Direct calculation of the spin stiffness of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on square, triangular, and cubic lattices using the coupled-cluster method

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We present a method for the direct calculation of the spin stiffness by means of the coupled-cluster method. For the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on square, triangular, and cubic lattices, we calculate the stiffness in high orders of approximation. For square and cubic lattices, our results are in very good agreement with the best results available in the literature. For the triangular lattice, our result is more precise than any other result obtained thus far by other approximate method.

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I. INTRODUCTION

The study of quantum magnetism has attracted much experimental and theoretical attention over many years (for an overview, see Ref. 1). The spin stiffness ρ_s constitutes, together with the spin-wave velocity, a fundamental parameter that determines the low-energy dynamics of magnetic systems.[2–4] In particular, in two-dimensional quantum antiferromagnets, where magnetically ordered as well as quantum disordered ground-state phases are observed, the ground-state stiffness measures the distance of the ground state from criticality[4] and can be used, in addition to the sublattice magnetization M, to test the existence or absence of magnetic long-range order (LRO).

Over the last 15 years in a series of papers, several methods, such as series expansion,[5,6] spin-wave theory,[6–11] quantum Monte Carlo,[12] exact diagonalization,[8,13,14] Schwinger-boson approach,[15–17] and renormalization group theory,[18] have been used to calculate the spin stiffness of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet (HAFM) on square, triangular, and cubic lattices. However, results for the triangular lattice seem to be less precise than those for the square lattice due to strong frustration. Published values therefore show significant variability.

The spin stiffness ρ_s measures the increase in the amount of energy when we rotate the order parameter of a magnetically long-range-order system along a given direction by a small angle θ per unit length, i.e.,

$$\frac{E(\theta)}{N} = \frac{E(\theta=0)}{N} + \frac{1}{2}\rho_s\theta^2 + \mathcal{O}(\theta^4) \qquad (1)$$

where $E(\theta)$ is the ground-state energy as a function of the imposed twist and N is the number of sites. In the thermodynamic limit, a positive value of ρ_s means that there is LRO in the system, while a value of zero reveals that there is no LRO.[19]

In this paper we present a method to calculate the spin stiffness for the quantum-spin HAFM using the coupled-cluster approach.[20–22] The coupled-cluster approach is a powerful and universal tool in quantum many-body physics, which has been applied in various fields, such as nuclear physics, quantum chemistry, strongly correlated electrons, etc.[20–22] More recently the coupled-cluster method (CCM) has been applied to quantum spin systems with much success, see, e.g., Refs. 23–34. In the field of magnetism an important advantage of this approach is its applicability to strongly frustrated quantum spin systems in any dimension, where some other methods (such as, e.g., the quantum Monte Carlo method) fail. Therefore, the method to calculate the spin stiffness described in this paper is quite generally applicable to spin systems also with noncollinear ground states.

To demonstrate the potential of the presented method we calculate the spin stiffness for the spin-$1/2$ HAFM with nearest-neighbor interaction on the cubic, square, and triangular lattices and compare our results to available data in the literature. Although for the square and cubic lattices accurate high-order spin-wave results are available that can be used to estimate the accuracy of the CCM results, the known results for the frustrated HAFM on the triangular lattice with a noncollinear ground state seem to be less reliable, since the used methods are less accurate. We argue that our result for the stiffness of the HAFM on the triangular lattice obtained by CCM in high order of approximation is better than the available results to date. We mention that some preliminary results for the spin stiffness of the so-called $J-J'$ model using the CCM can be found in Ref. 32.

II. THE METHOD

The model we consider is the spin-$\frac{1}{2}$ HAFM

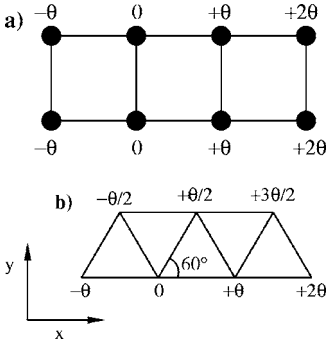

FIG. 1. Illustration of the twisted Néel state: (a) square lattice and (b) triangular lattice. The twist is introduced along rows in the x direction. The angles at the lattice sites indicated the twist of the spins with respect to the corresponding Néel state.

$$H = J\sum_{\langle i,j\rangle} \mathbf{s}_i \cdot \mathbf{s}_j. \tag{2}$$

In (2), the sum runs over all pairs of nearest neighbors $\langle i,j\rangle$. We now set $J=1$ henceforth.

We start with a brief illustration of the main features of the CCM. For a general overview on the CCM, the interested reader is referred, e.g., to Ref. 22 and, for details of the CCM computational algorithm for quantum spin systems (with spin quantum number $s=1/2$), to Refs. 26, 28, and 29. The starting point for a CCM calculation is the choice of a normalized model or reference state $|\Phi\rangle$, together with a set of mutually commuting multispin creation operators C_I^+, which are defined over a complete set of many-body configurations I. The operators C_I are the multispin destruction operators and are defined to be the Hermitian adjoints of the C_I^+. We choose $\{|\Phi\rangle; C_I^+\}$ in such a way that we have $\langle\Phi|C_I^+=0=C_I|\Phi\rangle$, $\forall I\neq 0$. Note that the CCM formalism corresponds to the thermodynamic limit $N\to\infty$.

For spin systems, an appropriate choice for the CCM model state $|\Phi\rangle$ is often a classical spin state, in which the most general situation is one in which each spin can point in an arbitrary direction.

We then perform a local coordinate transformation such that all spins are aligned in negative z direction in the new coordinate frame.[28,34] As a result, we have

$$|\Phi\rangle = |\cdots\downarrow\downarrow\downarrow\cdots\rangle; \quad C_I^+ = s_i^+,\ s_i^+s_j^+,\ s_i^+s_j^+s_k^+,\ \ldots, \tag{3}$$

(where the indices $i,j,k,\ldots$, denote arbitrary lattice sites) for the model state and the multispin creation operators, which now consist of spin-raising operators only. In the new coordinate system, the Hamiltonian reads[28]

$$H = J\sum_{\langle i,j\rangle}\left\{\tfrac{1}{2}\sin\varphi[s_i^+s_j^z - s_i^zs_j^+ + s_i^-s_j^z - s_i^zs_j^-] + \cos\varphi s_i^zs_j^z + \tfrac{1}{4}(\cos\varphi+1)[s_i^+s_j^- + s_i^-s_j^+] + \tfrac{1}{4}(\cos\varphi-1)[s_i^+s_j^+ + s_i^-s_j^-]\right\}, \tag{4}$$

with φ being the angle between the two spins, and $s^\pm \equiv s^x \pm i s^y$ are the spin-raising and spin-lowering operators. According to Fig. 1, we have, e.g., for the twisted Néel state on the square lattice $\varphi=\pi$ for nearest-neighbors along the y direction, but $\varphi=\pi+\theta$ along the x direction; and, for the twisted 120° Néel state on the triangular lattice, we have $\varphi=2\pi/3+\theta/2$ for nearest neighbors along the $\frac{1}{2}\vec{e}_x+\vec{e}_y$ direction, but $\varphi=4\pi/3+\theta$ along the x direction.

The CCM parametrizations of the ket and bra ground states are given by

$$H|\Psi\rangle = E|\Psi\rangle; \quad \langle\tilde{\Psi}|H = E\langle\tilde{\Psi}|,$$

$$|\Psi\rangle = e^S|\Phi\rangle; \quad S = \sum_{I\neq 0}\mathcal{S}_I C_I^+,$$

$$\langle\tilde{\Psi}| = \langle\Phi|\tilde{\mathcal{S}}e^{-S}; \quad \tilde{\mathcal{S}} = 1 + \sum_{I\neq 0}\tilde{\mathcal{S}}_I C_I^-. \tag{5}$$

The correlation operators S and $\tilde{S}$ contain the correlation coefficients $\mathcal{S}_I$ and $\tilde{\mathcal{S}}_I$ that we must determine. Using the Schrödinger equation, $H|\Psi\rangle=E|\Psi\rangle$, we can now write the ground-state energy as $E=\langle\Phi|e^{-S}He^S|\Phi\rangle$ and the sublattice magnetization is given by $M=-1/N\Sigma_i^N\langle\tilde{\Psi}|s_i^z|\Psi\rangle$, where s_i^z is expressed in the transformed coordinate system. To find the ket- and bra-state correlation coefficients, we require that the expectation value $\bar{H}=\langle\tilde{\Psi}|H|\Psi\rangle$ is a minimum with respect to the bra- and ket-state correlation coefficients, such that the CCM ket- and bra-state equations are given by

$$\langle\Phi|C_I^-e^{-S}He^S|\Phi\rangle = 0 \quad \forall\, I\neq 0 \tag{6}$$

$$\langle\Phi|\tilde{\mathcal{S}}e^{-S}[H,C_I^+]e^S|\Phi\rangle = 0 \quad \forall\, I\neq 0. \tag{7}$$

The problem of determining the CCM equations now becomes a *pattern-matching exercise* of the $\{C_I^-\}$ to the terms in $e^{-S}He^S$ in Eq. (6).

The CCM formalism is exact if we take into account all possible multispin configurations in the correlation operators S and $\tilde{S}$. This is, however, generally not possible for most quantum many-body models, including those studied here. We must therefore use the most common approximation scheme to truncate the expansion of S and $\tilde{S}$ in the Eqs. (6) and (7), namely, the LSUBn scheme, 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 adjacent (contiguous) lattice sites (for more details see Refs. 24, 28, and 29).

The spin stiffness considered in this paper is the stiffness of the Néel order parameter (sublattice magnetization). Hence, the corresponding model state $|\Phi\rangle$ is the Néel state. This is the ordinary collinear two-sublattice Néel state for the square and cubic lattices. The model state is a noncollinear 120° three-sublattice Néel state for the triangular lattice. Note that for the collinear Néel state, only LSUBn approximations with even n are relevant.[28,29] In order to calculate the spin stiffness directly using Eq. (1), we must modify the model (Néel) state by introducing an appropriate twist θ (see Fig. 1). Thus, the ket-state correlation coefficients $\mathcal{S}_I$ [after solving the CCM equations (6)] depend on θ and, hence, the ground-state energy E is also dependent on θ. Note that our numerical code for the CCM-LSUBn approximation allows

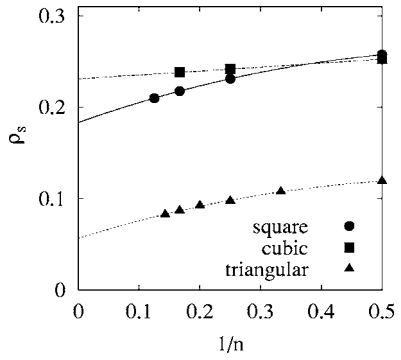

FIG. 2. Extrapolation of the CCM-LSUBn results for the stiffness. The points represent the CCM-LUBn results, and the lines correspond to the function (8) fitted to these data points.

us to calculate $E(\theta)$ with very high precision of about 14 digits. First, we have checked numerically that the ground-state energy calculated in LSUBn approximation does, indeed, fulfill the relation (1) with high precision for $\theta \lesssim 0.01$. The stiffness now can easily be calculated using numerical differentiation of $E(\theta)$, which was done using a three-point formula with $\theta = -10^{-4}, 0, +10^{-4}$.

Since the LSUBn approximation becomes exact for $n \to \infty$, it is useful to extrapolate the "raw" LSUBn results to the limit $n \to \infty$. Although we do not know the exact scaling of the LSUBn results, there is some empirical experience[26,28,29] how the ground-state energy and the order parameter for antiferromagnetic spin models scale with n. Based on this experience, we have tested several fitting functions for the stiffness and found that the best extrapolation is obtained by the fitting function

$$a = a_0 + a_1 \frac{1}{n} + a_2 \frac{1}{n^2}. \tag{8}$$

This law is known[28–31,33,34] to provide good extrapolated results for the order parameter. We show this extrapolation in Fig. 2.

III. RESULTS

Let us start with the results for the square lattice. Exploiting the lattice symmetries, we are able to perform calculations up to LSUB8, where for the twisted state 21 124 ket equations (6) have to be solved. The results for the stiffness are given in Table I. Using LSUBn with $n=2,4,6,8$, the extrapolated result is $\rho_s = 0.1831$. As known from the sublattice magnetization even better results can be obtained by excluding the LSUB2 data. Indeed the extrapolation using the LSUB4, LSUB6, and LSUB8 data yields $\rho_s = 0.1812$. Note that the corresponding extrapolated value for the sublattice magnetization[29] $M = 0.3114$ is in good agreement with other results.[29,35] A certain estimate of the accuracy can be obtained by an extrapolation using only LSUB2, LSUB4, and LSUB6, which yields $\rho_s = 0.1839$. We compare our results for ρ_s to some data obtained by other methods in Table II. Obviously, there is a significant variance in the data. In particular, the value obtained by quantum Monte Carlo seems to be surprisingly large. However, this might be connected with the fact, that in Ref. 12 the stiffness was not determined directly, but via the temperature dependence of the correlation length, which may lead to larger uncertainty. We think that the high-order spin-wave theory[6] is the most systematic approach, since one can see how the stiffness changes with increasing order of approximation. Assuming the third-order order spin-wave results as a benchmark, we find that our CCM result deviates by $\sim 3\%$.

TABLE I. Spin stiffness ρ_s for the spin-half Heisenberg antiferromagnet on the square lattice calculated by various CCM -LSUBn approximations and the result of the $n \to \infty$ extrapolation using LSUBn with $n=4,6,8$.

LSUBn	Number of equations	ρ_s
2	3	0.2574
4	40	0.2310
6	828	0.2176
8	21124	0.2097
Extrapolation	–	0.1812

For the triangular lattice, the twist we consider (see Fig. 1) corresponds to the in-plane spin stiffness. Because of the noncollinear structure of the three-sublattice Néel state, LSUBn approximations with odd n also appear. Furthermore, the number of ket equations in a certain level of approximation becomes larger then for the square lattice and, as a result the highest level of approximation we are able to consider is LSUB7. The results for different LSUBn approximations are given in Table III. The extrapolation of the LSUBn data according to Eq. (8) with $n=2,4,6$ leads to $\rho_s = 0.0604$ and with $n=2,3,4,5,6,7$ to $\rho_s = 0.0564$. Again, the difference in the two values can be considered as a certain estimate of the accuracy. As a by-product of our high-order calculation, we can give here improved values for the sublattice magnetization M. Thus far, results for M up to LSUB6[26,31] are published. We can add $M = 0.3152$ (LSUB7) and $M = 0.3018$ (LSUB8). The corresponding extrapolated value using Eq. (8) and LSUBn with $n=2,3,4,5,6,7,8$ is $M = 0.2134$, which is close to spin-wave[7,36] and Green's function Monte Carlo[37] results. The small values of the stiffness and the order parameter in comparison to the square lattice are attrib-

TABLE II. Collection of data for the spin stiffness ρ_s for the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice calculated by different methods.

First-order spin-wave theory[6,9]	0.191
Second-order spin-wave theory[6,9]	0.181
Third-order spin-wave theory[6]	0.175
Series expansion[6]	0.182
Exact diagonalization[14]	0.183
Quantum Monte Carlo[12]	0.199
Schwinger-boson approach I[15]	0.176
Schwinger-boson approach II[17]	0.153
CCM	0.181

TABLE III. In-plane spin stiffness ρ_s for the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the triangular lattice calculated by various CCM-LSUBn approximations and the result of the $n\to\infty$ extrapolation using LSUBn with $n=2,3,4,5,6,7$.

LSUBn	Number of equations	ρ_s
2	3	0.1188
3	14	0.1075
4	67	0.0975
5	370	0.0924
6	2133	0.0869
7	12878	0.0824
Extrapolation	–	0.0564

uted to the frustration leading to a noncollinear ground state and in combination with quantum fluctuations to a drastic weakening of magnetic order in the spin-$\frac{1}{2}$ HAFM.

We compare our results for ρ_s to available results from literature (see Table IV). Comparing the methods used to calculate ρ_s for the square lattice (Table II) and for the triangular lattice (Table IV), we see that the results for the triangular lattice are much less reliable, since here the accuracy of the methods used in Refs. 7, 8, and 17 is limited. Assuming the same tendency as for the square lattice, we can expect that the first-order spin-wave value for ρ_s[7,8] becomes smaller (and, therefore, closer to our CCM result) going to second- and third-order spin-wave theories. We believe that our result

TABLE IV. Collection of data for the spin stiffness ρ_s for the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the triangular lattice calculated by different methods.

Exact diagonalization[a]	0.05
First-order spin-wave theory[a,b]	0.080
Schwinger-boson approach[c]	0.088
CCM	0.056

[a]Reference 8.
[b]Reference 7.
[c]Reference 17.

TABLE V. Spin stiffness ρ_s for the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the cubic lattice calculated by various CCM-LSUBn approximations and the result of the $n\to\infty$ extrapolation using LSUBn with $n=2,4,6$.

LSUBn	Number of equations	ρ_s
2	4	0.2527
4	106	0.2416
6	5706	0.2380
Extrapolation	–	0.2312

is, indeed, of higher accuracy than data for ρ_s thus far available.

We now present our results for ρ_s for the simple cubic lattice (see Table V). Here, the highest level of approximation we can consider is LSUB6. From Fig. 2, it becomes obvious, that there is only a weak dependence on the level of CCM approximation n. Therefore, we expect that the extrapolation according to Eq. (8) yielding $\rho_s=0.2312$ is particularly accurate. Indeed, we find that our result is in very good agreement with the result obtained by second-order spin-wave theory[6] $\rho_s=0.2343$. Note that the $1/s$ spin-wave expansion seems to converge very rapidly,[6] and therefore, the second-order spin-wave theory is expected to yield a very precise result for ρ_s. For the sublattice magnetization, a corresponding extrapolation leads to $M=0.4181$,[29] coinciding to 1% with the high-precision third-order spin-wave result.[38]

IV. SUMMARY

In summary, we have presented a method for the direct calculation of spin stiffness within the framework of the coupled-cluster method. We obtain accurate values for the stiffness by applying this algorithm to high orders of LSUBn approximations for the spin-$\frac{1}{2}$ isotropic Heisenberg antiferromagnet on various lattices with and without frustration.

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