Spin-wave spectra of a Kagome stripe

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Abstract – We study ground-state degeneracy and spin-wave excitations in a 1D version of a Kagome antiferromagnet—a Heisenberg antiferromagnet on a Kagome stripe. We show that for nearest-neighbor interaction, the classical ground state is infinitely degenerate. For any spin configuration from the degenerate set, the classical spin-wave spectrum contains, in addition to Goldstone modes, a branch of zero-energy excitations, and a zero mode in another branch. We demonstrate that the interactions beyond nearest neighbors lift the degeneracy, eliminate a zero mode, and give a finite dispersion to formerly zero-energy branch, leaving only Goldstone modes as zero-energy excitations.

In the last few years, there has been a revival of interest in the studies of frustrated spin systems. One of the most intriguing aspects of spin frustration is the existence, in many cases, of extra zero modes in the excitation spectrum, in addition to Goldstone modes related to the breaking of a continuous symmetry. These zero modes are often associated with the local degeneracy of a classical ground state of a frustrated system with short-range interactions between nearest-neighbors, and are lifted either by fluctuations, thermal or quantum, or by longer-range interactions which include second, third, etc neighbors [1].

The most prominent example of a system with extra zero modes is a much studied 2D nearest-neighbor antiferromagnet on a Kagome lattice [2–5]. The Kagome lattice consists of corner-sharing hexagons, and can be obtained from a triangular lattice by removing a quarter of the spins. The classical spectrum of a Kagome antiferromagnet contains the whole branch of zero-energy excitations, associated with the local degeneracy of a classical ground state with respect to rotations of spins belonging to a particular hexagon. Quantum and thermal fluctuations remove the degeneracy and select a particular $\sqrt{3} \times \sqrt{3}$ configuration, same as in a triangular antiferromagnet [3,5,6]. The same selection, also accompanied by the lifting of zero modes, can be also achieved by adding interactions between next-nearest neighbors [4]. In this later case, the lifting of the degeneracy is a natural consequence of the fact that next-nearest-neighbor interaction connects spins belonging to different hexagons and adds an energy cost to local rotations. Another way to lift the degeneracy is to include lattice distortion, see ref. [7].

Most of the recent work on Kagome-type systems was devoted to the 3D version of a Kagome antiferromagnet, which is an antiferromagnet of the pyrochlore lattice [8]. Less attention was given to an “opposite” 1D version, which is an antiferromagnet on a Kagome stripe. This is a three-chain structure, consisting of top/bottom sharing hexagons (fig. 1b). Like its 2D parent, a Kagome-stripe antiferromagnet can be obtained from a three-chain triangular antiferromagnet by removing 1/6 of the spins (fig. 1a). The existing analytical [9,10] and numerical [11,12] works focused on $S = 1/2$ and primarily addressed the issue of a spin-disordered state with gapped spin-triplet excitations, and gapless spin-singlet excitations. Closely related three-spin ladder systems have been investigated in [13] by exact diagonalization.

![Fig. 1: (Color online) (a) A triangular three-chain stripe. The Kagome stripe (b) is obtained by taking out the spin in the middle.](67005-p1)
The directions of the spin quantization axes are labeled by A, B, C. The ordering of the whole system is uniquely determined by the ABC ordering in a given triangle.

In this letter, we analyze the properties of a Heisenberg Kagome stripe with a large spin $S \gg 1$. We will not discuss the destruction of long-range magnetic order by 1D fluctuations, which at $T = 0$ occurs only at exponentially small energies, but rather focus on the issue of the lifting of the ground-state degeneracy and corresponding zero modes by the interaction beyond nearest neighbors. We show that there are two different ground-state degeneracies in a Kagome stripe, besides a conventional global degeneracy which is broken by the long-range order and gives rise to Goldstone modes. One is a truly local degeneracy, which gives rise to a whole branch of zero-energy excitations. Another is an extra global degeneracy with gives rise to an extra zero mode at a particular momentum $k = 0$. We demonstrate that the local degeneracy is lifted by the interactions between spins in the middle chain (formally, third-neighbor interaction), while the extra global degeneracy is lifted by a second-neighbor interaction in the direction perpendicular to the direction of the chains.

The frustrated nature of the Kagome stripe can be most easily understood by comparing it with the triangular stripe in fig. 1. In both cases, the lowest energy of a particular triangle of spins is achieved by placing the spins 120° apart. For a triangular stripe with nearest-neighbor interaction, the 120° ordering of a particular triangle uniquely determines the ordering of the full system (see fig. 2). From this perspective, the triangular stripe of Heisenberg spins is non-frustrated. For a Kagome stripe with nearest-neighbor interaction, the 120° ordering of a particular triangle does not specify the global order for two reasons. First, the spins $D$ and $E$ in the triangle $DEC$, connected to the $ABC$ triangle by the spin $C$ in the middle chain (see fig. 1b), can freely rotate around the quantization axis of the middle-chain spin $C$ (such rotation is impossible in a triangular antiferromagnet as there the spins $D$ and $E$ are also connected to the neighboring spins in the middle chain, whose directions are fixed by the ordering in $ABC$ triangle). Second, the five spins in the next set of two triangles $FKL$ and $LMN$, sharing the spin $L$ in the middle chain, are connected to the triangle $ABC$ only via antiferromagnetic interaction between nearest neighbors $B$ and $F$ along the upper chain. This sets the direction of the spin $F$, but other four spins can rotate in various ways preserving a 120° ordering within triangles $FKL$ and $LMN$. This is clearly a frustrated system.

In fig. 3 we show three different ground-state configurations of a Kagome stripe. Each preserves a 120° ordering within each spin triangle, and antiparallel orientation of the coupled spins from different triangles. The directions $A$, $B$, $C$ and their opposites $\bar{A}$, $\bar{B}$, $\bar{C}$ are shown in panel (d). The configuration (b) is the 1D version of the $\sqrt{3} \times \sqrt{3}$ configuration of a 2D Kagome antiferromagnet. It is stabilized by the interactions between second and third neighbors. For nearest-neighbor interaction only, the spins in the configuration 2b can be moved without energy cost, as shown in figs. 4 and 5.

\[Fig. 2: (Color online) 120° spin ordering on a triangular stripe. The directions of the spin quantization axes are labeled by A, B, C. The ordering of the whole system is uniquely determined by the ABC ordering in a given triangle.\]

\[Fig. 3: (Color online) Different ground-state configurations on a Kagome stripe. Each preserves a 120° ordering within each spin triangle, and antiparallel orientation of the coupled spins from different triangles. The directions A, B, C and their opposites A, B, C are shown in panel (d). The configuration (b) is the 1D version of the $\sqrt{3} \times \sqrt{3}$ configuration of a 2D Kagome antiferromagnet. It is stabilized by the interactions between second and third neighbors. For nearest-neighbor interaction only, the spins in the configuration 2b can be moved without energy cost, as shown in figs. 4 and 5.\]
corner spins C can rotate around the common quantization axis of the spectrum. This degeneracy gives rise to a zero mode in the spin-wave from the lower chain, and is therefore a global rotation. Since the spins along the lower chain belonging to different obviously lifted by an interaction global involve all spins in the lower chain, and is therefore a boring triangles, interact antiferromagnetically and must obviously favors antiparallel orientation of the spins C and C and therefore stabilizes the configuration in fig. 3b. To this end, we consider a J1-J2-J3 model with Heisenberg interaction within a Kagome stripe (J1), in between two chains (J2), and between the spins in the middle chain (J3) (see fig. 6). The corresponding Hamiltonian is

$$H = J_1 \sum_{\langle i, i' \rangle} S_i S_{i'} - J_2 \sum_i S_i \bar{S}_i + J_3 \sum_{(j,j')} S_{j,m} S_{j',m},$$

where the summation \langle i, i' \rangle is over nearest neighbors, l, u, m denote spins from lower, upper, and middle chains, respectively, and the summation over \langle j, j' \rangle in the last term is over next neighbors along the middle chain. We obtain the spin-wave spectrum of this Hamiltonian and show explicitly that the interactions J2 and J3 lift the zero modes leaving only three Goldstone zero-energy excitations, associated with $\sqrt{3} \times \sqrt{3}$ ordering. These Goldstone modes are related to the breaking of $O(3) \times O(2)$ symmetry by $\sqrt{3} \times \sqrt{3}$ ordering [17], and are: i) a homogeneous rotation of A and B spins, in phase with respect to upper and lower chains, and out of phase with respect to A and B directions, ii) a homogeneous rotation of A, B, and C spins—in phase with respect to upper and lower chains, and in phase with respect to A and B, and C spins, and iii) a rotation with $k = \pi/2$, in phase with respect to upper and lower chains, and in phase with respect to A and B spins, but out of phase with respect to C vs. A and B spins.

We follow the conventional strategy of the large-S approach: introduce five different bosonic operators for five spins belonging to top/bottom sharing triangles, use Holstein-Primakoff transformation from spin operators to bosons, and diagonalize the quadratic form in boson operators. This is a straightforward, but quite cumbersome procedure. We label the five bosons as shown in fig. 7, set the distance between the sites along the chains to be one, and introduce Fourier components.

Fig. 4: (Color online) The “global” degeneracy of the $\sqrt{3} \times \sqrt{3}$ spin configuration. Spins along the lower chain can rotate around the common quantization axis of middle-chain spins C and C, while the spins along the upper chain remain intact. Since the spins along the lower chain belonging to different sets of top/bottom sharing triangles must remain antiparallel to each other, this rotation simultaneously involves all spins from the lower chain, and is therefore a global rotation. This degeneracy gives rise to a zero mode in the spin-wave spectrum.

Fig. 5: (Color online) The “local” degeneracy of the $\sqrt{3} \times \sqrt{3}$ spin configuration. Spins along the hexagon $\bar{B}, \bar{B}, \bar{C}, \bar{B}, \bar{B}$, $\bar{C}$ can rotate around the common quantization axis of the “corner” spins A and A, preserving the 120° orientations of spins in any triangle. This degeneracy is local as it only involves spins inside a particular hexagon. The local degeneracy gives rise to zero-energy branch of spin-wave excitations.

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Fig. 6: Kagome stripe with antiferromagnetic nearest-neighbor and third-neighbor interactions, $J_1$ and $J_3$, respectively, and a ferromagnetic second-neighbor exchange interaction $J_2$. The Hamiltonian for this model is given by eq. (1).

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as \[a_{m-1/4} = \sum_k e^{2ikm}\tilde{a}_k, b_{m+1/4} = \sum_k e^{2ikm}\tilde{b}_k, c_m = \sum_k e^{2ikm}\tilde{c}_k, \tilde{a}_{m-1/4} = \sum_k e^{2ikm}\tilde{a}_k, \tilde{b}_{m+1/4} = \sum_k e^{2ikm}\tilde{b}_k. \]

Substituting into the Hamiltonian, we obtain \(\hat{H} = \hat{H}_0 + \hat{H}_2 + \hat{H}_{\text{int}},\) where \(\hat{H}_0 = O(S^2)\) is the classical ground-state energy. \(\hat{H}_2 = O(S)\) describes non-interacting spin-waves, and \(\hat{H}_{\text{int}} = O(1),\) which we neglect below, describes the interaction between spin-waves.

For the spin-wave part, we obtain, explicitly
\[
H_2 = J_1 S \sum_k \left[ 2\tilde{a}_k^\dagger a_k + 2\tilde{c}_k^\dagger c_k + 2\tilde{b}_k^\dagger b_k + 2\tilde{a}_k^\dagger a_k \right.
+ 2\tilde{b}_k^\dagger b_k + \frac{1}{4} \left( a_k^\dagger b_k + a_k^\dagger c_k + b_k^\dagger c_k \right)
+ \tilde{a}_k^\dagger \tilde{b}_k + \tilde{a}_k^\dagger \tilde{c}_k + \tilde{b}_k^\dagger \tilde{c}_k + \text{h.c.}
- \frac{3}{4} \left( a_k b_{-k} + a_k c_{-k} + b_k c_{-k} + \tilde{a}_k \tilde{b}_{-k} \right)
+ \tilde{a}_k c_{-k} + \tilde{b}_k c_{-k} + \text{h.c.}
- \left( e^{-ik} b_k a_{-k} + e^{-ik} \tilde{b}_k \tilde{a}_{-k} + \text{h.c.} \right)
\left. + J_2 S \sum_k \left[ a_k^\dagger a_k + b_k^\dagger b_k + \tilde{a}_k^\dagger \tilde{a}_k + \tilde{b}_k^\dagger \tilde{b}_k \right.
- \left( a_k^\dagger \tilde{a}_k + b_k^\dagger \tilde{b}_k + \text{h.c.} \right) \right] + 2J_2 S \sum_k \left[ c_k^\dagger c_k - \frac{\cos(2k)}{2} (c_k c_{-k} + \text{h.c.}) \right].
\]

Introducing the combinations of operators
\[a_{1,2}(k) = \frac{1}{\sqrt{2}}(a_k \pm \tilde{a}_k), b_{1,2}(k) = \frac{1}{\sqrt{2}}(b_k \pm \tilde{b}_k),\]
we find that the quadratic form is decoupled into a quadratic form which involves \(a_1(k), b_1(k),\) and \(c_k\) operators (which describe in-phase rotations of the spins in the upper and lower chains), and the quadratic form which involves only \(a_2(k)\) and \(b_2(k)\) operators (it describes out-of-phase rotations of the spins in the upper and lower chains). We then have
\[H_2 = H_{2 \times 2} + H_{3 \times 3},\]

where
\[
H_{2 \times 2} = J_1 S \sum_k \left\{ 2a_k^\dagger(k)a_2(k) + 2b_k^\dagger(k)b_2(k) \right\} + \frac{1}{4} \left( a_2^\dagger(k)b_2(k) + \text{h.c.} \right)
- \left[ \left( \frac{3}{4} + e^{2ik} \right) a_2(k)b_2(-k) + \text{h.c.} \right] \right) + J_2 S \sum_k 2a_k^\dagger(k)a_2(k) + 2b_k^\dagger(k)b_2(k),
\]
\[
H_{3 \times 3} = J_1 S \sum_k \begin{cases} 2a_1^\dagger(k)a_1(k) + 2b_1^\dagger(k)b_1(k) \\
+ \frac{1}{4} \left( a_1^\dagger(k)b_1(k) + \text{h.c.} \right) \right) \\
- \left[ \left( \frac{3}{4} + e^{2ik} \right) a_1(k)b_1(-k) + \text{h.c.} \right] \right) + 2c_k^\dagger c_k + \frac{\sqrt{2}}{2} \left[ A_1^\dagger(k)c_k + B_1^\dagger(k)c_k + \text{h.c.} \right) \\
- 3\frac{\sqrt{2}}{4} \left[ a_1(k)c_{-k} + b_1(k)c_{-k} + \text{h.c.} \right) \right) + 2J_3 S \sum_k \left[ c_k^\dagger c_k - \frac{\cos(2k)}{2} (c_k c_{-k} + \text{h.c.}) \right].
\]

The \(H_{2 \times 2}\) part depends on \(J_1\) and \(J_2\) but not on \(J_3.\) As we said, it describes out-of-phase rotations of the spins in the upper and lower chains. Such rotations are not Goldstone modes, and generally the two spin-wave branches of \(H_{2 \times 2}\) must be gapped. This, however, happens only at a finite \(J_2;\) for only nearest-neighbor interaction, out-of-phase rotations give rise to an extra zero mode (see fig. 4).

The Hamiltonian \(H_{2 \times 2}\) can be diagonalized analytically. For this, we note that for a generic Hamiltonian
\[
H_{4 \times 4} = \sum_k C_1(k) \left( A_k^\dagger A_k + B_k^\dagger B_k \right) + C_2(k) \left( A_k^\dagger B_k + B_k^\dagger A_k \right) + \left( C_3(k)A_kB_{-k} + C_3^*(k)A_k^\dagger B_{-k}^\dagger \right),
\]
with real \(C_1,\) \(C_2\) and complex \(C_3,\) the excitation spectrum is
\[
e(k) = \left[ \sqrt{C_1^2(k) + (\text{Im}C_3(k))^2} + C_2(k) \right]^2 - (\text{Re}C_3(k))^2.
\]
In our case, we have \(C_1(k) = 2S(J_1 + J_2),\) \(C_2(k) = J_3 S/4,\) \(C_3(k) = -J_1 S (\frac{3}{4} + e^{2ik})\), such that \(\text{Re}C_3(k) = J_1 S (-3/4 - \cos(2k)),\) \(\text{Im}C_3(k) = -J_1 S \sin(2k).\) Substituting into (6), we obtain two branches of excitations with
and lower chains. The three Goldstone modes are among \( k \) linear in degeneracy. All three branches can be easily obtained for all \( k \). The dispersion removes the zero mode at \( k = 0 \).

The other dispersion branch, \( \epsilon \), the dispersion acquires a finite gap, as we anticipated. The diagonalization of the Hamiltonian is more involved as this Hamiltonian contains the diagonalization amounts to solving a 6 by 6 matrix which we did numerically. The results for \( J_3 = 0 \) and \( J_3 = 0.3 J_1 \) are plotted in fig. 9. There are three branches of magnon dispersion. They describe in-phase and out-of-phase rotations between \( A \), \( B \), and \( C \) spins —in all cases the rotations are symmetric with respect to spins in the upper and lower chains. The three Goldstone modes are among these excitations.

For \( J_3 = 0 \), one of the branches is gapped, another is linear in \( k \) near \( k = 0 \), and the third one is exactly zero for all \( k \)-points. This is the consequence of the local degeneracy. All three branches can be easily obtained analytically as at \( J_3 = 0 \), the zero-energy branch decouples from the other two branches, which are the same as \( \epsilon_{\pm}(k) \) for \( J_2 = 0 \). At a finite \( J_3 \), the local degeneracy is lifted, and the former zero-energy branch acquires a “\( \sin 2k \)”-like dispersion with finite energy at a generic \( k \), and Goldstone points at \( k = 0 \) and \( k = \pm \pi/2 \). The linear in \( k \) branch remains gapless and its velocity is only slightly affected by \( J_3 \).

The existence of three Goldstone modes at a finite \( J_3 \) agrees with what one should expect on general grounds. Furthermore, the Goldstone modes can be obtained analytically. For \( k = 0 \) and \( k = \pi/2 \), the out-of-phase mode \( p_+ = (a_1 - b_1)/\sqrt{2} \) is decoupled from the modes \( p_+ = (a_1 + b_1)/\sqrt{2} \) and \( c \). At \( k = 0 \), the energy of the \( p_- \) mode is zero (Goldstone), at \( k = \pi/2 \), it is \( J_1 S \sqrt{3} \), independent of \( J_3 \). For the remaining two coupled excitations, \( p_+ \) and \( c \), the Hamiltonian can be diagonalized in the same spirit as \( H_{2 \times 2} \). At \( k = 0 \), we obtain one solution at zero energy (Goldstone), and one at energy \( \epsilon_+(k = 0) = J_1 S \sqrt{2 + 8 J_3/J_1} \), at \( k = \pi/2 \), one solution has zero energy (Goldstone), another is at energy \( \epsilon_+(\pi/2) = J_1 S \sqrt{5 + 8 J_3/J_1} \). The combinations of \( p_+ \) and \( c \) for the Goldstone modes are \( 2 p_+ + c \) at \( k = 0 \) and \( p_+ - c \) at \( k = \pi/2 \).

In summary, in this paper, we considered a Heisenberg model on a Kagome stripe. We showed that for nearest-neighbor interaction, the quasiclassical excitation spectrum contains two special features associated with

Fig. 8: (Color online) The spectrum of \( H_{2 \times 2} \). The two branches \( \epsilon_{\pm} \) are shown for \( J_2 = 0 \) (full line and dash-dotted line), and for \( J_2/J_1 = 0.1 \) (dashed and dash-double-dotted lines). A finite \( J_2 \) removes the zero mode at \( k = 0 \).

Fig. 9: (Color online) The spectrum of \( H_{3 \times 3} \). Without \( J_3 \), the dispersion has one linear in \( k \) (Goldstone) branch, and one branch of zero-energy excitations. When \( J_3 \) is finite, the former zero-energy branch acquires a dispersion and yields two Goldstone modes at \( k = 0 \) and \( k = \pi/2 \). The third branch is gapped with and without \( J_3 \).
the extra degeneracies of a classical ground state, a zero-energy branch of excitations associated with a local degeneracy, and a single zero mode associated with an additional global degeneracy. We demonstrated that the zero mode and zero-energy branch are removed by second- and third-neighbor interactions, respectively. We obtained the full quasiclassical spin-wave spectrum for a model with the interaction between first, second, and third neighbors, and showed that it contains three Goldstone modes, precisely as it should be for a ground state which breaks $O(3) \times O(2)$ symmetry.

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