Direct calculation of the spin stiffness 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-half Heisenberg antiferromagnet on the square, the triangular and the cubic lattices we calculate the stiffness in high orders of approximation. For the square and the 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 so far by other approximate method.

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 \( \rho_s \) 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 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 like series expansion [5-11], quantum Monte Carlo [12], exact diagonalization [13,14], Schwinger-boson approach [15,16,17] and renormalization group theory [18] have been used to calculate the spin stiffness of the spin-half Heisenberg antiferromagnet (HAFM) on the square, the triangular and the 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 \( \rho_s \) measures the increase in the amount of energy when we rotate the order parameter of a magnetically long-range ordered system along a given direction by a small angle \( \theta \) per unit length, i.e.

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

(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 \( \rho_s \) 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 new method to calculate the spin stiffness for the quantum-spin HAFM using the coupled cluster approach [20,21,22]. The coupled cluster approach is a powerful and universal tool in quantum many-body physics which has been applied in various fields like nuclear physics, quantum chemistry, strongly correlated electrons etc. [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 non-collinear ground states.

To demonstrate the potential of the presented method we calculate the spin stiffness for the spin-\( \frac{1}{2} \) HAFM with nearest-neighbor interaction on the cubic, the square, and on the triangular lattices and compare our results with available data in the literature. While for the square and the cubic lattices accurate high order spin-wave results are available which can be used to estimate the accuracy of the CCM results, the known results for the frustrated HAFM on the triangular lattice with a non-collinear 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 so far available results. 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-half HAFM

\[
H = J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j.
\]

(2)
In (2) the sum runs over all pairs of nearest neighbors \((i,j)\). 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. \textsuperscript{22} and for details of the CCM computational algorithm for quantum spin systems (with spin quantum number \(s = 1/2\)) to Refs. \textsuperscript{20,26,28,29}. 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 \(C_I^+\) in such a way that we have \(|\Phi\rangle = \{C_I | I\rangle\} \), \(\forall I \neq 0\). 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.\textsuperscript{28} As a result we have

\[
|\Phi\rangle = |\cdots \downarrow \downarrow \cdots \rangle; \quad C_I^+ = s_i^+ s_j^+ + s_i^- s_j^-; \quad \cdots,
\]

(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

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

\[
+ \frac{1}{4} (\cos \varphi - 1) \left[ s_i^+ s_j^+ + s_i^- s_j^- \right],
\]

(4)

with \(\varphi\) being the angle between the two spins, and \(s^\pm = s^x \pm is^y\) the spin-raising and spin-lowering operators. According to Fig. we have e.g. for the twisted Néel state on the square lattice \(\varphi = \pi/2\) 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 \(\hat b\) direction but \(\varphi = 4\pi/3 + \theta\) along the \(x\) direction.

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

\[
H|\Psi\rangle = E|\Psi\rangle; \quad \langle \bar \Psi | H = E \langle \bar \Psi |; \quad |\Psi\rangle = e^S|\Phi\rangle; \quad S = \sum_{I \neq 0} S_I C_I^+ ;
\]

\[
\langle \bar \Psi | = \langle \Phi | \bar S e^{-S}; \quad \bar S = 1 + \sum_{I \neq 0} \bar S_I C_I^- .
\]

(5)

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

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

\[
\langle \Phi | \bar S e^{-S} [H, C_I^+] e^S | \Phi\rangle = 0 \quad \forall I \neq 0. \quad (7)
\]

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

The CCM formalism is exact if we take into account all possible multispin configurations in the correlating operators \(S\) and \(\bar S\). 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 \(\bar S\) in the Eqs. \(6\) and \(7\), namely the LSBg 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. \textsuperscript{24,28,29}).

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 the 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 LSBg approximations with even \(n\) are relevant.\textsuperscript{28} In order to calculate the spin stiffness directly using Eq. \(1\) we must modify the model (Néel) state by introducing an appropriate twist \(\theta\), see Fig. \(1\). Thus the ket-state correlation coefficients \(S_I\) (after solving the CCM equations \(5\)) depend on \(\theta\) and hence the ground-state energy \(E\) is also dependent on \(\theta\). Note that our numerical code for the CCM-LSBg approximation allows 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 LSBg 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 LSBg approximation becomes exact for \(n \to \infty\), it is useful to extrapolate the 'raw' LSBg results to the limit \(n \to \infty\). Although we do not know the exact scaling of the LSBg results, there is some empirical experience\textsuperscript{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 we have found...
the best extrapolation is obtained by the fitting function
\[ a = a_0 + a_1 \frac{1}{n} + a_2 \frac{1}{n^2}. \] (8)
This law is known to provide good extrapolated results for the order parameter. We show this extrapolation in Fig. 2.

TABLE I: Spin stiffness \( \rho_s \) 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 eqs. | \( \rho_s \) |
|-------|-------------|-------------|
| 2     | 3           | 0.2574      |
| 4     | 40          | 0.2310      |
| 6     | 828         | 0.2176      |
| 8     | 21124       | 0.2097      |
| extrapol. | –           | 0.1812      |

TABLE II: Collection of data for the spin stiffness \( \rho_s \) for the spin-half Heisenberg antiferromagnet on the square lattice calculated by different methods.

| Method                        | \( \rho_s \) |
|-------------------------------|-------------|
| first-order spin-wave theory  | 0.191       |
| second-order spin-wave theory | 0.181       |
| third-order spin-wave theory  | 0.175       |
| exact diagonalization         | 0.182       |
| quantum Monte Carlo           | 0.183       |
| Schwinger-boson approach I    | 0.176       |
| Schwinger-boson approach II   | 0.153       |
| CCM                           | 0.181       |

for the stiffness are given in Tab. 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, LSUB8 data yields \( \rho_s = 0.1812 \). Note that the corresponding extrapolated value for the sublattice magnetization \( M = 0.3114 \) is in good agreement with other results.28,35 A certain estimate of the accuracy can be obtained by an extrapolation using LSUB2, LSUB4, LSUB6, only, which yields \( \rho_s = 0.1839 \). We compare our results for \( \rho_s \) with some data obtained by other methods in Tab. 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 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 about 3%.

For the triangular lattice the twist we consider (see Fig. 1) corresponds to the in-plane spin stiffness. Due to the noncollinear structure of the three-sublattice Néel state also LSUBn approximations with odd \( n \) appear. Furthermore the number of ket equations in a certain

III. RESULTS

Let us start with the results for the square lattice. Exploiting the lattice symmetries we are able to perform calculations up to LSUBB8, where for the twisted state 21124 ket equations have to be solved. The results
TABLE III: In-plane spin stiffness $\rho_s$ for the spin-half Heisenberg antiferromagnet on the triangular lattice calculated by various CCM-LSUB$n$ approximations and the result of the $n \to \infty$ extrapolation using LSUB$n$ with $n = 2, 3, 4, 5, 6, 7$.

| LSUB$n$ | number eqs. | $\rho_s$ |
|---------|-------------|---------|
| 2       | 3           | 0.1188  |
| 3       | 14          | 0.1075  |
| 4       | 67          | 0.0975  |
| 5       | 370         | 0.0924  |
| 6       | 2133        | 0.0860  |
| 7       | 12878       | 0.0824  |
| extrapol.|             | 0.0564  |

TABLE IV: Collection of data for the spin stiffness $\rho_s$ for the spin-half Heisenberg antiferromagnet on the triangular lattice calculated by different methods.

| Method                  | $\rho_s$ |
|-------------------------|----------|
| exact diagonalization   | 0.05     |
| first-order spin-wave   | 0.080    |
| Schwinger-boson approach| 0.088    |
| CCM                     | 0.056    |

level of approximation becomes larger then for the square lattice and as a results the highest level of approximation we are able to consider is LSUB7. The results for different LSUB$n$ approximations are given in Tab. III. The extrapolation of the LSUB$n$ 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 byproduct of our high-order calculation we can give here improved values for the sublattice magnetization $M$. So far results for $M$ up to LSUB$n$=26 are published. We can add $M = 0.3152$ (LSUB7) and $M = 0.3018$ (LSUB8). The corresponding extrapolated value using Eq. (8) and LSUB$n$ with $n = 2, 3, 4, 5, 6, 7, 8$ is $M = 0.2134$, which is close to spin-wave and Green’s function Monte Carlo results. The small values of the stiffness and the order parameter in comparison with the square lattice are attributed to the frustration leading to a non-collinear ground state and in combination with quantum fluctuations to a drastic weakening of magnetic order in the spin-half HAFM.

We compare our results for $\rho_s$ with available results from literature, see Tab. IV. Comparing the methods used to calculate $\rho_s$ for the square lattice (Tab. III) and for the triangular lattice (Tab. IV) we see that the results for the triangular lattice are much less reliable, since here the accuracy of the methods used in Refs. 7,8,17 is limited. Assuming the same tendency as for the square lattice we can expect that the first-order spin-wave value for $\rho_s$ becomes smaller (and therefore closer to our CCM result) going to second- and third-order spin-wave theories. We believe that our result is indeed of higher accuracy than data for $\rho_s$ so far available.

We present now our results for $\rho_s$ for the simple cubic lattice, see Tab. 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 particular accurate. Indeed we find that our result is in very good agreement with the result obtained by second-order spin-wave theory of $\rho_s = 0.2343$. Note that the $1/s$ spin-wave expansion seems to converge very rapidly and therefore the second-order spin-wave theory is expected to yield a very precise result for $\rho_s$. For the sublattice magnetization a corresponding extrapolation leads to $M = 0.4181$ coinciding to 1% with the high precision third-order spin-wave result.

### IV. SUMMARY

In summary, we have presented a method for the direct calculation of the 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 LSUB$n$ approximations for the spin-half isotropic Heisenberg antiferromagnet on various lattices with and without frustration.

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