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LOW-ENERGY SINGLET DYNAMICS OF SPIN-1/2 KAGOMÉ HEISENBERG ANTIFERROMAGNETS

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We suggest a new approach for description of the low-energy sector of the spin-$\frac{1}{2}$ kagomé Heisenberg antiferromagnets (KAFs). We show that a kagomé lattice can be represented as a set of blocks containing 12 spins, having the form of stars and arranged in a triangular lattice. Each of these stars has two degenerate singlet ground states that can be considered in terms of pseudospin $\frac{1}{2}$. Using symmetry consideration, we show that the KAF lower singlet band is made by the inter-star interaction from these degenerate states. We demonstrate that this band is described by the effective Hamiltonian of a magnet in the external magnetic field. The general form of this Hamiltonian is established. The Hamiltonian parameters are calculated up to the third order of the perturbation theory. The ground state energy calculated in the model considered is lower than those evaluated numerically in the previous finite clusters studies. A way of experimental verification of this picture using neutron scattering is discussed. It is shown that the approach presented cannot be directly extended to KAFs with larger spin values.

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1. INTRODUCTION

Unusual low-temperature properties of kagomé antiferromagnets (KAFs) attracted much attention of both theorists and experimenters in the last decade. Apparently the most intriguing features were observed in specific heat C measurements of SrCrGaO (spin-$\frac{3}{2}$ kagomé material) [1]. A peak at $T \approx 5$ K has been revealed that is practically independent of the magnetic field up to 12 T and C appeared to be proportional to T^2 at $T \lesssim 5$ K.

There is no appropriate theory describing the low-energy KAF sector. Qualitative understanding of the low-temperature spin-$\frac{1}{2}$ KAF physics is based mostly on results of numerous finite-cluster investigations [2–6]. They revealed a gap separating the ground state from the upper triplet levels and a band of nonmagnetic singlet excitations with a very small or zero gap inside the spin gap. The number of states in the band increases with the number of sites N as α^N. It was obtained for samples with up to 36 sites that $\alpha = 1.15$ and 1.18 for even and odd N, respectively [2, 5]. It is now believed that this wealth of singlets is responsible for a low-T specific heat peak and explains its field independence [1, 7].

The origin of the singlet band and the nature of the ground state are still under debate. Previous exact diagonalization studies of clusters with $N \leq 36$ [4, 8] revealed an exponential decay of the spin–spin and dimer–dimer correlation functions, and therefore the point of view that KAF is a spin liquid is widely accepted [2, 4–12].

A quantum dimer model (QDM) is now considered the best candidate for description of low-energy KAF properties [6, 9, 13–15]. In QDMs proposed for the kagomé problem in some recent papers [6, 13–16], the spin Hilbert space is restricted to the states in which spins are paired into first-neighbor singlets. The main argument to support this restriction is the coincidence of the low-energy spectrum and the number of lower singlet excitations in samples with up to 36 sites with the exact diagonalization results [13, 15, 16]. At the same time, it was noted that further studies are required to analyze this problem. As was recently demonstrated in Ref. [15], an effective Hamiltonian describing the low-energy KAF singlet sector can be writ-

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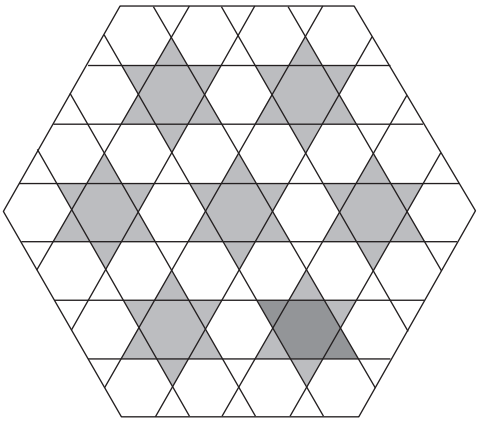

Fig. 1. Kagomé lattice (KL). There is a spin at each lattice site. The KL can be considered as a set of stars arranged in a triangular lattice. Each star contains 12 spins. A unit cell is also presented (dark region). There are four unit cells per star

ten in this approach. Unfortunately, it appears to be quite cumbersome and allows one to obtain the result under a number of crude approximations only [14, 15].

In our recent paper [17], we have suggested another approach for spin-$\frac{1}{2}$ KAF that differs from the QDMs discussed above. We proposed to consider a kagomé lattice as a set of stars with 12 spins arranged in a triangular lattice (see Fig. 1). Numerical diagonalization has shown that a single star has two degenerate singlet ground states separated from the upper triplet levels by a gap. These states form a singlet energy band as a result of the inter-star interaction. It was assumed that this band determines the low-energy KAF singlet sector. We have shown that it is described by the Hamiltonian of a magnet in the external magnetic field where degenerate states of the stars are represented in terms of two projections of pseudospin $\frac{1}{2}$.

This picture possibly reflects only the lowest part of the lower singlet sector because the number of states in the band within our approach is $2^{N/12} \approx 1.06^N$ [17], whereas it is now believed that it should be scaled by the 1.15^N law obtained numerically for clusters with $N \leq 36$ [13, 16].

In the present, more comprehensive paper, we develop this star concept. Using symmetry considerations presented in Sec. 2, we prove that the singlet band arising from the star ground states does determine the KAF lower singlet sector. This band is studied in Sec. 3, where the general form of the effective Hamiltonian is established. The Hamiltonian parameters are calculated up to the third order of the perturbation theory. The ground state energy calculated in the model considered is lower than these energies evaluated numerically in the previous finite cluster studies. A comparison between our model and the QDM is carried out. We demonstrate that our approach cannot be directly extended to KAFs with larger spin values. A way of experimental verification of this picture using neutron scattering is discussed. We summarize our results in Sec. 4.

2. SYMMETRY CONSIDERATION

We start with the Hamiltonian of the spin-$\frac{1}{2}$ kagomé Heisenberg antiferromagnet,

$$\mathcal{H}_0 = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{(i,j)} \mathbf{S}_i \cdot \mathbf{S}_j, \qquad (1)$$

where $\langle i,j \rangle$ and (i,j) denote nearest and next-nearest neighbors on the kagomé lattice, respectively, shown in Fig. 1. The case where $|J_2| \ll J_1$ is considered in this paper. We discuss the possibility of both signs of the next-nearest-neighbor interactions, the ferromagnetic and the antiferromagnetic one. As shown below, although the second term in Eq. (1) is small, it can be important for the low-energy properties.

A kagomé lattice can be represented as a set of stars arranged in a triangular lattice (see Fig. 1). We first neglect the interaction between stars and put $J_2 = 0$ in Eq. (1). A star is a system of 12 spins. We now consider its properties in detail.

Because Hamiltonian (1) commutes with all the projections of the total spin operator, all the star levels are classified by the values of S, irreducible representations (IRs) of its symmetry group, and are degenerate with respect to S_z. The star symmetry group C_{6v} contains six rotations and reflections with respect to six lines passing through the center. There are four one-dimensional and two two-dimensional IRs, which are presented in Appendix A. In their basis, the matrix of the Hamiltonian has a block structure. Each block has been diagonalized numerically.

As a result, it was obtained that the star has a doubly degenerate singlet ground state separated from the lower triplet level by a gap $\Delta \approx 0.26 J_1$. Ground state wave functions can be represented as

$$\Psi_+ = \frac{1}{\sqrt{2+1/16}}(\phi_1 + \phi_2), \qquad (2)$$

$$\Psi_- = \frac{1}{\sqrt{2-1/16}}(\phi_1 - \phi_2), \qquad (3)$$

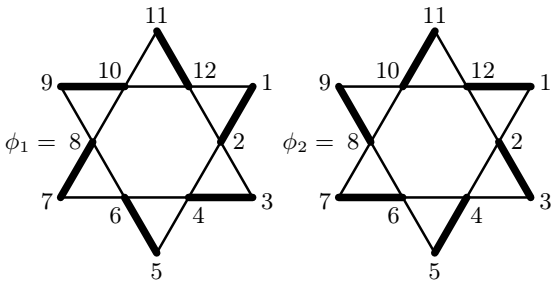

Fig. 2. Schematic representation of the two singlet ground state wave functions ϕ_1 and ϕ_2 of a star. The bold line shows the singlet state of two neighboring spins, i.e., $(|\uparrow\rangle_i|\downarrow\rangle_j - |\downarrow\rangle_i|\uparrow\rangle_j)/\sqrt{2}$

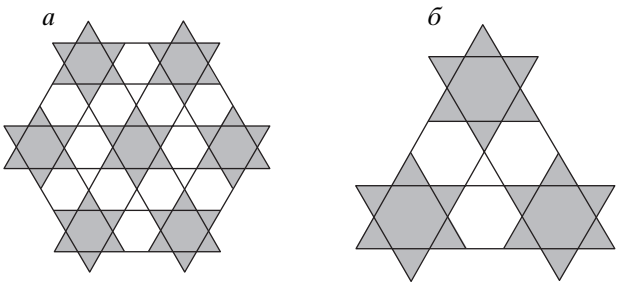

Fig. 3. *а*) A cluster where the operator of the interaction between stars has the same symmetry group C_{6v} as the whole cluster; *b*) the only configuration of three stars giving a nonzero contribution to the third term in the perturbation expansion

where functions ϕ_1 and ϕ_2 are shown schematically in Fig. 2. The bold line there represents the singlet state of the corresponding two spins, i.e. $(|\uparrow\rangle_i|\downarrow\rangle_j - |\downarrow\rangle_i|\uparrow\rangle_j)/\sqrt{2}$.

It can be shown that ϕ_1 and ϕ_2 are not orthogonal: their scalar product is $(\phi_1\phi_2) = 1/32$. They contain six singlets, each having the energy $-S(S+1)J_1 = -3/4J_1$. It can be shown that the interaction between singlets does not contribute to the energy of the ground states, which is consequently equal to $-4.5J_1$.

The functions ϕ_1 and ϕ_2 are invariant under rotations of the star and transform into each other under reflections. Hence, Ψ_+ is invariant under all the symmetry group transformations. In contrast, the function Ψ_- is invariant under rotations, changes sign under reflections, and is transformed under representation (A.3). Therefore, the ground state has accidental degeneracy. As shown in the next section, the next-nearest neighbor interaction, which has the same symmetry as the original Hamiltonian, lifts this degeneracy.

The KAF containing $\mathcal{N}$ noninteracting stars has the energy spectrum with a large level degeneracy when $\mathcal{N} \gg 1$. For example, the ground state degeneracy is $2^{\mathcal{N}}$ and that of the lowest triplet level is $3\mathcal{N}2^{(\mathcal{N}-1)}$. Interaction between stars gives rise to an energy band from every such group of levels, and it is a very difficult task to follow their evolution. On the other hand, group theory allows making some conclusions about the KAF low-energy sector. We now show that the singlet band stemming from the ground state cannot be overlapped by those originating from the upper singlet levels.

We consider a cluster with seven stars shown in Fig. 3*a*, and we begin with neglecting the interaction between them. The symmetry group of the cluster is also C_{6v}. The ground state has the degeneracy $2^7 = 128$. The corresponding wave functions transformed under IRs of C_{6v} are constructed as linear combinations of products containing Ψ_+ or Ψ_- for each star. Using the standard procedure of constructing bases in irreducible representations ([18, 19] and Appendix A), it is easy to show that there are at least two ground state wave functions of the cluster discussed, transformed under any given IR.

It is important to mention that the operator of the inter-star interaction in the cluster has the same symmetry as the intra-star one, which is a sum of the star Hamiltonians. The interaction between stars then commutes with the square of the total spin operator. Therefore, if we increase the inter-star interaction from zero, all the levels move by energy, but their classification cannot be changed. Levels can cross each other as the interaction rises from 0 to J_1, but the crossing is forbidden for levels of the same symmetry. This is a consequence of a symmetry theorem proved in Refs. [18, 19]. Hence, we can conclude that the lower singlet sector of the cluster is formed by states that stem from the original 128 lower levels.

We can obtain the same conclusions considering clusters of the symmetry C_{6v} with a large number of stars. We therefore assume in what follows that the KAF low-energy singlet sector is formed by the states originating from those in which each star is in one of the states Ψ_+ or Ψ_-. Because bands with $S \neq 0$ can overlap the singlet bands under discussion, we have to suppose that the KAF low-energy properties are determined by the lowest states in this singlet band.

Because the interaction between stars commutes with the square of the total spin operator, bands of different S can be studied independently. The KAF lower singlet sector is considered in detail in the next section. Investigation of states with $S \neq 0$ is outside the scope of this paper.

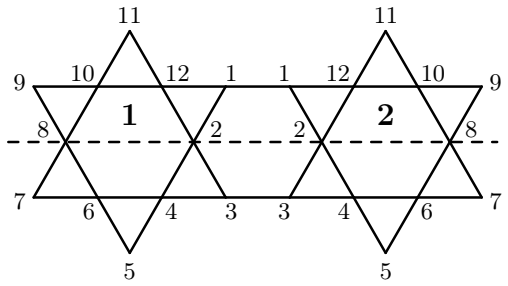

Fig. 4. Interactions between two stars: $V = J_1(\mathbf{S}_1^{(1)} \cdot \mathbf{S}_1^{(2)} + \mathbf{S}_3^{(1)} \cdot \mathbf{S}_3^{(2)})$ and $\tilde{V} = J_2(\mathbf{S}_1^{(1)} \cdot \mathbf{S}_2^{(2)} + \mathbf{S}_2^{(1)} \cdot \mathbf{S}_1^{(2)} + \mathbf{S}_2^{(1)} \cdot \mathbf{S}_3^{(2)} + \mathbf{S}_3^{(1)} \cdot \mathbf{S}_2^{(2)})$, where the superscripts label the stars. The system is symmetric under reflection with respect to the dotted line

3. SINGLET DYNAMICS

In this section, we derive the general form of the effective Hamiltonian describing the lower singlet sector. The inter-star interaction is considered a perturbation. Although it is not small compared to the intra-star interaction, there are reasons presented below to use the perturbation expansion here.

Two-star coupling. We begin with considering the interaction between two nearest stars, still neglecting the second term in Eq. (1). Initially, there are four fold degenerate ground state with the wave functions $\{\Psi_{n_1}^{(1)}\Psi_{n_2}^{(2)}\}$ (where $n_i = +, -$ and the superscript labels the stars) and the energy

$$E_{n_1n_2}^{(0)} = E_{n_1}^{(0)} + E_{n_2}^{(0)} = -9J_1.$$

As can be seen from Fig. 4, the interaction has the form

$$V = J_1(\mathbf{S}_1^{(1)} \cdot \mathbf{S}_1^{(2)} + \mathbf{S}_3^{(1)} \cdot \mathbf{S}_3^{(2)}). \tag{4}$$

According to the standard theory [18], the following conditions should be satisfied to consider V as a perturbation:

$$\left|C_{m_1m_2}^{n_1n_2}\right| = \left|\frac{V_{n_1n_2;m_1m_2}}{E_{n_1n_2}^{(0)} - E_{m_1m_2}^{(0)}}\right| \ll 1, \tag{5}$$

where $V_{n_1n_2;m_1m_2} = \langle\Psi_{n_1}^{(1)}\Psi_{n_2}^{(2)}|V|\Psi_{m_1}^{(1)}\Psi_{m_2}^{(2)}\rangle$, m_1m_2 denotes excited singlet levels of the two stars, and $n_i = +, -$. We have calculated $C_{m_1m_2}^{n_1n_2}$ for $n_i = +, -$ using wave functions obtained numerically and found that all of these coefficients do not exceed 0.09. Conditions (5) are therefore satisfied. Then the maximum value of the sum $\sum_{m_1m_2}|C_{m_1m_2}^{n_1n_2}|^2$ is 0.28, which is also sufficiently small. Thus, the interaction between stars is considered a perturbation in what follows.

We proceed with calculations of corrections to the initial ground state energy of two stars. For this, because the state is fourfold degenerate, we must solve a secular equation [18]. The corresponding matrix elements in the third order of perturbation theory are given by [18]

$$H_{n_1n_2;k_1k_2} = V_{n_1n_2;k_1k_2} + \sum_{m_1,m_2} \frac{V_{n_1n_2;m_1m_2}V_{m_1m_2;k_1k_2}}{E_{n_1n_2}^{(0)} - E_{m_1m_2}^{(0)}} + \sum_{m_1,m_2}\sum_{q_1,q_2} \frac{V_{n_1n_2;m_1m_2}V_{m_1m_2;q_1q_2}V_{q_1q_2;k_1k_2}}{(E_{n_1n_2}^{(0)} - E_{m_1m_2}^{(0)})(E_{n_1n_2}^{(0)} - E_{q_1q_2}^{(0)})}, \tag{6}$$

where $n_i, k_i = +, -$. Obviously, the first term in Eq. (6) is zero and the second term can be represented as

$$H_{n_1n_2;k_1k_2} = -i\int_0^\infty dt\, e^{-\delta t + iE_{n_1n_2}^{(0)}t} \times \langle\Psi_{n_1}^{(1)}\Psi_{n_2}^{(2)}|Ve^{-it(\mathcal{H}_0^{(1)}+\mathcal{H}_0^{(2)})}V|\Psi_{k_1}^{(1)}\Psi_{k_2}^{(2)}\rangle, \tag{7}$$

where $\mathcal{H}_0^{(i)}$ are Hamiltonians of the corresponding stars. The third term in Eq. (6) is to be considered later. Using the symmetry of the functions Ψ_+ and Ψ_- discussed above and the invariance of the system under reflection with respect to the dotted line in Fig. 4, it can be shown that the only nonzero elements belong to the first and the second diagonals (i.e., with $n_1 = k_1$, $n_2 = k_2$ and with $n_1 \neq k_1$, $n_2 \neq k_2$). We have calculated them numerically with a very high precision by expansion of the operator exponent up to the power 150[1)]. The results can be represented as

$$H_{++;++} = -a_1 + a_2 - a_3, \tag{8}$$

$$H_{+-;+-} = -a_1 + a_3, \tag{9}$$

$$H_{-+;-+} = -a_1 + a_3, \tag{10}$$

$$H_{--;--} = -a_1 - a_2 - a_3, \tag{11}$$

where $a_1 = 0.256J_1$, $a_2 = 0.015J_1$, and $a_3 = 0.0017J_1$. The terms of the second diagonal $H_{++;--} = H_{--;++} = -H_{+-;-+} = -H_{-+;+-} = a_4 = -0.0002J_1$ are much smaller than a_1, a_2, and a_3. The interaction therefore shifts all the levels by the value $-a_1$ and lifts their degeneracy. The constants a_2, a_3, and a_4 determine the level splitting. It is seen that the splitting is very small compared to the shift.

[1)] Difference of these results from those obtained by the expansion of the exponent up to the power 149 is of the order 10^{-5} %. Therefore, the method gives nearly precise values. The results would be the same if the calculations are done with the more common expression in Eq. (6) and eigenfunctions of the star obtained numerically.

Contributions to the parameters of effective Hamiltonian (13) from the terms V^1, V^2, and V^3 of the perturbation expansion. The interaction J_2 has been taken into account in V^1 and V^2 terms only. $\mathcal{N}$ is the number of stars in the lattice

	V^1	V^2	$V^{3\,a}$		Totals
			two-stars	three-stars	
$\mathcal{J}_z$	0	$-0.007J_1 + 0.002J_2$	$-0.013J_1$	$0.010J_1$	$-0.010J_1 + 0.002J_2$
$\mathcal{J}_y$	0	$-0.001J_1 + 0.007J_2$	$-0.001J_1$	$0.001J_1$	$-0.001J_1 + 0.007J_2$
$\mathcal{J}_x$	0	0	$0.067J_1$	0	$0.067J_1$
h	$-0.563J_2$	$-0.092J_1 - 0.218J_2$	$-0.161J_1$	$0.080J_1$	$-0.173J_1 - 0.781J_2$
$\Delta\mathcal{C}^b$	$-0.009J_2\mathcal{N}$	$-0.768J_1\mathcal{N} + 1.530J_2\mathcal{N}$	$-0.361J_1\mathcal{N}$	$0.304J_1\mathcal{N}$	$-0.825J_1\mathcal{N} + 1.521J_2\mathcal{N}$

[a] This term implies the two-star coupling shown in Fig. 4 and the three-star interaction in the configuration presented in Fig. 3*b*.
[b] Correction to the value $\mathcal{C}_0 = -4.5J_1\mathcal{N}$ for noninteracting stars.

The KAF therefore appears to be a set of two-level interacting systems, and the low-energy singlet sector of the Hilbert space can naturally be represented in terms of pseudospins: $|\uparrow\rangle = \Psi_-$ and $|\downarrow\rangle = \Psi_+$. It follows from Eqs. (8)–(11) that in these terms, the interaction between stars is described by the Hamiltonian of a ferromagnet in the external magnetic field,

$$\mathcal{H} = \sum_{\langle i,j\rangle} [\mathcal{J}_z s_i^z s_j^z + \mathcal{J}_y s_i^y s_j^y] + h \sum_i s_i^z + \mathcal{C}, \qquad (12)$$

where $\langle i,j\rangle$ now labels nearest-neighbor pseudospins, arranged in a triangular lattice formed by the stars, $\mathbf{s}$ is the spin-$\frac{1}{2}$ operator, $\mathcal{C} = -5.268J_1\mathcal{N}$, $\mathcal{J}_z = 4a_3 = -0.007J_1$, $\mathcal{J}_y = 4a_4 = -0.001J_1$, and $h = -6a_2 = -0.092J_1$. Here, $\mathcal{N} = N/12$ is the number of stars in the lattice. The factor 6 appears in the expression for h because each star interacts with 6 neighbors. We see that the magnetic field in effective Hamiltonian (12) is much larger than the exchange. In this approximation, the stars therefore behave as almost free spins in the external magnetic field and the ground state of the KAF has a long-range singlet order, which settles on the triangular star lattice and is formed by stars in Ψ_- states.

V^3 corrections. The field remains the largest term in the effective Hamiltonian and the KAF ground state has the same long-range order if we take the V^3 terms in the perturbation series into account. For the two-star coupling, the V^3 corrections have the form given by Eq. (6). The V^3 terms also require analyzing the three-star interaction. Nonzero contributions from them are only obtained for the configuration presented in Fig. 3*b*. The secular matrix for three stars is of the size 8×8. We have calculated the V^3 corrections with a very high precision using the integral representation similar to that in Eq. (7) for the second term in Eq. (6). All the operator exponents were expanded up to the power 150. As a result, the low-energy properties of the KAF are described by the effective Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j\rangle} \left[\mathcal{J}_z s_i^z s_j^z + \mathcal{J}_x s_i^x s_j^x + \mathcal{J}_y s_i^y s_j^y\right] + h \sum_i s_i^z + \mathcal{C}, \qquad (13)$$

where all parameters are given in the Table. It describes two-star coupling. We omit the three-pseudospin terms in Eq. (13) that have the form $s_i^z s_j^z s_k^z$ and $s_i^z s_j^y s_k^y$ and describe the three-star interaction. The corresponding coefficients are of the order of $10^{-3}J_1$ and $10^{-4}J_1$, respectively, and are negligible in comparison with those of the retained terms. We stress that within our precision, the Hamiltonian in Eq. (13) is an exact mapping of the original Heisenberg model to the low-energy sector (the excitation energy $\omega \sim \max\{\mathcal{J}_z, \mathcal{J}_y, \mathcal{J}_x, h\} \ll J_1$).

As follows from the study of the V^3 corrections in the Table, the common shift given by them remains much larger than the level splitting in both cases of the two- and three-star coupling. At the same time, the values of the V^3 perturbation terms are approximately two times smaller than those of the V^2 ones. The change in the effective Hamiltonian from the V^3 terms is therefore significant and analysis of the perturbation series cannot be finished at this point for correct determination of the effective Hamiltonian. Unfortunately, such a work requires great computer capacity

that is not at our disposal. We have to restrict ourself with this precision here.

One can judge about the applicability of the perturbation series from the values of the ground state energy of two interacting stars, shown in Fig. 4, obtained numerically and using the first two orders of the perturbation theory. The ground state energy of two noninteracting stars is $-9J_1$. That of two interacting stars calculated numerically by the power method [20] is $-9.62J_1$. On the other hand, the ground state energy obtained using the Table is $-9.42J_1$ (the respective contributions of the V^2 and V^3 terms are $-0.27J_1$ and $-0.15J_1$).

Effective Hamiltonian structure. Although the perturbation theory works badly in the star model and many perturbation terms are to be taken into account, we can now show that Eq. (13) is the most general form of the effective Hamiltonian assuming that n-pseudospin couplings with $n > 2$ are small, as this was in the case of $n = 3$ discussed above. We consider possible terms of the form $s_i^z s_j^+$, $s_i^z s_j^-$, s_i^+, and s_i^-. In these cases, the numbers of functions Ψ_+ and Ψ_- to the right of the corresponding matrix elements differ from those to the left by unity. As has been pointed out above, a kagomé lattice contains lines of symmetry reflections, and the star Hamiltonian and the inter-star interaction are invariant under these reflections. Because Ψ_+ are invariant and Ψ_- change sign under these transformations, the matrix elements are equal to themselves with the opposite sign and must therefore be zero. Another possible term

$$s_i^x s_j^y = -\frac{i}{4}(s_i^+ s_j^+ - s_i^- s_j^- + s_i^- s_j^+ - s_i^+ s_j^-)$$

cannot appear in the effective Hamiltonian because the corresponding matrix elements should be imaginary.

Ground state. As is clear from the Table, $\mathcal{J}_x$ and h are the largest parameters of Hamiltonian (13) in our approximation. Therefore, the KAF behaves as the Ising antiferromagnet in the perpendicular magnetic field. In this case, the classical value of the field at which spin flip occurs is $h_{s-f} = \mathcal{J}_x$, which is approximately 2.6 times smaller than h. The ground state must therefore remain ordered with all the stars in the Ψ_- state.

The ground state energy and that of the upper edge of the singlet band calculated using the Table are

$$(-4.5J_1 + \Delta\mathcal{C} + h/2 + 3\mathcal{J}_z/4)\mathcal{N} = -0.452J_1N$$

and

$$(-4.5J_1 + \Delta\mathcal{C} - h/2 + 3\mathcal{J}_z/4)\mathcal{N} = -0.437J_1N,$$

respectively. Corrections from $\mathcal{J}_x$ to these values in the first nonzero order of the perturbation theory are given by $(3/16)\mathcal{N}\mathcal{J}_x^2/h$ and are negligible. At the same time, the ground state energy of the largest cluster with $N = 36$ that has previously been considered numerically is $-0.438J_1N$ [5]. Hence, we believe that clusters used in the previous studies were too small to reflect the Heisenberg KAF low-energy sector at $J_2 = 0$ properly.

Interaction J_2. We now show that in spite of its smallness, the next-nearest neighbor interaction can play an important role for low-energy properties. We have calculated J_2 corrections to the parameters of effective Hamiltonian (13) for the first and the second terms in Eq. (6) only. There are 12 intrinsic J_2 interactions in each star, which splits the doubly degenerate ground state and, as is seen from the Table, gives a contribution to the magnetic field h and to the constant $\mathcal{C}$.

As is clear from Fig. 4, the two-star coupling is now given by the operator

$$\tilde{V} = J_2(\mathbf{S}_1^{(1)} \cdot \mathbf{S}_2^{(2)} + \mathbf{S}_2^{(1)} \cdot \mathbf{S}_1^{(2)} + \mathbf{S}_2^{(1)} \cdot \mathbf{S}_3^{(2)} + \mathbf{S}_3^{(1)} \cdot \mathbf{S}_2^{(2)}).$$

Corrections proportional to J_2 were calculated in the same way as above and are also presented in the Table. It is seen that the contribution of the next-nearest interactions to the magnetic field becomes significant if $|J_2| \sim 0.1J_1$. If $J_2 < 0$ (ferromagnetic interaction), they can even change the sign of h.

The effect of the next-nearest ferromagnetic coupling for KAF properties was previously studied in Ref. [2] numerically on finite clusters with $N \leq 27$ in a wide range of the values of J_2. It was shown there that at $|J_2|/J_1 \sim 1$, the ground state has the $\sqrt{3} \times \sqrt{3}$ magnetic structure. At $|J_2|/J_1 \ll 1$, the ground state is disordered and there is a band of singlet excitations inside the triplet gap. As we demonstrated above, this band is a result of the star ground state degeneracy in our approach.

T^2 specific heat behavior. There have been many speculations on the low-temperature dependence of the KAF specific heat $C \propto T^2$ observed experimentally for $S = 3/2$ (see Refs. [7, 21] and references therein). As we obtained above, low-T properties are described by effective Hamiltonian (13) of a magnet, which has the spectrum of the form $\epsilon_{\mathbf{q}} = \sqrt{(cq)^2 + \Delta'^2}$ at $q \ll 1$ and can be in the ordered or disordered phases depending on particular values of the parameters. Small Δ' here implies the proximity to the quantum critical point at which $C \propto T^2$. Such a situation arises in the singlet dynamics of the model of interactive plaquets [21]. We do not present the corresponding analysis here because parameters of the effective

Hamiltonian could be changed in the next orders of the perturbation theory.

Experimental verification. In both cases of the ordered and disordered ground state, the approach presented in this paper can be checked by inelastic neutron scattering: the corresponding intensity for the singlet–triplet transitions should have the periodicity in the reciprocal space corresponding to the star lattice. This picture is similar to that observed in the dimerized spin-Pairls compound $CuGeO_3$ [22]. In this case, inelastic magnetic scattering has a periodicity that corresponds to the dimerized lattice.

Comparison with QDMs. We point out that states in which all the stars are in the Ψ_- or Ψ_+ state can be presented as linear combinations of some first-neighbor dimer states proposed in Refs. [15, 16] for the QDM. But our approach to the kagomé problem is not equivalent to the QDM. In particular, we take all the intermediate states into account in considering the star interaction via perturbation theory in Eq. (6), whereas the QDM is restricted to the first-neighbor dimer subspace as regards the dimer dynamics.

Unfortunately, we cannot carry out a complete comparison between the QDM and the star approach at the present stage. The effective Hamiltonian derived in Ref. [15] was analyzed under crude approximations only. At the same time, the model presented here also requires further studies of the perturbation theory applicability for description of the inter-star interaction. We also note that some present-day results obtained within these two approaches contradict each other. For example, our model gives the ordered ground state, whereas the authors of Ref. [15] suggest that it is not ordered.

Cases of $S > 1/2$. We finally note that our consideration of the $S = 1/2$ KAF cannot be extended directly to the cases of larger spins. Although functions presented in Fig. 2, where the bold line shows the singlet state of the corresponding two spins, remain eigenfunctions of the Hamiltonian for $S > 1/2$, we have found numerically that they are not ground states of the star with $S = 1$ and $S = 3/2$. All details of calculations are presented in Appendix B. Another approach to KAFs with $S > 1/2$ should therefore be proposed.

4. CONCLUSION

In this paper, we present a model of the low-energy physics of spin-$\frac{1}{2}$ kagomé Heisenberg antiferromagnets (KAFs). The spin lattice can be represented as a set of stars that are arranged in a triangular lattice and contain 12 spins (see Fig. 1). Each star has two degenerate singlet ground states with a different symmetry, which can be described in terms of pseudospin. It is shown that the interaction between the stars leads to the band of singlet excitations that determines the low-energy KAF properties. The low-energy dynamics is described by the Hamiltonian of a spin-$\frac{1}{2}$ magnet in the external magnetic field given by Eq. (13). The Hamiltonian parameters are calculated in the first three orders of perturbation theory and are summarized in the Table. Within our precision, the KAF has an ordered singlet ground state with all the stars in the state given by Eq. (3). The ground state energy is lower than that calculated in the previous finite cluster studies. We show that our model cannot be extended directly to KAFs with $S > 1/2$.

The approach discussed in this paper can be verified experimentally on inelastic neutron scattering: the corresponding intensities for singlet–triplet transitions should have the periodicity in the reciprocal space corresponding to the star lattice.

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APPENDIX A

Irreducible representations of the group C_{6v}

The symmetry group C_{6v} contains six rotations C^k by the angles $2\pi k/6$ ($k = 0, 1, \ldots, 5$) and six reflections, which can be written as $C^k u_1$, where u_1 is the operator of a reflection. One-dimensional irreducible representations can be presented as follows [18, 19]:

$$C^k \sim 1, \qquad u_1 \sim 1, \qquad \text{(A.1)}$$

$$C^k \sim (-1)^k, \qquad u_1 \sim 1, \qquad \text{(A.2)}$$

$$C^k \sim 1, \qquad u_1 \sim -1, \qquad \text{(A.3)}$$

$$C^k \sim (-1)^k, \qquad u_1 \sim -1. \qquad \text{(A.4)}$$

For two-dimensional representations, we have [18, 19]

$$C^k \sim \begin{pmatrix} e^{i\frac{2\pi l}{6}k} & 0 \\ 0 & e^{-i\frac{2\pi l}{6}k} \end{pmatrix}, \qquad u_1 \sim \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{A.5}$$

where two inequivalent representations are given by $l = 1$ and $l = 2$.

APPENDIX B

Star with $S = 1$ and $S = 3/2$

In this Appendix, we give the details of numerical calculations showing that functions presented in Fig. 2, where the bold line shows the singlet state of the corresponding two spins, are not ground states of the star with $S = 1$ and $S = 3/2$, as this was for $S = 1/2$.

A simple numerical method for determination of the eigenvalue of a Hermitian operator H of the maximum modulus (power method [20]) was used. It is based on the following statement. We consider a state of the system $f = \sum_i c_i \psi_i$, where the sum may not include all the H eigenfunctions. For a given f, the eigenvalue E_{extr} of the maximum modulus is determined by

$$\lim_{n\to\infty} \frac{\langle f|H^{n+1}|f\rangle}{\langle f|H^n|f\rangle} = E_{extr}. \tag{B.1}$$

This becomes evident by noting that $\langle f|H^n|f\rangle = \sum_i |c_i|^2 E_i^n$.

Equation (B.1) can be used in numerical calculations as follows. The corresponding expression is calculated for $n = 1, 2, \ldots, n_{max}$. Convergence can therefore be controled by comparing results with different n. Studying a full set of vectors f and taking n_{max} large enough to match the necessary precision, one can find the eigenvalue of H with the largest modulus.

In the case of the star, the maximum eigenvalue of the Hamiltonian is $E_{max} = 18S^2 J_1$ (this energy has the state in which all the spins are along the same direction) and the energy of singlet states shown in Fig. 2 is $E_{ss} = -6S(S+1)J_1$. Because $E_{max} > |E_{ss}|$ for $S > 1/2$, we have to take $H = \mathcal{H}_0 - WI$ to investigate the lower $\mathcal{H}_0$ levels, where $\mathcal{H}_0$ is the star Hamiltonian given by Eq. (1), I is the unit matrix, and $W = (E_{max} + E_{ss})/2 + J_1$. Eigenvalues of H are therefore shifted down relative to those of $\mathcal{H}_0$ by the same value W such that the H eigenvalue with the largest modulus becomes equal to the $\mathcal{H}_0$ ground state energy minus W.

We have not found the ground state energy for the star with $S = 1$ and $S = 3/2$ by this method because the full set of vectors f should be examined for that. This operation requires much computer time. But studying a number of vectors f, we have obtained that there are states lower than those discussed above by the energy $1.8J_1$ at least. The method has given E_{extr} with the prescribed precision to the second decimal position at $n_{max} = 100$–300 depending on f and S.

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