
|---|---|---|---|---|---|
| $A_1$ | 1 | 1 | 1 | 1 | 1 |
| $A_2$ | 1 | -1 | -1 | -1 | 2 |
| $E$ | 2 | -1 | 0 | 0 | 0 |
| $T_1$ | 3 | 0 | -1 | -1 | 4 |
| $T_2$ | 3 | 0 | 1 | -1 | 5 |

The decomposition (4) directly gives the number of states that belong both to $D_S$ and $\Gamma_\nu$, i.e., that are compatible with both the SO(3) and $\mathcal{O}$ symmetries, as required for the QDJS. It should be emphasized that for a given $S$ value the number of such states is $n(S) = \sum_{\nu=1}^{5} n_\nu(S) \dim \Gamma_\nu = 2S + 1$, as expected for a complete SO(3) breaking.

We stress that (4) relies only on group theory and that it makes no reference to the representation space.

Now, if we are to find the total content of each spin sector of the Anderson’s tower of states, we should treat the whole $\mathcal{O}_h$ group, not limiting ourselves to the rotational symmetry-breaking $SO(3) \to \mathcal{O}$ as in (4).

This is particularly simple since $\mathcal{O}_h$ is the direct product of $\mathcal{O}$ with the group $\{Id, i\}$, and the spin flip being also a symmetry of the Hamiltonian, there is no compatibility issue here. Thus, everytime an IR $\Gamma_\nu$ appears in (4) we actually get two copies of it associated to the two IRs.
of the \{Id,i\} group (Table I). Since these two IRs differ only in their parity under the spin flip operation, which itself transforms any order parameter into its \(Z_2\) image, this double quasidegeneracy is clearly reminiscent of the \(Z_2\) symmetry breaking observed classically.

We thus have formally determined the number and symmetries of the QDJS appearing in each spin sector of the tower of states. However, for a given total spin, their symmetries are given in terms of the IRs of \(O_h\) while exact diagonalizations provide eigenstates of given symmetry under the lattice symmetry group.

It thus remains to map the IRs of \(O_h\) onto those of the lattice symmetry group, namely \(G_N = T_N \wedge P_N\), where \(T_N\) contains the \(N/3\) translations by a Bravais lattice vector and \(P_N\) is the point group of the sample (in general, \(P_N\) is a subgroup of \(C_{6v}\), the point group of the infinite kagomé lattice).

Such a mapping clearly exists since the labeling of the 12 vertices of the cuboctahedron induces a labeling of the lattice (Fig. 2). Applying an element of \(O_h\) to a cuboctahedral means permuting its 12 labels, which itself is equivalent to a lattice transformation.

We thus have a mapping between \(O_h\) and some elements of \(G_N\). Note that while the mapping between the group elements is not necessarily one-to-one, and in fact it is a one-to-many mapping for all the elements of the subgroup \(O\), the resulting mapping between the IRs of the two groups is one-to-one, as is explicit in Table III.

A notable exception is the spin flip, which is exactly mapped onto the rotation of the lattice \(R_\pi\) by angle \(\pi\) around the center of an empty hexagon. Hence, the parity of an eigenstate of the Hamiltonian (1) under \(R_\pi\) is directly equal to its parity under the spin flip. Thus, if ever the thermodynamic ground state has the classical 12-sublattice structure, we are able to find the number and degeneracies of the expected QDJS using Table II and the one-to-one mapping between the IRs of \(O_h\) and those of \(G_N\) (Table III).

However, there is still one subtlety. Indeed, in order not to artificially frustrate the 12-sublattice order, we choose samples containing multiples of 12 spins, \(i.e., N=12, 24,\) and 36 spins. The representation spaces of these three samples have different properties since the total spin on each sublattice is \(N/24\), which may be integer or half-integer.

To be more specific, we want to write down the matrix \(\tilde{U}(g)\in SU(2)\) associated with a particular rotation \(g\in O\) that acts on the wave function \(\ket{\text{cuboc}}\) of a cuboc-ordered state. The Hilbert space that contains such states is a subspace of \(\bigotimes_{i=1}^{12} D_{N=24}\), where \(D_{N=24}\) is the Hilbert space of one spin \(N/24\). Thus, a natural choice for \(\tilde{U}(g)\) would be the tensor product of 12 \(\tilde{U}_{N=24}(g)\) matrices, each one of them representing \(g\) in \(D_{N=24}\).

Now, we know that in each subspace \(D_{N=24}\), if \(N/24\) is a half-integer, \(\tilde{U}_{N=24}(g)\) and \(-\tilde{U}_{N=24}(g)\) are equally suitable choices, and we cannot decide between them other than arbitrarily, due to the double connectedness of \(SO(3)\).

Let us choose 12 such matrices anyway and form their tensor product \(\tilde{U}(g)\). When acting on a particular order parameter, named \(\ket{\text{cuboc}}\), we get

\[
\tilde{U}(g)|\text{cuboc}\rangle = \varphi(g)|\text{cuboc}\rangle,
\]

6

where \(\varphi(g)\) represents the order parameter obtained by applying the global rotation \(g\in O\) on \(\text{cuboc}\), and \(\varphi(g)\) is an overall phase factor that we cannot get rid of since it embeds the arbitrariness of our choice of the matrices \(\tilde{U}_{N=24}(g)\).

Recall, however, that \(\tilde{U}(g)\) acts in a subspace of \(\bigotimes_{i=1}^{12} D_{N=24}\), which is known from spin algebra to contain states with integer spins only, whatever \(N/24\), integer, or half-integer. Hence \(\tilde{U}(g)\) is always a true representation of \(g\), \(i.e.,\) no ambiguity should remain in it and consequently in \(\varphi(g)\). Thus the group law should be exactly verified by \(\varphi(g)\), which is then simply a one-dimensional, thus irreducible, representation of \(O\).

Direct computation for \(N=12, 24,\) and 36 spins indeed shows that \(\varphi(g) = \chi_{\nu_0}(g)\), where \(\nu_0=1\) for \(N=24\) spins, and \(\nu_0=2\) for \(N=12\) and 36 spins.

Finally, to embed this subtlety in the decomposition (4), one simply has to permute \(A_1 \leftrightarrow A_2\) and \(T_1 \leftrightarrow T_2\) in Table II for \(N=12\) and 36 spins, as can be seen directly on the character table of \(O\) (Table I). Note that no additional ambiguity arises from the consideration of the

| \(O\) | \(k\) | \(R_{2\pi/3}\) | \(\nu\) |
|---|---|---|---|
| \(A_1\) | 0 | 1 | 1 |
| \(A_2\) | 0 | 1 | -1 | 2 |
| \(E\) | 0 | \(j, j^2\) | 3 |
| \(T_1\) | \(X_{1,2,3}\) | -1 | 4 |
| \(T_2\) | \(X_{1,2,3}\) | 1 | 5 |
part of $O_h$, since the whole discussion relies on the double connectedness of $SO(3)$ that is irrelevant here.

C. Analysis of exact $N=36$ spectrum

We determine the number and degeneracies of the QDJS expected for a sample with $N=36$ spins and compare this to the exact diagonalization result. We first compute the decomposition (4) for total spin $S \leq 6$, the approximate maximum spin of the QDJS for $N=36$. As stated earlier, we just have to take Table II and perform the relevant permutations $A_1 \leftrightarrow A_2$ and $T_1 \leftrightarrow T_2$. In order to take the whole $O_h$ group into account we recall that each one of the IRs of the decomposition should actually appear twice with the two possible parities under the spin flip operation. Then we map these IRs onto those of $G_N$ and here we need to specify the shape of the sample we diagonalize (Fig. 7). The mapping is readily done since the $N=36$ sample has the full $C_{6v}$ symmetry and we may directly use Table III. Hence we have obtained the full composition of the Anderson’s tower of states in the lowest spin sectors $0 \leq S \leq 6$ (Table IV). Again we stress that each QDJS appearing in Table IV should actually appear twice with the two possible parities under the $Z_2$ symmetry breaking observed classically.

The comparison with the exact spectrum of the Hamiltonian (1) for the $N=36$ sample is straightforward (Fig. 8 and Table V). Indeed, one clearly notes a set of low-energy eigenstates, well separated from the magnon excitations for total spin $S \leq 6$, which scale reasonably as $S(S+1)$. But the main point is that for each total spin $S$ the number and symmetries of the low-lying eigenstates are exactly those obtained from our symmetry analysis, as can be readily verified in Table V.

In particular, we note that we have $2(2S+1)$ QDJS in each total spin $S$ sector, consistently with a complete $SU(2)$ breaking in the thermodynamic limit, with the factor 2 coming from the two replica $R_x = \pm 1$ of each QDJS and taking care of the $Z_2$ symmetry breaking. The same analysis has been made for $N=12$ and 24 non-frustrating samples, leading to the same result. These symmetry arguments are strong enough to claim that, at least in a certain range of parameters, quantum fluctuations do not destroy the complicated 12-sublattice classical long-range order and that there exists a quantum $cuboc$ phase in the thermodynamic limit, in the sense of a ground state consisting of the classical $cuboc$ state.
renormalized by quantum fluctuations, as explained earlier. However, it can be objected that long-wavelength quantum fluctuations, which cannot be accounted for on the small samples we diagonalized, may wipe out the cuboc order.

IV. SEMICLASSICAL APPROACH

Now that we are convinced that the 12-sublattice Néel order observed in the classical cuboc phase also exists in small samples of spins 1/2, we may compute the effect of long-wavelength quantum fluctuations on the energy, sublattice magnetization, and chiral order parameter in the ground state using the spin-wave approximation. The route to compute the quantum deviations to a classical cuboc state is straightforward: at each site of the kagomé lattice we define a local frame in spin space whose z axis is aligned with the local spin in the classical ground state. Thus, in this frame the classical cuboc ground state is simply a ferromagnetic state to which one can readily apply the Holstein-Primakov transformation. First, we choose a particular cuboc state, say, the one of Fig. 2. At a given site \( i \) of the kagomé lattice we define the local frame \( (x_i, y_i, z_i) \) with \( z_i \) the unit vector parallel to the local classical spin \( S_i \). To choose \( x_i \) we note that each site of the kagomé lattice belongs to two triangles pointing toward opposite directions. Consider the other two spins on the downward triangle and label them \( j \) and \( k \), with \( (i,j,k) \) turning clockwise. The directions of the two spins \( j,k \) in our cuboc state are \( z_j \) and \( z_k \) and one can easily verify that \( x_i = (z_k - z_j)/\sqrt{2} \) is indeed a unit vector orthogonal to \( z_i \). We completely determine the local frame by imposing \( y_i = z_i \wedge x_i \).

This construction is translationally invariant and repeating it for all the sites of the kagomé lattice will lead to 12 different local frames associated to the 12 sublattices of the classical ground state. Hence, using the appropriate transition matrix \( R_i \) from the reference frame \( (x,y,z) \) to the local frame \( (x_i,y_i,z_i) \), we may compute the components of the spin at site \( i \) in its local frame \( S_i^x = (S_i^{x_i}, S_i^{y_i}, S_i^{z_i}) \) from \( S_i = R_i S_i' \) (Remark: there are only 12 different \( R_i \) matrices).

Before computing the Hamiltonian (1) in the local frame, we note that it can be rewritten as a sum over the N/3 empty hexagons (Fig. 9):

\[
\mathcal{H} = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle \langle i,k \rangle \rangle} S_i \cdot S_k, \quad (7)
\]

where \( \langle i,j \rangle \) and \( \langle \langle i,k \rangle \rangle \) are now, respectively, the six nearest and six next-nearest neighbor pairs of sites enclosed in the empty hexagon \( \bigcirc \). Now, using \( S_i \cdot S_j = S_i^x T_{ij} S_j^x \), with \( T_{ij} = \langle R_i R_j \rangle \), we may rewrite (7) in the local frame as

\[
\mathcal{H} = J_1 \sum_{\bigcirc \langle i,j \rangle} S_i^x T_{ij} S_j^x + J_2 \sum_{\langle \langle i,k \rangle \rangle} S_i^x T_{ik} S_k^x. \quad (8)
\]

Now, we are able to quantize the fluctuations around the classical cuboc state using Holstein-Primakov bosons. Up to quadratic order the transformation at site \( i \) is written as

\[
\begin{cases}
S_i^{x+} = S_i^{e_{x_i}} + j S_i^{e_{y_i}} = \sqrt{2S - n_i} c_i \simeq \sqrt{2S} c_i, \\
S_i^{x-} = S_i^{e_{x_i}} - j S_i^{e_{y_i}} = c_i^\dagger \sqrt{2S - n_i} \simeq \sqrt{2S} c_i^\dagger, \\
S_i^{z} = S_i^{e_{z_i}} = S - n_i,
\end{cases}
\]

where \( c_i^\dagger \) and \( c_i \), respectively, create and annihilate a Holstein-Primakov boson at site \( i \), with \( S \) the length of the classical local spin and \( n_i = c_i^\dagger c_i \).

Inserting (9) into (8) we obtain the quantized version of the original Hamiltonian (1) up to quadratic order. As usual we Fourier-transform \( c_i \) and \( c_i^\dagger \) according to

\[
c_i = \sqrt{\frac{3}{N}} \sum_q e^{-jq(R_i + e_{n_i})} c_q, \quad (10)
\]
is the column vector \((\text{three sites per Bravais cell on the kagomé lattice. We where the sum runs over the entire first Brillouin zone, } V_\mu \text{ a vector of the Bravais lattice, and }\nu \text{ associated with the three sites per Bravais cell on the kagomé lattice. We may finally bring the Hamiltonian to matrix form as})

\[
\mathcal{H} = (J_1 - J_2)NS(S + 1) + \sum_q V_\mu^\dagger M_q V_\mu,
\]

where the sum runs over the entire first Brillouin zone, \(V_\mu\) is a column vector of the Bravais lattice, and \(\mu = \alpha, \beta, \gamma\) indicates one of the three possible sites in the Bravais cell (Fig. 9). Again, in the local frame the complicated 12 sublattice order is just a ferromagnetic state, so that we need only three flavors of bosons \(\mu = \alpha, \beta, \gamma\) associated with the three sites per Bravais cell on the kagomé lattice. We may define the three Goldstone modes in the thermodynamic limit. One indeed verifies that the lowest branch vanishes at each one of the three edge centers of the first Brillouin zone giving exactly three Goldstone modes in the thermodynamic limit, as expected for a complete \(SU(2)\) symmetry breaking. We may then compute the renormalization of the magnetization in the local basis,

\[
m_N^N = \frac{1}{NS} \left( \sum_{i=1}^N S_i^\dagger S_i - 1 \right) = 1 + \frac{1}{S} \left( 1 - \frac{1}{N} \sum_{i,j=1}^N \left( P_q^{ij} \right)^2 \right),
\]

where the prime denotes a sum over the first Brillouin zone deprived of its three edge centers and where \(P_q^{ij}\) is the \((i,j)\)th matrix element of the matrix \(P_q\).

Another quantity of interest to us is the renormalization of the scalar chirality on a triangle. It is naturally normalized by its value in the classical ground state, so that we define \(\xi_\Delta = \frac{2}{\sqrt{3}} (S_i \wedge S_j) \cdot S_k\) on each triangle \((i,j,k)\), with \((i,j,k)\) turning clockwise. We may then compute the renormalization of the alternate scalar chirality in the ground state as

\[
m_\xi^N = \frac{3}{2N} \sum_\Delta (-1)^\alpha \xi_\Delta |0\rangle = 1 + \frac{3}{S} \left( 1 - \frac{1}{N} \sum_q \Omega_q \right),
\]

where the sum runs over the \(2N/3\) triangles of the kagomé lattice, while \(\alpha_\Delta\) is, respectively, 0 and 1 on upward and
downward triangles, and
\[
\mathcal{D}_q = \sum_{i,j=1}^{3} (P_i^{j,i})^2 \left( \begin{array}{c}
\cos q_{a}(P_{q}^{2,j} + P_{q}^{5,j})(P_{q}^{3,j} + P_{q}^{6,j}) \\
+ \cos q_{b}(P_{q}^{1,j} + P_{q}^{4,j})(P_{q}^{3,j} + P_{q}^{6,j}) \\
+ \cos q_{c}(P_{q}^{1,j} + P_{q}^{4,j})(P_{q}^{2,j} + P_{q}^{5,j}) \\
+ \frac{\sqrt{3}}{3} \sin q_{a}(P_{q}^{5,j} P_{q}^{6,j} - P_{q}^{2,j} P_{q}^{3,j}) \\
+ \frac{\sqrt{3}}{3} \sin q_{b}(P_{q}^{4,j} P_{q}^{6,j} - P_{q}^{1,j} P_{q}^{3,j}) \\
+ \frac{\sqrt{3}}{3} \sin q_{c}(P_{q}^{4,j} P_{q}^{5,j} - P_{q}^{1,j} P_{q}^{2,j}) \end{array} \right) \right) \tag{18}
\]

These quantities were numerically computed on finite size samples with linear sizes \( L \leq 10^2 \) Bravais lattice spacings. As usual, the leading correction to the classical value comes from the first magnon excitation whose energy scales as \( 1/L \). We find very good agreement with the expected scaling laws for \( e_0^N \sim (1/L^3) \), \( m_0^N \sim (1/L) \), and \( m_0^N \sim (1/L) \), and perform the extrapolation to the thermodynamic limit.

We first note in (Fig. 10) that in the thermodynamic limit \( m_0^\infty \) and \( m_0^\infty \) remain finite in a large region around the point where exact diagonalizations were performed, thus showing the stability of the cuboc phase against long-wavelength quantum fluctuations. For \( J_2/|J_1| = 0.5 \) we find to lowest order in the spin wave approximation that \( m_0^\infty \) and \( m_0^\infty \) are renormalized by 16% and 50%, respectively.

However, upon increasing \( J_2 \), both quantities decrease drastically. For \( J_2/|J_1| \geq 3 \) the chirality disappears which casts a strong doubt on the stability of the 12-sublattice state itself in this range of parameters.

\section{V. A Gapped Phase for \( J_2/|J_1| = 5.0 \)}

Exact spectra for \( J_2/|J_1| = 5.0 \) differ notably from spectra of an ordered phase as described in Sec. III. First of all, their low-lying levels in each \( S \) sector do not scale as \( S(S + 1) \) but rather as \( S \), as can be seen in Fig. 11. Second, the gap to the first excitation seemingly does not close to zero with the system size, as shown in Fig. 12. This second result is consistent with the first one: in a gapped phase a finite magnetic field \( H_c \) is needed to close the gap. This critical field is directly proportional to the first derivative of the energy versus \( S \). For this given model in this range of parameters, the available sizes of exact spectra are large enough to infer the presence of a 12 sublattice Néel order and confirm the existence of a gapped phase. However they are too small to discriminate between a true spin liquid or a valence bond crystal, and to decide if there is one or two different gapped phases in this range of parameter.

\section{VI. Conclusion}

In this paper we have studied the \( J_1 - J_2 \) model on the kagomé lattice with \( J_1 < 0 \) and \( J_2 > 0 \). We have found a 12-sublattice ordered phase for \( J_1 < 0 \) and \( J_2/|J_1| > 1/3 \). This new phase was shown to resist quantum fluctuations. On the exact spectra of small size samples we found the complete signature of this complicated Néel order, \( \alpha \), the number and symmetries of the QDJS in the tower of states, based on a very general group-theoretical approach. Moreover, in the spin wave approximation, long-wavelength quantum fluctuations were found to renormalize the order parameter to a finite value in a finite
FIG. 12: (Color online) Left: Finite size scaling of the spin gap $\Delta E$ for $J_2/|J_1| = 5.0$, in the supposed to be gapped phase. Right: The same gap in the 12-sublattice Néel phase, for $J_2/|J_1| = 0.5$, closes as $1/N$, as expected for the à la Néel $SU(2)$ symmetry breaking (Sec. III A).

range of parameters up to $J_2/|J_1| \simeq 3$.

The noncoplanarity of the 12 sublattices in the cuboc phase was shown to induce a chiral symmetry breaking, to which we associated a chiral order parameter. Classically, we showed that this $Z_2$ symmetry was restored at finite temperature, consistently with the Mermin-Wagner theorem, though the exact nature of the transition remains to be investigated. We were also able to find the signature of this discrete symmetry breaking on exact spectra.

Finally, we showed in the spin-wave approach that the 12 sublattice order is wiped out by quantum fluctuations for $J_2/|J_1| \gtrsim 3$. Exact diagonalizations indeed confirm the existence of a spin-gap phase, with short-range order in spin-spin correlations. For this model the largest available sizes ($N = 36$) are too small to give more information on the nature of this quantum phase.

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24 In our problem the representation space is $E \equiv \bigotimes_{i=1}^{12} D_{N/24}$. For large values of $S$ the subspace of $E$ with total spin $S$ has a dimension smaller than $2S + 1$ and can only display a limited set of the states appearing in the decomposition (4). However, at least up to $S < \sqrt{N}$, it can be verified by direct inspection that the number of states in $E$ with total spin $S$ is much larger than $(2S + 1)$.