

Heisenberg antiferromagnet on the kagome lattice with arbitrary spin: A higher-order coupled cluster treatment

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Starting with the $\sqrt{3} \times \sqrt{3}$ and the $q = 0$ states as reference states, we use the coupled cluster method to high orders of approximation to investigate the ground state of the Heisenberg antiferromagnet on the kagome lattice for spin quantum numbers $s = 1/2, 1, 3/2, 2, 5/2$, and 3 . Our data for the ground-state energy for $s = 1/2$ are in good agreement with recent large-scale density-matrix renormalization group and exact diagonalization data. We find that the ground-state selection depends on the spin quantum number s . While for the extreme quantum case, $s = 1/2$, the $q = 0$ state is energetically favored by quantum fluctuations, for any $s > 1/2$ the $\sqrt{3} \times \sqrt{3}$ state is selected. For both the $\sqrt{3} \times \sqrt{3}$ and the $q = 0$ states the magnetic order is strongly suppressed by quantum fluctuations. Within our coupled cluster method we get vanishing values for the order parameter (sublattice magnetization) M for $s = 1/2$ and $s = 1$, but (small) nonzero values for M for $s > 1$. Using the data for the ground-state energy and the order parameter for $s = 3/2, 2, 5/2$, and 3 we also estimate the leading quantum corrections to the classical values.

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I. INTRODUCTION

The investigation of the low-energy physics of the Heisenberg antiferromagnet (HAFM)

$$H = \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \quad (1)$$

on the kagome lattice is one of the most challenging problems in the field of frustrated quantum magnetism. The sum over $\langle i, j \rangle$ runs over all nearest-neighbor pairs of sites on the lattice, counting each bond once only, and $\mathbf{s}_i \equiv (s_i^x, s_i^y, s_i^z)$ is the spin operator on site i . Although, there has been an intensive discussion of the problem over many years applying various theoretical methods (see, e.g., Refs. 1–34), no conclusive answer on the nature of the ground state (GS) and the existence of a spin gap has been found.

While for many years a spin-liquid GS was favored,^{5,10,12} recently arguments have been given for a valence-bond crystal GS with a large unit cell of 36 sites that breaks the symmetry of the underlying kagome lattice.^{16,20,21} However, very recently this valence-bond picture has been rechecked by large-scale numerics^{28,29,31} and once again the spin-liquid GS is favored.

Although large-scale density-matrix renormalization group (DMRG) and exact diagonalization (ED) calculations seem to be most effective to study the low-energy physics of the kagome HAFM, complementary methods (see, e.g., Refs. 27, 30, 33, and 34), are highly desirable to shed further light on this challenging problem.

A method which has been successfully applied to strongly frustrated quantum magnets is the coupled cluster method (CCM) (see, e.g., Refs. 14, 26, and 35–42). In the present paper we apply the CCM in high orders of approximation to the kagome HAFM.

II. COUPLED CLUSTER METHOD

For the sake of brevity we illustrate here only some relevant features of the coupled cluster method (CCM). For more general information on the methodology of the CCM, see, e.g., Refs. 43–48.

We first mention that the CCM approach yields results directly in the thermodynamic limit $N \rightarrow \infty$, where N is the number of lattice sites (and hence spins). The starting point for a CCM calculation is the choice of a normalized reference state $|\Phi\rangle$ that is typically a classical GS of the model. For the kagome HAFM we choose the $\sqrt{3} \times \sqrt{3}$ and the $q = 0$ states illustrated in Fig. 1 (see also, e.g., Refs. 2, 7, and 33 for further details). Then we perform a rotation of the local axes of each of the spins such that all spins in the reference state align along the negative z axis. In this new set of local spin coordinates a complete set of mutually commuting multispin creation operators $C_I^+ \equiv (C_I^-)^\dagger$ related to this reference state is defined by

$$|\Phi\rangle = |\downarrow\downarrow\downarrow\cdots\rangle, \quad C_I^+ = s_n^+, s_n^+ s_m^+, s_n^+ s_m^+ s_k^+, \dots, \quad (2)$$

where $s_n^+ \equiv s_n^x + i s_n^y$, the indices n, m, k, \dots denote arbitrary lattice sites, and the components of the spin operators are defined in the local rotated coordinate frames. Note that for spins of quantum number s , each site index in each configuration index I in Eq. (2) can be repeated up to a maximum of $2s$ times. With the set $\{|\Phi\rangle, C_I^+\}$ thus defined, the CCM parametrizations of the ket and bra GS eigenvectors $|\Psi\rangle$ and $\langle\tilde{\Psi}|$ of the spin system are given by

$$|\Psi\rangle = e^S |\Phi\rangle, \quad S = \sum_{I \neq 0} a_I C_I^+, \quad (3)$$

$$\langle\tilde{\Psi}| = \langle\Phi| \tilde{S} e^{-S}, \quad \tilde{S} = 1 + \sum_{I \neq 0} \tilde{a}_I C_I^-. \quad (4)$$

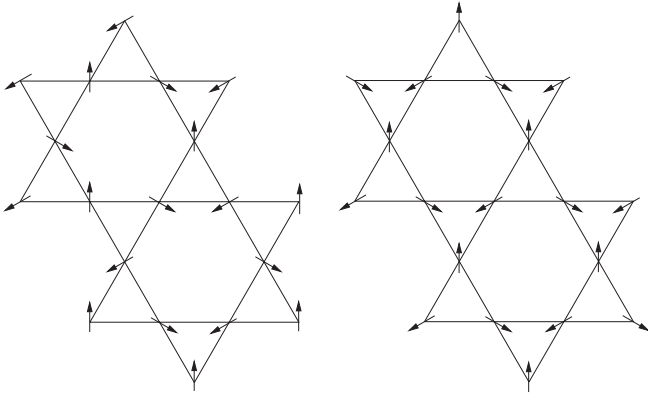


FIG. 1. Illustration of the $\sqrt{3} \times \sqrt{3}$ (left) and the $q = 0$ (right) classical GS of the kagome HAFM.

We have defined $C_0^+ \equiv 1$, and the normalization of the states is clearly such that $\langle \tilde{\Psi} | \Psi \rangle = \langle \Phi | \Psi \rangle = \langle \Phi | \Phi \rangle \equiv 1$. The CCM correlation operators S and \tilde{S} contain the correlation coefficients a_I and \tilde{a}_I , which can be determined by the CCM ket-state and bra-state equations

$$\langle \Phi | C_I^- e^{-S} H e^S | \Phi \rangle = 0, \quad \forall I \neq 0, \quad (5)$$

$$\langle \Phi | \tilde{S} e^{-S} [H, C_I^+] e^S | \Phi \rangle = 0, \quad \forall I \neq 0. \quad (6)$$

Equations (5) and (6) are fully equivalent to the GS Schrödinger equations for the ket and bra states. They follow readily from the requirement that the GS energy functional $\langle \tilde{\Psi} | H | \Psi \rangle$ be stationary with respect to variations in all of the correlation coefficients \tilde{a}_I and a_I , respectively ($\forall I \neq 0$). Each ket-state or bra-state equation belongs to a certain configuration index I , i.e., it corresponds to a certain set (configuration) of lattice sites n, m, k, \dots , as in Eq. (2). Using the Schrödinger equation, $H | \Psi \rangle = E | \Psi \rangle$, we can now write the GS energy as $E = \langle \Phi | e^{-S} H e^S | \Phi \rangle$. The magnetic order parameter (sublattice magnetization) is given by $M = -\frac{1}{N} \sum_{i=1}^N \langle \tilde{\Psi} | s_i^z | \Psi \rangle$, where s_i^z is expressed in the transformed coordinate system, and $N (\rightarrow \infty)$ is the number of lattice sites.

If we would be able to consider all creation and annihilation operators C_I^+ and C_I^- , i.e., all sets (configurations) of lattice sites, in the CCM correlation operators S and \tilde{S} we would get, in principle, the exact eigenstate.⁴⁴ However, for the many-body quantum system under consideration it is necessary to use approximation schemes in order to truncate the expansions of S and \tilde{S} in Eqs. (3) and (4) in a practical calculation. Then the approximate results for the GS energy E and the order parameter M will depend certainly on the choice of the reference state.

We use for spin quantum number $s = 1/2$ the so-called LSUB n approximation scheme to truncate the expansions of S and \tilde{S} in Eqs. (3) and (4), where we include only n or fewer correlated spins in all configurations (or lattice animals in the language of graph theory) which span a range of no more than n contiguous lattice sites, where a set of sites is defined to be contiguous if every site has at least one other in the set as a nearest neighbor (for more details see Refs. 43 and 46–48). Using efficient parallelized CCM code⁴⁹ we are able to solve the CCM equations up to LSUB10 for $s = 1/2$ (where,

e.g., for the $q = 0$ reference state a set of 238 010 coupled ket-state equations has to be solved), which goes significantly beyond earlier CCM calculations for the kagome HAFM.^{14,26} Moreover, we also use the CCM to consider spin quantum numbers $s > 1/2$.

Since the LSUB n approximation becomes exact for $n \rightarrow \infty$ (as does the alternative SUB n - n scheme that we introduce and use in Sec. III B for values of the spin quantum number $s > 1/2$), it is useful to extrapolate the “raw” LSUB n (or SUB n - n) data to the limit $n \rightarrow \infty$. There is ample experience regarding how one should extrapolate the GS energy per site $e_0(n) \equiv E(n)/N$ and the magnetic order parameter $M(n)$. For the GS energy per spin, $e_0(n) = a_0 + a_1(1/n)^2 + a_2(1/n)^4$ is a very well-tested extrapolation ansatz.^{35–38,40,46,48} An appropriate extrapolation rule for the magnetic order parameter of highly frustrated systems is^{37,38,40} $M(n) = b_0 + b_1(1/n)^{1/2} + b_2(1/n)^{3/2}$. Moreover, we know from Refs. 37, 38, and 40 that low levels of approximation conform poorly to these rules. Hence, we exclude the $n = 2$ and $n = 3$ data from the extrapolations.

For the solution of the CCM equations we rewrite the Hamiltonian (1) in the rotated coordination frame of the local quantization axis

$$H_\lambda = \sum_{\langle i \rightarrow j \rangle} \left(-\frac{1}{2} (\lambda s_i^x s_j^x + s_i^z s_j^z) + \lambda s_i^y s_j^y + \frac{\sqrt{3}}{2} \lambda (-s_i^x s_j^z + s_i^z s_j^x) \right), \quad (7)$$

where we have further introduced an anisotropy parameter λ that now multiplies the non-Ising terms, similar to what was done in Refs. 6 and 45. Note that the symbols $\langle i \rightarrow j \rangle$ on the sum in Eq. (7) now indicate directionality of the nearest-neighbor bonds (see, e.g., Refs. 6, 39, and 45), which is different for the $\sqrt{3} \times \sqrt{3}$ and the $q = 0$ reference states. Starting at $\lambda = 0$, where the corresponding reference states are eigenstates of H_λ , we can slowly increase λ and hence trace the CCM solutions out to the true kagome point at $\lambda = 1$. Moreover, λ can be understood as a parameter that tunes the strength of the quantum fluctuations.

III. RESULTS

A. The extreme quantum case: $s = 1/2$

We start with the CCM investigation of the kagome HAFM for spin quantum number $s = 1/2$. At a given finite level of the CCM LSUB n scheme, the treatment of quantum effects is performed in an approximate manner. Certainly, the treatment of quantum effects becomes better as the level of approximation n is increased. In previous studies of the GS selection based on an expansion around the classical limit,^{4,7,11} the $\sqrt{3} \times \sqrt{3}$ state was found to be selected by quantum fluctuations. We present our results for the GS energy per site in Fig. 2, where the dependence on the anisotropy parameter λ of the difference in the energies per site between the two states considered, $\Delta e \equiv e_0^{\sqrt{3} \times \sqrt{3}} - e_0^{q=0}$, is shown for various LSUB n approximations. Interestingly, the GS selection depends on the LSUB n truncation index n . Just as in linear spin-wave theory,^{2,11} there is also no GS selection

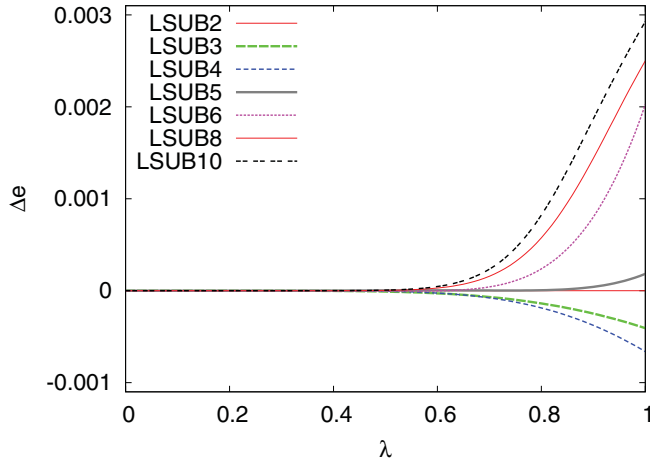


FIG. 2. (Color online) Difference of GS energies per site, $\Delta e \equiv e_0^{\sqrt{3} \times \sqrt{3}} - e_0^{q=0}$, between the $\sqrt{3} \times \sqrt{3}$ and $q = 0$ states of the spin-1/2 kagome HAFM, for various CCM-LSUB n approximations and spin quantum number $s = 1/2$.

(i.e., $\Delta e = 0$) at the CCM-LSUB2 level, thereby indicating a poor consideration of quantum effects at the lowest LSUB n order. As the level of approximation n is increased we first find

that $\Delta e < 0$ for $n = 3$ and $n = 4$ (i.e., the $\sqrt{3} \times \sqrt{3}$ state is selected in accordance with previous findings^{7,11}), but as n is further increased we then find that $\Delta e > 0$ for $n > 4$ (i.e., the $q = 0$ state is selected). Bearing in mind that quantum effects are better taken into account at higher LSUB n levels, we might argue that strong quantum fluctuations indeed favor the $q = 0$ state. Note that this line of argument is also supported by our CCM results below for spin quantum numbers $s > 1/2$ (i.e., generally speaking, where quantum fluctuations are weaker), where in all levels of approximations the $\sqrt{3} \times \sqrt{3}$ state is selected (see our discussion below in Sec. III B).

In Fig. 3 we show the magnetic order parameter as a function of the anisotropy parameter λ . At $\lambda = 0$ we have $M = s = 1/2$, since the corresponding reference state is the exact GS of $H_{\lambda=0}$. As λ is increased the order parameter decreases monotonically. At a certain value of λ , near the true kagome point $\lambda = 1$, the extrapolated order parameter vanishes, thus indicating that the GS is magnetically disordered. The difference in the two variants of the extrapolation (including or excluding LSUB4 and LSUB5) may be considered as an error bar for the extrapolated order parameter.

To illustrate the quality of the extrapolations of the “raw” LSUB n data in the limit $n \rightarrow \infty$, we show corresponding plots for the $q = 0$ state and various values of the anisotropy parameter λ in Fig. 4. It is obvious that the LSUB n data are well fitted by the applied extrapolation functions.

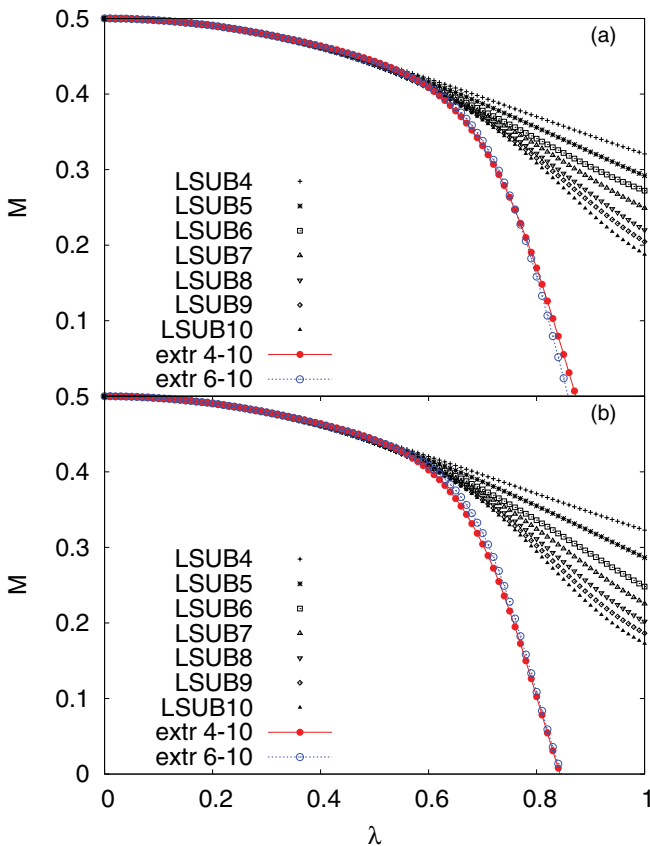


FIG. 3. (Color online) CCM-LSUB n data for the magnetic order parameter M versus λ for the spin-1/2 kagome HAFM, for (a) the $\sqrt{3} \times \sqrt{3}$ reference state and (b) the $q = 0$ reference state. For the extrapolations to $n \rightarrow \infty$ according to $M(n) = b_0 + b_1(1/n)^{1/2} + b_2(1/n)^{3/2}$ we have used LSUB n data for $n = 4, 5, \dots, 10$ as well as for $n = 6, 7, \dots, 10$.

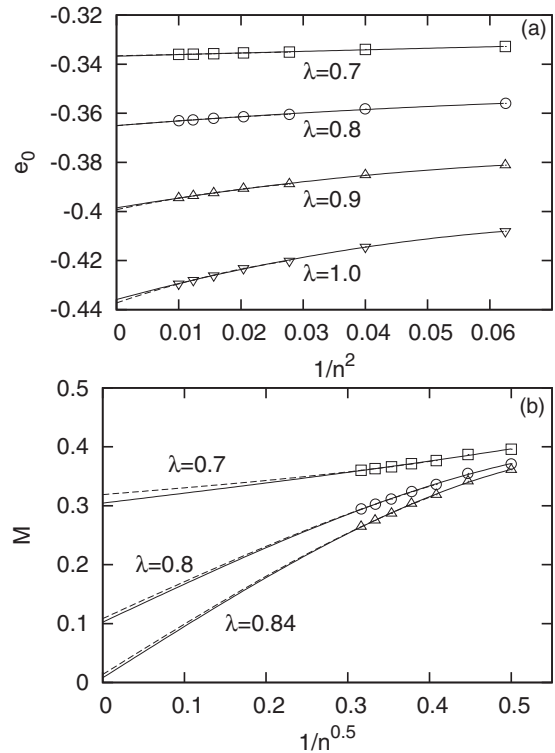


FIG. 4. Illustration of the extrapolation of the CCM-LSUB n data (symbols) for (a) the ground-state energy e_0 and (b) the magnetic order parameter M for the $q = 0$ state of the spin-1/2 kagome HAFM. For the extrapolations to $n \rightarrow \infty$ according to $e_0(n) = a_0 + a_1(1/n)^2 + a_2(1/n)^4$ and $M(n) = b_0 + b_1(1/n)^{1/2} + b_2(1/n)^{3/2}$ we have used LSUB n data for $n = 4, 5, \dots, 10$ (solid lines) as well as for $n = 6, 7, \dots, 10$ (dashed lines).

TABLE I. CCM results for the spin-1/2 HAFM on the kagome lattice (i.e., at $\lambda = 1$). The quantity $e_0 \equiv E/N$ is the GS energy per spin and M is the magnetic order parameter (sublattice magnetization). The LSUBn results are extrapolated to $n \rightarrow \infty$ according to $e_0(n) = a_0 + a_1(1/n)^2 + a_2(1/n)^4$ and $M(n) = b_0 + b_1(1/n)^{1/2} + b_2(1/n)^{3/2}$ using LSUBn data for $n = 4, 5, \dots, 10$ as well as for $n = 6, 7, \dots, 10$.

$\sqrt{3} \times \sqrt{3}$	e_0	M
LSUB4	-0.408 728	0.320 702
LSUB5	-0.414 235	0.291 917
LSUB6	-0.418 052	0.272 109
LSUB7	-0.420 677	0.248 989
LSUB8	-0.423 554	0.219 994
LSUB9	-0.424 962	0.204 661
LSUB10	-0.426 485	0.187 634
Extrapolated (4–10)	-0.4318	<0
Extrapolated (6–10)	-0.4336	<0
$q = 0$	e_0	M
LSUB4	-0.408 066	0.322 860
LSUB5	-0.414 418	0.286 462
LSUB6	-0.420 078	0.248 078
LSUB7	-0.423 126	0.225 356
LSUB8	-0.426 054	0.202 074
LSUB9	-0.427 952	0.186 435
LSUB10	-0.429 413	0.172 742
Extrapolated (4–10)	-0.4357	<0
Extrapolated (6–10)	-0.4372	<0
Other recent results		
Ref. 20	-0.433	–
Ref. 27	-0.4322	–
Ref. 29, $N = 42$ (type a)	-0.437 999	–
Ref. 29, $N = 42$ (type b)	-0.438 143	–
Ref. 28	-0.4379	–

Next we analyze the model for $\lambda = 1$ in more detail. The CCM-LSUBn data, as well as the extrapolated data, are listed in Table I. Moreover, we present results for the GS energy obtained by other methods for comparison. While the values $e_0 = -0.4322$ obtained in Ref. 27 and $e_0 = -0.4332$ obtained in Ref. 28 can be considered as rigorous upper bounds of the GS energy, the large-scale DMRG result $e_0 = -0.4379$ obtained in Ref. 28 seems to be the most accurate estimate presently available. The lowest extrapolated CCM energy is $e_0 = -0.4372$, obtained for the $q = 0$ reference state using CCM-LSUBn results for $n = 6, 7, 8, 9$, and 10 for the extrapolation. This CCM estimate is very close to the DMRG result of Ref. 28.

B. Higher spin quantum numbers: $s > 1/2$

Although several magnetic kagome compounds carry spins with $s > 1/2$, such as the $s = 3/2$ magnet $\text{KCr}_3(\text{OH})_6(\text{SO}_4)_2$,⁵⁰ or the $s = 5/2$ compound $(\text{H}_3\text{O})\text{Fe}_3(\text{OH})_6(\text{SO}_4)_2$,⁵¹ far fewer theoretical results are available for those higher-spin quantum numbers. In the classical limit $s \rightarrow \infty$, thermal fluctuations may lead to $\sqrt{3} \times \sqrt{3}$ long-range order as $T \rightarrow 0$.^{3,23} In most papers dealing with large-spin quantum models it has been found that quantum fluctuations select the $\sqrt{3} \times \sqrt{3}$ state.^{4,7,11,32}

Moreover, magnetic long-range order might be possible for higher spin values.^{4,32}

For our CCM approach for $s > 1/2$ we use (instead of the LSUBn scheme) the alternative SUBn-m approximation scheme to truncate the expansions of S and \tilde{S} in Eqs. (3) and (4). This is because as s increases the number of fundamental configuration I retained at a given LSUBn level also increases, since each spin at any site i may be raised up to $2s$ times by its raising operator s_i^+ , and hence each site index i may be repeated up to $2s$ times in the operators C_i^+ of Eq. (2). In the SUBn-m scheme we include no more than n spin flips spanning a range of no more than m contiguous lattice sites.^{47,48} In what follows we consider the case $n = m$, i.e., SUBn-n, which for $s = 1/2$ is identical to the LSUBn scheme. Since the number of coupled ket-state equations for a certain level of SUBn-n approximation increases with increasing spin quantum number s , the highest level of approximation we can consider is SUB8-8 for $s = 1, 3/2, 2, 5/2$, and 3. The maximum number of ket-state equations we have to take into account is 416 126 for $s = 3$. For the extrapolation to $n \rightarrow \infty$ we use the same extrapolation formulas as for $s = 1/2$, and consider the SUBn-n data for $n = 4, 5, 6, 7$, and 8.

First we discuss the GS selection. In Fig. 5 we present the dependence on the anisotropy parameter λ of the energy difference per site, $\Delta e \equiv e_0^{\sqrt{3} \times \sqrt{3}} - e_0^{q=0}$, for the highest level of approximation that we have performed (viz., SUB8-8), and for values of the spin quantum number $s = 1/2, 1, \dots, 3$. We find that the $\sqrt{3} \times \sqrt{3}$ state is selected for all values $s > 1/2$. This is in agreement with previous studies based on an expansion around the classical limit,^{4,7,11} but it is in contrast to our findings for the extreme quantum case $s = 1/2$. Hence, interestingly, our results suggest that for the frustrated quantum spin system under consideration the $s = 1/2$ case and the cases $s > 1/2$ may exhibit different behavior. It is interesting to note that a similar effect has also been observed for a frustrated quantum spin chain.⁵² We see clearly that the energy difference Δe scaled by s^2 decreases monotonically with increasing s ,

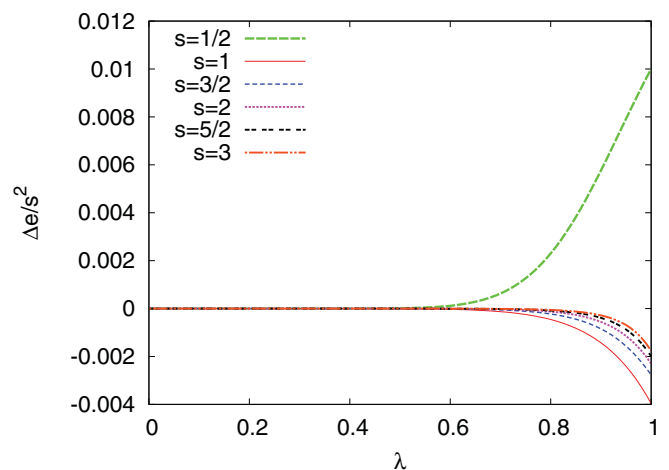


FIG. 5. (Color online) Difference of the GS energies per site, $\Delta e \equiv e_0^{\sqrt{3} \times \sqrt{3}} - e_0^{q=0}$, between the $\sqrt{3} \times \sqrt{3}$ and $q = 0$ states of the kagome HAFM, calculated for the CCM SUB8-8 approximation and for spin quantum numbers $s = 1/2, 1, 3/2, 2, 5/2$, and 3.

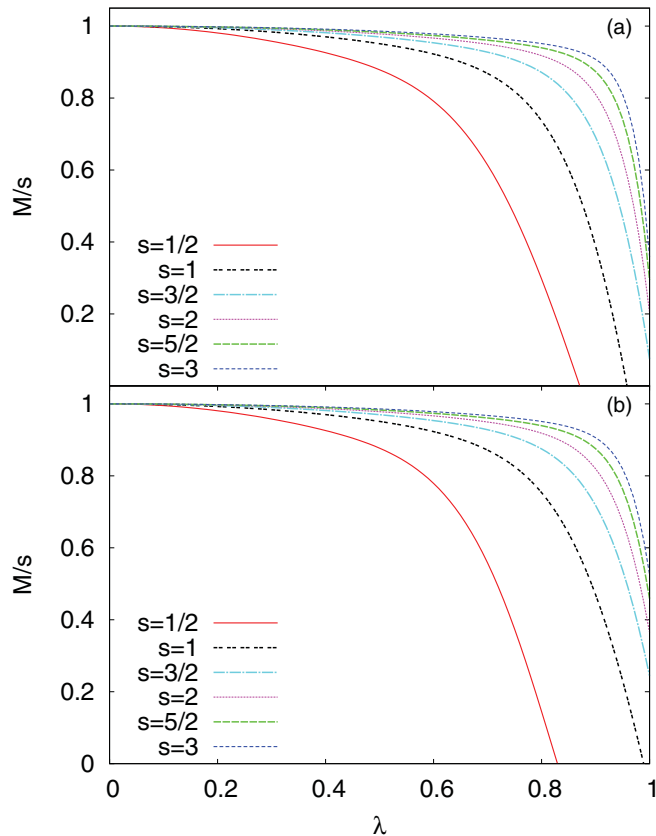


FIG. 6. (Color online) Extrapolated magnetic order parameter M/s versus λ for (a) the $\sqrt{3} \times \sqrt{3}$ reference state and (b) the $q = 0$ reference state of the kagome HAFM, for various values of the spin quantum number s . For the extrapolations to $n \rightarrow \infty$ according to $M(n) = b_0 + b_1(1/n)^{1/2} + b_2(1/n)^{3/2}$ we have used SUB n - n data for $n = 4, 5, \dots, 8$. [Note that even for the $s = 1/2$ case we have excluded the (available) LSUB9 and LSUB10 data here to be consistent with the $s > 1/2$ cases.]

thereby demonstrating that for $s \rightarrow \infty$ the $\sqrt{3} \times \sqrt{3}$ and the $q = 0$ states become degenerate.

Next we discuss the magnetic order parameter M . To compare results for various values of s it is useful to consider M/s . Since for $s \rightarrow \infty$ the chosen reference state is an eigenstate, we would get $M/s = 1$ within our CCM approach in this classical limit. Hence, we may expect that by increasing the spin quantum number the quantity M/s becomes nonzero for a certain value $s > s_0$ in the whole range $0 \leq \lambda \leq 1$ (see, e.g., Ref. 4). In Fig. 6 we show the extrapolated magnetic order parameter for both reference states as a function of the anisotropy parameter λ , for values $s = 1/2, 1, \dots, 5/2, 3$. For large values of s the scaled order parameter becomes almost constant, $M/s \sim 1$, over a wide range of λ values. However, as the true kagome point at $\lambda = 1$ is approached we find a steep decay of M/s . Nevertheless, only for $s = 1/2$ (as discussed already above) and for $s = 1$ does the extrapolated order parameter vanish at $\lambda = 1$, whereas M/s remains nonzero for $s \geq 1$. Hence, our data suggest that for higher values of s a $\sqrt{3} \times \sqrt{3}$ magnetic order might be possible. To provide more detailed information on the GS properties of the kagome HAFM, we present in Table II CCM-SUB8-8 data as well

TABLE II. CCM results for the HAFM on the kagome lattice (i.e., at $\lambda = 1$) for spin quantum numbers $s = 1, 3/2, 2, 5/2, 3$. The quantity $e_0 \equiv E/N$ is the GS energy per spin and M is the magnetic order parameter (sublattice magnetization). The SUB n - n results are extrapolated to $n \rightarrow \infty$ according to $e_0(n) = a_0 + a_1(1/n)^2 + a_2(1/n)^4$ and $M(n) = b_0 + b_1(1/n)^{1/2} + b_2(1/n)^{3/2}$ using SUB n - n data for $n = 4, 5, 6, 7$, and 8.

	$\sqrt{3} \times \sqrt{3}$		$q = 0$	
$s = 1$	e_0/s^2	M/s	e_0/s^2	M/s
SUB8-8	-1.383 644	0.580 079	-1.379 680	0.607 293
extr4-8	-1.4031	<0	-1.3965	<0
$s = 3/2$	e_0/s^2	M/s	e_0/s^2	M/s
SUB8-8	-1.257 354	0.690 229	-1.254 588	0.709 167
extr4-8	-1.2680	0.0744	-1.2643	0.2438
$s = 2$	e_0/s^2	M/s	e_0/s^2	M/s
SUB8-8	-1.195 442	0.735 642	-1.193 145	0.754 580
extr4-8	-1.2026	0.2029	-1.2000	0.3645
$s = 5/2$	e_0/s^2	M/s	e_0/s^2	M/s
SUB8-8	-1.157 697	0.766 290	-1.155 703	0.785 822
extr4-8	-1.1627	0.2942	-1.1607	0.4586
$s = 3$	e_0/s^2	M/s	e_0/s^2	M/s
SUB8-8	-1.132 263	0.788 722	-1.130 497	0.808 862
extr4-8	-1.1360	0.3583	-1.1344	0.5256
$s \rightarrow \infty$	e_0/s^2	M/s	e_0/s^2	M/s
Exact	-1	1	-1	1

as extrapolated data at $\lambda = 1$, for values of the spin quantum number $s = 1, 3/2, 3, 5/2$, and 3. We see clearly that the scaled GS energy per spin approaches the classical value, $e_0/s^2 = -1$, quite rapidly as s is increased. On the other hand, even for the largest spin considered here (viz., $s = 3$) the extrapolated order parameter remains relatively small, particularly for the $\sqrt{3} \times \sqrt{3}$ state.

Our CCM data for e_0 and M , available up to $s = 3$, together with the known results in the classical limit, $\lim_{s \rightarrow \infty} e_0/s^2 = -1$ and $\lim_{s \rightarrow \infty} M/s = 1$, also allow us to discuss the s dependence of e_0/s^2 and M/s in the large- s limit. In spin-wave theories one typically obtains expansions for e_0 and M in powers of $1/s$.^{53,54} For the GS energy of the kagome HAFM the standard linear spin-wave theory yields for both the $\sqrt{3} \times \sqrt{3}$ and the $q = 0$ states, $e_0/s^2 = -1 - 0.4412/s$ (see Refs. 2 and 9). On the other hand, due to the presence of the flat zero mode in the kagome HAFM, the integral for the order parameter diverges.^{9,55} Using an effective spin-wave theory, in which short-wavelength fluctuations are neglected, Asakawa and Suzuki⁹ obtained $M/s = 1 - 0.336/s$, whereas Chubukov⁷ found fluctuation corrections proportional to $s^{-2/3}$ (in contrast to conventional spin-waves) by using a self-consistent spin-wave approach.

Here we use our extrapolated CCM data for $s = 3/2, 2, 5/2$, and 3 to find the leading corrections to the classical values. By fitting the extrapolated GS energy e_0/s^2 with a fitting function $f(s) = -1 + a_1 s^{-a_2}$, we obtain a value for the exponent a_2 very close to one for both reference states. Hence, finally we have fitted the extrapolated CCM data for e_0/s^2 using $f(s) = -1 + x_1 s^{-1} + x_2 s^{-2}$. The fits yield the corresponding values $x_1 = -0.414$ (-0.410) and $x_2 = 0.018$ (0.020) for the $\sqrt{3} \times \sqrt{3}$ ($q = 0$) reference states, as shown in Fig. 7(a). Obviously,

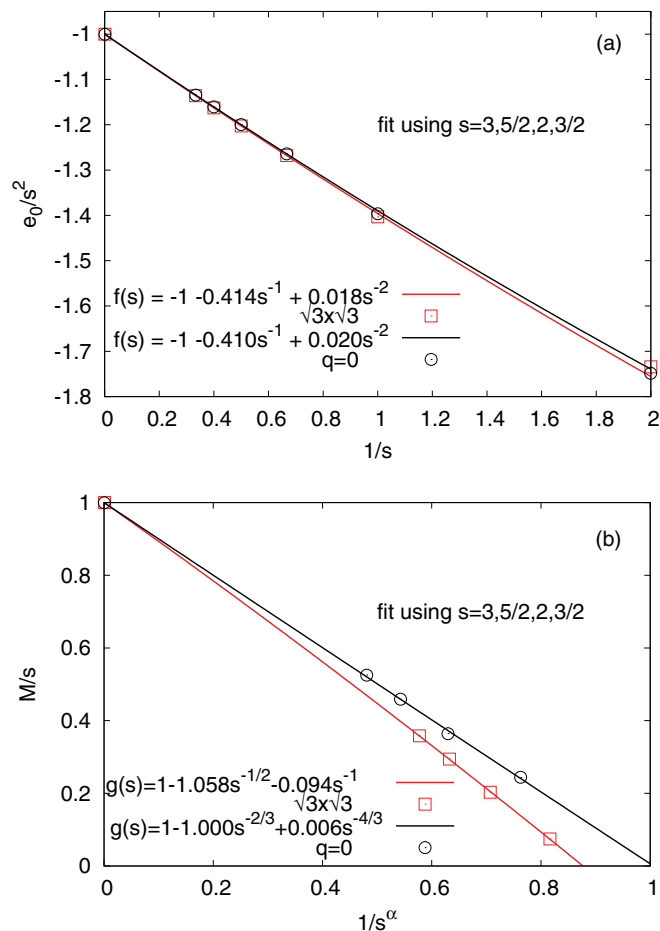


FIG. 7. (Color online) Dependence on the spin quantum number s of (a) the extrapolated scaled GS energy per spin, e_0/s^2 , and (b) the extrapolated scaled magnetic order parameter, M/s , of the kagome HAFM. For M/s the exponent $\alpha = 1/2$ for the $\sqrt{3} \times \sqrt{3}$ state and $\alpha = 2/3$ for the $q = 0$ state. (Symbols are CCM data points; lines are fits to the data points).

the $\frac{1}{s}$ prefactor is close to that of the linear spin-wave theory, and the contribution of the next order is small. Note, however, that if the fitting function $f(s)$, with the above given values for x_1 and x_2 , is applied to the $s = 1/2$ case, it does not reproduce the GS selection of the $q = 0$ state in this extreme quantum case [c.f., Fig. 7(a) at the value $1/s = 2$].

Next we use $g(s) = 1 + b_1 s^{-b_2}$ as a fitting function to fit the extrapolated CCM order parameters M/s , again using data for $s = 3/2, 2, 5/2$, and 3 . For the exponent b_2 we get the values $b_2 = 0.529$ for the $\sqrt{3} \times \sqrt{3}$ reference state and $b_2 = 0.666$ for the $q = 0$ reference state. Clearly, the leading correction is not proportional to s^{-1} ; rather

Chubukov's result⁷ of a leading correction proportional to $s^{-2/3}$ is confirmed for the $q = 0$ state. By contrast, for the $\sqrt{3} \times \sqrt{3}$ reference state our results are in favor of a leading correction for the order parameter proportional to $s^{-1/2}$. Hence, finally we have fitted the extrapolated CCM data for M/s using the fitting functions $g(s) = 1 + y_1 s^{-1/2} + y_2 s^{-1}$ [$g(s) = 1 + y_1 s^{-2/3} + y_2 s^{-4/3}$] for the $\sqrt{3} \times \sqrt{3}$ [$q = 0$] reference states. The fits yield the corresponding values $y_1 = -1.058$ [-1.000] and $y_2 = -0.094$ [0.006], as shown in Fig. 7(b).

IV. SUMMARY

In the present investigation we present data for the GS energy per spin, e_0 , and the order parameter (sublattice magnetization), M , of the kagome HAFM for spin quantum numbers $s = 1/2, 1, 3/2, 2, 5/2$, and 3 , using high-order CCM-SUB n - n calculations based on the $\sqrt{3} \times \sqrt{3}$ and the $q = 0$ reference states. Our best estimate of the GS energy for the $s = 1/2$ case, viz., $e_0 = -0.4372$, is clearly below rigorous upper bounds reported recently,^{27,28} and it also agrees well with recent accurate DMRG²⁸ and ED²⁹ results. We find that the GS selection by quantum fluctuations depends on the spin quantum number s . While for $s = 1/2$ the $q = 0$ state is selected, for all values $s > 1/2$ the $\sqrt{3} \times \sqrt{3}$ state has lower energy. Using CCM data for $s = 3/2, 2, 5/2$ and 3 we determine also the leading quantum corrections to the classical values of the GS energy and the order parameter.

For the order parameter M/s obtained by an appropriate extrapolation of the CCM-SUB n - n data we get small (but nonzero) values $M/s > 0$ for all values of the spin quantum number $s > 1$. For $s = 1/2$ and $s = 1$ the situation is different. Clearly, in any SUB n - n approximation for finite n we have a magnetic quantum ground state (i.e., a finite M/s) with the corresponding symmetry of the classical ground state. Extrapolating to $n \rightarrow \infty$ we get a nonmagnetic ground state (vanishing order parameter) but locally the magnetic correlations still fit to the symmetry of the classical ground state. However, they can be extremely short ranged; i.e., the ground state can be considered as a spin-liquid state with spin correlations on a very short-ranged length scale. However, the true kagome ground state might have also an admixture of contributions of other classical ground states renormalized by quantum fluctuations.

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