Absence of long-range order in a spin-half Heisenberg antiferromagnet on the stacked kagomé lattice

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We study the ground state of a spin-half Heisenberg antiferromagnet on the stacked kagomé lattice by using a spin-rotation-invariant Green's function method. Since the pure two-dimensional kagomé antiferromagnet is most likely a magnetically disordered quantum spin liquid, we investigate the question whether the coupling of kagomé layers in a stacked three-dimensional system may lead to a magnetically ordered ground state. We present spin-spin correlation functions and correlation lengths. For comparison we apply also linear spin wave theory. Our results provide strong evidence that the system remains short-range ordered independent of the sign and the strength of the interlayer coupling.

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I. INTRODUCTION

In frustrated quantum spin lattices the interplay of quantum and frustration effects causes interesting physics, see, e.g., the recent reviews.[1–4] Special attention was focused on the problem of the ground state (GS) nature of the Heisenberg antiferromagnet (HAFM) on the two-dimensional (2D) kagomé lattice. In the classical limit the GS of the HAFM on the kagomé lattice exhibits a huge nontrivial degeneracy (see, e.g., Refs. 2 and 5–7). Intensive work over the last decade on the spin-half quantum version of the model[5,8–26] led to the conclusion that for the quantum HAFM the GS is most likely a short-range ordered spin liquid without any kind of long-range order (LRO). However, we mention that the GS properties in the quantum case are far from being fully understood, yet. Most of the conclusions are drawn from finite-lattice results of up to $N=36$ sites. Very recently, the rotation-invariant Green's function method introduced by Kondo and Yamaji[27] has been successfully applied on the spin-half HAFM on the 2D kagomé lattice.[22,23] In the framework of this approach one obtains also a spin-liquid GS with an energy per spin $E_0/JN=-0.4296$ which agrees well with the best available results obtained by other methods like the exact diagonalization[4,8,17,18] ($E_0/JN=-0.4344$) and the coupled-cluster method[21] ($E_0/JN=-0.4252$). Note that additional second-neighbor couplings may lead to a magnetically ordered GS phase.[17,28,29]

It is well-known that the dimensionality is crucial for the existence of order. Roughly spoken one can say, the higher the dimensionality of the spin system the more the influence of quantum or thermal fluctuations is suppressed. For the GS of quantum spin systems one finds several examples, where the physical properties change basically going from one to two dimensions or from two to three dimensions. For instance, the transition from the linear-chain to the square-lattice HAFM was studied in Refs. 30–33. Another example is the frustrated J_1-J_2 HAFM, which exhibits a magnetically disordered quantum paramagnetic GS phase around $J_2 \sim 0.5J_1$ for the 2D square lattice (see, e.g., Refs. 34–40 and references therein) but does not show this kind of quantum phase for the 3D body-centered cubic lattice.[41,42] Moreover, we know from the Mermin-Wagner theorem[43] that the interlayer coupling in quasi-2D Heisenberg magnets is crucial for magnetic ordering at finite temperatures. The role of the interlayer coupling in quasi-2D systems becomes particularly interesting if the decoupled layers themselves are magnetically disordered, e.g., due to strong frustration. Though this question is relevant for real 3D solids with a layered arrangement of magnetic atoms it has been less studied to date.

In this paper we address this question for the HAFM on a congruently stacked kagomé lattice. For such a system it is not known, whether an appropriate interlayer coupling may lead to a semiclassically ordered magnetic GS. However, one can expect that in the special limit of infinite ferromagnetic interlayer coupling the physics of the classical $O(3)$ kagomé antiferromagnet is obtained (see Sec. V B). We emphasize that the Lanczos exact diagonalization of finite lattices being the most powerful method to study the HAFM in the pure 2D kagomé case is inappropriate in 3D. Therefore we will discuss this question in our paper by the above-mentioned spin-rotation-invariant Green's function method, having in mind that this method was successfully applied to the pure 2D case. In particular, we will calculate the correlation functions and the correlation lengths. In addition, we will discuss the linear spin-wave theory (LSWT) for comparison.

II. MODEL

We consider congruently stacked kagomé layers shown in Fig. 1. The vertices of this stacked lattice are occupied by N spins one-half interacting via the Heisenberg exchange coupling

$$H=\frac{1}{2}\sum_{m\alpha,n\beta} J_{m\alpha,n\beta}\mathbf{S}_{m\alpha}\mathbf{S}_{n\beta}, \tag{1}$$

where the sum runs over all unit cells (labeled by m and n) and all spins within a unit cell (labeled by running indices α

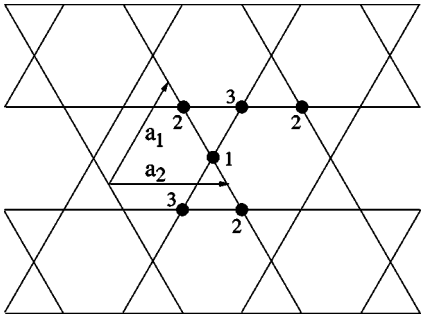

FIG. 1. Sketch of one kagomé layer in the congruently stacked lattice with its in-plane geometrical unit vectors $\mathbf{a}_1=(0,2,0)$, $\mathbf{a}_2=(\sqrt{3},1,0)$.The out-of plane unit vector $\mathbf{a}_3=(0,0,1)$ is not shown. Within a geometrical unit cell the spins are distinguished by a running index $\alpha=1,2,3$.

and β, see Fig. 1). One unit cell contains three spins, therefore the number of cells is $N/3$. The exchange coupling $J_{m\alpha,n\beta}$ is nonzero for nearest neighbors (NN), only. We introduce two different exchange parameters $J_\parallel$ and $J_\perp$ according to $J_{m\alpha,n\beta}\rightarrow J_\parallel(1-\delta_{\alpha,\beta})+J_\perp\delta_{\alpha,\beta}$.Since we are interested in the stacked kagomé HAFM, we consider $J_\parallel>0$ but allow both signs for $J_\perp$.

III. CLASSICAL GROUND STATE AND LINEAR SPIN WAVE THEORY

We start with a brief discussion of the classical GS of Eq. (1). Because there is no additional frustration caused by $J_\perp$, the classical GS within a certain layer is not modified, and the nontrivial huge degeneracy due to corner-sharing triangles[2,5–7] is not lifted. The only effect of a ferromagnetic (antiferromagnetic) interlayer coupling $J_\perp$ is the parallel (antiparallel) orientation of interacting spins of adjacent layers. Thus for a certain classical GS the spin configurations in all layers are identical. Two particular variants for the classical GS, namely, the so-called $\sqrt{3}\times\sqrt{3}$ state and the so-called $q=0$ state (see, e.g., Fig. 17 in Ref. 4), are often used for discussing possible magnetic LRO in the kagomé lattice. These two particular planar states can also be considered as variants of possible GS ordering for the stacked kagomé lattice.

Let us remind the reader of the fact, that starting from the $\sqrt{3}\times\sqrt{3}$ state as well as from the $q=0$ state the linear spin-wave theory (LSWT) for the pure 2D kagomé HAFM (Refs. 5 and 16) leads to one flat zero mode and two degenerate modes producing divergent integrals in the sublattice magnetization, which might be taken as a hint on the absence of semi-classical magnetic order.

For the stacked (3D) system we start also from both the $\sqrt{3}\times\sqrt{3}$ state and the $q=0$ state and perform the LSWT as usual. Taking into account that we have three spins per unit cell we have to introduce three different kinds of magnons. As in the 2D case[5,16] the spin wave spectrum is equivalent for all coplanar classical GS configurations because the directional cosine of in-plane neighbors is always $-1/2$ while the directional cosine of out-of-plane neighbors is either 1 or -1 depending on the sign of $J_\perp$. For $J_\perp>0$ we obtain for the spin-wave dispersions

$$\omega_{1\mathbf{q}}=s\sqrt{4J_\perp^2(1-\cos^2 q_z)+6J_\parallel J_\perp(1+\cos q_z)}, \tag{2}$$

$$\omega_{2\mathbf{q}}=s\sqrt{a_\mathbf{q}+b_\mathbf{q}},\quad \omega_{3\mathbf{q}}=s\sqrt{a_\mathbf{q}-b_\mathbf{q}}, \tag{3}$$

with

$$a_\mathbf{q}=4J_\parallel^2\left(2\cos^2\frac{q_y}{2}+\left(\cos^2\frac{\sqrt{3}q_x}{2}+\cos^2\frac{q_y}{2}\right)\left(1-2\cos^2\frac{q_y}{2}\right)\right)$$
$$+4J_\perp^2(1-\cos^2 q_z)+3J_\parallel J_\perp(3-\cos q_z), \tag{4}$$

$$b_\mathbf{q}=J_\parallel J_\perp(1-3\cos q_z)D_\mathbf{q}, \tag{5}$$

$$D_\mathbf{q}=\sqrt{9+16\cos^4\frac{q_y}{2}+16\cos^2\frac{\sqrt{3}q_x}{2}\cos^2\frac{q_y}{2}-8\cos^2\frac{\sqrt{3}q_x}{2}-24\cos^2\frac{q_y}{2}}. \tag{6}$$

For $J_\perp<0$ we find

$$\omega_{1\mathbf{q}}=s\sqrt{4J_\perp^2(1-\cos q_z)^2-6J_\parallel J_\perp(1-\cos q_z)}, \tag{7}$$

$$\omega_{2\mathbf{q}}=s\sqrt{a_\mathbf{q}+b_\mathbf{q}},\quad \omega_{3\mathbf{q}}=s\sqrt{a_\mathbf{q}-b_\mathbf{q}}, \tag{8}$$

with

$$a_\mathbf{q}=4J_\parallel^2\left(2\cos^2\frac{q_y}{2}+\left(\cos^2\frac{\sqrt{3}q_x}{2}+\cos^2\frac{q_y}{2}\right)\left(1-2\cos^2\frac{q_y}{2}\right)\right)$$
$$+4J_\perp^2(1-\cos q_z)^2-9J_\parallel J_\perp(1-\cos q_z), \tag{9}$$

$$b_\mathbf{q}=J_\parallel J_\perp(1-\cos q_z)D_\mathbf{q}. \tag{10}$$

The quantity s in Eqs. (2), (3), (7), and (8) is the spin quantum number which can be considered as parameter of the model (1) within the LSWT. If $J_\perp$ goes to zero, the known flat zero mode as well as the both degenerate modes[5,16] are recovered. But even for nonzero $J_\perp$ we have a flat zero mode $\omega_{1\mathbf{q}}$ and degenerate $\omega_{2\mathbf{q}}$ and $\omega_{3\mathbf{q}}$ in the q_x-q_y plane for certain q_z. For $J_\perp>0$, $\omega_{1\mathbf{q}}$ is a flat zero mode at $q_z=\pi$, and $\omega_{2\mathbf{q}}$ and $\omega_{3\mathbf{q}}$ become degenerate at any q_x,q_y for $q_z=\arccos 1/3$.For $J_\perp<0$, $\omega_{1\mathbf{q}}$ becomes a flat zero mode in the q_x-q_y plane for $q_z=0$, and $\omega_{2\mathbf{q}}$ and $\omega_{3\mathbf{q}}$ are degenerate at any q_x,q_y also for $q_z=0$. Thus, in both cases there is no finite

sublattice magnetization due to the resulting logarithmic divergencies in the involved integrals. We conclude, that the LSWT yields very similar behavior for the pure 2D and the 3D stacked case.

For completeness we give the expression for the GS energy per spin E_0/N

$$\frac{E_0}{N} = -(J_\parallel + |J_\perp|)s(s+1) + \frac{1}{2N}\sum_{\mathbf{q}}\sum_{m=1}^{3}\omega_{m\mathbf{q}}, \tag{11}$$

where the $\omega_{m\mathbf{q}}$ are the respective spin wave dispersions from Eqs. (2) and (3) or (7) and (8).

IV. SPIN-ROTATION-INVARIANT GREEN'S-FUNCTION THEORY

The Green's function method is one of the most powerful techniques for the investigation of quantum many-body systems and was successfully applied to spin systems over many decades. The rotation-invariant decoupling scheme was introduced by Kondo and Yamaji[27] to study the one-dimensional Heisenberg antiferromagnet and ferromagnet at finite temperatures. This decoupling scheme was developed to improve the description of magnetic short-range order and allows us to describe magnetic order-disorder transitions driven by quantum fluctuations as well as by thermal fluctuations. Later on the spin-rotation-invariant Green's function theory was used to discuss several two-dimensional models, for example, the pure HAFM,[44,45] the frustrated J_1-J_2 HAFM,[38,46] and the spatially anisotropic HAFM on the square lattice[32] as well as the doped square-lattice HAFM (t-J-model).[47,48] The quasi-two-dimensional and the three-dimensional HAFM have been investigated, too.[49,50]

Let us outline the main ideas of this method based on the equation-of-motion technique. To evaluate the relevant correlation functions we have to calculate a set of Fourier-transformed Green's functions $\langle\langle S^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega$ which are related to the dynamic spin susceptibilities by $\chi^{+-}_{\mathbf{q}\alpha\beta}(\omega) = -\langle\langle S^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega$. Their equation of motion reads

$$\omega\langle\langle S^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega = \langle[S^+_{\mathbf{q}\alpha}, S^-_{-\mathbf{q}\beta}]_-\rangle + \langle\langle i\dot{S}^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega. \tag{12}$$

Supposing rotational symmetry we have $\langle S^z_{m\alpha}\rangle = 0$ for any spin and, as a result, $\langle[S^+_{\mathbf{q}\alpha}, S^-_{-\mathbf{q}\beta}]_-\rangle \equiv 0$. Furthermore, we have $\langle S^z_{m\alpha} S^z_{n\beta}\rangle = \frac{1}{2}\langle S^+_{m\alpha} S^-_{n\beta}\rangle$, i.e., it is sufficient to calculate $\langle S^+_{m\alpha} S^-_{n\beta}\rangle$ to know all components of the correlation function $\langle \mathbf{S}_{m\alpha}\mathbf{S}_{n\beta}\rangle$. Going beyond the random-phase approximation (RPA) decoupling[51] we consider in a second step the equation of motion for $\langle\langle i\dot{S}^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega$,

$$\omega\langle\langle i\dot{S}^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega = \langle[i\dot{S}^+_{\mathbf{q}\alpha}, S^-_{-\mathbf{q}\beta}]_-\rangle + \langle\langle -\ddot{S}^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega. \tag{13}$$

The combination of Eqs. (12) and (13) yields

$$\omega^2\langle\langle S^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega = \langle[i\dot{S}^+_{\mathbf{q}\alpha}, S^-_{-\mathbf{q}\beta}]_-\rangle + \langle\langle -\ddot{S}^+_{\mathbf{q}\alpha}; S^-_{-\mathbf{q}\beta}\rangle\rangle_\omega. \tag{14}$$

The operator $-\ddot{S}^+_{\mathbf{q}\alpha} = [[S^+_{\mathbf{q}\alpha}, H], H]$ contains products of three spin operators along NN sequences. Those operator products were treated in the spirit of the decoupling scheme by Shimahara and Takada.[44] This decoupling is performed in the site representation of the Green's functions. For example, the operator product $S^-_A S^+_B S^+_C$ is replaced by $\eta_{A,B}\langle S^-_A S^+_B\rangle S^+_C + \eta_{A,C}\langle S^-_A S^+_C\rangle S^+_B$, where A, B, C represent spin sites. The quantities $\eta_{\gamma,\mu}$ are vertex parameters introduced to improve the approximation scheme. In the minimal version of the theory we introduce just as many vertex parameters as independent conditions for them that can be formulated. Because there are just two such conditions (see below) we consider two different parameters $\eta_\parallel$ and $\eta_\perp$ attached to intralayer and interlayer correlators, respectively. After the decoupling we write Eq. (14) in a compact matrix form omitting the running indices α and β

$$(\omega^2 - F_{\mathbf{q}})\chi^{+-}_{\mathbf{q}}(\omega) = -M_{\mathbf{q}}, \tag{15}$$

where $F_{\mathbf{q}}$ and $M_{\mathbf{q}}$ are the frequency and momentum matrices, respectively. Since the unit cell contains three spins, $F_{\mathbf{q}}$, $M_{\mathbf{q}}$, and $\chi^{+-}_{\mathbf{q}}$ are 3×3-matrices. For the sake of brevity we do not give the lengthy expressions for the matrix elements of $F_{\mathbf{q}}$ and $M_{\mathbf{q}}$ but give their eigenvalues, only. Both matrices are hermitean and commute with each other. Hence, the solution of Eq. (15) in terms of the common set of normalized eigenvectors $|j\mathbf{q}\rangle$of $\chi^{+-}_{\mathbf{q}}$ reads

$$\chi^{+-}_{\mathbf{q}}(\omega) = -\sum_{j=1}^{3}\frac{m_{j\mathbf{q}}}{\omega^2 - \omega^2_{j\mathbf{q}}}|j\mathbf{q}\rangle\langle j\mathbf{q}|. \tag{16}$$

For the eigenvalues $m_{j\mathbf{q}}$ of $M_{\mathbf{q}}$ and $\omega^2_{j\mathbf{q}}$ of $F_{\mathbf{q}}$ we find

$$m_{1\mathbf{q}} = -12J_\parallel c_{1,0,0} - 4J_\perp c_{0,0,1}(1-\cos q_z), \tag{17}$$

$$\begin{aligned}\omega^2_{1\mathbf{q}} = {} & 3J^2_\parallel[1 + 2\eta_\parallel(2c_{1,0,0} + c_{1,1,0} + c_{2,0,0})] + J^2_\perp(1-\cos q_z)\\ & \times[1 + 2\eta_\perp(c_{0,0,1} + c_{0,0,2}) - 4\eta_\perp c_{0,0,1}(1+\cos q_z)]\\ & + 4J_\parallel J_\perp[\eta_\perp c_{0,0,1}(1-\cos q_z) - 2\eta_\perp c_{1,0,1}(1+\cos q_z)\\ & + 7\eta_\perp c_{1,0,1} - 3\eta_\parallel c_{1,0,0}\cos q_z],\end{aligned} \tag{18}$$

$$m_{2\mathbf{q}} = -6J_\parallel c_{1,0,0} - 4J_\perp c_{0,0,1}(1-\cos q_z) - 2J_\parallel c_{1,0,0} D_{\mathbf{q}}, \tag{19}$$

$$\omega_{2\mathbf{q}}^2 = J_\parallel^2\left[\frac{3}{2} + 3\eta_\parallel(2c_{1,0,0} + c_{1,1,0} + c_{2,0,0}) + 8\eta_\parallel c_{1,0,0}\left(2\cos^4\frac{q_y}{2} + 2\cos^2\frac{\sqrt{3}q_x}{2}\cos^2\frac{q_y}{2} - \cos^2\frac{\sqrt{3}q_x}{2} - 3\cos^2\frac{q_y}{2}\right)\right] + J_\perp^2(1-\cos q_z)$$
$$\times[1 + 2\eta_\perp(c_{0,0,1} + c_{0,0,2}) - 4\eta_\perp c_{0,0,1}(1+\cos q_z)] + J_\parallel J_\perp[-8\eta_\perp c_{1,0,1}(1+\cos q_z) - 2\eta_\perp c_{0,0,1}(1-\cos q_z) - 6\eta_\parallel c_{1,0,0}\cos q_z$$
$$+ 22\eta_\perp c_{1,0,1}] + \frac{J_\parallel}{2}\{J_\parallel[1 + 2\eta_\parallel(2c_{1,0,0} + c_{1,1,0} + c_{2,0,0})] + 4J_\perp[\eta_\perp c_{0,0,1}(1-\cos q_z) + \eta_\perp c_{1,0,1} - \eta_\parallel c_{1,0,0}\cos q_z]\}D_{\mathbf{q}}, \quad (20)$$

$$m_{3\mathbf{q}} = -6J_\parallel c_{1,0,0} - 4J_\perp c_{0,0,1}(1-\cos q_z) + 2J_\parallel c_{1,0,0}D_{\mathbf{q}}, \quad (21)$$

$$\omega_{3\mathbf{q}}^2 = J_\parallel^2\left[\frac{3}{2} + 3\eta_\parallel(2c_{1,0,0} + c_{1,1,0} + c_{2,0,0}) + 8\eta_\parallel c_{1,0,0}\left(2\cos^4\frac{q_y}{2} + 2\cos^2\frac{\sqrt{3}q_x}{2}\cos^2\frac{q_y}{2} - \cos^2\frac{\sqrt{3}q_x}{2} - 3\cos^2\frac{q_y}{2}\right)\right] + J_\perp^2(1-\cos q_z)$$
$$\times[1 + 2\eta_\perp(c_{0,0,1} + c_{0,0,2}) - 4\eta_\perp c_{0,0,1}(1+\cos q_z)] + J_\parallel J_\perp[-8\eta_\perp c_{1,0,1}(1+\cos q_z) - 2\eta_\perp c_{0,0,1}(1-\cos q_z) - 6\eta_\parallel c_{1,0,0}\cos q_z$$
$$+ 22\eta_\perp c_{1,0,1}] - \frac{J_\parallel}{2}\{J_\parallel[1 + 2\eta_\parallel(2c_{1,0,0} + c_{1,1,0} + c_{2,0,0})] + 4J_\perp[\eta_\perp c_{0,0,1}(1-\cos q_z) + \eta_\perp c_{1,0,1} - \eta_\parallel c_{1,0,0}\cos q_z]\}D_{\mathbf{q}}, \quad (22)$$

where $D_{\mathbf{q}}$ is defined in Eq. (6). The correlators $c_{l,k,m}$ have to be determined self-consistently; their indices correspond to a vector $\mathbf{R} = l\mathbf{a}_1/2 + k\mathbf{a}_2/2 + m\mathbf{a}_3$ connecting two spins, i.e., $c_{l,k,m} = c_{\mathbf{R}} = \langle S_0^+ S_{\mathbf{R}}^-\rangle = \frac{2}{3}\langle \mathbf{S}_0\mathbf{S}_{\mathbf{R}}\rangle$. Using the NN correlators $c_{1,0,0}$ and $c_{0,0,1}$ the GS energy per spin E_0/N is given by $E_0/N = 3J_\parallel c_{1,0,0} + 3J_\perp c_{0,0,1}/2$. Equations (17)–(22) contain eight parameters $c_{1,0,0}$, $c_{1,1,0}$, $c_{2,0,0}$, $c_{0,0,1}$, $c_{1,0,1}$, $c_{0,0,2}$, $\eta_\parallel$, and $\eta_\perp$, which must be determined self-consistently. The relation between the correlators and the corresponding Green's functions is given by the spectral theorem.[51,52] Its application to the correlators $c_{l,k,m}$ leads to six equations, a seventh one is the sum rule $c_{0,0,0} = 1/2$. One additional equation is obtained requiring that the matrix of the static susceptibility $\chi_{\mathbf{q}}^{+-} = \chi_{\mathbf{q}}^{+-}(\omega = 0)$ is isotropic in the limit $\mathbf{q} \to 0$,[32] i.e., $\lim_{q_x\to 0, q_y\to 0}\chi_{\mathbf{q}}^{+-}|_{q_z=0} = \lim_{q_z\to 0}\chi_{\mathbf{q}}^{+-}|_{q_x=q_y=0}$. From that constraint we obtain

$$c_{1,0,0}\{J_\perp[1 - 2\eta_\perp(3c_{0,0,1} - c_{0,0,2})] + 8J_\parallel\eta_\perp(c_{1,0,1} - c_{0,0,1})\}$$
$$- c_{0,0,1}\{J_\parallel[1 - 2\eta_\parallel(4c_{1,0,0} - c_{1,1,0} - c_{2,0,0})]$$
$$+ 4J_\perp(\eta_\perp c_{1,0,1} - \eta_\parallel c_{1,0,0})\} = 0. \quad (23)$$

For the discussion of the magnetic GS ordering we consider the spin-spin correlation functions $\langle \mathbf{S}_{m\alpha}\mathbf{S}_{n\beta}\rangle$. A possible magnetic LRO in the system is described via $\langle \mathbf{S}_{m\alpha}\mathbf{S}_{n\beta}\rangle$ at large distances $\mathbf{R}_n - \mathbf{R}_m$. More precisely, we consider, as in Refs. 44 and 45, a condensation term $C_{\mathbf{Q}\alpha\beta}$ in the Fourier transformation $S_{\alpha\beta}(\mathbf{q})$ of $\langle \mathbf{S}_{m\alpha}\mathbf{S}_{n\beta}\rangle$ according to

$$\langle \mathbf{S}_{m\alpha}\mathbf{S}_{n\beta}\rangle = \frac{3}{N}\sum_{\mathbf{q}\neq\mathbf{Q}} S_{\alpha\beta}(\mathbf{q})\exp(-i\mathbf{q}\mathbf{r}_{m\alpha,n\beta})$$
$$+ \frac{3}{2}C_{\mathbf{Q}\alpha\beta}\exp(-i\mathbf{Q}\mathbf{r}_{m\alpha,n\beta}), \quad (24)$$

where $\mathbf{Q}$ is the corresponding wave vector of the magnetic order and $S_{\alpha\beta}(\mathbf{q})$ is given by

$$S_{\alpha\beta}(\mathbf{q}) = \frac{3}{2}\sum_{j=1}^{3}\frac{m_{j\mathbf{q}}}{2\omega_{j\mathbf{q}}}\langle\alpha|j\mathbf{q}\rangle\langle j\mathbf{q}|\beta\rangle. \quad (25)$$

The existence of $C_{\mathbf{Q}\alpha\beta} \neq 0$ is accompanied by a diverging static susceptibility $\chi_{\mathbf{q}}^{+-}$ at the magnetic wave vector $\mathbf{Q}$.

To describe the magnetic order in a short-range ordered phase we use in addition to the spin-spin correlation functions the correlation length ξ_ν along a certain direction $\mathbf{e}_\nu$. To calculate ξ_ν we apply the procedure illustrated in Refs. 44 and 45. We expand that eigenvalue of the static susceptibility $\chi_{\mathbf{q}}^{+-}$, which is largest at the magnetic wave vector $\mathbf{Q}$ around this point $\mathbf{Q}$. The relevant magnetic wave vector $\mathbf{Q}$ in the short-range ordered phase is that vector, where the largest eigenvalue of the static susceptibility has its maximum. Then the square of the correlation length along $\mathbf{e}_\nu$ is given by the factor in front of the square of the corresponding component of the $\mathbf{q}$ vector $q_\nu = \mathbf{e}_\nu(\mathbf{Q} - \mathbf{q})$. For illustration we give the expression for the intralayer correlation length $\xi_\parallel$ in the pure kagomé limit ($J_\perp = 0$), $\xi_\parallel^2 = -2\eta_\parallel c_{1,0,0}/[1 + 2\eta_\parallel(2c_{1,0,0} + c_{1,1,0} + c_{2,0,0})]$, and omit the lengthy general expressions for the inter- and intralayer correlation lengths.

V. RESULTS

A. Antiferromagnetic interlayer coupling $J_\perp > 0$

Solving the set of the eight self-consistency equations we find that there is no solution with a nonzero condensation term. Therefore we conclude that within the applied rotation-invariant Green's function decoupling scheme there is no indication of magnetic LRO for the stacked 3D kagomé HAFM with antiferromagnetic interlayer coupling. This remarkable result is in accordance with the findings within the LSWT (see Sec. III). To study the influence of the interlayer coupling on the GS magnetic short-range order we calculate the spin-spin correlation functions and the correlation lengths. For convenience we set $J_\parallel = 1$. In Fig. 2 we show several first, second, and third neighbor correlation func-

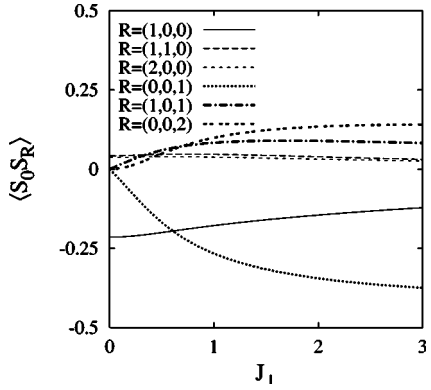

FIG. 2. First, second, and third neighbor intralayer [$\mathbf{R}=(1,0,0);(1,1,0);(2,0,0)$] and interlayer [$\mathbf{R}=(0,0,1);(1,0,1);(0,0,2)$] correlation functions in dependence on the antiferromagnetic interlayer coupling $J_\perp$.

tions. The strongest change is seen in the strengths of the interlayer correlators which increase in the interval $0 \leqslant J_\perp \leqslant 1$, for $J_\perp \approx 1$ their values are already close to those of the pure linear chain. The change in the intralayer correlators is small. While the NN intralayer correlator shows some decrease in strength, the second and third neighbor correlators are weakly increased for small $J_\perp$. Remarkably, already for $J_\perp < 1$ the interlayer correlators become stronger than the intralayer correlators. Note that in the limit $J_\perp = 0$ our values for the GS energy as well as for the correlators coincide with available results reported in Refs. 22 and 23.

As illustrated above, to calculate the inter- and intralayer correlation lengths $\xi_\perp$ and $\xi_\parallel$ we have to expand the extreme eigenvalue of the static susceptibility around $\mathbf{Q}$, which is $\mathbf{Q}=(0,0,\pi)$ for all $J_\perp > 0$. The results for the intra- and interlayer correlation lengths are shown in Fig. 3. The intralayer correlation length is of the order of the NN separation $d=1$ in the pure 2D limit. It increases up to a maximal value of about $\xi_\parallel \approx 2.5d$ for $J_\perp \approx 1$ and goes to zero for $J_\perp \to \infty$. The increase of the interlayer correlation length is stronger. Though we expect a diverging $\xi_\perp$ for the isolated chain, it remains finite for any $J_\perp > 0$. This behavior is a drawback of the Green's function decoupling, which is not able to describe the critical GS with a power-law decay of the correlation functions of the linear-chain HAFM.

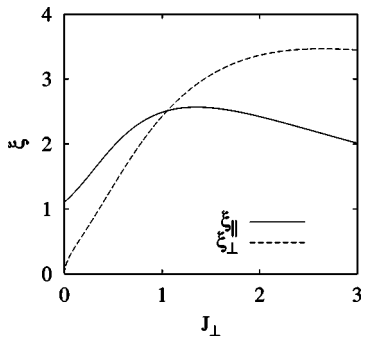

FIG. 3. Intralayer ($\xi_\parallel$) and interlayer ($\xi_\perp$) correlation lengths in dependence on the antiferromagnetic interlayer coupling $J_\perp$.

B. Ferromagnetic interlayer coupling $J_\perp < 0$

Now we turn to the case $J_\perp < 0$ which appears to be more complicated from the numerical point of view. Starting from $J_\perp = 0$ we find a solution of the self-consistency equations with zero condensation term until $J_\perp \approx -J_\parallel = -1$. That means we can conclude that for ferromagnetic interlayer coupling there is no indication for magnetic LRO for $|J_\perp| \lesssim 1$, too. Beyond this point our numerical procedure fails because of numerical instabilities in the $\mathbf{q}$ space integrals. The reason for that consists in the specific behavior of the dispersion relations $\omega_{\alpha\mathbf{q}}$ from Eqs. (18), (20), and (22). Increasing the strength of the ferromagnetic interlayer coupling beyond $|J_\perp| \gtrsim 1$ we find that $\omega_{1\mathbf{q}}$ becomes more and more a flat zero mode in the q_x-q_y plane at $q_z=0$, and at the same time $\omega_{2\mathbf{q}}$ and $\omega_{3\mathbf{q}}$ become more and more degenerate leading to divergent terms in $\mathbf{q}$ integrals. This behavior of the $\omega_{\alpha\mathbf{q}}$ is in coincidence with our findings within the LSWT, where we have found a flat zero-mode and two degenerate modes in the $q_x - q_y$-plane at $q_z=0$ (see Sec. III). We believe that the physical interpretation of this behavior is connected with the classical limit (large quantum number s) of the pure 2D kagomé HAFM. In the large s limit the results of the LSWT theory become reliable. In the 3D stacked kagomé lattice with ferromagnetic $J_\perp$ the spins along the chains become stronger coupled with increasing $|J_\perp|$ and can be considered as large s (quasiclassical) composite spins. These quasiclassical spins are coupled kagomélike with each other, thus we are most likely faced with the classical HAFM on the kagomé lattice with its huge nontrivial degeneracy of the GS. Though we do not have rigorous statements on the zero-temperature correlation functions of the classical kagomé HAFM, presumably at $T=0$ the average of the spin-spin correlation over the set of all ground states does not exhibit magnetic LRO.[2,4,6] Hence we may conclude that the zero-temperature spin-spin correlation functions within a kagomé layer do not exhibit LRO for any ferromagnetic $J_\perp$.

However, the subtile interplay between the tendency to form large s (quasiclassical) composite spins and the still remaining (weak) quantum fluctuations may lead to order by disorder effects. As it was argued in Refs. 6, 7, 53, and 54 for the pure 2D classical HAFM on the kagomé lattice at low temperatures $T \to 0$, the entropy of fluctuations may lead to different relative Boltzmann weights of the classical ground states this way favoring planar ordered ground states. Presumably there is a nematic LRO but an algebraic decay of the spin-spin correlation for $T \to 0$.[6,53] Hence, for the stacked system considered in this paper at $T=0$ and for $J_\perp \to -\infty$, due to remaining quantum fluctuations a nematic order accompanied by an algebraic decay in the intralayer spin-spin correlation functions is possible.

To describe the magnetic GS in more detail we present, similar to the case $J_\perp > 0$, the spin-spin correlation functions and the correlation lengths in Figs. 4 and 5. Due to the above-mentioned numerical problems our data are restricted to $0 \leqslant |J_\perp| \leqslant J_\parallel = 1$. Several first, second, and third neighbor correlation functions are shown in Fig. 4. Again the change in the intralayer correlators is very small, whereas the strengths of interlayer correlation functions increase with growing $|J_\perp|$ and become larger than those of intralayer cor-

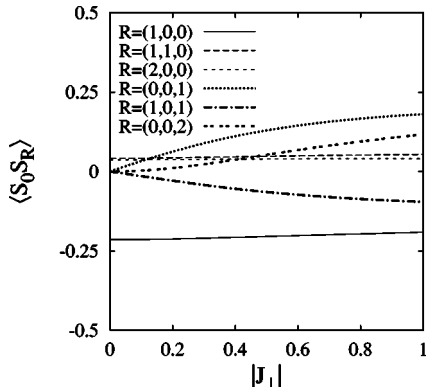

FIG. 4. First, second, and third neighbor intralayer [$\mathbf{R}=(1,0,0);(1,1,0);(2,0,0)$] and interlayer [$\mathbf{R}=(0,0,1);(1,0,1);(0,0,2)$] correlation functions in dependence on the strength of the ferromagnetic interlayer coupling $|J_\perp|$.

relation functions except for the NN correlation.

The correlation lengths for $J_\perp<0$ belong to $\mathbf{Q}=(0,0,0)$. We show the intra- ($\xi_\parallel$) and interlayer ($\xi_\perp$) correlation lengths in Fig. 5. $\xi_\parallel$ and $\xi_\perp$ increase in the parameter region shown but are still of the order of the NN separation d. Obviously, the increase in $\xi_\perp$ (i.e., along the chains) is significantly stronger. We expect that $\xi_\perp$ diverges for large $|J_\perp|$. As discussed above, a diverging $\xi_\parallel$ for $J_\perp\to-\infty$ would also be possible indicating an algebraic decay of the correlation functions.

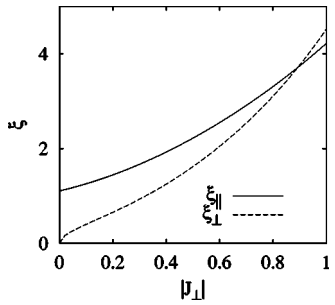

FIG. 5. Intralayer ($\xi_\parallel$) and interlayer ($\xi_\perp$) correlation lengths in dependence on the strength of the ferromagnetic interlayer coupling $|J_\perp|$.

VI. SUMMARY

In this paper we have investigated the GS of the stacked three-dimensional kagomé spin-half Heisenberg antiferromagnet for ferromagnetic and antiferromagnetic interlayer coupling. To study the magnetic GS order we have applied a second-order Green's function decoupling scheme going beyond the RPA. Though one could expect that an increase in the dimension from two to three would stabilize magnetic order, we find some evidence that the interlayer coupling is not able to create magnetic LRO within the antiferromagnetic kagomé layers. These findings based on the Green's function scheme are supported by linear spin wave theory.

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[1] C. Lhuillier, P. Sindzingre, and J.-B. Fouet, Can. J. Phys. **79**, 1525 (2001).
[2] R. Moessner, Can. J. Phys. **79**, 1283 (2001).
[3] G. Misguich and C. Lhuillier, cond-mat/0310405 (unpublished).
[4] J. Richter, J. Schulenburg, and A. Honecker, in *Quantum Magnetism in Two Dimensions: From Semi-Classical Néel Order to Magnetic Disorder*; Quantum Magnetism, Lecture Notes in Physics, Vol. 645 edited by U. Schollwöck, J. Richter, D. J. J. Farnell, and R. F. Bishop (Springer, Berlin, 2004), pp. 85–153; http://www.tu-bs.de/~honecker/papers/2dqm.ps.gz.
[5] A. B. Harris, C. Kallin, and A. J. Berlinsky, Phys. Rev. B **45**, 2899 (1992).
[6] J. T. Chalker, P. C. W Holdsworth, and E. F. Shender, Phys. Rev. Lett. **68**, 855 (1992).
[7] D. A. Huse and A. D. Rutenberg, Phys. Rev. B **45**, 2899 (1992).
[8] C. Zeng and V. Elser, Phys. Rev. B **42**, 8436 (1990).
[9] R. R. P. Singh and D. A. Huse, Phys. Rev. Lett. **68**, 1766 (1992).
[10] J. T. Chalker and J. F. G. Eastmond, Phys. Rev. B **46**, 14201 (1992).
[11] A. Chubukov, Phys. Rev. Lett. **69**, 832 (1992).
[12] S. Sachdev, Phys. Rev. B **45**, 12377 (1992).
[13] P. W. Leung and V. Elser, Phys. Rev. B **47**, 5459 (1993).
[14] K. Yang, L. K. Warman, and S. M. Girvin, Phys. Rev. Lett. **70**, 2641 (1993).
[15] P. Sindzingre, P. Lecheminant, and C. Lhuillier, Phys. Rev. B **50**, 3108 (1994).
[16] H. Asakawa and M. Suzuki, Physica A **205**, 687 (1994).
[17] P. Lecheminant, B. Bernu, C. Lhuillier, L. Pierre, and P. Sindzingre, Phys. Rev. B **56**, 2521 (1997).
[18] C. Waldtmann, H.-U. Everts, B. Bernu, P. Sindzingre, C. Lhuillier, P. Lecheminant, and L. Pierre, Eur. Phys. J. B **2**, 501–507 (1998).
[19] F. Mila, Phys. Rev. Lett. **81**, 2356 (1998).
[20] P. Sindzingre, C. Misguich, C. Lhuillier, B. Bernu, L. Pierre, C. Waldtmann, and H.-U. Everts, Phys. Rev. Lett. **84**, 2953 (2000).
[21] D. J. J. Farnell, R. F. Bishop, K. A. Gernoth, Phys. Rev. B **63**, 220402(R) (2001).
[22] W. Yu and S. Feng, Eur. Phys. J. B **13**, 265 (2000).
[23] B. H. Bernhard, B. Canals, and C. Lacroix, Phys. Rev. B **66**, 024422 (2002).
[24] J. Schulenburg, A. Honecker, J. Schnack, J. Richter, and H.-J. Schmidt, Phys. Rev. Lett. **88**, 167207 (2002).
[25] A. V. Syromyatnikov and S. V. Maleyev, Phys. Rev. B **66**, 132408 (2002); J. Phys.: Condens. Matter **16**, S843 (2004).
[26] P. Nikolic and T. Senthil, Phys. Rev. B **68**, 214415 (2003).
[27] J. Kondo and K. Yamaji, Prog. Theor. Phys. **47**, 807 (1972).
[28] R. Shankar and D. Shubashree, Phys. Rev. B **61**, 12126 (2000).
[29] Y. Narumi, K. Katsumata, Z. Honda, J.-C. Domenge, P. Sindzingre, C. Lhuillier, Y. Shimaoka, T. C. Kobayashi, and K. Kindo, Europhys. Lett. **65**, 705 (2004).

[30] I. Affleck, M. Gelfand, and R. Singh, J. Phys. A **27**, 7313 (1994); **28**, 1787(E) (1995).
[31] A. Fledderjohann, K.-H. Mütter, M.-S. Yang, and M. Karbach, Phys. Rev. B **57**, 956 (1998).
[32] D. Ihle, C. Schindelin, A. Weiße, and H. Fehske, Phys. Rev. B **60**, 9240 (1999).
[33] O. Derzhko, T. Verkholyak, R. Schmidt, and J. Richter, Physica A **320**, 407 (2003).
[34] P. Chandra and B. Doucot, Phys. Rev. B **38**, 9335 (1988).
[35] H. J. Schulz and T. A. L. Ziman, Europhys. Lett. **18**, 355 (1992); H. J. Schulz, T. A. L. Ziman, and D. Poilblanc, J. Phys. I **6**, 675 (1996).
[36] J. Richter, Phys. Rev. B **47**, 5794 (1993).
[37] L. Capriotti and S. Sorella, Phys. Rev. Lett. **84**, 3173 (2000).
[38] L. Siurakshina, D. Ihle, and R. Hayn, Phys. Rev. B **64**, 104406 (2001).
[39] O. P. Sushkov, J. Oitmaa, and Zheng Weihong, Phys. Rev. B **63**, 104420 (2001).
[40] L. Capriotti, Int. J. Mod. Phys. B **15**, 1799 (2001).
[41] R. Schmidt, J. Schulenburg, J. Richter, and D. D. Betts, Phys. Rev. B **66**, 224406 (2002).
[42] J. Oitmaa and Zheng Weihong, Phys. Rev. B **69**, 064416 (2004).
[43] N. Mermin and H. Wagner, Phys. Rev. Lett. **17**, 1133 (1966).
[44] H. Shimahara and S. Takada, J. Phys. Soc. Jpn. **60**, 2394 (1991).
[45] S. Winterfeldt and D. Ihle, Phys. Rev. B **56**, 5535 (1997); **59**, 6010 (1999).
[46] A. F. Barabanov and V. M. Berezovskii, J. Phys. Soc. Jpn. **63**, 3974 (1994).
[47] S. Feng and Y. Song, Phys. Rev. B **55**, 642 (1997).
[48] S. Winterfeldt and D. Ihle, Phys. Rev. B **58**, 9402 (1998).
[49] L. Siurakshina, D. Ihle, and R. Hayn, Phys. Rev. B **61**, 14601 (2000).
[50] D. Ihle, C. Schindelin, and H. Fehske, Phys. Rev. B **64**, 054419 (2001).
[51] S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967).
[52] K. Elk and W. Gasser, *Die Methode der Greenschen Funktionen in der Festkörperphysik* (Akademie-Verlag Berlin, 1979).
[53] J. N. Reimers and A. J. Berlinsky, Phys. Rev. B **48**, 9539 (1993).
[54] M. E. Zhitomirsky, Phys. Rev. Lett. **88**, 057204 (2002).