Order versus Disorder in the Quantum Heisenberg Antiferromagnet on the Kagomé lattice: an approach through exact spectra analysis.

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Abstract

A group symmetry analysis of the low lying levels of the spin-1/2 kagomé Heisenberg antiferromagnet is performed for small samples up to $N = 27$. This new approach allows to follow the effect of quantum fluctuations when the sample size increases. The results contradict the scenario of “order by disorder” which has been advanced on the basis of large S calculations. A large enough second neighbor ferromagnetic exchange coupling is needed to stabilize the $\sqrt{3} \times \sqrt{3}$ pattern: the finite size analysis indicates a quantum critical transition at a non zero coupling.
I. INTRODUCTION

There are very few simple two dimensional magnets which fail to order at $T = 0$. There is now a large amount of evidence that the $S = 1/2$ nearest neighbor Heisenberg antiferromagnet is ordered not only on the square lattice but also on the triangular lattice (THA). The reduction of the order parameter by quantum fluctuations is about 40% for the square lattice and of the order of 50% for the triangular lattice: frustration indeed enhances the role of the quantum fluctuations but the relatively high coordination number plays against them. The kagomé lattice which can be seen as a diluted triangular lattice (see Fig. 1) exhibits both frustration and low coordination number and the $S = 1/2$ Heisenberg antiferromagnet on the kagomé (KAH) is a good candidate for a disordered two dimensional quantum liquid.

Exact diagonalizations on periodic samples have shown that the spin-spin correlations decrease indeed very rapidly with distance. Series expansion from the Ising limit and high temperature series point to the absence of magnetic order. Large-N approaches, using Sp(N) bosons, find a disordered ground-state with unbroken symmetry for small enough spin while, using SU(N) fermions, a spin-Peierls phase or a chiral phase is suggested. The best variational energies for the N=36 sample are built from the short-ranged dimerized basis.

On the other hand, semiclassical approaches plead in favor of a magnetic order (the $\sqrt{3} \times \sqrt{3}$ state, see Fig. 1) induced by quantum fluctuations (“order by disorder”). This kind of phenomenon has already been seen in much simpler situations where there is a classical degeneracy between two kinds of orders. The $J_1 - J_2$ model on the triangular lattice for large enough $J_2$ ($J_2/J_1 > 1/8$) possesses classically degenerate ordered ground-states with respectively two and four sublattices. Large spin calculations have predicted that quantum fluctuations should select the two sublattices order. The study of small samples spectra has confirmed this prediction and shown the mechanism of this selection.
The kagomé antiferromagnet is a more problematic issue because of the infinite number of classically degenerate ground-states \[30,31\]. The linear spin wave approach for the kagomé antiferromagnet does not lift the extensive degeneracy of the classical ground-state (at this order the spectrum of magnetic excitations possesses a whole branch of zero modes \[18,30,31\]). One has to invoke non linear processes to stabilize the \(\sqrt{3} \times \sqrt{3}\) ordered solution \[19,20,22\]. On the other hand, one should note that in this class of problem there exist some situations where the “order by disorder” phenomenon fails for systems with a ground-state manifold associated with an extensive entropy. An example is the quantum Heisenberg antiferromagnet on the triangular Husimi cactus \[32\] where the system prefers to remain a spin liquid rather than localizing in a particular ordered state that breaks the degeneracy of the classical ground state manifold. Moreover, the possibility of a quantum tunnelling between different classical states might prevent the system from localizing in a particular ordered solution \[33,34\].

This paper is a scrutiny of the conjecture of selection of order by quantum fluctuations based on the study of the low lying levels of exact spectra. The paper is organized as follows: A brief presentation of our method to investigate the finite size properties of an ordered antiferromagnet is given in the next section. In Sec. III, we apply this method to the search of the selection of the \(\sqrt{3} \times \sqrt{3}\) state by quantum fluctuations. In Sec. IV, we introduce a second neighbor ferromagnetic exchange coupling \((J_2 < 0)\) and show that for large enough \(|J_2|\), the system orders through the \(\sqrt{3} \times \sqrt{3}\) state. The rigidity of the KHA and the hypothesis of an incommensurable planar order are investigated in Sec. V. Section VI, finally, summarizes our results and lists some open questions.

**II. REVIEW OF THE METHOD**

The presence of order in a quantum antiferromagnet is readily seen by examination of the low lying levels of its spectrum. The method used in this work has been described in details in \[4,7,29\], we give here a summary of its most important features. The first characteristic of an
ordered antiferromagnet (classical or quantum) is the existence of ferromagnetic sublattices: the total spin of each ferromagnetic sublattice is the collective variable relevant for the description of the low energy spectrum of the system. On a finite lattice with $p$ sublattices of $Q$ sites (the total number of sites being $N = pQ$), the $p$ identical spins $Q/2$ couple to form the rotationally invariant states that are the low lying eigenstates of the Hamiltonian. These $p$ coupled spins form a “generalized top” which precesses freely: elementary mechanics (confirmed by the non-linear sigma model approach [35–37]) indicates that the leading term of this precession is:

$$H_{\text{eff}} = \frac{S^2}{2I_N}.$$  (1)

In an ordered system, $I_N$, the inertia of the top is an extensive quantity, proportional to the perpendicular susceptibility of the magnet [4,37]. In a disordered system with a gap this quantity is asymptotically constant, and at the quantum critical point between this two regimes $I_N$ is expected to vary as $N^{-1/2}$ [37]. The coupling of the $pQ/2$ spins gives $N_S(N, S, p)$ states for each $S$ value of the total spin of the sample and a total of $(Q + 1)^p$ levels obeying the effective dynamics of Eq. (1). These levels form the quantum counterpart of the classical ground-state: they represent the tower of states indicated by Anderson in his 1952 famous paper [38]. In our spectral representation where the eigenstate energies are displayed as a function of $S(S+1)$ in order to exhibit the free precession (Eq. (1)), the tower is in fact a “Pisa Tower” with a slope decreasing with the sample size. In the thermodynamic limit, all these low lying levels (called QDJS in Ref. [4] for quasi-degenerate joint states) collapse to the absolute ground-state as $N^{-1}$. An experimental proof of these levels has recently been reported in the analysis of macroscopic quantum coherence in antiferromagnets [39]. It could be noticed that in the thermodynamic limit these levels give a ground-state entropy proportional to $\ln(N^p)$. Above these first family of levels, the spectrum of an ordered antiferromagnet exhibits the magnon spectrum; the low lying levels of this part of the spectrum collapse more slowly than the QDJS to the ground-state with a scaling law $N^{-1/2}$. Three features of the “Pisa Tower” of QDJS are thus essential:
i) the overall effective dynamics of a finite family of levels (of the order of $N^p$) and its finite size scaling leading to a clear cut separation from the first inhomogeneous magnon excitations (the absence of separation between the scaling laws would sign a quantum critical behaviour [37]),

ii) the numbers of levels $N_S(N, S, p)$ in each $S$ subset which for given $N$ and $S$ is determined by the number $p$ of ferromagnetic sublattices of the underlying Néel order,

iii) the spatial symmetries of these $N_S(N, S, p)$ levels: The number and nature of the space group irreducible representations (S.G.I.R.) that appear in each $S$ subspace are uniquely determined by the geometrical symmetries of the Néel order.

The exact diagonalization of the Heisenberg hamiltonian on small samples enables us to examine these features and to determine the nature of the ordering. This approach has been used for the quantum Heisenberg antiferromagnet on the triangular lattice [4,7] and the $J_1 - J_2$ problem on the triangular lattice [29].

III. THE LOW LYING LEVELS OF THE KAH

The hamiltonian of the KAH, including further neighbor interactions, has the form:

$$H = 2J_1 \sum_{<i,j>} S_i \cdot S_j + 2J_2 \sum_{<<i,k>>} S_i \cdot S_k$$

(2)

where the $S_i$ are spin-1/2 quantum operators on the sites of the kagomé lattice and $<i,j>$ (resp. $<<i,k>>$) denotes a sum over first (resp. second) neighbors. In this section, we shall only consider first neighbor exchange interactions ($J_2 = 0$). At first sight, the spectrum of the KAH has one feature which is common to all the Heisenberg antiferromagnet spectra that we have been studying: the absolute ground-state has a total spin $S = 0$ or $1/2$ depending on the number of sites of the sample ($N = 9, 12, 15, 18, 21, 24, 27$) and the ground-state energy $E_0(S)$ of the $S$ sectors order with increasing $S$ values. Lieb and Mattis [40] have shown that this result is exact for bipartite lattices: our numerical results tend to indicate an extremely robust property (the theorem seems to be true for the Heisenberg antiferromagnet on the
triangular and kagomé lattices and for the $J_1 - J_2$ problem: none of these situations can be reduced to a bipartite problem). Taken apart this feature the spectra of the KAH appear totally different from the spectra of the TAH. In Fig. 2 the low lying levels of the TAH and of the KAH are shown for the 27 sites samples:

$i)$ whereas the “Pisa Tower” is easily seen on the TAH spectrum, well separated from the magnons spectrum, there is absolutely no such scales in the KAH one,

$ii)$ the effective dynamics of the low lying levels of the KAH spectrum do not scale as $S(S+1)$,

$iii)$ the symmetries of the lowest lying levels of each $S$ subspace do not allow the description of an ordered structure: for $N = 27$, all the S.G.I.R., but one, appear in the low lying doublet states below the first $S = 3/2$ eigenstates, whereas their number $N_S$ and nature are strictly determined in the case of an ordered solution.

One could argue that the proliferation of these low lying levels are the quantum counterpart of the infinite degeneracy of the classical ground state with respect to local spin rotations. The real question is: do the quantum fluctuations show any trend to select a specific Néel order?

We have looked to this question for the so-called $\mathbf{q} = 0$ order, the $\sqrt{3} \times \sqrt{3}$ order and for any planar order (see section V). The $\mathbf{q} = 0$ order is studied in Ref. [41]. We give here the details of the analysis concerning the $\sqrt{3} \times \sqrt{3}$ order, which is the favored solution found in the semi classical approaches [18–22]. The smallest lattices where periodic boundary conditions are compatible with this order are $N = 9, 27$ and 36 sites. In this section, we shall consider explicitly the $N = 27$ sample since the $N = 9$ sites is too small and the $N = 36$ sample is too large to compute all the levels in each $S$ sector. The QDJS associated with the $\sqrt{3} \times \sqrt{3}$ state are homogeneous on each ferromagnetic sublattices (their wave-vectors are either $\mathbf{k} = 0$ or $\mathbf{k} = \pm \mathbf{k}_0$: corners of the Brillouin zone). They do not break the $C_{3v}$ symmetry of the lattice. The three irreducible representations characterizing the $\sqrt{3} \times \sqrt{3}$ order are the following:
Γ₁ : \[ \{ k = 0, R_{\pi} \Psi = \Psi, R_{2\pi/3} \Psi = \Psi, \sigma_x \Psi = \Psi \} \]

Γ₂ : \[ \{ k = 0, R_{\pi} \Psi = -\Psi, R_{2\pi/3} \Psi = \Psi, \sigma_x \Psi = \Psi \} \]  
(3)

Γ₃ : \[ \{ k = \pm k_0, R_{2\pi/3} \Psi = \Psi, \sigma_x \Psi = \Psi \} , \]

where \( R_\phi \) is a rotation of angle \( \phi \) and \( \sigma_x \) denotes an axial symmetry. The numbers \( N_S(N,S,p = 3) \) of levels in the “Pisa Tower” for each value of the total spin are given by the coupling of three \( N/6 \) spins:

\[
D^{N/6} \otimes D^{N/6} \otimes D^{N/6} = \sum_{S=0}^{N/6} (2S + 1) D^S + \sum_{S=N/6+1}^{N/2} (N/2 - S + 1) D^S
\]  
(4)

where \( D^S \) denotes the irreducible representation for a spin \( S \). Therefore, one obtains the numbers \( N_S(N,S,p = 3) \):

\[
N_S(N,S,p = 3) = (2S + 1) \min(2S + 1, N/2 - S + 1).
\]  
(5)

We notice that in each \( S \) sector, an ordered solution contains a number of levels which is strictly related to the number of sublattices of the selected order: in the lower \( S \) subspace this number is independent of the sample size for \( p \leq 3 \) (it is the Hilbert space dimension of a rotator or a symmetric top for \( p = 2 \) (respectively \( p = 3 \))). In each \( S \) subspace, amongst the \( N_S(N,S,p = 3) \) levels, the number of appearance \( (n_{\Gamma_i}^{(S)}) \) of the \( \Gamma_i \) IR can be computed following Refs. [7,29]:

\[
n_{\Gamma_i}^{(S)} = \frac{1}{6} \sum_k \text{Tr} (R_k|_S) \chi_i(k) N_{el}(k)
\]  
(6)

where the summation index \( k \) runs through the classes of the \( S_3 \) group (isomorphic to \( C_{3v} \)); \( \chi_i(k), N_{el}(k) \) denotes respectively the characters of the \( \Gamma_i \) IR and the number of elements in the class \( k \) (see Table I). The traces of the permutations of \( S_3 \) in the \( S \)-subspace, denoted \( \text{Tr} (R_k|_S) \), are determined as:

\[
\text{Tr} (R_k|_S) = \text{Tr} \left( R_k \bigg|_{S_z=S} \right) - \text{Tr} \left( R_k \bigg|_{S_z=S+1} \right),
\]  
(7)

and
\[
\begin{align*}
\text{Tr} \left( I_d \bigg|_{S_z} \right) &= \sum_{t,v,x=-N/6}^{N/6} \delta_{t+v+x,S_z} \\
\text{Tr} \left( (A, B) \bigg|_{S_z} \right) &= \sum_{t,v=-N/6}^{N/6} \delta_{2t+v,S_z} \\
\text{Tr} \left( (A, B, C) \bigg|_{S_z} \right) &= \sum_{t=-N/6}^{N/6} \delta_{3t,S_z},
\end{align*}
\]

where \((A, B)\) (respectively \((A, B, C)\)) stands for a two-body (respectively three-body) permutation of \(S_3\). The final results of the computation of the \(n_{\Gamma_i}^{(S)}\) are given for the \(N = 27\) sample in Table I.

The lowest levels in the first \(S\) subspaces of the \(N = 27\) sample spectrum are given in Table II. The levels which have the good symmetries to describe a \(\sqrt{3} \times \sqrt{3}\) antiferromagnet are displayed with an asterisk: most of these \(N_S(N = 27, S, p = 3)\) levels are rather far in the spectrum and many levels belonging to other S.G.I.R. proliferate between them. In fact, in the odd \(N\) samples, the number of low lying \(S = 1/2\) states below the first \(S = 3/2\) states increases very rapidly with the system size, the trend seems the same in the even samples (see Fig. 3). Altogether these numbers of low lying levels grow seemingly roughly as \(\alpha^N\) with \(\alpha \simeq 1.18\) (resp. \(\alpha \simeq 1.14\)) in the odd (resp. even) samples. Note that these numbers lay between the ground-state degeneracy of the three states Potts model \([42]\) (\(\alpha \simeq 1.134\)) and the degeneracy of the Dimer model \([43]\) (\(\alpha = 2^{1/3} \simeq 1.26\)). This exponential proliferation of low lying levels with all spatial symmetries is certainly the deepest proof of the absence of long range antiferromagnetic order: it signs both the absence of a finite number of ordered sublattices (that is the absence of an antiferromagnetic order parameter) and the impossibility of a Néel symmetry breaking.

The selection of order by quantum fluctuations previously observed in the \(J_1 - J_2\) model on a triangular lattice is quite different \([29]\). In that last model the four-sublattice QDJS family is perfectly pure on the smallest non frustrating sample spectra: the two-sublattice QDJS family is a subset of the first family. Quantum fluctuations just stabilize this subset relatively to the entire four-sublattice family and thus build a simpler structure with an
order parameter of higher symmetry: They do not create the order parameter, but just
renormalize it and increase its intrinsic symmetry.

IV. ORDERING WITH A SECOND NEIGHBOR FERROMAGNETIC
EXCHANGE COUPLING

In order to ascertain our conclusion and reinforce the credibility of the method, we have
studied with the same protocol the problem of the kagomé lattice with a first neighbor an-
tiferromagnetic interaction $J_1$ and a second neighbor ferromagnetic interaction $J_2$ (see Eq.
(4)) favouring the existence of a $\sqrt{3} \times \sqrt{3}$ order. For large enough $J_2 < 0$, the spectrum
has all the expected features of a “Pisa Tower” of QDJS (dynamics, number of states and
symmetries) associated with this order (see Fig. 4 for the $N = 9$ sample). When $|J_2|/J_1$
decreases the “Pisa Tower” disappears, indicating the existence of a quantum phase transi-
tion. The estimate of the critical value of $J_2/J_1$ is a difficult task requiring a study of finite
size effects. The smallest sizes compatible with the $\sqrt{3} \times \sqrt{3}$ order are $N = 9, 27, 36$ sites:
computing time and memory requirements for such an extensive study remain prohibitive.
However, using appropriate twisted boundary conditions ($\pm 2\pi/3$ around the $z$-axis, see Ref.
7 and Appendix A), we can use the intermediate $N = 12, 21$ samples. The twisted bound-
ary conditions break the rotational spin symmetry of the hamiltonian and fix the Néel plane
perpendicular to the twist axis. The helicity of Néel order is thus fixed along the $z$-axis and
the free dynamics of the system reduces to the precession of the total spin around $z$. The
effective hamiltonian reads:

$$H_{\text{eff}} = \frac{S_z^2}{2I_3},$$

where $I_3$ is the inertia of the top along the $z$-axis. The degeneracy of each $S_z^2$ subspace is
2 ($\pm S_z$). The IR characterizing the $\sqrt{3} \times \sqrt{3}$ order is $\Gamma_1 : [k = 0, R_{2\pi/3}\Psi = \Psi, \sigma_z\Psi = \Psi]$.
Fig. 5 shows the tower of states associated with the $\sqrt{3} \times \sqrt{3}$ order for the $N = 21$ sample
with $|J_2/J_1| = 1$. 

9
The order parameter or the spin stiffness of these levels scale as $N^{-1/2}$, whereas the slope of the “Pisa Tower” scales as $N^{-2}$. At first sight, it seems thus more efficient to use this information to look at the transition between order and disorder as $|J_2|/J_1$ is decreased. This can be done in a rather naive way by looking at the spin gap between the ground-state of $S_{z,min}$ and $S_{z,min}+1$: in the ordered phase this quantity should scale as $N^{-1}$ (respectively $N^{-1/2}$ and $N^0$ in the critical and disordered phase): this study is done in Fig. 6 for the case $|J_2/J_1| = 0$ (pure KAH). It shows thanks to the trends in the larger sample sizes that the KAH is certainly not ordered, probably not critical but truly disordered.

This naive use of the “Pisa Tower” does not account for the whole qualitative information contained in the QDJS family which is described both by the effective hamiltonian and by the space group symmetry of the levels. This information is incorporated in the index $R$ measuring the “degree of order” present in the low lying levels, and defined as follows:

i) First, we consider the ordered phase (with $|J_2/J_1| \geq 1$) and concentrate on all the low lying levels of the “Pisa Tower” that are lower in energy than the softest magnons: for each sample size this determinates the number of $S_z$ sectors which give a consistent picture of the “quasi-classical ground-state”. Precisely we search for the lower level of the spectrum with a non zero wave vector in the magnetic Brillouin zone ($E_{min}(k)$) and determine $S_{z,max}$ as the largest value of $S_z$ such that $E_0(S_{z,max}+1) \leq E_{min}(k)$. By definition $E_0(S_{z,max}+1)$ is thus smaller than the energy of the softest magnon of the sample and in the thermodynamic limit $S_{z,max}$ grows roughly as $N^{1/4}$.

ii) In each $S_z$ subspace considering all the levels in the energy range $[E_0(S_z),E_0(S_z+1)]$ we define $r_{S_z}$ as the ratio of the number of levels compatible with $\sqrt{3} \times \sqrt{3}$ order to the total number of levels of this range ($r_{S_z}$ is a number between 0 and 1).

iii) We then compute the index $R$ measuring the degree of order of the sample as the average of the ratios $r_{S_z}$ for $S_z$ running from 0 (resp. 1/2) up to $S_{z,max}$.

This index is equal to one if the lowest levels form a true “Pisa Tower” and decreases when other IRs appear in the low lying levels of the spectrum when $|J_2/J_1|$ is decreased. $R$
is thus a measure of the breakdown of order which includes qualitative information on the
low lying levels. It stands on the quantities that scale the more rapidly with the system size.

The variations of this index as a function of $|J_2|/J_1$ and of the sample size are given in
Fig. 7. When $|J_2/J_1| = 0$ this index goes very rapidly to zero with $N$: this conforts the
idea that the KAH is indeed disordered and that quantum fluctuations show no tendency
to select “order from disorder” in the disordered phase. More unexpected, the finite size
scaling on $R$ indicates that a small ferromagnetic exchange is not sufficient to establish long
range order in the system and that the value of the critical ratio $(|J_2|/J_1)_{c}$ is probably larger
than 0.5.

V. INCOMMENSURATE MAGNETIC ORDER

The previous study discards the hypothesis of a $\sqrt{3} \times \sqrt{3}$ order in the pure KAH (we did
the same check with the same conclusion for the $\mathbf{q} = \mathbf{0}$ order in Ref. [41]). Using twisted
boundary conditions $\mathbf{S}_{\alpha} = \mathcal{R}(\Phi_\alpha)\mathbf{S}_{\alpha}$ across the sample defined by the vectors
$\mathbf{T}_{\alpha=1,2}$ (see the appendix for more details), we have extended our search to any planar
antiferromagnetically ordered configurations, either commensurate or incommensurate. The
existence of a planar order, if any, would be signed by a minimum of the ground-state energy
for a given pair of twist angles $(\Phi_1, \Phi_2)$ and the appearence of a “Pisa Tower” for this couple
of parameters [7]. A typical result of a set of diagonalizations is shown in Fig. 8 for the
$N = 21$ sample. Sweeping the Brillouin zone for $(\Phi_1, \Phi_2)$, we have studied in this way the
spectra of the $N = 9, 12, 15, 18, 21, 24, 27$ samples. We observe the following properties:
i) the influence of the twisted boundary conditions is very small, much smaller than for the
TAH: on the $N = 21$ sample the effect of the twist on the ground-state of the KAH is only
8% of the same effect on the TAH. This is coherent with the picture of a disordered, liquid
system,
ii) we do not find a signature of any planar antiferromagnetic order for any size. Very
shallow minima appear in the spectra, but they are never associated with a tower of QDJS
and the position of these minima changes from place to place with the sample size, 

(iii) the “spin-gap” between the ground-state energy of the $S_z = 0$ (or $1/2$) subspace and the ground-state energy of the $S_z + 1$ subspace ($\Delta E_s = E_0(S_z + 1) - E_0(S_z)$) has only small variations with the twists (Fig. [3]). These variations appear systematic, and show a different trend in the even and odd samples: this could be related to the fact that the odd samples only accommodate spin-1/2 excitations of the thermodynamic absolute ground-state which is a true singlet. (This hypothesis is examined in a companion paper [14]).

VI. CONCLUSION

Using the analysis of the low lying levels of the Heisenberg antiferromagnet on a kagomé lattice we have shown new evidences that the system has no planar antiferromagnetic long range order at $T = 0$. Introducing a small second neighbor ferromagnetic exchange coupling does not seem to be sufficient to establish long range order: from the experimental point of view this is good news as it could perhaps enlarge the number of candidates for a spin liquid behaviour.

The theoretical study of the tower of low lying levels (“Pisa Tower”) that we have developed in this paper seems potentially useful to give an approximate location of the transition from order to disorder even on small samples: its advantage on other approaches stands on the finite size scaling of the parameter we are looking at and on the inclusion in this parameter of qualitative information on the macroscopic ground-state.

According to our present results, this spin-1/2 model exhibits a quantum critical point at a non zero $|J_2|/J_1$. It would be interesting to investigate the universality class of this quantum critical point and see how it may compare to the theoretical predictions of the non linear sigma model for canted antiferromagnets [15].

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APPENDIX A: TWISTED BOUNDARY CONDITIONS

For a sample defined by the two vectors:

\[
\begin{align*}
T_1 &= 2(l + m)u_1 + 2mu_2 \\
T_2 &= 2lu_1 + 2(l + m)u_2
\end{align*}
\]  

(A1)

where \(u_1\) and \(u_2\) are two unit vectors of the kagomé lattice, and \(m\) and \(n\) are two integers related to the number of sites of the sample by: \(N = 3(l^2 + m^2 + lm)\), the boundary conditions are defined through:

\[
S_{r_i + T_{\alpha=1,2}} = R_z(\Phi_{\alpha=1,2})S_{r_i}
\]  

(A2)

where \(r_i\) denotes the sites of the kagome lattice. In order to recover the translation invariance that seems to be broken by these boundary conditions, the spin frame at the point \(r_i + u_1\) (resp. \(r_i + u_2\)) is rotated with respect to the spin frame at point \(r_i\) by an angle \(\theta_1\) (resp. \(\theta_2\)). The boundary angles \(\Phi_{\alpha=1,2}\) are related to \(\theta_{\alpha=1,2}\) by the relations:

\[
\begin{align*}
\Phi_1 &= 2(l + m)\theta_1 + 2m\theta_2 \\
\Phi_2 &= 2l\theta_1 + 2(l + m)\theta_2.
\end{align*}
\]  

(A3)

The hamiltonian in the new frame reads:

\[
H = 2J_1 \sum_{\substack{i=1,N \\mu=1,3}} \tilde{S}_{r_i} R_z(\theta_{\mu}) \tilde{S}_{r_i + u_{\mu}}.
\]  

(A4)

\(\theta_1\) and \(\theta_2\) are changed step by step so that \(\Phi_1\) and \(\Phi_2\) sweep the appropriate fraction of the “Brillouin zone” of this problem.
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### TABLE I. Character table of the permutation group \( S_3 \). First line indicates classes of permutations. The number of elements in each class is \( N_{el} \).

| \( S_3 \) | \( I \) | \( (A, B, C) \) | \( (A, B) \) |
|----------|--------|---------------|---------------|
| \( N_{el} \) | 1      | 2             | 3             |
| \( \Gamma_1 \) | 1      | 1             | 1             |
| \( \Gamma_2 \) | 1      | 1             | -1            |
| \( \Gamma_3 \) | 2      | -1            | 0             |

### TABLE II. Number of occurrences \( n_{\Gamma_i}^{(S)} \) of each irreducible representation \( \Gamma_i \) \((i = 1, 2, 3)\) with respect to the total spin \( S \).

\[
\begin{array}{lcccccccccccccccc}
\hline
2S & 1 & 3 & 5 & 7 & 9 & 11 & 13 & 15 & 17 & 19 & 21 & 23 & 25 & 27 \\
\hline
n_{\Gamma_1}^{(S)} & 0 & 1 & 1 & 1 & 2 & 2 & 1 & 2 & 1 & 1 & 1 & 1 & 0 & 1 \\
n_{\Gamma_2}^{(S)} & 0 & 1 & 1 & 1 & 2 & 1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \\
n_{\Gamma_3}^{(S)} & 1 & 1 & 2 & 3 & 3 & 3 & 3 & 2 & 2 & 2 & 1 & 1 & 1 & 0 \\
\hline
\end{array}
\]
| \(N = 27\) | \(<2S_i S_j>\) | \(2S\) | deg. | \(k\) | \(R_{2\pi/3}\) | \(R_{\pi}\) | \(\sigma_x\) |
|---|---|---|---|---|---|---|---|
| -0.43627796 | 1 | 4 | 0 | 0 | -1 | 1 | 0 |
| * -0.43627796 | 1 | 4 | 3 | 6 | 1 | 0 | 1 |
| -0.43622206 | 1 | 12 | 0 | 3 | 0 | 0 | -1 |
| -0.43593382 | 1 | 12 | 0 | 3 | 0 | 0 | 1 |
| -0.43591527 | 1 | 8 | 3 | 6 | -1 | 0 | 0 |
| -0.43563229 | 1 | 12 | 0 | 3 | 0 | 0 | 1 |
| -0.42632327 | 3 | 8 | 0 | 0 | -1 | 1 | 0 |
| * -0.42632327 | 3 | 8 | 3 | 6 | 1 | 0 | 1 |
| -0.42630998 | 1 | 8 | 3 | 6 | -1 | 0 | 0 |
| -0.42615931 | 3 | 16 | 3 | 6 | -1 | 0 | 0 |
| * -0.42577308 | 3 | 4 | 0 | 0 | 1 | 1 | 1 |
| -0.42562690 | 3 | 8 | 0 | 0 | -1 | 1 | 0 |
| -0.42562690 | 3 | 8 | 3 | 6 | 1 | 0 | 1 |
| -0.42485791 | 1 | 8 | 3 | 6 | -1 | 0 | 0 |
| -0.42483901 | 1 | 4 | 0 | 0 | -1 | 1 | 0 |
| -0.42483901 | 1 | 4 | 3 | 6 | 1 | 0 | 1 |
| -0.42479279 | 1 | 4 | 0 | 0 | -1 | -1 | 0 |
| -0.42479279 | 1 | 4 | 3 | 6 | 1 | 0 | -1 |
| -0.42455077 | 3 | 24 | 0 | 3 | 0 | 0 | 1 |
| -0.42419453 | 3 | 16 | 3 | 6 | -1 | 0 | 0 |
| -0.42419310 | 3 | 4 | 0 | 0 | 1 | 1 | 1 |
| -0.42417083 | 1 | 2 | 0 | 0 | 1 | 1 | 1 |
| -0.42405358 | 1 | 2 | 0 | 0 | 1 | 1 | -1 |
| -0.42405358 | 1 | 2 | 0 | 0 | 1 | -1 | 1 |
TABLE III. Lowest eigenenergies (with degeneracy and quantum numbers) of the \(N = 27\) sample spectrum. Components of \(k\) are in units \(6\pi/N\). In the 3 last columns, 1 stands for invariant under the symmetry, 0 for no symmetry and -1 for a non trivial phase factor under the above mentioned symmetry (i.e. \(e^{i2\pi/3}\) for the rotation of \(2\pi/3\) and -1 for the two others). Stars indicate states possessing the symmetries associated with the \(\sqrt{3} \times \sqrt{3}\) state. The double horizontal bar indicates the omission of 127 \(S = 1/2\) states before the first levels in the \(S = 3/2\) subspace.
FIGURES

FIG. 1. Two classical planar states of the KAH: the $\sqrt{3} \times \sqrt{3}$ and $q = 0$ states.

FIG. 2. The low lying energy levels of the TAH and KAH spectrum of the $N = 27$ sample. The levels which possess the symmetry expected for an ordered solution are denoted by a star. The “Pisa Tower” of the TAH is easily seen, well distinct from the first magnon excitations. In the KAH on the contrary the levels candidate for the building of a tower of states are mixed with other representations in a continuum of excitations.

FIG. 3. Logarithm of the number $\Delta_N$ of $S = 1/2$ levels below the first $S = 3/2$ level as a function of the sample size $N$ (black triangles). This number which does not take into account the two-fold magnetic degeneracy is compared to the same quantity (square symbols) for the even $N$ samples (i.e. number of $S = 0$ levels below the first $S = 1$ level).

FIG. 4. Low lying spectrum of the $N = 9$ sample with $|J_2|/J_1 = 1$ and periodic boundary conditions, as a function of $S(S+1)$. Note the “Pisa Tower” associated with the $\sqrt{3} \times \sqrt{3}$ state.

FIG. 5. Low lying spectrum of the $N = 21$ sample with $|J_2|/J_1 = 1$ as a function of $S_z^2$. A twist of $2\pi/3$ in the boundary conditions is applied to accommodate the $\sqrt{3} \times \sqrt{3}$ state with the sample size. Due to the boundary conditions, the “Pisa Tower” reduces to one IR for each $S_z$ value.

FIG. 6. Finite size study of the “spin gap” $\Delta E_s = E_0(S_{z,\text{min}} + 1) - E_0(S_{z,\text{min}})$ of the pure KAH ($J_2 = 0$) as a function of the sample size. This energy is $O(N^\alpha)$ with $\alpha = -1, -1/2$ or 0 whether the system is ordered, critical or disordered. Continuous lines (resp. broken lines) are guides for the eye through the even $N$ (resp. odd $N$) results. The comparison of the three quantities $\Delta E_s$, $N^{1/2} \times \Delta E_s$ and $N \times \Delta E_s$ versus $N^{-1}$ favors the hypothesis of spin disorder.

FIG. 7. Behavior of the “index of order” ($R$) as a function of $|J_2|/J_1$ and of the system size.
FIG. 8. Variation of the energy per link $\langle 2S_i S_j \rangle$ of the low lying levels of the $N = 21$ sample versus twisted boundary conditions $\Phi_1$ ($\Phi_2 = 0$). $O_i$ are the points where $\Phi_1 = 0 \pmod{2\pi}$. $O_7$ is the first point where the twist per link is $0 \pmod{2\pi}$. The points $A_k$ ($\Phi_1 = \pi \pmod{2\pi}$) are in the middle of $O_i$ and $O_{i+1}$. Because the figure is symmetric with respect to $A_3$, the part $A_3 - O_7$ is not represented here. Note that most of the levels do not come back to their original assignation after a $2\pi$ twist of the boundary conditions. In fact on this small size sample, due to an extra-symmetry when $\Phi_i = 0$, the uniform $k=0$ ground-state is degenerate with the first star of $k \neq 0$ eigenstates. Only the $k=0$ states and their continuation have been shown in $OA_1$. The 6 other $k \neq 0$ in $OA$ are found by folding the $O_i A_i$ onto $OA$. Full lines stand for states going continuously to $k=0$ chiral states (complex IRs of $C_3$), dashed lines stand for states going continuously to the first star of $k \neq 0$ eigenstates the $k=0$ non chiral states (trivial IR of $C_3$); bold line: the first $S_z = 3/2$ level.

FIG. 9. Variations of the “spin gap” with boundary conditions: the small horizontal tick gives the value of the gap for periodic boundary conditions. There is a systematic effect: the $\Delta S = 1$ excitation energy decreases with the twists of the boundary conditions in the even $N$ samples and increases in the odd $N$ ones.
$E_i/2N$

$S_z$

$J_2/J_1 = -1$

$N = 21$
